



HOKKAIDO UNIVERSITY

Title	Global search for low-lying crystal structures using the artificial force induced reaction method : A case study on carbon
Author(s)	Takagi, Makito; Taketsugu, Tetsuya; Kino, Hiori et al.
Citation	Physical Review B, 95(18), 184110 https://doi.org/10.1103/PhysRevB.95.184110
Issue Date	2017-05-30
Doc URL	https://hdl.handle.net/2115/67066
Rights	©2017 American Physical Society
Type	journal article
File Information	Supplemental material.pdf



Supplemental Material for:

Global search for low-lying crystal structures using the artificial force induced reaction method: A case study on carbon

Makito Takagi,¹ Tetsuya Taketsugu,² Hiori Kino,^{3,4} Yoshitaka Tateyama,³ Kiyoyuki Terakura,³ and Satoshi Maeda^{2,*}

¹ Graduate School of Chemical Sciences and Engineering, Hokkaido University, Kita 13, Nishi 8, Kita-ku, Sapporo 060-8628, Japan

² Department of Chemistry, Faculty of Science, Hokkaido University, Kita 10, Nishi 8, Kita-ku, Sapporo 060-0810, Japan

³ Center for Materials Research by Information Integration, National Institute for Materials Science, 1-2-1, Sengen, Tsukuba 305-0047, Japan

⁴ ESICMM, National Institute for Materials Science, Tsukuba, 1-2-1, Sengen, Ibaraki 305-0047, Japan

* smaeda@eis.hokudai.ac.jp

CONTENTS:

S1. The full list of references on carbon crystal structures

S2. The derivation of Eq. (1)

S3. Initial structures

S4. Cartesian coordinate of all obtained MINs

S5. Primitive lattice of 3D-min10, 3D-min12, and 3D-min13

S6. Phonon dispersion curve of 3D-min10, 3D-min12, and 3D-min13

S7. Symmetry k-points of 3D-min10, 3D-min12, and 3D-min13

S1. The full list of references on carbon crystal structures

Carbon can take various forms,^[1-247] such as diamond,^[22-24] graphite,^[25,47] lonsdaleite (hexagonal diamond),^[27] fullerene^[29,38] (or fullerite^[44]) and related structures,^[81-124] carbon nanotube (CNT)^[41] and related structures,^[125-139] graphene^[60] and related structures,^[140-172] graphene nanoribbon (GNR),^[66,173-176] q-carbon,^[77] carbyne,^[79] graphyne^[80] and related structures,^[177-202] n-diamond,^[203-214] and amorphous carbon.^[215-247]

Furthermore, many stable structures have been predicted theoretically.^[248-460] M-carbon,^[313,324] 8-tetra(2,2) tubulane^[127] (or bct C₄^[293,329]) or other names^[132,288,305,308,332,334,348]) Cco-C₈^[343] (or Z-carbon^[345]), and so forth have been predicted recently from first principles.

- [1] I. V. Stankevich, M. V. Nikerov, and D. A. Bochvar, *Russ. Chem. Rev.* **53**, 640 (1984).
- [2] R. C. DeVries, *Ann. Rev. Mater. Sci.* **17**, 161 (1987).
- [3] A. T. Balaban, *Comput. Math. Appl.* **17**, 397 (1989).
- [4] Y. Tanabe and E. Yasuda, *J. Ceram. Soc. Jpn.* **99**, 1069 (1991).
- [5] F. Diederich and Y. Rubin, *Angew. Chem. Int. Ed.* **31**, 1101 (1992).
- [6] R. B. Heimann, S. E. Evsvukov, and Y. Koga, *Carbon* **35**, 1654 (1997).
- [7] J. M. D. Tascón, *Opt. Pura Apl.* **40**, 149 (2007).
- [8] V. V. Pokropivny and A. L. Ivanovskii, *Russ. Chem. Rev.* **77**, 899 (2008).
- [9] A. L. Ivanovskii, *Russ. J. Inorg. Chem.* **53**, 2083 (2008).
- [10] V. V. Ivanovskaya and A. L. Ivanovskii, *J. Superhard Mater.* **32**, 67 (2010).
- [11] A. T. Balaban and K. P. C. Vollhardt, *Open Org. Chem. J.* **5**, 117 (2011).
- [12] V. A. Greshnyakov, E. A. Belenkov, and V. M. Berezin, *Crystalline Structure and Properties of Carbon Diamond Like Phases*, South-Ural State University, Chelyabinsk, (2012).
- [13] A. L. Ivanovskii, *J. Superhard Mater.* **35**, 1 (2013).
- [14] C. He, L. Z. Sun, and J. Zhong, *J. Superhard Mater.* **34**, 386 (2012).
- [15] A. R. Oganov, R. J. Hemley, R. M. Hazen, and A. P. Jones, *Rev. Mineral. Geochem.* **75**, 47 (2013).
- [16] E. A. Belenkov and V. A. Greshnyakov, *Phys. Sol. State* **55**, 1754 (2013).
- [17] E. A. Belenkov and V. A. Greshnyakov, *New Carbon Mater.* **28**, 273 (2013).
- [18] V. Georgakilas, J. A. Perman, J. Tucek, and R. Zboril, *Chem. Rev.* **115**, 4744 (2015).
- [19] E. A. Belenkov and A. E. Kochengin, *Phys. Sol. State* **57**, 2126 (2015).
- [20] J. Zhai, A. Wan, and W. Wu, *Mod. Phys. Lett. B* **29**, 1530011 (2015).
- [21] J. Zhang, M. Terrones, C. R. Park, R. Mukherjee, M. Monthieux, N. Koratkar, Y. S. Kim, R. Hurt, E. Frackowiak, T. Enoki, Y. Chen, Y. Chen, and A. Bianco, *Carbon* **98**, 708 (2016).
- [22] S. Tennant, *Roy. Soc. (London) A* **87**, 123 (1797).

- [23] W. H. Bragg and W. L. Bragg, *Nature* **91**, 557 (1913).
- [24] W. H. Bragg and W. L. Bragg, *Proc. R. Soc. London Ser. A* **89**, 277 (1913).
- [25] A. W. Hull, *Phys. Rev.* **10**, 661 (1917).
- [26] R. B. Aust and H. G. Drickamer, *Science* **140**, 817 (1963).
- [27] F. P. Bundy and J. S. Kasper, *J. Chem. Phys.* **46**, 3437 (1967).
- [28] A. El Gorsey and G. Donnay, *Science* **161**, 363 (1968).
- [29] E. Osawa, *Kagaku* **25**, 854 (1970).
- [30] A. G. Whittaker and G. M. Wolten, *Science* **178**, 54 (1972).
- [31] V. E. Strel'nitskii, V. G. Padalka, and S. I. Vakula, *Sov. Phys. Tech. Phys.* **23**, 222 (1978).
- [32] A. G. Whittaker, *Carbon* **17**, 21 (1979).
- [33] N. N. Matyushenko, V. E. Strel'nitskii, and V. A. Gausev, *JETP Lett.* **30**, 199 (1979).
- [34] V. M. Mel'nichenko, A. M. Sladkov, and Y. N. Nikulin, *Russ. Chem. Rev.* **51**, 421 (1982).
- [35] V. M. Melnitchenko, Y. N. Nikulin, and A. M. Sladkov, *Carbon* **23**, 3, (1985).
- [36] L. S. Palatnik, M. B. Guseva, V. G. Babaev, N. F. Savchenko, and I. I. Fal'ko, *Sov. Phys. JETP* **60**, 520, (1984).
- [37] D. V. Fedoseev, V. P. Varnin, and B. V. Deryagin, *Russ. Chem. Rev.* **53**, 435 (1984).
- [38] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, and R. E. Smalley, *Nature* **318**, 162 (1985).
- [39] F. Diederich, Y. Rubin, C. B. Knobler, R. L. Whetten, K. E. Schriver, K. N. Houk, and Y. Li, *Science* **245**, 1088 (1989).
- [40] J. J. Cuomo, J. P. Doyle, J. Bruley, and J. C. Liu, *J. Vac. Sci. Technol. A* **9**, 2210 (1991).
- [41] S. Iijima, *Nature* **354**, 56 (1991).
- [42] W. Utsumi and T. Yagi, *Science* **252**, 1542 (1991).
- [43] H. Hirai and K. Kondo, *Science* **253**, 772 (1991).
- [44] C. S. Yoo and W. J. Nellis, *Chem. Phys. Lett.* **198**, 379 (1992).
- [45] M. Miki-Yoshida, L. Rendon, and M. Jose-Yacaman, *Carbon* **31**, 843 (1993).
- [46] R. J. Lagow, J. J. Kampa, H.-C. Wei, S. L. Battle, J. W. Genge, D. A. Laude, C. J. Harper, R. Bau, R. C. Stevens, J. F. Haw, and E. Munson, *Science* **267**, 362 (1995).
- [47] E. D. Miller, D. C. Nesting, and J. V. Badding, *Chem. Mater.* **9**, 18 (1997).
- [48] S. M. Jarkov, Y. N. Titarenko, and G. N. Churilov, *Carbon* **36**, 595 (1998).
- [49] C. Piskoti, J. Yarger, and A. Zettl, *Nature* **393**, 771 (1998).
- [50] Y.-K. Kwon, D. Tománek, and S. Iijima, *Phys. Rev. Lett.* **82**, 1470 (1999).
- [51] I. Alexandrou, H.-J. Scheibe, C. J. Kiely, A. J. Papworth, G. A. J. Amaratunga, and B. Schultrich, *Phys. Rev. B* **60**, 10903 (1999).

- [52] V. N. Khabashesku, Z. Gu, B. Brinson, J. L. Zimmerman, J. L. Margrave, V. A. Davydov, L. S. Kashevarova, and A. V. Rakhmanina, *J. Phys. Chem. B* **106**, 11155 (2002).
- [53] Z. Iqbal, Y. Zhang, H. Grebel, S. Vijayalakshmi, A. Lahamer, G. Benedek, M. Bernasconi, J. Cariboni, I. Spagnolatti, R. Sharma, F. J. Owens, M. E. Kozlov, K. V. Rao, and M. Muhammed, *Eur. Phys. J. B* **31**, 509 (2003).
- [54] W. L. Mao, H.-K. Mao, P. J. Eng, T. P. Trainor, M. Newville, C.-C. Kao, D. L. Heinz, J. Shu, Y. Meng, and R. J. Hemley, *Nature* **302**, 425 (2003).
- [55] T. Irifune, A. Kurio, S. Sakamoto, T. Inoue, and H. Sumiya, *Nature* **421**, 599 (2003).
- [56] K. Yamada, *Carbon* **41**, 1309 (2003).
- [57] A. El. Goresy, L. S. Dubrovinsky, P. Gillet, S. Mostefaoui, G. Graup, M. Drakopoulos, A. S. Simionovici, V. Swamy, and V. L. Masaitis, *C. R. Geoscience* **335**, 889 (2003).
- [58] C. S. Casari, A. Li Bassi, L. Ravagnan, F. Siviero, C. Lenardi, P. Piseri, G. Bongiorno, C. E. Bottani, and P. Milani, *Phys. Rev. B* **69**, 075422 (2004).
- [59] P. J. F. Harris, *Philos. Mag.* **84**, 3159 (2004).
- [60] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, *Science* **306**, 666 (2004).
- [61] V. N. Inkin, A. Y. Kolpakov, S. I. Oukhanov, V. I. Barbakov, M. E. Galkina, and I. U. Goncharov, *Diam. Relat. Mater.* **13**, 1474 (2004).
- [62] Y. M. Korolev, *Dokl. Phys.* **49** (2004).
- [63] I. Konyashin, V. Khvostov, V. Babaev, M. Guseva, J. Mayer, and A. Sirenko, *Int. J. Refra.* **24**, 17 (2006).
- [64] Z. Wang and Y. Zhao, *Science* **312**, 1149 (2006).
- [65] L. Sun, F. Banhart, A. V. Krashennnikov, J. A. Rodríguez-Manzo, M. Terrones, and P. M. Ajayan, *Science* **312**, 1199 (2006).
- [66] M. Y. Han, B. Özyilmaz, Y. Zhang, and P. Kim, *Phys. Rev. Lett.* **98**, 206805 (2007).
- [67] J. C. Meyer, A. K. Geim, M. I. Katsnelson, K. S. Novoselov, T. J. Booth, and S. Roth, *Nature* **446**, 60 (2007).
- [68] P. Liu, H. Cui, and G. W. Yang, *Cryst. Growth Des.* **8**, 581 (2008).
- [69] A. Y. Basharin, V. S. Dozhikov, V. T. Dubinchuk, A. V. Kirillin, I. Y. Lysenko, and M. A. Turchaninov, *Tech. Phys. Lett.* **35**, 428 (2009).
- [70] M. D. Knudson, M. P. Desjarlais, and D. H. Dolan, *Science* **322**, 1822 (2008).
- [71] C. Jin, H. Lan, L. Peng, K. Suenaga, and S. Iijima, *Phys. Rev. Lett.* **102**, 205501 (2009).
- [72] J. Bai, X. Zhong, S. Jiang, Y. Huang, and X. Duan, *Nat. Nanotech.* **5**, 190 (2010).
- [73] A. Kuc, T. Heine, G. Seifert, *Phys. Rev. B* **81**, 085430 (2010).

- [74] L. Zhang, P. Mohanty, N. Coombs, Y. Fei, H.-K. Mao, and Kai Landskron, *Proc. Natl. Acad. Sci. USA* **107**, 13593 (2010).
- [75] P. Németh, L. A. J. Garvie, T. Aoki, N. Dubrovinskaya, L. Dubrovinsky, and P. R. Buseck, *Nat. Commun.* **5**, 5447 (2014).
- [76] Y. Wu, N. Yi, L. Huang, T. Zhang, S. Fang, H. Chang, N. Li, J. Oh, J. A. Lee, M. Kozlov, A. C. Chipara, H. Terrones, P. Xiao, G. Long, Y. Huang, F. Zhang, L. Zhang, X. Lepró, C. Haines, M. D. Lima, N. P. Lopez, L. P. Rajukumar, A. L. Elias, S. Feng, S. J. Kim, N. T. Narayanan, P. M. Ajayan, M. Terrones, A. Aliev, P. Chu, Z. Zhang, R. H. Baughman, and Y. Chen, *Nat. Commun.* **6**, 6141 (2015).
- [77] J. Narayan and A. Bhaumik, *Apl. Mater.* **3**, 100702, (2015).
- [78] P. Németh, L. A. J. Garvie, and P. R. Buseck, *Sci. Rep.* **5**, 18381 (2015).
- [79] L. Shi, P. Rohringer, K. Suenaga, Y. Niimi, J. Kotakoski, J. C. Meyer, H. Peterlik, M. Wanko, S. Cahangirov, A. Rubio, Z. J. Lapin, L. Novotny, P. Ayala, and T. Pichler, *Nat. Mater.* **15**, 634 (2016).
- [80] N. Han, H. Liu, S. Zhou, and J. Zhao, *J. Phys. Chem. C* **120**, 14699 (2016).
- [81] H. Terrones, M. Terrones, and W. K. Hsu, *Chem. Soc. Rev.* **24**, 341 (1995).
- [82] B. I. Yakobson and R. E. Smalley, *Am. Sci.* **85**, 324 (1997).
- [83] B. Sundqvist, *Adv. Phys.* **48**, 1 (1999).
- [84] X. Lu and Z. Chen, *Chem. Rev.* **105**, 3643 (2005).
- [85] A. San-Miguel, *Chem. Soc. Rev.* **35**, 876 (2006).
- [86] V. V. Brazhkin and A. G. Lyapin, *J. Superhard Mater.* **34**, 400 (2012).
- [87] W. Krätschmer, L. D. Lamb, K. Fostiropoulos, and D. R. Huffman, *Nature* **347**, 354 (1990).
- [88] M. O'Keeffe, *Nature* **352**, 674 (1991).
- [89] W. I. F. David, R. M. Ibberson, J. C. Matthewman, K. Prassides, T. J. S. Dennis, J. P. Hare, H. W. Kroto, R. Taylor, and D. R. M. Walton, *Nature* **353**, 147 (1991).
- [90] R. Ettl, I. Chao, F. Diederich, and R. L. Whetten, *Nature* **353**, 149 (1991).
- [91] G. B. Adams, O. F. Sankey, J. B. Page, M. O'keeffe, and D. A. Drabold, *Science* **256**, 1792 (1992).
- [92] C. S. Yoo, W. J. Nellis, M. L. Sattler, and R. G. Musket, *Appl. Phys. Lett.* **61**, 273 (1992).
- [93] W. I. F. David, R. M. Ibberson, T. J. S. Dennis, J. P. Hare, and K. Prassides, *Europhys. Lett.* **18**, 219 (1992).
- [94] L. Zeger and E. Kaxiras, *Phys. Rev. Lett.* **70**, 2920 (1993).
- [95] M. Yoshida and E. Osawa, *J. Fullerene Sci. Tech.* **1**, 55 (1993).
- [96] P. W. Fowler, and S. J. Austin, *J. Chem. Inform. Comput. Sci.*, **34**, 264 (1994).
- [97] E. Kaxiras, L. M. Zeger, A. Antonelli, and Y.-M. Juan, *Phys. Rev. B* **49**, 8446 (1994).

- [98] M. Núñez-Regueiro, L. Marques, J.-L. Hodeau, O. Béthoux, and M. Perroux, *Phys. Rev. Lett.* **74**, 278 (1995).
- [99] G. Oszlanyi and L. Forro, *Solid State Commun.* **93**, 265 (1995).
- [100] Y. Iwasa, T. Arima, R. M. Fleming, T. Siegrist, O. Zhou, R. C. Haddon, L. J. Rothberg, K. B. Lyons, H. L. Carter, A. F. Hebard Jr., R. Tycko, G. Dabbagh, J. J. Krajewski, G. A. Thomas, and T. Yagi, *Science* **264**, 1570 (1995).
- [101] S. Itoh, P. Ordejón, D. A. Drabold, and R. M. Martin, *Phys. Rev. B* **53**, 2132 (1996).
- [102] L. Marques, J.-L. Hodeau, M. Núñez-Regueiro, and M. Perroux, *Phys. Rev. B* **54**, R12633 (1996).
- [103] D. Porezag, G. Jungnickel, T. Frauenheim, G. Seifert, A. Ayuela, and M. R. Pederson, *Appl. Phys. A* **64**, 321 (1997).
- [104] G.-W. Wang, K. Komatsu, Y. Murata, and M. Shiro, *Nature* **387**, 583 (1997).
- [105] P. W. Fowler, D. Mitchell, R. Taylor, and G. Seifert, *J. Chem. Soc. Perkin Trans.* **2**, 1901 (1997).
- [106] M. Côté, J. C. Grossman, M. L. Cohen, and S. G. Louie, *Phys. Rev. Lett.* **81**, 697 (1998).
- [107] V. D. Blank, S. G. Buga, G. A. Dubitsky, N. R. Serebryanaya, M. Y. Popov, and B. Sundqvist, *Carbon* **36**, 319 (1998).
- [108] S. Okada, S. Saito, and A. Oshiyama, *Phys. Rev. Lett.* **83**, 1986 (1999).
- [109] S. Okada and S. Saito, *Phys. Rev. B* **59**, 1930 (1999).
- [110] J. C. Grossman, S. G. Louie, and M. L. Cohen, *Phys. Rev. B* **60**, R6941 (1999).
- [111] Y. Miyamoto and M. Saito, *Phys. Rev. B* **63**, 161401(R) (2001).
- [112] A. G. Glazov, V. V. Mukhamad'yarov, V. V. Brazhkin, A. G. E. Lyapin, E. L. Gromnitskaya, O. V. Stal'gorova, and S. V. Popova, *JETP Lett.* **73**, 552 (2001).
- [113] S. Okada, Y. Miyamoto, and M. Saito, *Phys. Rev. B* **64**, 245405 (2001).
- [114] V. V. Pokropivny and A. V. Pokropivny, *Phys. Sol. State* **46**, 392 (2004).
- [115] G. Seifert, A. N. Enyashin, and T. Heine, *Phys. Rev. B* **72**, 012102 (2005).
- [116] A. E. Belenkov, A. L. Ivanovskii, S. N. Ul'yanov, and F. K. Shabiev, *J. Struct. Chem.* **46**, 961, (2005).
- [117] S. Yamanaka, A. Kubo, K. Inumaru, K. Komaguchi, N. S. Kini, T. Inoue, and T. Irifune, *Phys. Rev. Lett* **96**, 076602 (2006).
- [118] A. Enyashin, S. Gemming, T. Heine, G. Seifert, and L. Zhechkov, *Phys. Chem. Chem. Phys.* **8**, 3320 (2006).
- [119] A. L. Ivanovskii, *Russ. J. Inorg. Chem.* **53** 1274 (2008).
- [120] S. Yamanaka, N. S. Kini, A. Kubo, S. Jida, and H. Kuramoto, *J. Am. Chem. Soc.* **130**, 4303 (2008).
- [121] A. N. Enyashin and A. L. Ivanovskii, *Phys. Rev. B* **77**, 113402 (2008).
- [122] M. Maruyama and S. Okada, *J. Phys. Soc. Jpn.* **82**, 043708 (2013).
- [123] J. Li and R.-Q. Zhang, *Carbon*, **63** 571 (2013).

- [124] R. P. Kaur, R. S. Sawhney, and D. Engles, *Int. J. Comput. Mater. Sci. Eng.* **5**, 1650009 (2016).
- [125] J.-C. Charlier X. Blase, and S. Roche, *Rev. Mod. Phys.* **79**, 677 (2007).
- [126] Y. Segawa, H. Ito, and K. Itami, *Nat. Rev. Mater.* **1**, 15002 (2016).
- [127] R. H. Baughman and D. S. Galvgão, *Chem. Phys. Lett.* **211**, 110 (1993).
- [128] T. W. Ebbesen, *Acc. Chem. Res.* **31**, 558 (1998).
- [129] T. Yildirim, O. Gülseren, Ç. Kılıç, and S. Ciraci, *Phys. Rev. B* **62**, 12648 (2000).
- [130] X. Zhao, Y. Liu, S. Inoue, T. Suzuki, R. O. Jones, and Y. Ando, *Phys. Rev. Lett.* **92**, 125502 (2004).
- [131] Z. Wang, Y. Zhao, K. Tait, X. Liao, D. Schiferl, C. Zha, R. T. Downs, J. Qian, Y. Zhu, and T. Shen, *Proc. Natl. Acad. Sci. USA* **101**, 13699 (2004).
- [132] H. S. Domingos, *J. Phys.: Cond. Matter* **16**, 9083 (2004).
- [133] Y. Omata, Y. Yamagami, K. Tadano, T. Miyake, and S. Saito, *Physica E* **29**, 454 (2005).
- [134] G. Kim, B. W. Jeong, and J. Ihm, *Appl. Phys. Lett.* **88**, 193107 (2006).
- [135] J. Kotakoski, A. V. Krashenninnikov, and K. Nordlund, *Phys. Rev. B* **74**, 245420 (2006).
- [136] S. Park, K. Kittimanapun, J.-S. Ahn, Y.-K. Kwon, and D. Tománek, *J. Phys.: Cond. Matter* **22**, 334220 (2010).
- [137] P. A. S. Autreto, S. B. Legoas, M. Z. S. Flores, and D. S. Galvao, *J. Chem. Phys.* **133**, 124513 (2010).
- [138] R. Zhou, R. Liu, L. Li, X. Wu, and X. C. Zeng, *J. Phys. Chem. C* **115**, 18174 (2011).
- [139] Z. S. Zhao, X.-F. Zhou, M. Hu, D. L. Yu, J. L. He, H.-T. Wang, Y. J. Tian, and B. Xu, *J. Superhard Mater.* **4**, 371 (2012).
- [140] H. Terrones and M. Terrones, *New J. Phys.* **5**, 126 (2003).
- [141] M. J. Allen, V. C. Tung, and R. B. Kaner, *Chem. Rev.* **110**, 132 (2010).
- [142] A. L. Mackay and H. Terrones, *Nature* **352**, 762 (1991).
- [143] D. Vanderbilt and J. Tersoff, *Phys. Rev. Lett.* **68**, 511 (1992).
- [144] T. Lenosky, X. Gonze, M. Teter, and V. Elser, *Nature* **355**, 333 (1992).
- [145] S. Iijima, T. Ichihashi, and Y. Ando, *Nature* **356**, 776 (1992).
- [146] H. Terrones and A. L. Mackay, *Carbon* **30**, 1251 (1992).
- [147] S. J. Townsend, T. J. Lenosky, D. A. Muller, C. S. Nichols, and V. Elser, *Phys. Rev. Lett.* **69**, 921 (1992).
- [148] R. Phillips, D. A. Drabold, T. Lenosky, G. B. Adams, and O. F. Sankey, *Phys. Rev B* **46**, 1941, (1992).
- [149] M.-Z. Huang, W. Y. Ching, and T. Lenosky, *Phys. Rev. B* **47**, 1593 (1993).
- [150] H. Terrones and A. L. Mackay, *Chem. Phys. Lett.* **207**, 45 (1993).
- [151] M. Fujita, T. Umeda, and M. Yoshida, *Phys. Rev. B* **51**, 13778 (1995).
- [152] I. Spagnolatti, M. Bernasconi, and G. Benedek, *Eur. Phys. J. B* **32**, 181 (2003).
- [153] F. Valencia, A. H. Romero, E. Hernández, M. Terrones, and H. Terrones, *New J. Phys.* **5**, 123 (2003).

- [154] G. K. Dimitrakakis, E. Tylianakis, and G. E. Froudakis, *Nano Lett.* **8**, 3166 (2008).
- [155] R. S. Ruoff, *MRS bulletin* **37**, 1314 (2012).
- [156] M. Tagami, Y. Liang, H. Naito, Y. Kawazoe, and M. Kotani, *Carbon* **76**, 266 (2014).
- [157] S. K. Ameri, P. K. Singh, and S. R. Sonkusale, *Carbon* **79**, 572 (2014).
- [158] F. Xu, H. Yu, A. Sadrzadeh, and B. I. Yakobson, *Nano Lett.* **16**, 34 (2015).
- [159] J. R. Owens, C. Daniels, A. Nicolai, H. Terrones, and V. Meunier, *Carbon* **96**, 998 (2016).
- [160] F. Banhart, J. Kotakoski, and A. V. Krasheninnikov, *ACS Nano* **5**, 26 (2010).
- [161] R. H. Telling, C. P. Ewels, A. A. El-barbary, and M. I. Heggie, *Nat. Mat.* **2**, 333 (2003).
- [162] E. Ertekin, D. C. Chrzan and M. S. Daw, *Phys. Rev. B* **79**, 155421 (2009).
- [163] M. T. Lusk, D. T. Wu, and L. D. Carr, *Phys. Rev. B* **81**, 155444 (2010).
- [164] R. Grantab, V. B. Shenoy, and R. S. Ruoff, *Science* **330**, 946 (2010).
- [165] J. Lahiri, Y. Lin, P. Bozkurt, I. I. Oleynik, and M. Batzill, *Nat. Nanotech.* **5**, 326 (2010).
- [166] D. J. Appelhans, Z. Lin, and M. T. Lusk, *Phys. Rev. B* **82**, 073410 (2010).
- [167] D. J. Appelhans, L. D. Carr, and M. T. Lusk, *New J. Phys.* **12**, 125006 (2010).
- [168] S. Okada, T. Kawai, and K. Nakada, *J. Phys. Soc. Jpn.* **80**, 013709 (2011).
- [169] J. Kotakoski, A. V. Krasheninnikov, U. Kaiser, and J. C. Meyer, *Phys. Rev. Lett.* **106**, 105505 (2011).
- [170] A. R. Botello-Méndez, X. Declerck, M. Terrones, H. Terronesa, and J.-C. Charlier, *Nanoscale* **3**, 2868 (2011).
- [171] A. Lherbier, Simon M.-M. Dubois, X. Declerck, S. Roche, Y.-M. Niquet, and J.-C. Charlier, *Phys. Rev. Lett.* **106**, 046803 (2011).
- [172] T. Fujimori, L. R. Radovic, A. B. Silva-Tapia, M. Endo, and K. Kaneko, *Carbon* **50**, 3274 (2012).
- [173] N. Hamada, S.I. Sawada, and A. Oshiyama, *Phys. Rev. Lett.* **68**, 1579 (1992).
- [174] K. Nakada, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, *Phys. Rev. B* **54**, 17954 (1996).
- [175] Y.-W. Son, M. L. Cohen, and S. G. Louie, *Phys. Rev. Lett.* **97**, 216803 (2006).
- [176] M. Y. Han, B. Ozyilmaz, Y. Zhang, and P. Kim, *Phys. Rev. Lett.* **98**, 206805 (2007).
- [177] F. Diederich, *Nature* **369**, 199 (1994).
- [178] U. H. F. Bunz, Y. Rubin, and Y. Tobe, *Chem. Soc. Rev.* **28**, 107 (1999).
- [179] A. Hirsch, *Nat. Mat.* **9**, 868 (2010).
- [180] Y. Li, L. Xu, H. Liua, and Y. Li, *Chem. Soc. Rev.* **43**, 2572 (2014).
- [181] Q. Peng, A. K. Dearden, J. Crean, L. Han, S. Liu, X. Wen, and S. De, *Nanotech. Sci. Appl.* **7**, 1 (2014).
- [182] E. A. Belenkov, V. V. Mavrinskii, T. E. Belenkova, and V. M. Chernov, *J. Exp. Theor. Phys.* **120**, 820 (2015).
- [183] D. Sundholm, L. N. Wirzb, and P. Schwerdtfeger, *Nanoscale* **7**, 15886 (2015).
- [184] A. T. Balaban, C. C. Rentia and E. Ciupitu, *Rev. Roum. Chim.* **13**, 231 (1968).

- [185] R. H. Baughman, H. Eckhardt, and M. Kertesz, *J. Chem. Phys.* **87**, 6687 (1987).
- [186] R. H. Baughman, D. S. Galvão, C. Cui, Y. Wang, and D. Tomádněk, *Chem. Phys. Lett.* **204**, 8 (1993).
- [187] N. Narita, S. Nagai, S. Suzuki, and K. Nakao, *Phys. Rev. B* **58**, 11009 (1998).
- [188] V. R. Coluci, S. F. Braga, S. B. Legoas, D. S. Galvão, and R. H. Baughman, *Phys. Rev. B* **68**, 035430 (2003).
- [189] V. R. Coluci, S. F. Braga, S. B. Legoas, D. S. Galvao, and, R. H. Baughman, *Nanotech.* **15**, S142 (2004).
- [190] J.-X. Jiang, F. Su, H. Niu, C. D. Wood, N. L. Campbell, Y. Z. Khimyak, and A. I. Cooper, *Chem. Commun.* **4**, 486 (2008).
- [191] G. Li, Y. Li, H. Liu, Y. Guo, Y. Lia, and D. Zhu, *Chem. Commun.* **46**, 3256 (2010).
- [192] M. Wu, X. Wu, Y. Pei, Y. Wang, and X. C. Zeng, *Chem. Commun.* **47**, 4406 (2011).
- [193] Y.-Q. Zhang, N. Kepčija, M. Kleinschrodt, K. Diller, S. Fischer, A. C. Papageorgiou, F. Allegretti, J. Björk, S. Klyatskaya, F. Klappenberger, M. Ruben, and J. V. Barth, *Nat. Commun.* **3**, 1286 (2012).
- [194] S. W. Cranford, D. B. Brommer, and M. J. Buehler, *Nanoscale* **4**, 7797 (2012).
- [195] H. Huang, W. Duan, and Z. Liu, *New J. Phys.* **15**, 023004 (2013).
- [196] A. T. Balaban, *Open Chem. Phys. J.* **5**, 1 (2013).
- [197] W.-J. Yin, Y.-E. Xie, L.-M. Liu, R.-Z. Wang, X.-L. Wei, L. Lau, J.-X. Zhong, and Y.-P. Chen, *J. Mater. Chem. A* **1**, 5341 (2013).
- [198] M. Hu, J. He, Q. Wang, Q. Huang, D. Yu, Y. Tian, and B. Xu, *J. Superhard Mater.* **36**, 257 (2014).
- [199] X. Qian, H. Liu, C. Huang, S. Chen, L. Zhang, Y. Li, J. Wang, and Y. Li, *Sci. Rep.* **5**, 7756 (2015).
- [200] M. Hu, Y. Pan, K. Luo, J. He, D. Yu, and B. Xu, *Carbon* **91**, 518 (2015).
- [201] H. Kim, Y. Kim, J. Kim, and W. Y. Kim, *Carbon* **98**, 404 (2016).
- [202] J.-T. Wang, C. Chen, H.-D. Li, H. Mizuseki, and Y. Kawazoe, *Sci. Rep.* **6**, 24665 (2016).
- [203] H. Vora and T. J. Moravec, *J. Appl. Phys.* **52**, 6151 (1981).
- [204] N. R. Greiner, D.S. Phillips, J. D. Johnson, and F. Volk, *Nature* **333**, 440 (1988).
- [205] M. Frenklach, R. Kematich, D. Huang, W. Howard, K. E. Spear, A. W. Phelps, and R. Koba, *J. Appl. Phys.* **66**, 395 (1989).
- [206] H. Hirai, K. Kondo, and H. Sugiura, *Appl. Phys. Lett.* **61**, 414 (1992).
- [207] M. Rossi, G. Vitali, M. L. Terranova, and V. Sessa, *Appl. Phys. Lett.* **63**, 2765 (1993).
- [208] K. Yamada and A. B. Sawaoka, *Carbon* **32**, 665 (1994).
- [209] M. L. Terranova, M. Rossi, V. Sessa, and G. Vitali, *Solid State Commun.* **91**, 55, (1994).
- [210] A. Grill, *Diam. Relat. Mater.* **8**, 428 (1999).

- [211] I. Konyashin, A. Zern, J. Mayer, F. Aldinger, V. Babaev, V. Khvostov, and M. Guseva, *Diam. Relat. Mater.* **10**, 99 (2001).
- [212] P. Santiago, G. A. Camacho-Bragado, M. Marin-Almazo, J. Murgich, and M. José'-Yacaman, *Energy Fuels* **18**, 390 (2004).
- [213] M. J. Bucknum, I. Stanarin, and E. A. Castro, *Mol. Phys.* **103**, 2707 (2005).
- [214] D. J. Kennett, J. P. Kennett, A. West, C. Mercer, S. S. Q. Hee, L. Bement, T. E. Bunch, M. Sellers, and W. S. Wolbach, *Science* **323**, 94 (2009).
- [215] J. Robertson, *Prog. Sol. State Chem.* **21**, 199 (1991).
- [216] J. Robertson, *Mat. Sci. Eng. R Rep.* **37**, 129 (2002).
- [217] L. A. Pesin, *J. Matter. Sci.* **37**, 1 (2002).
- [218] J. Gibson, M. Holohan, and L. Riley, *J. Chem. Soc.* 456 (1946).
- [219] J. Robertson and E. P. O'Reilly, *Phys. Rev. B* **35**, 2946 (1987).
- [220] D. J. H. Cockayne and D. R. McKenzie, *Acta Cryst. A* **44**, 870, (1988).
- [221] A. F. Goncharov, I. N. Makarenko, and S. M. Stishov, *Sov. Phys. JETP* **69**, 380 (1989).
- [222] D. R. McKenzie, D. Muller, and B. A. Pailthorpe, *Phys. Rev. Lett.* **67**, 773 (1991).
- [223] P. H. Gaskell, A. Saeed, P. Chieux, and D. R. McKenzie, *Phys. Rev. Lett.* **67**, 1286 (1991).
- [224] P. C. Kelires, *Phys. Rev. Lett.* **68**, 1854 (1992).
- [225] P. C. Kelires, *Phys. Rev. B* **47**, 1829 (1993).
- [226] T. Frauenheim, P. Blaudeck, U. Stephan, and G. Jungnickel, *Phys. Rev. B* **48**, 4823 (1993).
- [227] C. Z. Wang and K. M. Ho, *Phys. Rev. Lett.* **71**, 1184 (1993).
- [228] C. Z. Wang, and K. M. Ho, *J. Phys.: Cond. Matter* **6**, L239 (1994).
- [229] C. H. Lee, W. R. L. Lambrecht, B. Segall P. C. Kelires T. Frauenheim, and U. Stephan, *Phys. Rev. B* **49**, 11448 (1994).
- [230] D. A. Drabold, P. A. Fedders, and Petra Stumm, *Phys. Rev. B* **49**, 16415 (1994).
- [231] U. Stephan, T. Frauenheim, P. Blaudeck, and G. Jungnickel, *Phys. Rev. B* **50**, 1489 (1994).
- [232] C. Z. Wang and K. M. Ho, *Phys. Rev. B* **50**, 12429 (1994).
- [233] P. C. Kelires, *Phys. Rev. Lett.* **73**, 2460 (1994).
- [234] K. W. R. Gilkes, P. H. Gaskell, and J. Robertson, *Phys. Rev. B* **51**, 12303 (1995).
- [235] B. R. Djordjevic, M. F. Thorpe and F. Wooten, *Phys. Rev. B* **52**, 5685 (1995).
- [236] D. A. Drabold, P. A. Fedders, and M. P. Grumbach, *Phys. Rev. B* **54**, 5480 (1996).
- [237] N. A. Marks, D. R. McKenzie, B. A. Pailthorpe, M. Bernasconi, and M. Parrinello, *Phys. Rev. B* **54**, 9703 (1996).
- [238] N. A. Marks, D. R. McKenzie, B. A. Pailthorpe, M. Bernasconi, and M. Parrinello, *Phys. Rev. Lett.* **76**, 768 (1996).

- [239] S. J. Clark, J. Crain, and G. J. Ackland, *Phys. Rev. B* **55**, 14059 (1997).
- [240] P. A. Schultz and E. B. Stechel, *Phys. Rev. B* **57**, 3295 (1998).
- [241] J. P. Sullivan, T. A. Friedmann, M. P. de Boer, D. A. LaVan, R. J. Hohlfelder, C. I. H. Ashby, M. T. Dugger, M. Mitchell, R. G. Dunn, and A. J. Magerkurth, *Mat. Res. Soc. Symp. Proc.* **657**, EE7.1.1 (2001).
- [242] M. G. Fyta, I. N. Remediakis, and P. C. Kelires, *Phys. Rev. B* **67**, 035423 (2003).
- [243] D. S. Grierson, A. V. Sumant, A. R. Konicek, T. A. Friedmann, J. P. Sullivan, and R. W. Carpick, *J. Appl. Phys.* **107**, 033523 (2010).
- [244] V. Kapko, D. A. Drabold, and M. F. Thorpe, *Phys. Status Solidi B* **247**, 1197 (2010).
- [245] Y. Lin, L. Zhang, H.-K. Mao, P. Chow, Y. Xiao, M. Baldini, J. Shu, and W. L. Mao, *Phys. Rev. Lett.* **107**, 175504 (2011).
- [246] B. A. Fairchild, S. Rubanov, D. W. M. Lau, M. Robinson, I. Suarez-Martinez, N. Marks, A. D. Greentree, D. McCulloch, and S. Praver, *Adv. Mater.* **24**, 2024 (2012).
- [247] F. Legrain, K. Kotsis, and S. Manzhos, *J. Phys. Chem. C* **119**, 13496 (2015).
- [248] J. R. Platt, *Z. Kristallogr* **109**, 226 (1957).
- [249] A. M. Sladkov, and Y. P. Kudryavtsev, *Priroda* **5**, 88 (1964).
- [250] J. Kakinoki, *Acta. Cryst.* **18**, 578 (1965).
- [251] I. Bally, E. Ciornei, and A. T. Balaban, *Rev Roum. Chem.* **13**, 1507 (1968).
- [252] D. A. Bochvar and E. G. Gal'pern, *Sov. Phys. Dokl.* **18**, 239 (1973).
- [253] V. V. Korshak, Yu. P. Kudryavtsev, and A. M. Sladkov, *Vestn. Akad. Nauk SSSR* **1**, 70 (1978).
- [254] M. V. Nikerov, D. A. Bochvar, and I. V. Stankevich, *Izv. Akad. Nauk SSSR, Ser. Khim.* **5**, 1117 (1981).
- [255] M. V. Nikerov, D. A. Bochvar, and I. V. Stankevich, *Zh. Strukt. Khim.* **23**, 13 (1982).
- [256] M. V. Nikerov, D. A. Bochvar, and I. V. Stankevich, *Zh. Strukt. Khim.* **23**, 177 (1982).
- [257] V. M. Melnitchenko, Y. N. Nikulin, and A. M. Sladkov, *Dokl. Akad. Nauk SSSR.* **267** (1982).
- [258] R. Hoffmann, T. Hughbanks, and M. Kertisz, *J. Am. Chem. Soc.* **105**, 4831 (1983).
- [259] M. T. Yin and M. L. Cohen, *Phys. Rev. Lett.* **50**, 2006 (1983).
- [260] J. R. Dias, *Carbon* **22**, 107 (1984).
- [261] V. S. Ivan, M. V. Nikerov, and D. A. Bochvar, *Russ. Chem. Rev.* **53**, 640 (1984).
- [262] M. T. Yin, *Phys. Rev. B* **30**, 1773 (1984).
- [263] J. K. Burdett and S. Lee, *J. Am. Chem. Soc.* **107**, 3063 (1985).
- [264] R. Biswas, R. M. Martin, R. J. Needs and O. H. Nielsen, *Phys. Rev. B* **35**, 9559 (1987).
- [265] K. M. Merz, Jr., R. Hoffmann, and A. T. Balabant, *J. Am. Chem. Soc.* **109**, 6742 (1987).
- [266] R. L. Johnston and R. Hoffmann, *J. Am. Chem. Soc.* **111**, 810 (1989).

- [267] R. L. Johnston and R. Hoffmann, *Polyhedron* **9**, 1901 (1990).
- [268] K. E. Spear, A. W. Phelps, and W. B. White, *J. Mat. Res.* **5**, 2277 (1990).
- [269] M. A. Tamor and K. C. Hass, *J. Mater. Res.* **5**, 2273 (1990).
- [270] H. R. Karfunkel and T. Dressler, *J. Am. Chem. Soc.* **114**, 2285 (1992).
- [271] M. O'Keeffe, G. B. Adams, and O. F. Sankey, *Phys. Rev. Lett.* **68**, 2325 (1992).
- [272] R. Nesper, K. Vogel, and P. E. Blöchl, *Angew. Chem. Int. Ed.* **32**, 701 (1993).
- [273] A. T. Balaban, D. J. Klein, and C. A. Folden, *Chem. Phys. Lett.* **217**, 266 (1994).
- [274] H. W. Kroto, *Nature* **359**, 670 (1992).
- [275] R. H. Baughman and C. Cui, *Synth. Met.* **55**, 315, (1993).
- [276] R. H. Baughman and D. S. Galvao, *Nature* **365**, 735 (1993).
- [277] N. Shima and H. Aoki, *Phys. Rev. Lett.* **71**, 4389 (1993).
- [278] H. Terrones, J. Fayos, and J. L. Aragon, *Acta Metall. Mater.* **42**, 2687 (1994).
- [279] H. Zhu, A. T. Balaban, D. J. Klein, and T. P. Živković, *J. Chem. Phys.* **101**, 5281 (1994).
- [280] K. Nakada, K. Takeda, and H. Hosoya, *Theochem. J. Mol. Struc.* **311**, 79 (1994).
- [281] M. J. Bucknum and R. Hoffmann, *J. Am. Chem. Soc.* **116**, 11456 (1994).
- [282] S. Scandolo, M. Bernasconi, G. L. Chiarotti, P. Focher, and E. Tosatti, *Phys. Rev. Lett.* **74**, 4015 (1995).
- [283] G. Benedek, E. Galvani, S. Sanguinetti, and S. Serra, *Chem. Phys. Lett.* **244**, 339 (1995).
- [284] S. J. Clark, G. J. Ackland, and J. Crain, *Phys. Rev. B* **52**, 15035 (1995).
- [285] S. Scandolo, G. L. Chiarotti, and E. Tosatti, *Phys. Rev. B* **53**, 5051 (1996).
- [286] V. H. Crespi, L. X. Benedict, M. L. Cohen, and S. G. Louie, *Phys. Rev. B* **53**, R13303 (1996).
- [287] G. Benedek, L. Colombo, S. Gaito, E. Galvani, and S. Serra, *J. Chem. Phys.* **106**, 2311 (1997).
- [288] R. H. Baughman, A. Y. Liu, C. Cui, and P. J. Schields, *Synth. Met.* **86**, 2371, (1997).
- [289] G. Jungnickel, P. K. Sitch, T. Frauenheim, B. R. Eggen, M. I. Heggie, C. D. Latham, and C. S. G. Cousins, *Phys. Rev. B* **57**, 661 (1998).
- [290] M. Côté, J. C. Grossman, M. L. Cohen, and S. G. Louie, *Phys. Rev. B* **58**, 664 (1998).
- [291] S. Gaito, L. Colombo, and G. Benedek, *Europhys. Lett.* **44**, 525 (1998).
- [292] M. O'Keeffe and G. B. Adams, *Philos. Mag. Lett.* **78**, 21, (1998).
- [293] P. A. Schultz, K. Leung, and E. B. Stechel, *Phys. Rev. B* **59**, 733 (1999).
- [294] P. W. Fowler, T. Heine, K. M. Rogers, J. P. B. Sandall, G. Seifert, and F. Zerbetto, *Chem. Phys. Lett.* **300**, 369 (1999).
- [295] J. Fayos, *J. Solid State Chem.* **148**, 278 (1999).
- [296] B. Winkler, C. J. Pickard, V. Milman, W. E. Klee, and G. Thimm, *Chem. Phys. Lett.* **312**, 536 (1999).

- [297] H. Terrones, M. Terrones, E. Hernández, N. Grobert, J. C. Charlier, and P. M. Ajayan, *Phys. Rev. Lett.* **84**, 1716 (2000).
- [298] M. Deza, P. W. Fowler, M. Shtogrin, and K. Vietze, *J. Chem. Inform. Comput. Sci.* **40**, 1325 (2000).
- [299] N. Park and J. Ihm, *Phys. Rev. B* **62**, 7614 (2000).
- [300] E. Scholtzová, L. T. Nagy, and K. Putyera, *J. Chem. Inform. Comput. Sci.* **41**, 451 (2001).
- [301] B. Winkler, C. J. Pickard, V. Milman, and G. Thimm, *Chem. Phys. Lett.* **337**, 36 (2001).
- [302] M. J. Bucknum, *Chem. Preprint Arch.* **2001**, 75 (2001).
- [303] K. Umemoto, S. Saito, S. Berber, and D. Tománek, *Phys. Rev. B* **64**, 193409 (2001).
- [304] E. G. Gal'pern, A. R. Sabirov, I. V. Stankevich, A. L. Chistyakov and L. A. Chernozatonskii, *Phys. Solid State* **44**, 623 (2002).
- [305] J. V. Badding and T. J. Scheidemantel, *Solid State Commun.* **122**, 473 (2002).
- [306] X. Blase, *Phys. Rev. B* **67**, 035211 (2003).
- [307] S. Okada and A. Oshiyama, *Phys. Rev. B* **68**, 235402 (2003).
- [308] R. T. Strong, C. J. Pickard, V. Milman, G. Thimm, and B. Winkler, *Phys. Rev. B* **70**, 045101 (2004).
- [309] X. Rocquefelte, G.-M. Rignanese, V. Meunier, H. Terrones, M. Terrones, and J.-C. Charlier, *Nano Lett.* **4**, 805 (2004).
- [310] A. L. Chistyakov, I. V. Stankevich, and A. A. Korlyukov, *Phys. Sol. State* **47**, 191 (2005).
- [311] M. J. Bucknum, I. Stamatina, and E. A. Castro, *Mol. Phys.* **103**, 2707 (2005).
- [312] F. J. Ribeiro, P. Tangney, S. G. Louie, and M. L. Cohen, *Phys. Rev. B* **72**, 214109 (2005).
- [313] A. R. Oganov and C. W. Glass, *J. Chem. Phys.* **124**, 244704 (2006).
- [314] B. Wen, J. Zhao, T. Li, and C. Dong, *New J. Phys.* **8**, 62 (2006).
- [315] F. J. Ribeiro, P. Tangney, S. G. Louie, and M. L. Cohen, *Phys. Rev. B* **74**, 172101 (2006).
- [316] A. Kuc and G. Seifert, *Phys. Rev. B* **74**, 214104 (2006).
- [317] M. J. Bucknum and E. A. Castro, *J. Chem. Theor. Comput.* **2**, 775 (2006).
- [318] A. N. Enyashin and A. L. Ivanovskii, *JETP Lett.* **86**, 537 (2007).
- [319] M. J. Bucknum and E. A. Castro, *Solid State Sci.* **10**, 1245 (2008).
- [320] T. Sunada, *Not. Am. Math. Soc.* **55**, 208 (2008).
- [321] G.-M. Rignanese and J.-C. Charlier, *Phys. Rev. B* **78**, 125415 (2008).
- [322] M. Itoh, M. Kotani, H. Naito, T. Sunada, Y. Kawazoe, and T. Adschiri, *Phys. Rev. Lett.* **102**, 055703 (2009).
- [323] J. Sun, D. D. Klug, and R. Martončák, *J. Chem. Phys.* **130**, 194512 (2009).
- [324] Q. Li, Y. Ma, A. R. Oganov, H. Wang, H. Wang, Y. Xu, T. Cui, H.-K. Mao, and G. Zou, *Phys. Rev. Lett.* **102**, 175506 (2009).
- [325] A. N. Enyashin and A. L. Ivanovskii, *Chem. Phys. Lett.* **473**, 108 (2009).

- [326] T. Singh, M. J. Behr, E. S. Aydil and D. Maroudas, Chem. Phys. Lett. **474**, 168 (2009).
- [327] C. J. Pickard and R. J. Needs, Phys. Rev. B **81**, 014106 (2010).
- [328] K. Iyakutti, M. Rajarajeswari, and Y. Kawazoe, Physica B **405**, 3324 (2010).
- [329] K. Umemoto, R. M. Wentzcovitch, S. Saito, and T. Miyake, Phys. Rev. Lett. **104**, 125504 (2010).
- [330] P. Melinon and A. Miguel, Handbook of Nanophysics **43**, 1 (2010).
- [331] M. D. Corato, M. Bernasconi, L. D'Alessio, O. Ori, M. V. Putz, and G. Benedek, Topology. Model. Nanostr. Ext. Systems **7**, 105 (2013).
- [332] X.-F. Zhou, G.-R. Qian, X. Dong, L. Zhang, Y. Tian, and H.-T. Wang, Phys. Rev. B **82**, 134126 (2010).
- [333] M. J. Bucknum, B. Wen and E. A. Castro, J. Math. Chem. **48**, 816 (2010).
- [334] V. A. Greshnyakov and E. A. Belenkov, J. Exp. Theor. Phys. **113**, 86 (2011).
- [335] A. J. Karttunen, T. F. Fassler, M. Linnolahti and T. A. Pakkanen, Inorg. Chem. **50**, 1733 (2011).
- [336] J.-T. Wang, C. Chen, and Y. Kawazoe, Phys. Rev. Lett. **106**, 075501 (2011).
- [337] X.-L. Sheng, Q.-B. Yan, F. Ye, Q.-R. Zheng, and G. Su, Phys. Rev. Lett. **106**, 155703 (2011).
- [338] E. A. Belenkov and V. A. Ali-Pasha, Russ. Phys. J. **53**, 1280 (2011).
- [339] P. B. Sorokin, H. Lee, L. Y. Antipina, A. K. Singh, and B. I. Yakobson, Nano Lett. **11**, 2660 (2011).
- [340] Q. Zhu, A. R. Oganov, M. A. Salvadó, P. Pertierra, and A. O. Lyakhov, Phys. Rev. B **83**, 193410 (2011).
- [341] J.-T. Wang, C. Chen, and Y. Kawazoe, Phys. Rev. B **84**, 012102 (2011).
- [342] Y. Liu, G. Wang, Q. Huang, L. Guo, and X. Chen, Phys. Rev. Lett. **108**, 225505 (2012).
- [343] Z. Zhao, B. Xu, X.-F. Zhou, L.-M. Wang, B. Wen, J. He, Z. Liu, H.-T. Wang, and Y. Tian, Phys. Rev. Lett. **107**, 215502 (2011).
- [344] A. O. Lyakhov and A. R. Oganov, Phys. Rev. B **84**, 092103 (2011).
- [345] M. Amsler, J. A. Flores-Livas, L. Lehtovaara, F. Balima, S. A. Ghasemi, D. Machon, S. Pailhès, A. Willand, D. Caliste, S. Botti, A. San Miguel, S. Goedecker, and M. A. L. Marques, Phys. Rev., Lett. **108**, 065501 (2012).
- [346] A. N. Enyashin, V. G. Bamburov, and A. L. Ivanovskii, Dokl. Phys. Chem. **442**, 1 (2012).
- [347] D. Selli, I. A. Baburin, R. Martoňák, and S. Leoni, Phys. Rev. B **84**, 161411(R) (2011).
- [348] Z. Zhao, B. Xu, L.-M. Wang, X.-F. Zhou, J. He, Z. Liu, H.-T. Wang, and Y. Tian, Acs Nano **5**, 7226 (2011).
- [349] J.-T. Wang, C.-F. Chen, and Y. Kawazoe, Phys. Rev. B **85**, 214104 (2012).
- [350] G. Brunetto, P. A. S. Autreto, L. D. Machado, B. I. Santos, R. P. B. dos Santos, and D. S. Galvão, J. Phys. Chem. C **116**, 12810 (2012).
- [351] D. Li, K. Bao, F. Tian, Z. Zeng, Z. He, B. Liu, and T. Cui, Phys. Chem. Chem. Phys. **14**, 4347 (2012).

- [352] J.-T. Wang, C. Chen, and Y. Kawazoe, *Phys. Rev. B* **85**, 033410 (2012).
- [353] H. Niu, X.-Q. Chen, S. Wang, D. Li, W. L. Mao, and Y. Li, *Phys. Rev. Lett.* **108**, 135501 (2012).
- [354] R. C. Andrew, R. E. Mapasha, A. M. Ukpong, and N. Chetty, *Phys. Rev. B* **85**, 125428 (2012).
- [355] F. Tian, X. Dong, Z. Zhao, J. He, and H.-T. Wang, *J. Phys.: Cond. Matter* **24**, 165504 (2012).
- [356] M. J. Bucknum, E. A. Castro, and Bin Wen, *J. Math Chem.* **50**, 2281 (2012).
- [357] C.-P. Tanga and S.-J. Xiong, *AIP Adv.* **2**, 042147 (2012).
- [358] C. He, L. Z. Sun, C. X. Zhang, K. W. Zhang, X. Peng, and J. Zhong, *Phys. Chem. Chem. Phys.* **14**, 8410 (2012).
- [359] R. Zhou and X. C. Zeng, *J. Am. Chem. Soc.* **134**, 7530 (2012).
- [360] M. Amsler, J. A. Flores-Livas, S. Botti, M. A. L. Marques, and S. Goedecker, *Eur. Phys. J. B* **86**, 383 (2013).
- [361] Q. Zhu, Q. Zeng, and A. R. Oganov, *Phys. Rev. B* **85**, 201407(R) (2012).
- [362] C. He, L. Sun, C. Zhang, X. Peng, K. Zhang, and J. Zhong, *Solid State Commun.* **152**, 1560 (2012).
- [363] J.-T. Wang, C. Chen, and Y. Kawazoe, *J. Chem. Phys.* **137**, 024502 (2012).
- [364] Z. Zhao, F. Tian, X. Dong, Q. Li, Q. Wang, H. Wang, X. Zhong, B. Xu, D. Yu, J. He, H.-T. Wang, Y. Ma, and Y. Tian, *J. Am. Chem. Soc.* **134**, 12362 (2012).
- [365] J. Y. Jo and B. G. Kim, *Phys. Rev. B* **86**, 075151 (2012).
- [366] X.-Q. Wang, H.-D. Li, and J.-T. Wang, *Phys. Chem. Chem. Phys.* **14**, 11107 (2012).
- [367] X.-L. Sheng, H.-J. Cui, F. Ye, Q.-B. Yan, Q.-R. Zheng, and G. Su, *J. Appl. Phys.* **112**, 074315 (2012).
- [368] Z. Zhu and D. Tománek, *Phys. Rev. Lett.* **109**, 135501 (2012).
- [369] M. Hu, F. Tian, Z. Zhao, Q. Huang, B. Xu, L.-M. Wang, H.-T. Wang, Y. Tian, and J. He, *J. Phys. Chem. C* **116**, 24233 (2012).
- [370] J. Nisar, X. Jiang, B. Pathak, J. Zhao, T. W. Kang, and R. Ahuja, *Nanotech.* **23**, 385704 (2012).
- [371] L. Yang, H. Y. He, and B. C. Pan, *J. Chem. Phys.* **138**, 024502 (2013).
- [372] Q. Song, B. Wang, K. Deng, X. Feng, M. Wagner, J. D. Gale, K. Mullen, and L. Zhi, *J. Mater. Chem. C* **1**, 38 (2013).
- [373] X.-Q. Wang, H.-D. Li, and J.-T. Wang, *Phys. Chem. Chem. Phys.* **15**, 2024 (2013).
- [374] C. He, L. Sun, C. Zhang, and J. Zhong, *Phys. Chem. Chem. Phys.* **15**, 680 (2013).
- [375] H. Bu, M. Zhao, Y. Xi, X. Wang, H. Peng, C. Wang and X. Liu, *EPL* **100**, 56003 (2012).
- [376] K. Srinivasu, and S. K. Ghosh, *J. Phys. Chem. C* **116**, 25015 (2012).
- [377] S. Botti, M. Amsler, J. A. Flores-Livas, P. Ceria, S. Goedecker, and M. A. L. Marques, *Phys. Rev. B* **88**, 014102 (2013).
- [378] M. Hu, Z. Zhao, F. Tian, A. R. Oganov, Q. Wang, M. Xiong, C. Fan, B. Wen, J. He, D. Yu, H.-T. Wang, B. Xu, and Y. Tian, *Sci. Rep.* **3**, 1331 (2013).

- [379] M. J. Bucknum, D. Prasad and E. A. Castro, *J. Math. Chem.* **51**, 868 (2013).
- [380] X. Jiang, C. Århammar, P. Liu, J. Zhao, and R. Ahuja, *Sci. Rep.* **3**, 1877 (2013).
- [381] H. -Y. Zhao, J. Wang, Q. -M. Ma and Y. Liu, *J. Chem. Phys.* **138**, 164703 (2013).
- [382] L. Huang, Z. Xiang, and D. Cao, *J. Mater. Chem. A* **1**, 3851 (2013).
- [383] X. Zhang, Y. Wang, J. Lv, C. Zhu, Q. Li, M. Zhang, Q. Li, and Y. Ma, *J. Chem. Phys.* **138**, 114101 (2013).
- [384] H. Bu, X. Wang, Y. Xi, X. Zhao, and M. Zhao, *Diam. Relat. Mater.* **37**, 55 (2013).
- [385] C. He, L. Z. Sun, C. X. Zhang, and J. X. Zhong, *arXiv:1302.6430* (2013).
- [386] A. J. Karttunen and T. F. Fassler, *Chem. Phys. Chem.* **14**, 1807 (2013).
- [387] C. Su, H. Jiang, and J. Feng, *Phys. Rev. B* **87**, 075453 (2013).
- [388] B. G. Kim, H. Sim and J. Park, *Solid State Commun.* **169**, 50 (2013).
- [389] X. Jiang, J. Zhao, Y.-L. Li, and R. Ahuja, *Adv. Funct. Mater.* **10**, 5846 (2013).
- [390] L. Öhrström and M. O'Keeffe, *Z. Kristallogr. Cryst. Mater.* **228**, 343 (2013).
- [391] M. Zhang, H. Liu, Y. Du, X. Zhang, Y. Wang, and Q. Li, *Phys. Chem. Chem. Phys.* **15**, 14120 (2013).
- [392] D. L. V. K. Prasad, N. M. Gerovac, M. J. Bucknum, and R. Hoffmann, *J. Chem. Theor. Comput.* **9**, 3855 (2013).
- [393] S. Bahmann, T. Weißbach, and J. Kortus, *Phys. Status Solidi RRL* **7**, 639 (2013).
- [394] E. A. Belenkov and V. A. Greshnyakov, *J. Struct. Chem.* **55**, 409 (2014).
- [395] S. Zhang, Q. Wanga, X. Chen, and P. Jena, *Proc. Natl. Acad. Sci. USA* **110**, 18809 (2013).
- [396] L. F. C. Pereira, I. Savić, and D. Donadio, *New J. Phys.* **15**, 105019 (2013).
- [397] M. Maruyama and S. Okada, *Appl. Phys. Expr.* **6**, 095101 (2013).
- [398] L.-C. Xu, R.-Z. Wang, M.-S. Miao, X.-L. Wei, Y.-P. Chen, H. Yan, W.-M. Lau, L.-M. Liu and Y.-M. Ma, *Nanoscale* **6**, 1113 (2014).
- [399] Y. A. Kvashnina, A. G. Kvashnin, and P. B. Sorokin, *J. Appl. Phys.* **114**, 183708 (2013).
- [400] C. He and J. Zhong, *Solid State Commun.* **181**, 24 (2014).
- [401] J.-T. Wang, C. Chen, E. Wang, and Y. Kawazoe, *Sci. Rep.* **4**, 4339 (2013).
- [402] M. Liu, V. I. Artyukhov, H. Lee, F. Xu, and B. I. Yakobson, *Acs Nano* **7**, 10075 (2013).
- [403] H. Bu, M. Zhao, W. Dong, S. Lua, and X. Wang, *J. Mater. Chem. C* **2**, 2751 (2014).
- [404] M. Hu, Q. Huang, Z. Zhao, B. Xu, D. Yu and J. He, *Diam. Relat. Mater.* **46**, 15 (2014).
- [405] M. Maruyama and S. Okada, *Jpn. J. Appl. Phys.* **53**, 06JD02 (2014).
- [406] J.-T. Wang, C. Chen, and Y. Kawazoe, *Sci. Rep.* **3**, 3077 (2013).
- [407] C.-Y. Niu, X.-Q. Wang, and J.-T. Wang, *J. Chem. Phys.* **140**, 054514 (2014).
- [408] E. A. Belenkov, M. M. Brzhezinskaya, and V. A. Greshnyakov, *Diam. Relat. Mater.* **50**, 9 (2014).
- [409] E. A. Belenkov and V. A. Greshnyakov, *J. Exp. Theor. Phys.* **119**, 101 (2014).

- [410] M. C. Nguyen, X. Zhao, C.-Z. Wang, and K.-M. Ho, *Phys. Rev. B* **89**, 184112 (2014).
- [411] Y. Liu, M. Lu, and M. Zhang, *Phys. Lett. A* **378**, 3326 (2014).
- [412] M. Hu, X. Dong, Y. Pan, B. Xu, D. Yu, and J. He, *J. Phys.: Cond. Matter* **26**, 235402 (2014).
- [413] D. Li, F. Tian, D. Duan, Z. Zhao, Y. Liu, B. Chu, X. Sha, L. Wang, B. Liu and T. Cui, *RSC Adv.* **4**, 17364 (2014).
- [414] Y. Chen, Y. Y. Sun, H. Wang, D. West, Y. Xie, J. Zhong, V. Meunier, M. L. Cohen, and S. B. Zhang, *Phys. Rev. Lett.* **113**, 085501 (2014).
- [415] S. Zhang, J. Zhou, Q. Wang, X. Chen, Y. Kawazoe, and P. Jena, *Proc. Natl. Acad. Sci. USA* **112**, 2372 (2015).
- [416] H. -Y. Zhao, J. Wang, X. -J. Su, D. -B. Zhang and Y. Liu, *J. Phys. Chem. C* **118**, 27502 (2014).
- [417] B. R. Sharma, A. Manjanath, and A. K. Singh, *Sci. Rep.* **4**, 7164 (2014).
- [418] Z. Zhang, H. Liu, and M. Zhang, *EPL* **108**, 46006 (2014).
- [419] I. A. Baburin, D. M. Proserpio, V. A. Saleev, and A. V. Shipilov, *Phys. Chem. Chem. Phys.* **17**, 1332 (2015).
- [420] C. Cheng, Z.-L. Lv, Y. Cheng, X.-R. Chen, and L.-C. Cai, *Diam. Relat. Mater.* **43**, 49 (2014).
- [421] L.-C. Xu, X.-J. Song, R.-Z. Wang, Z. Yang, X.-Y. Li, and H. Yan, *Appl. Phys. Lett.* **107**, 021905 (2015).
- [422] Ning Xu, J.-F. Li, B.-L. Huang, and B.-L. Wang, *Chin. Phys. B* **25**, 016103 (2015).
- [423] G. Wen-Feng, W. Ling-Sheng, L. Zhi-Ping, X. Mei-Rong, and G. Fa-Ming, *Chin. Phys. Lett.* **32**, 096201 (2015).
- [424] X. Meng-Jiang, L. Bin-Hua, Y. Zheng-Tao, and C. Qi, *Commun. Theor. Phys.* **64**, 237 (2015).
- [425] D. Li, F. Tian, B. Chu, D. Duan, X. Sha, Y. Lv, H. Zhang, N. Lu, B. Liu, and T. Cui, *Sci. Rep.* **5**, 13447 (2015).
- [426] Z.-Z. Li, C.-S. Lian, J. Xu, L.-F. Xu, J.-T. Wang, and C. Chen, *Phys. Rev. B* **91**, 214106 (2015).
- [427] X. Dong, M. Hu, J. He, Y. Tian and H.-T. Wang, *Sci. Rep.* **5**, 10713 (2015).
- [428] D. Li, F. Tian, B. Chu, D. Duan, S. Wei, Yu. Lv, H. Zhang, L. Wang, N. Lu, B. Liu, and T. Cui, *J. Mater. Chem. A* **3**, 10448 (2015).
- [429] W.-J. Yin, Y.-P. Chen, Y.-E. Xie, L.-M. Liu, and S. B. Zhang, *Phys. Chem. Chem. Phys.* **17**, 14083 (2015).
- [430] A. Mujica, C. J. Pickard, and R. J. Needs, *Phys. Rev. B* **91**, 214104 (2015).
- [431] M. Hu, X. Dong, B. Yang, B. Xu, D. Yu and J. He, *Phys. Chem. Chem. Phys.* **17**, 13028 (2015).
- [432] S. Xu, L. Wang, Y. Liu, R. Yuan, X. Xu, and Y. Cai, *Phys. Lett. A* **379**, 2116 (2015).
- [433] K. Ohno, H. Satoh, and T. Iwamoto, *Chem. Phys. Lett.* **633**, 120 (2015).
- [434] E. A. Belenkov and V. A. Greshnyakov, *J. Mater. Sci.* **50**, 7627 (2015).

- [435] K. Ohno, H. Tokoyama, and H. Yamakado, Chem. Phys. Lett. **635**, 180 (2015).
- [436] M. Xing, B. Li, Z. Yu, and Q. Chen, J. Mater. Sci. **50**, 7104 (2015).
- [437] Z. Wang, X.-F. Zhou, X. Zhang, Q. Zhu, H. Dong, M. Zhao, and A. R. Oganov, Nano Lett. **15**, 6182 (2015).
- [438] W. Liu, M.-S. Miaobe, and J.-Y. Liu, RSC Adv. **5**, 70766 (2015).
- [439] J. Luöder, C. Puglia, H. Ottosson, O. Eriksson, B. Sanyal, and B. Brena, J. Chem. Phys. **144**, 024702 (2016).
- [440] Y. Chen, Y. Xie, S. A. Yang, H. Pan, F. Zhang, M. L. Cohen, and S. Zhang, Nano Lett. **15**, 6974 (2015).
- [441] M. Xing, B. Li, Z. Yu, and Q. Chen, Structural, Eur. Phys. J. B **89**, 9 (2016).
- [442] Y. Cheng, J. Du, R. Melnik, Y. Kawazoe, and B. Wen, Carbon **98**, 468 (2016).
- [443] K. Ohno, H. Satoh, T. Iwamoto, H. Tokoyama, and H. Yamakado, Chem. Phys. Lett. **639**, 178 (2015).
- [444] C.-X. Zhao, C.-Y. Niu, Z.-J. Qin, X. Y. Ren, J.-T. Wang, J.-H. Cho, and Y. Jia, Sci. Rep. **6**, 21879 (2016).
- [445] Y. Cheng, R. Melnik, Y. Kawazoe, and B. Wen, Cryst. Growth Des. **16**, 1360 (2016).
- [446] Z. Li, M. Hu, M. Ma, Y. Gao, B. Xu, J. He, D. Yu, Y. Tian, and Z. Zhao, Carbon **105**, 151 (2016).
- [447] M. J. Xing, B. H. Li, Z. T. Yu, and Q. Chen, RSC Adv. **6**, 32740 (2016).
- [448] C. Zhong, Y. Chen, Y. Xie, S. A. Yang, M. L. Cohenc, and S. B. Zhang, Nanoscale **8**, 7232 (2016).
- [449] J.-T. Wang, H. Weng, S. Nie, Z. Fang, Y. Kawazoe, and C. Chen, Phys. Rev. Lett. **116**, 195501 (2016).
- [450] M. Hu, M. Ma, Z. Zhao, D. Yu, and J. He, AIP Adv. **6**, 055020 (2016).
- [451] C. He, C.-X. Zhang, H. Xiao, L. Meng, and J.-X. Zhong, Carbon **112**, 91 (2017).
- [452] Y. Cai, H. Wang, S. Xu, Y. Hu, N. Liu, and X. Xu, AIP Adv. **6**, 065225 (2016).
- [453] Y.-Y. Zhang, S. Chen, H. Xiang, and X.-G. Gong, Carbon **109**, 246 (2016).
- [454] J. Liu, S. Zhang, Y. Guo, and Q. Wang, Sci. Rep. **6**, 37528 (2016).
- [455] M. Xing, B. Li, Z. Yu, and Q. Chen, Materials **9**, 484 (2016).
- [456] Z.-J. Wei, H.-Y. Zhao, J. Wang, and Y. Liu, J. Appl. Phys. **120**, 165101 (2016).
- [457] J.-Q. Wang, C.-X. Zhao, C.-Y. Niu, Q. Sun, and Y. Jia, J. Phys.: Cond. Matter **28**, 475402 (2016).
- [458] X. Zhu and M. Wang, RSC Adv. **6**, 112035 (2016).
- [459] Z.-Z. Li, J.-T. Wang, L.-F. Xu, and C. Chen, Phys. Rev. B **94**, 174102 (2016).
- [460] Q. Wei, Q. Zhang, H. Yan, and M. Zhang, J. Mater. Sci. **52**, 2385 (2017).

S2. The derivation of Eq. (1)^[S1]

Suppose the unit cell h_0 with its volume $V_0 = \det h_0$. When an infinitesimal strain tensor (3×3) ε is applied to the system, the total energy E changes. The stress tensor (3×3) σ is defined as a conjugate intensive tensor to the strain. In this case, the energy change ΔE is described as,

$$\Delta E|_{h_0} = \text{Tr}(\sigma \varepsilon) V_0 = V_0 \sum_{i,j} \sigma_{ij} \varepsilon_{ji}$$

$$\sigma_{ij}|_{h_0} = - \frac{1}{V_0} \frac{\partial E}{\partial \varepsilon_{ij}} \bigg|_{h_0}$$

In the case, the unit cell matrix h with the strain ε is described as,

$$h = (\mathbf{I} + \varepsilon) h_0$$

where

$$h \equiv \{a_1, a_2, a_3\} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

$$\varepsilon = h h_0^{-1} - \mathbf{I}$$

$$\varepsilon_{kl} = \sum_m h_{km} (h_0^{-1})_{ml} - \delta_{kl}$$

$$\frac{\partial}{\partial h_{ij}} = \sum_{k,l} \frac{\partial \varepsilon_{kl}}{\partial h_{ij}} \frac{\partial}{\partial \varepsilon_{kl}} = \sum_{k,l} \sum_m \delta_{ki} \delta_{mj} (h_0^{-1})_{ml} \frac{\partial}{\partial \varepsilon_{kl}} = \sum_l (h_0^{-1})_{jl} \frac{\partial}{\partial \varepsilon_{il}}$$

$$\frac{\partial E}{\partial h_{ij}} = \sum_l (h_0^{-1})_{jl} \frac{\partial E}{\partial \varepsilon_{il}} = -V_0 \sum_l (h_0^{-1})_{jl} \sigma_{il}$$

[S1] Y. Tateyama, Ph.D. thesis, The University of Tokyo, 1998.

S3. Initial structures

(i) 3D: random structure

C	0.137308413163	0.506599825145	-1.868353596046
C	0.454881030641	0.261893055938	-0.459650647353
C	-0.038572922682	-0.582719939072	1.856101415009
C	-0.553616521124	-0.185772942013	0.471902828391
TV	2.403797389080	0.633328610945	-0.618894291773
TV	-0.000000000000	2.485867546525	0.618802310954
TV	0.000000000000	-0.000000000000	4.655918444073

(ii) 3D: optimized structure from the random structure (i)

C	0.092861193378	0.549889344723	-1.863216378662
C	0.512456418314	0.219972286613	-0.457163965076
C	-0.092850046223	-0.549905060801	1.863215315444
C	-0.512467565473	-0.219956570536	0.457165028293
TV	2.421958222986	0.587673818868	-0.584585848161
TV	0.000000000000	2.492272339496	0.584417956901
TV	-0.000000000000	0.000000000000	4.640726338585

(iii) 2D: random structure

C	0.842413738951	-0.699941099220	-1.536504084107
C	-0.150809902139	0.330402959125	-0.417816714320
C	-0.668202549609	0.989342176372	0.929799430199
C	-0.023401287203	-0.619804036277	1.024521368228
TV	2.970616288560	0.000000000000	0.000000000000
TV	0.000000000000	3.149283275592	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

(iv) 2D: optimized structure from the random structure (iii)

C	0.980565465842	-0.000102994868	-1.199464635400
C	-0.326823115063	0.000028326091	-0.611024974393
C	-0.326844680284	0.689777160123	0.905223289939
C	-0.326897670489	-0.689702491349	0.905266319858
TV	2.614795654964	-0.000098341352	-0.000000000000
TV	-0.000000000000	2.724424929913	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

(v) 1D: random structure

C	1.156776368568	-0.019423438428	-0.006132277899
C	-0.000010435852	0.268348498411	-0.851570760546
C	0.000010488915	-0.229477135115	0.863831443902
C	-1.156776421628	-0.019447924867	-0.006128405456
TV	3.696192700632	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

(vi) 1D: optimized structure from the random structure (v)

C	1.144569087036	-0.069925312093	-0.020371337496
C	0.000009423911	0.310333337432	-0.807407316215
C	-0.000013133539	-0.170501186304	0.848170586744
C	-1.144565377405	-0.069906839033	-0.020391933034
TV	3.665894106167	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

S4. Cartesian coordinate of all obtained MINs

(i) 3D

Geometry of 3D-min0

C	1.147842342502	1.700352278037	-1.329375344457
C	0.428767591338	1.709003411360	-0.079152785827
C	-0.428741552599	-1.708991305308	1.320779273830
C	-1.147833049317	-1.700370464390	0.083533552347
C	1.147857918577	1.700402713041	1.158112265234
C	0.428725431963	1.708954131732	2.408313505717
C	-0.428762182926	-1.708981430634	3.808246706383
C	-1.147856499557	-1.700369333837	2.570996721426
TV	2.149992471718	-0.025740779877	1.238180962191
TV	0.000000000000	6.856836876772	-0.032611172401
TV	0.000000000000	-0.000000000000	4.974956273322

Energy = -45.570529730612 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min1

C	0.405369110385	0.552763705506	-1.824959361196
C	0.675571709636	0.112802143854	-0.362985362802
C	-0.405386411479	-0.550303999130	1.828868758790
C	-0.675439475849	-0.110274787025	0.366895068197
C	0.405366875369	2.977482038234	-1.095083402545
C	0.675573217955	2.537421249362	0.366863329458
C	-0.405465713987	1.874491466655	2.558520124925
C	-0.675589312031	2.314442884398	1.096520780613
TV	2.161987717042	1.326069148902	-0.000024381284
TV	-0.000000000000	4.849473585721	1.459415318269
TV	0.000000000000	0.000000000000	4.383515387665

Energy = -45.570244519236 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min2

C	0.605432750131	0.141260014007	-1.793105037990
C	0.605283799848	0.142115020721	-0.359307236904
C	-0.567227799250	-0.271446927687	1.792801566677
C	-0.567028465128	-0.272383616585	0.359017090652
C	2.950421925038	0.968718524912	-1.794263836776
C	2.950234725945	0.969685527814	-0.360475329362
C	1.777723039434	0.556044005542	1.791613250002
C	1.777904061989	0.555152929177	0.357810154968
TV	4.689891146422	1.654886230197	-0.002315819788
TV	0.000000000000	3.600048323482	-0.831403469444
TV	0.000000000000	0.000000000000	4.303045447497

Energy = -45.567833103166 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min3

C	0.444237167204	0.590494860246	-2.218197461915
C	1.168783875360	0.231477167647	-0.874471879349
C	-0.441555463037	-0.594171165173	2.214955959401
C	-1.166112077459	-0.235201547121	0.871237934065
C	2.377669225420	2.068775356942	-2.865652205534
C	3.102201319859	1.709782757150	-1.521916916538
C	1.491873792950	0.884095177567	1.567601360268
C	0.767307103894	1.243103620098	0.223896040019
TV	3.866840585532	2.956615427991	-1.294765113512
TV	0.000000000000	2.436282337615	0.650742739695
TV	0.000000000000	-0.000000000000	4.883867163692

Energy = -45.562067504289 hartree

```

Spin(**2) = 0.000000000000
Geometry of 3D-min4
C      1.212176941906      -0.093808709661      -2.578292416218
C      1.354923417360      -0.810307803587      -1.194246233594
C      0.415609237428      -1.044423141151      2.004990391184
C      -0.266570247377      -0.398401440109      0.755815236717
C      2.833853349290      1.735814926358      -3.368451845660
C      2.151632854407      0.140290723453      -0.285570276543
C      2.631086628638      0.222339670170      2.302671035584
C      -0.063993606487      1.115214185905      0.576680030028
TV      3.830369343544      3.094887565191      -0.489932551609
TV      -0.000000000000      2.241509634113      1.159891031977
TV      -0.000000000000      0.000000000000      5.491927687343
Energy   = -45.531893603257 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min5
C      2.189149416060      0.158812099638      -2.205207354864
C      1.774908934721      -1.469191860881      -0.324506390126
C      1.578693141590      -1.186248053872      4.816780525732
C      -0.626202822465      0.063223822916      -1.703057192653
C      1.939068526338      1.796314932780      -4.134613194723
C      1.828504905812      -0.377526071080      0.595686125444
C      1.992901858590      0.441898590256      2.936017891070
C      0.064046165099      1.281735018525      -1.446779463805
TV      4.329982939335      2.519475374174      0.079661162215
TV      -0.000000000000      2.445925134671      0.468339829334
TV      -0.000000000000      -0.000000000000      6.618565158163
Energy   = -45.522840925808 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min6
C      0.680589377711      -0.097183438006      -2.501549746526
C      1.603626449773      -0.662811942458      -1.436053846654
C      -0.117983997144      -1.069842914003      2.038212277085
C      -0.085348797439      -0.288273288562      0.565584616178
C      2.525567010527      1.370316234592      -2.561680430851
C      2.493307330709      0.588595142802      -1.088932112058
C      1.726816246300      0.397666125054      1.978290573898
C      0.804237528095      0.963170724985      0.912537641614
TV      3.968769930673      2.775725591636      0.179254095906
TV      0.000000000000      2.240643224156      1.188579449957
TV      -0.000000000000      -0.000000000000      5.412386335325
Energy   = -45.521115656061 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min7
C      0.434642467764      0.585751164355      -1.434825044893
C      1.549272270506      0.166195014333      -0.402145817505
C      -0.434650557144      -0.581237745477      1.435756324619
C      -1.549338980702      -0.161679014351      0.403130446457
C      0.434681723552      2.919873158648      -0.485605182465
C      1.549334266881      2.500343251205      0.547036672146
C      -0.434692757143      1.752911406671      2.384938981545
C      -1.549345380370      2.172529667664      1.352314804705
TV      3.098717902982      1.167293055634      0.474647601280
TV      -0.000000000000      4.668350826935      1.898463346967
TV      -0.000000000000      -0.000000000000      3.345159985802
Energy   = -45.515956494259 hartree
Spin(**2) = 0.000000000000

```

Geometry of 3D-min8

C	0.605676167110	0.469837520152	-0.943358510340
C	1.494772744147	-0.314941464229	0.087441235918
C	-0.618406249520	-0.315327711287	1.910379675544
C	-1.507296029662	0.469629257761	0.879417238687
C	-0.158458021227	2.662028019789	-1.829347067009
C	2.258920575785	1.877390037998	0.973090256569
C	0.145675601640	1.877228012310	2.796020710399
C	-2.271441196513	2.661861705837	-0.006400660672
TV	3.306325540160	0.000401636668	0.490518091109
TV	0.000000000000	4.384756331796	-0.000339110841
TV	-0.000000000000	-0.000000000000	3.342638348226

Energy = -45.512974765684 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min9

C	1.465203757298	0.274401334650	-1.774549946771
C	0.624092824785	-0.381044809390	-0.589518983294
C	-1.154779536211	-0.113085783197	1.325718607425
C	-0.313584947219	0.542320632303	0.140641769861
C	2.836813798386	2.002393744022	-0.161069549227
C	3.690280397451	3.091894663588	-0.808969774429
C	0.623984119444	-2.042322532815	1.189495364966
C	1.477301333208	-0.952474540542	0.542064827573
TV	4.003659608196	0.888512838190	0.829671302154
TV	-0.000000000000	3.454217430539	-0.236837359590
TV	0.000000000000	0.000000000000	3.462413900379

Energy = -45.512927947066 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min10

C	2.136402982649	0.158049361446	-3.679661372793
C	1.059492142464	-1.013887670602	0.179651657614
C	1.707645353553	-1.241523626776	5.234918810659
C	0.648861323044	-0.593531199539	-1.203533334750
C	1.568633011207	1.974670024174	-5.349054009244
C	1.217841304813	-0.013112750680	1.193179809833
C	1.726560586248	0.579092359354	3.551677618173
C	1.077746055289	0.806093454566	-1.503428624014
TV	3.221635236593	3.139231726558	-1.722025205550
TV	0.000000000000	2.396185854581	0.727728020202
TV	0.000000000000	0.000000000000	8.614812782519

Energy = -45.504929533754 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min11

C	1.341397852353	-1.048617893022	-1.379103125827
C	0.621256443074	-0.303606881619	-0.417575928865
C	-0.669589855731	0.866733232556	1.147959122773
C	-0.689048059087	-0.213070889066	0.107633232012
C	2.754173348843	-0.542565753572	-1.357148803440
C	2.773004226800	0.537628118631	-0.317239300477
C	0.743077023255	1.372647760513	1.169683904236
C	1.462743470544	0.627822236440	0.207758911948
TV	4.515656684151	1.570829793917	0.023211946237
TV	0.000000000000	3.430159178244	-1.485003379439
TV	0.000000000000	0.000000000000	4.812796978416

Energy = -45.500391031008 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min12

C	2.740750343098	-0.240644765646	0.118692092223
C	0.617790029518	-1.407088222927	-0.357738198707
C	1.994638403756	-1.407445391064	2.981734111647
C	-1.341759869145	0.181044590711	-0.916291536797
C	4.117709963704	2.092968988831	-2.268335426186
C	-0.188620663359	-0.240180526603	0.118041409142
C	4.924187464632	0.925997541698	0.595296915940
C	-1.341592095382	1.672097872761	-1.235206450355
TV	7.418989494500	3.500285722298	-1.910025935294
TV	-0.000000000000	2.333822584529	0.951787500582
TV	0.000000000000	-0.000000000000	3.339271987206
Energy = -45.496013269734 hartree			
Spin(**2) = 0.015380859375			
Geometry of 3D-min13			
C	2.584713085332	0.150977112963	-1.309410765998
C	0.814647411994	-1.443118293242	-0.591913056108
C	1.680735538543	-0.990733068438	1.892935719528
C	-1.369639220483	-0.123232164825	-0.405316760588
C	2.895847437299	2.022064718831	-2.802570294938
C	1.369048141474	-0.490411762193	0.488080352588
C	3.450666033668	0.604043424293	1.175382552001
C	-0.684948302073	0.979428510880	0.087133199590
TV	6.320093595183	3.046124012115	-1.152437956193
TV	-0.000000000000	2.370732181092	0.844850425698
TV	-0.000000000000	-0.000000000000	3.743104937331
Energy = -45.494461750714 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min14			
C	0.728394362085	-0.331222774423	-1.849159152283
C	0.728346011775	-0.331330819059	-0.436432927647
C	-0.640909513456	-0.330913305859	1.766418649283
C	-0.640931204532	-0.330946144533	0.193928852156
C	3.309667139158	-0.331773334279	-1.929009781441
C	3.309674698622	-0.331820006310	-0.356440293856
C	1.940370749067	-0.331603252200	1.686409465481
C	1.940272251733	-0.331691561442	0.273711510514
TV	4.719209632579	-1.303900273699	-0.000095664302
TV	-0.000000000000	2.606067978978	-0.000084629449
TV	-0.000000000000	-0.000000000000	4.245699041938
Energy = -45.491477155693 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min15			
C	0.573286827500	0.443199188233	-2.196201804195
C	0.604863042491	0.396922609287	-0.620225346997
C	-0.036815094160	-0.935744413933	2.772099836616
C	-0.902134739025	0.350847444807	-0.320235206037
C	0.598731220642	2.690982893282	-1.472255955126
C	0.579820669481	2.719396739971	0.744122932962
C	-0.294357039749	1.733130249271	2.966849086054
C	-0.643971521577	2.252567793485	1.573240444753
TV	2.117230493444	1.424837361761	-0.000522063017
TV	0.000000000000	4.570322195256	2.088477607211
TV	0.000000000000	-0.000000000000	5.267894587602
Energy = -45.489765078948 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min16			
C	1.206348012942	-0.207991239666	-2.597912466368

C	1.305932442615	-0.912468045678	-1.252108092004
C	0.374767200236	-1.161309200759	1.985622923566
C	0.275020470744	-0.457227046624	0.639807068184
C	2.831259180199	1.669681922014	-3.424829660771
C	1.685853419918	-0.134360943001	0.022580125878
C	2.635752762530	0.118957356527	2.299851864933
C	-0.104670555960	1.033655371066	0.552577082572
TV	3.885758268228	3.158236214823	-0.512852001163
TV	0.000000000000	2.269032612186	1.187431766168
TV	0.000000000000	-0.000000000000	5.523178162857
Energy = -45.487520026995 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min17			
C	2.590099679054	-0.227559403549	-0.177796906202
C	0.409171770359	-1.469774978001	-0.448040995473
C	1.895887253886	-1.424808810435	2.924677959836
C	-1.320550876472	-0.056989900339	-0.619646690758
C	4.031040506129	2.168459310513	-2.896761743750
C	-0.266759141680	-0.500838997379	0.530401118905
C	4.725375329273	1.021914316906	0.074508893366
C	-0.644691070746	1.318152127689	-0.694001154880
TV	7.532618830826	3.468181931760	-2.008135941180
TV	0.000000000000	2.344004755483	0.904278236248
TV	0.000000000000	0.000000000000	3.489119091286
Energy = -45.487394454610 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min18			
C	2.715860969186	-0.640915839647	-1.262438433536
C	0.545596387009	-1.692550773732	-1.963633814212
C	1.900596906294	-1.691999446727	2.585656686551
C	-2.226547365819	0.839029443807	-1.201655990337
C	3.825878541541	-0.019530820761	-2.192462192933
C	-0.269596398551	-0.641713227846	-1.260923945198
C	4.672794032258	0.839745587182	3.347165964496
C	-1.379543779984	2.081777686129	-0.786466743879
TV	6.052399165702	0.000483694551	2.273416153854
TV	-0.000000000000	2.102135599854	1.404476740296
TV	-0.000000000000	-0.000000000006	4.550185802624
Energy = -45.486786878307 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min19			
C	1.964379883144	1.483350915231	-4.950862436638
C	0.798699974743	-2.716290515858	3.516703237648
C	1.964426326512	-0.067285443686	-0.398898641011
C	-0.804466597285	-0.618138797110	0.414820289192
C	3.228154426725	3.581376790695	-5.791607185985
C	0.798485612549	-2.161942307341	4.957712549722
C	3.228216991291	2.030941326544	-1.239747283497
C	-0.804432910472	-0.063731337462	1.855934184841
TV	5.198492389804	4.196082642127	-3.941274003988
TV	0.000000000000	2.098230371687	1.419551414208
TV	0.000000000000	0.000000000000	4.520612723925
Energy = -45.486323910529 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min20			
C	2.847938174009	0.559537988219	-2.752698069453
C	1.846366945078	-1.053508944448	-1.108067369649

C	2.467653527630	-0.814676388937	4.004117407435
C	-0.686930795957	-1.306439856046	0.138545217937
C	2.045094005130	2.200054828127	-4.530582799973
C	1.466218719339	0.027960994627	-0.138420259849
C	2.270318347697	0.843472236302	2.138578172690
C	-0.030323176537	-0.041088822932	0.204031278998
TV	5.031619094293	4.391126326074	-2.733661860841
TV	0.000000000000	2.455850942775	0.499675023103
TV	-0.000000000000	-0.000000000000	6.287008656834
Energy	= -45.483380070490 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min21			
C	2.507964424628	0.093185196234	-1.168898393994
C	0.786022130730	-1.502478627921	-0.426527884847
C	1.648399488188	-1.037267765099	2.114585542030
C	-1.293961555618	-0.025103193656	-0.825889953770
C	2.807300673187	2.023674359936	-2.885186473100
C	1.349109896953	-0.539590117581	0.668087026344
C	3.666914033808	0.758622667438	0.789597007669
C	-0.730678966119	0.937975958919	0.268554075738
TV	5.260297298204	2.681362340601	-0.004660543439
TV	0.000000000000	2.395646971541	0.824880535436
TV	-0.000000000000	-0.000000000000	3.891582588991
Energy	= -45.480509839315 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min22			
C	0.183000306146	0.613787879244	-1.710696606777
C	2.016927839182	-0.288822135061	0.280022407723
C	-0.194566046712	-0.700332763906	2.130702660439
C	-2.028254165691	0.202132584447	0.140264155520
C	0.523755741524	2.875321105135	-0.668405337419
C	1.548675372160	2.239415912725	0.414851516399
C	-0.535178317797	1.851555370521	2.158919576283
C	-1.560206834139	2.487308447306	1.075682524851
TV	3.269828667321	0.608576126477	0.652917130555
TV	-0.000000000000	4.813418833090	1.070436107689
TV	-0.000000000000	-0.000000000000	3.389464345615
Energy	= -45.480291879171 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min23			
C	0.691946108924	0.088530948981	-3.668353467313
C	2.639460117258	0.087358332347	-1.720653424735
C	2.639291866389	-1.176266139231	2.725112524968
C	-0.668761615952	-2.438513746465	1.585877783247
C	1.500883956835	1.352113401376	-3.667978935711
C	2.639891277128	0.087359301898	-0.360157155830
C	2.639817620682	1.351249921539	0.448821662398
C	-1.477796503689	-1.174855421400	1.585603743356
TV	5.255595090023	2.526657615249	0.001620556440
TV	0.000000000000	2.527504520661	0.000021919636
TV	0.000000000000	0.000000000000	5.254828735573
Energy	= -45.479469466415 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min24			
C	-0.092137360674	0.524008224653	-1.775953012458
C	1.098337533188	0.159856279964	0.622057546612
C	0.089967029153	-0.318775348811	2.791036259311

C	-1.100542796086	0.045334625608	0.392868217483
C	0.551725479154	2.921407306422	-1.041226049143
C	1.742232771553	2.557136355640	-0.112943940288
C	-0.554168591537	1.915375899251	2.055975111151
C	-1.744565378761	2.279448481307	1.127525874028
TV	3.304819114453	1.120626937809	-0.000049812486
TV	-0.000000000000	4.631268966482	-0.000428347125
TV	0.000000000000	-0.000000000000	3.326383285654
Energy = -45.479159596253 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min25			
C	1.487129926801	0.232847425251	-1.794637064327
C	0.568024701411	-0.347069448465	-0.631517051857
C	-1.607831082993	0.890596814404	0.513677976693
C	-0.218675852982	0.856465092747	-0.107375609132
C	2.739058557852	1.881022626857	-0.210296094391
C	4.128263665401	1.915510371856	0.410572219161
C	0.666207860375	-2.080112203454	1.151984030638
C	1.487133971285	-0.927177970576	0.531403909317
TV	4.346945383297	0.000385955644	1.710703300752
TV	-0.000000000000	3.465859130157	-0.144426062284
TV	0.000000000000	-0.000000000000	3.422616713523
Energy = -45.479030238690 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min26			
C	0.630501536095	0.394760667460	-1.006540188534
C	1.537193961129	-0.348504192163	0.033313203476
C	-0.637069353365	-0.333509422278	1.976156719196
C	-1.563591103149	0.409746471650	0.953810363357
C	-0.225207143699	2.684484635233	-1.961268523078
C	1.873229850389	1.932980707700	1.400995432600
C	0.701211736717	1.941172583344	2.448132235161
C	-2.399753351004	2.699459372051	-0.018595342185
TV	3.366197411024	-0.023238675977	0.379635853287
TV	0.000000000000	4.420642892757	-0.032925980872
TV	0.000000000000	-0.000000000000	3.387020818595
Energy = -45.477590988805 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min27			
C	0.613302864264	0.110325500959	-1.866158604252
C	0.751804716970	0.544259921552	-0.441560829345
C	-0.256685063835	1.195994778157	1.700729829669
C	-0.549919342676	0.760503727800	0.268331498401
C	3.169036343645	0.123471214235	-1.823950689156
C	3.307671180478	0.557326558353	-0.399254872742
C	1.943365324846	-0.124183702644	1.664688462849
C	1.977367548770	0.791716124593	0.371944037024
TV	4.727457594032	1.107921977282	-0.660770486370
TV	0.000000000000	2.396680539955	-0.728493260239
TV	0.000000000000	0.000000000000	4.302241985688
Energy = -45.475639931313 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min28			
C	0.477633719501	0.512981629094	-1.483476008794
C	1.583789442287	0.141548099461	-0.437746381315
C	-0.438943074212	-0.621815804360	1.473396384943
C	-1.567098438478	-0.258803577613	0.448356169821

C	0.511321768061	2.982877679736	-0.437631810544
C	1.023388238282	2.386967915535	0.863211694354
C	-0.073376418128	1.973060657061	1.899556189734
C	-1.511142042234	2.219515779653	1.473344853342
TV	3.141565229032	1.185711341942	0.414771200136
TV	0.000000000000	4.754521713963	1.898828532381
TV	-0.000000000000	0.000000000000	3.383051400278

Energy = -45.470826800991 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min29

C	0.234133466259	1.428679246598	-1.260032013467
C	0.494977740141	0.658550622511	0.001265552220
C	-0.234146065517	-1.428691857142	1.262375168376
C	-0.495001060696	-0.658568586012	0.001036674620
C	0.234123101224	1.428689909809	1.262615129026
C	0.494992039055	0.658565951129	2.523912434384
C	-0.234097786070	-1.428680566590	3.785026456133
C	-0.494981434420	-0.658544720327	2.523703956450
TV	2.561772141209	0.832762127440	2.522413548399
TV	-0.000000000000	4.133578060858	0.000117248557
TV	-0.000000000000	-0.000000000000	5.045330412955

Energy = -45.470132643319 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min30

C	-0.377548437954	1.096206708388	-1.365193187687
C	1.271435326983	-1.635666260866	0.156172394759
C	-1.020865567380	0.256943455094	3.574212493927
C	-2.519480492506	0.587500016965	0.258755689901
C	1.721503581243	3.903925731690	-1.538174316097
C	0.768069233292	2.727323121531	0.292511655922
C	-1.373750217606	2.218611307941	1.916452043199
C	-0.730546980603	3.057847074708	0.708080882719
TV	2.372210676140	-0.523244115257	0.898769230464
TV	0.000000000000	5.638892114913	-0.449724796424
TV	-0.000000000000	-0.000000000000	3.730978854909

Energy = -45.468301021076 hartree

Spin(**2) = 0.066405687500

Geometry of 3D-min31

C	2.873964243882	0.398432626535	-1.925859375573
C	-0.136275802771	-1.833745488897	0.616306896254
C	2.045104735949	-0.718122366030	1.196672142523
C	-1.157335893449	0.062795281687	-0.758357635030
C	3.895021077617	2.294892843602	-3.300179537247
C	0.692635895918	-0.717245430215	1.195463607337
C	3.895043278319	0.735479814157	0.606407254690
C	-1.157332510329	0.737139296622	0.604385749928
TV	6.408287407878	2.231806031476	-0.691330058615
TV	0.000000000000	2.233506416522	1.157504787964
TV	-0.000000000000	0.000000000000	3.701678398173

Energy = -45.467700647637 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min32

C	1.098282583314	0.086617644207	-3.364009381248
C	2.290906372912	0.086354613919	-2.200457553289
C	2.899049445377	-1.172010256773	2.563429655111
C	-0.355932029159	-2.429548319271	2.280652050483
C	1.706733504885	1.344849037070	-3.987574078689

C	2.069354442312	0.086749759724	-0.740557030500
C	1.928836549907	1.345106893270	-0.060579170273
C	-1.032498041994	-1.171142773115	2.437368238798
TV	5.385683126789	-0.000567880776	-0.130922093111
TV	0.000000000000	2.516638142091	-0.000321587865
TV	0.000000000000	-0.000000000000	5.386945860513
Energy = -45.464469464761 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min33			
C	0.296515563306	-0.660661137102	-1.174069665025
C	0.960513836814	0.319980935136	-0.173724663710
C	-0.085066384147	-0.126172697766	0.957816361512
C	-0.748977838769	-1.106738427340	-0.042647006441
C	0.296511491531	1.719368849039	-0.236203775538
C	0.960558373960	2.699988898047	0.764123036000
C	-0.085038016212	2.253869528974	1.895654094925
C	-0.748972043092	1.273281624519	0.895233339372
TV	3.207234794508	1.368069044752	0.017099844300
TV	-0.000000000000	4.760066681133	1.875721058391
TV	-0.000000000000	0.000000000000	3.487636197121
Energy = -45.463158139216 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min34			
C	0.646248714271	-0.124881907718	-1.775871539520
C	0.646216348065	-0.280500521281	-0.331631165128
C	-0.573989113657	0.142946627780	1.771123293975
C	-0.574096087331	-0.547810732864	0.452458306017
C	3.074010856593	-0.549392949768	-1.713120351179
C	3.074129581403	0.141275493129	-0.394465786106
C	1.853780857203	-0.281263923710	1.833938735114
C	1.853767068154	-0.125473794046	0.389745789611
TV	4.641886589545	1.587791542579	-0.470755560274
TV	-0.000000000000	3.178564869059	-0.940758645119
TV	-0.000000000000	0.000000000000	4.331156453739
Energy = -45.462466076255 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min35			
C	0.545673839836	-0.018637084190	-1.856891036026
C	0.679794426705	0.233508927215	-0.389388839827
C	-0.309128080364	1.085411489972	1.753357822179
C	-0.590044084804	0.566895537105	0.330006193937
C	3.035335018113	-0.387377990869	-1.868202666070
C	3.169469647162	-0.135221336487	-0.400668502578
C	1.866922158987	-0.112890759637	1.752295465156
C	1.848237513209	-0.040941512317	0.315460175405
TV	4.614135435429	0.788812367802	-0.679420082055
TV	-0.000000000000	2.595068684754	-0.663718592194
TV	0.000000000000	0.000000000000	4.325316904111
Energy = -45.458932630324 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min36			
C	2.458814227963	1.124626494191	-2.568558553320
C	2.450976879806	-0.326834974994	-0.035069933983
C	2.457089282713	-0.327120372777	4.952236604278
C	-0.779225877394	-1.270396156337	-0.531340403716
C	2.442514154389	1.858458738942	-6.314946595017
C	2.444656737576	1.124439055999	-0.074994750143

C	2.446846485137	1.124534981925	2.418919602697
C	-0.867497567981	-0.078557341034	-1.044076392652
TV	6.553505776633	2.200926944046	1.199722023496
TV	-0.000000000000	2.185699711940	-1.292416869575
TV	0.000000000000	0.000000000001	7.481052821104
Energy = -45.456334785017 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min37			
C	2.194872234520	1.738074619349	-5.669884913960
C	0.295296223551	-2.082501635772	3.233625223478
C	1.935210949085	0.255995799254	-0.710370114601
C	0.008354055676	-0.673288783682	0.856637357441
C	2.907490096463	3.879448526713	-6.823637210408
C	-0.069871081210	-2.091327955104	5.708223417094
C	2.647825422577	2.397812487165	-1.864742073122
C	-0.357843174017	-0.682690259217	3.331093255492
TV	4.904517733956	4.742813203042	-5.542486083632
TV	-0.000000000000	2.157013564481	1.278897745258
TV	0.000000000000	0.000000000000	4.917962792061
Energy = -45.456231298966 hartree			
Spin(**2) = 0.015380859375			
Geometry of 3D-min38			
C	1.995608841000	1.719497301529	-1.770840216177
C	1.992809736273	-1.049882148420	-0.846712006629
C	1.996302488602	0.610843161692	3.857015034307
C	-1.400639172531	-1.708133604799	-1.844013563523
C	1.994338726153	2.269974164690	-4.569246032630
C	1.992611221754	0.058913234164	0.090172765455
C	1.995384923652	0.888684000252	2.442303557678
C	-1.242331408287	-0.483496106089	-1.483332488414
TV	6.629780105298	3.540030934128	0.845378535733
TV	-0.000000000001	2.490056411825	0.490878811877
TV	-0.000000000000	0.000000000001	6.564502716793
Energy = -45.456171213848 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min39			
C	3.334984550256	0.314878455659	-1.887159829486
C	1.315319044850	-1.049006633129	-1.358631429970
C	2.673106734789	-0.975769096138	5.330422405602
C	-1.349329944848	-1.201751471478	-0.355892382912
C	1.954119969686	2.065176666491	-4.596422894403
C	0.653340011936	0.168694129071	-0.928205432855
C	1.950099391187	0.842304989809	2.183909608489
C	-0.692487134271	0.091142469654	-0.418234541369
TV	6.029624958036	4.102489051537	-1.658749865873
TV	0.000000000000	2.508380955366	0.383478063682
TV	0.000000000000	0.000000000000	7.170214817165
Energy = -45.456056225265 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min40			
C	4.01555749826	0.813284338194	-2.439377455781
C	2.079806408921	-0.521820626980	-1.609937655750
C	3.382014009665	-0.475592051548	5.131459976980
C	-0.509697863266	-0.610701856911	-0.420747792765
C	1.130107033629	0.574385263373	-4.676061743095
C	1.439137601857	0.722127377077	-1.221901769158
C	1.192452895029	-0.683330567803	2.403111215351

C	0.127919208427	0.677401788256	-0.624453982521
TV	5.823452691892	4.002359805388	-2.454301201889
TV	0.000000000000	2.531411365309	0.190006949342
TV	0.000000000000	-0.000000000000	7.357752974787
Energy = -45.455930395635 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min41			
C	2.384044636641	1.886152128172	-2.184186679076
C	2.377430784846	0.217397276396	-0.327486496044
C	2.383925451490	-2.005006123398	4.322532798492
C	-0.818677925266	-1.454937475481	-1.473707322222
C	2.374527444993	1.051556706223	-4.536127675831
C	2.375027695225	-1.170839297672	0.113856552536
C	2.376997573521	-0.336625173917	2.466924885713
C	-0.820218241477	-0.272159573903	-1.238493153256
TV	6.394783429002	0.814093971765	2.360168828075
TV	-0.000000000000	2.502993838846	0.496152581474
TV	-0.000000000000	-0.000000000000	6.561514434140
Energy = -45.455918525609 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min42			
C	2.359348923297	0.905237881345	-3.131483259656
C	2.360949251264	-0.763423472117	-1.276133827491
C	2.360113256752	-0.483003556501	3.870442982096
C	-0.865164515233	-1.616749830233	-0.020093799677
C	2.358727618803	2.574362597618	-4.986853299730
C	2.360534965789	0.351438717861	-0.338502115625
C	2.358315820837	1.186066612405	2.015188416103
C	-0.865280566800	-0.433909829210	0.212678184577
TV	6.451797148388	2.477218601002	0.548833280284
TV	0.000000000000	2.502999939562	0.496443574799
TV	0.000000000000	-0.000000000000	6.560712521630
Energy = -45.45565400566 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min43			
C	1.332666040747	-1.346985887596	-1.018635070647
C	0.621977873763	-0.484757900970	-0.183756320418
C	-0.767394007742	0.939379128727	1.214041625950
C	-0.813054251095	-0.266344062600	0.131069311909
C	2.836892203491	-1.055578052370	-0.872512843258
C	2.882887579692	0.149843285058	0.210635583200
C	0.736957680223	1.230710726740	1.359880716584
C	1.447877188092	0.367612151309	0.526045600629
TV	4.370994066379	1.777834748511	-0.305820836755
TV	0.000000000000	3.564216978271	-0.399471628937
TV	-0.000000000000	-0.000000000000	3.566371783013
Energy = -45.454845629572 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min44			
C	2.403203824661	0.087444843790	-1.770160094662
C	1.347272702931	-1.552778239122	-0.200084292626
C	1.659626972181	-1.237979842639	4.475461595557
C	-0.293470874876	0.250722758326	-2.516139543482
C	1.661222566391	1.736954081015	-3.382290372015
C	1.347971950715	-0.426548912452	0.753666186011
C	2.404456423774	0.411297173192	2.864200492573
C	0.539555916854	1.488964604932	-2.245310555956

TV	4.018628337194	2.475462695431	0.543247856412
TV	-0.000000000000	2.477131547612	0.539706677082
TV	0.000000000000	0.000000000000	6.121679226638
Energy	= -45.454149597685 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min45			
C	1.952936732713	-1.330576676248	-3.549868594817
C	1.962200989100	-1.880533602625	-0.749926528897
C	1.949563881739	-2.708375653923	3.464736367337
C	-1.254742232741	1.666109866185	0.565407375669
C	1.967521317034	0.325159625967	-5.412919071396
C	1.956016768050	-0.502793814944	-1.198004841323
C	1.964868440883	-1.052668976971	1.601704466548
C	-1.251321349515	2.858880509466	1.056719918177
TV	6.412106318023	-0.796520262734	-2.362050631443
TV	-0.000000000000	2.483776600420	0.487749793457
TV	-0.000000000000	0.000000000001	6.566065623459
Energy	= -45.453519751301 hartree		
Spin(**2)	= 0.312500000000		
Geometry of 3D-min46			
C	2.368818754859	-0.077274563779	-3.159914478276
C	2.371918429400	-1.734113519426	-1.296628468794
C	2.370189359873	-1.455486830154	3.855759280766
C	-0.860652961678	0.460973929557	0.688523116763
C	2.367840056920	1.578230511810	-5.022907764321
C	2.371090509405	-0.628049768136	-0.360460877515
C	2.367079214586	0.200302267645	1.991919329007
C	-0.854903458667	1.750564551771	0.689612190090
TV	6.452323315576	2.429836934135	0.625556790223
TV	0.000000000000	2.484260377706	0.487676632386
TV	0.000000000000	0.000000000000	6.566556064111
Energy	= -45.453340341181 hartree		
Spin(**2)	= 0.312500000000		
Geometry of 3D-min47			
C	2.304492528556	-0.139214087953	-2.528749744310
C	2.304637596583	-1.799493853670	-0.668595044163
C	2.304814868928	-1.520759607832	4.480878281437
C	-1.082110595283	-1.573666937933	-1.402711815624
C	2.304161311946	2.630216124617	-3.452813843678
C	2.304598719606	-0.690432904688	0.268106954192
C	2.304327946465	1.521332598502	2.173627443141
C	-0.927918799353	-0.313050823573	-1.234489607400
TV	6.625817500084	1.109545188698	0.229800564127
TV	0.000000000000	2.490590366810	0.490692856810
TV	-0.000000000000	-0.000000000000	6.563896915275
Energy	= -45.453090703134 hartree		
Spin(**2)	= 0.750000000000		
Geometry of 3D-min48			
C	2.529149305403	0.082068785694	-2.944725857443
C	2.526485825606	-1.578578531946	-1.083676926597
C	2.527704874888	-1.299838423036	4.064896187958
C	-0.854564336301	-0.183779192449	0.688978578164
C	2.531038850202	1.742667345880	-4.805098039467
C	2.527721034208	-0.469350974250	-0.147209651730
C	2.531220361396	0.360989774474	2.203909178820
C	-0.727812196830	1.084808499308	0.819710103725
TV	6.653867585728	0.118815679068	-0.194305089873

TV	0.000000000000	2.490901346543	0.490836578541
TV	0.000000000000	0.000000000000	6.563220582255
Energy	=	-45.453070380767 hartree	
Spin(**2)	=	0.750000000000	
Geometry of 3D-min49			
C	2.167378768917	0.753963638118	-4.223927846795
C	0.266298287607	-2.209760916002	0.413738834951
C	2.167225638547	-0.774183603353	-0.198362951383
C	-0.738895183841	-0.345515193012	-0.993494128007
C	3.494283481455	3.019288194313	-1.066170650992
C	1.162179391069	-1.109815695438	1.018538436102
C	3.494393085041	1.359324090882	2.898704393672
C	-0.739061526771	0.326197429285	0.407665463867
TV	5.560069810158	3.298905102563	1.814130599484
TV	-0.000000000000	2.199922764946	1.210035560601
TV	0.000000000000	-0.000000000000	3.834545754402
Energy	=	-45.452946609099 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min50			
C	2.317782928818	-0.050678627345	-0.959490161544
C	0.632986002775	-1.700664010968	-0.050291199343
C	1.366995359088	-1.326508624720	3.769778271316
C	-0.657665030054	-0.068062945490	-2.101476320844
C	2.486533073274	1.322010218151	-3.007359632474
C	1.027177158263	-0.816174882557	1.231099826112
C	3.123018259282	1.666013373692	1.015975567692
C	0.293036801326	1.207935723509	-1.664451752628
TV	3.949759066775	3.106430497717	1.069510023749
TV	0.000000000000	2.398363795281	0.924942654468
TV	0.000000000000	0.000000000000	5.165695758192
Energy	=	-45.450188867554 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min51			
C	3.035254898904	1.076385041895	-0.271416508313
C	1.604558620768	-1.446248511060	-0.734094557260
C	3.035310418044	1.076593886871	1.167009792362
C	-1.212159933006	-1.446461514238	-1.479399646916
C	0.782101961248	2.338608948624	-2.628770007116
C	0.781955075911	-0.184704736603	-0.328785168481
C	1.604606174687	1.077063461386	1.629890339025
C	-0.307541859956	-0.184836573875	-1.479087193245
TV	5.216440289919	2.522911921464	0.000501581829
TV	0.000000000000	2.523363679957	0.000144057144
TV	-0.000000000000	0.000000000000	3.853991062115
Energy	=	-45.449899466757 hartree	
Spin(**2)	=	0.015380859375	
Geometry of 3D-min52			
C	0.079285171884	0.430167229963	-0.563157913443
C	1.063785823509	-0.219265653546	0.454337684523
C	-0.078574229239	-0.219389663906	1.560336448239
C	-1.062931220314	0.430113575074	0.542840967947
C	-0.078714733977	2.647154321613	-1.914116800448
C	2.408303708315	1.997777318697	0.657342584666
C	0.079241919570	1.997597774856	2.911178247491
C	-2.407737068193	2.646873775682	0.339724457854
TV	3.471440615696	0.000402752233	0.114545756768
TV	0.000000000000	4.433868226694	-0.000064395953

TV	0.000000000000	0.000000000000	3.474345321287
Energy	= -45.449508931864 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min53			
C	0.340377671945	-0.779465303224	-1.942527474259
C	0.340333098066	-0.779388107330	-0.348424461840
C	-0.021149739346	0.544037246671	1.742151377402
C	-0.021082538685	0.544160068065	0.328359127039
C	2.180694505131	2.353740527432	-1.845309453757
C	2.180987922123	2.353956600183	-0.446078836726
C	1.780518786921	-1.116722636849	1.843291605389
C	1.780424339592	-1.116752993029	0.227516414307
TV	2.508840425509	0.681551703357	0.000051681539
TV	0.000000000000	4.936781646770	-2.181240768361
TV	0.000000000000	-0.000000000000	4.361760171908
Energy	= -45.447974942264 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min54			
C	1.802400226834	0.770341270804	-1.230071288045
C	1.108278619028	-0.140670610696	-0.356915053428
C	-1.062985702003	-0.836755621201	0.834025575069
C	-0.344149787006	0.153995390092	-0.114830369148
C	3.255197612591	2.203576132613	0.333250223173
C	3.973789908143	3.194429311471	-0.615711584768
C	1.108494731252	-1.973269878265	1.292590628287
C	1.802789066432	-1.062019536413	0.419751896845
TV	4.318067380490	1.834941957266	1.804499366943
TV	0.000000000000	3.560353480002	0.155254671315
TV	-0.000000000000	0.000000000000	3.564319639490
Energy	= -45.447840403049 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min55			
C	0.615862947842	0.236955199399	-1.825632215055
C	0.622716329785	0.372762971313	-0.411217607827
C	-0.577818121388	0.530103388180	1.756526899194
C	-0.725135807122	0.327287631984	0.282219423540
C	3.068622216794	-0.022255158153	-1.770325049283
C	3.204845575942	0.477315590205	-0.370413932727
C	1.837035238668	-0.166454308071	1.679539535555
C	1.855909782971	0.725574670123	0.397378364528
TV	4.821252270645	1.538861400389	-0.636779054395
TV	-0.000000000000	2.480729862850	-0.739297529069
TV	0.000000000000	-0.000000000000	4.285880495010
Energy	= -45.446804476815 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min56			
C	-0.453726031387	0.752156250575	-2.410241029025
C	2.575509895773	-1.147721743439	-1.224536925404
C	-0.453438379417	-0.363794451422	3.058153200165
C	-0.205948432537	0.681371968875	0.744958328424
C	-0.205961928428	2.693791329944	-0.781069922007
C	0.556336517152	1.828667582258	0.167999049538
C	-0.700648412888	2.145735580549	2.675602938379
C	-1.462897829695	3.011124608529	1.726770005568
TV	3.276180148284	-0.854969386752	-1.127452844947
TV	-0.000000000000	4.451143636059	1.246511845100
TV	0.000000000000	-0.000000000000	4.622054681802

```

Energy   = -45.445323920709 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min57
C         -0.992080712678      -1.778575517484      -1.771768332765
C         0.847421971430      -0.155122780651      -0.416758065801
C        -0.443935048956      -0.545969140945      1.829883535627
C        -0.443828769859      -0.545959455209      0.278927515965
C         4.526043503027      -0.614846691819      -1.772083186013
C         2.686684941419      1.468263101377      -0.416590980176
C         2.138661166251      0.235536691946      1.829796069648
C         2.138758804116      0.235313769919      0.278881721492
TV        3.678635052333      3.246933699705      0.000023194043
TV        -0.000000000000      3.706541919990      0.000124781490
TV        0.000000000000      -0.000000000000      4.297218654262
Energy   = -45.445252627052 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min58
C         0.610534267626      0.111046930830      -2.204622031744
C         1.365437008258      -0.265996640525      -0.902064472265
C        -0.243172823904      -0.887428343904      1.914886006445
C        -0.370395402003      0.024901662579      0.679867209283
C         2.650597018349      1.187908514891      -2.438140682747
C         2.778309076925      0.275547517062      -1.203329205507
C         1.796792045448      0.189324853637      1.681303938007
C         1.042307244180      0.566052713135      0.378475001755
TV        4.244804301969      2.432223881656      -0.084435732030
TV        -0.000000000000      2.360562612610      1.043295670858
TV        0.000000000000      0.000000000000      4.919467331913
Energy   = -45.442832868889 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min59
C         0.642867024575      -0.021025578309      -2.133542469391
C         1.376571298234      -0.734648903323      -0.938073758633
C        -0.221006365580      -1.066233876513      1.985035227999
C        -0.463365565510      -0.310287600314      0.553444466279
C         2.628510071427      1.459698786875      -2.482723949094
C         2.871228075826      1.376209142352      -0.866173990543
C         1.764720940619      0.249341904809      1.590434593615
C         1.031285668930      0.248582768835      0.198008852444
TV        4.109048284086      2.760873783517      -0.615435751992
TV        0.000000000000      2.409109041524      0.663612085049
TV        0.000000000000      -0.000000000000      4.705966903985
Energy   = -45.441430478560 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min60
C         1.722492981400      -0.280420566116      -1.986710102705
C         0.363328133833      0.372640192989      -1.879777112092
C        -1.250775066099      -0.238358424609      -0.093343806536
C        -0.390788287747      0.947818662808      -0.636802588986
C         3.254017171934      2.135095601597      0.600101345220
C         3.970898527243      2.705773058210      -0.641449090152
C         0.363369721303      -1.990593553893      0.613080373834
C         1.722582509848      -1.337240382019      4.281737933358
TV        4.504711454034      0.001398308165      1.779909211315
TV        0.000000000002      3.513448034195      -0.006910340079
TV        -0.000000000001      0.000000000000      3.562474359689
Energy   = -45.440495098432 hartree

```

```

Spin(**2) = 0.000000000000
Geometry of 3D-min61
C      0.275163723372      0.632804847361      -1.834736113430
C      2.176629821890      -0.148343355404      0.339723316909
C      -0.164419830733      -0.688989399648      1.960468414953
C      -1.814741614886      0.025187305350      0.059152891080
C      0.052857682767      3.167370338884      -1.269983824065
C      1.749013697138      2.293630649004      0.763195463487
C      -0.592099838645      1.753075019971      2.383898506748
C      -1.592294482563      2.223933374200      1.134306571543
TV      3.123760734572      0.946722118368      0.834666737536
TV      -0.000000000000      4.733130381360      1.639086838588
TV      -0.000000000000      0.000000000000      3.663487738529
Energy   = -45.439610101606 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min62
C      2.579180636400      -0.383503122872      -1.790523091199
C      0.438589885697      -1.452540304055      -2.481830761742
C      1.803848609376      -1.452413231060      2.201922280285
C      -2.251688506489      1.087438603907      -1.718303571887
C      3.942157209945      -0.785634958008      -1.169616714900
C      -0.366829505207      -0.383669434283      -1.789412010873
C      4.657563837846      0.047716439283      4.570804904937
C      -1.536266979714      2.392430041230      -1.390536331707
TV      6.193516131950      -1.068477824968      3.990133474466
TV      0.000000000000      2.138166582091      1.384177522162
TV      -0.000000000000      -0.000000000006      4.684337814829
Energy   = -45.437334988718 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min63
C      1.122742942070      -0.762008634269      -2.426363577860
C      1.605346405070      -0.534715696533      -1.031784550540
C      -0.141190826256      -0.614944551821      2.371262458567
C      -0.623566542384      -0.842184442879      0.976610580344
C      2.335430006836      1.520401992402      -3.057444103309
C      3.459262063907      1.247623369742      -1.921907967666
C      2.369129489906      0.327126341055      1.066545152032
C      1.245357876474      0.599391826534      -0.069074452184
TV      3.722950536610      3.224029498273      -1.935686410361
TV      0.000000000000      2.569004258055      0.285174194867
TV      0.000000000000      -0.000000000000      5.171868368123
Energy   = -45.435461325267 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min64
C      0.936486327358      -0.925451207559      -2.072328605690
C      0.936536248654      -0.925536122942      -0.494815872952
C      -0.471995235092      -0.925465012674      1.701961721316
C      -0.471854161061      -0.925473214390      0.111528106886
C      3.159129715685      0.364982473583      -2.698869047090
C      3.159293570951      0.364929210769      0.132063278117
C      1.603220134911      0.365068203636      1.721582735952
C      1.603365438236      0.365018044666      0.090633380127
TV      4.468731346593      -0.000138414057      -0.000078875516
TV      0.000000000000      2.580985204334      -0.000373451241
TV      -0.000000000000      0.000000000000      4.380139363710
Energy   = -45.433933656548 hartree
Spin(**2) = 0.000000000000

```

Geometry of 3D-min65

C	0.186700131315	0.620370826578	-1.762148526168
C	2.081483632632	-0.240453518828	0.278163375394
C	-0.206687736460	-0.640806130733	2.231113296278
C	-2.098540886448	0.220314711458	0.188198753434
C	0.145084899745	2.744691949502	-0.242733753259
C	1.510830971503	2.214470354442	0.259722620775
C	-0.634489262675	1.839120852906	2.090755305552
C	-1.040699011293	2.537004338048	0.769221449760
TV	3.338258734142	0.584314623670	0.590757873455
TV	0.000000000000	4.865365342065	0.997684032556
TV	0.000000000000	0.000000000000	3.439966376702

Energy = -45.432820446521 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min66

C	0.638361204664	-0.075126072082	-1.684575311217
C	0.638361996165	-0.331203443108	-0.289583359494
C	-0.607036149236	0.370158737162	1.632061414970
C	-0.606971259436	-0.776503937714	0.458271627166
C	3.106801247202	-0.776337527606	-1.573932307468
C	3.106914371297	0.370157576567	-0.400241411573
C	1.861783450302	-0.330789425387	1.742620542974
C	1.861853363743	-0.075457616309	0.347556087433
TV	4.884051136053	1.276512212482	0.213216279257
TV	-0.000000000000	2.553048272077	0.426540796263
TV	0.000000000000	0.000000000000	4.064390452498

Energy = -45.432445419836 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min67

C	0.582553974096	-0.140948041488	-1.850521119456
C	0.582515237553	0.308276146951	-0.477517948762
C	-0.667187261205	-0.175019657924	1.602883869850
C	-0.667222328827	0.341705876204	0.294334724185
C	3.081836191222	0.893194021465	-4.472291896261
C	3.081918661182	-0.726405919946	2.144155326406
C	1.832358119478	-0.174957258283	1.602885948245
C	1.832341618646	0.341718068666	0.294362041217
TV	4.998701900495	0.000067039003	-0.000084595517
TV	0.000000000000	2.884310026442	1.135165995175
TV	-0.000000000000	-0.000000000000	4.225305676904

Energy = -45.432169763280 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min68

C	2.596056362630	0.000841426918	-1.980389811183
C	1.091240940025	-0.506113730619	-0.554244798421
C	1.201305163847	0.000654048829	1.794184091076
C	-1.681014577845	-0.748818851874	0.131209029849
C	2.705738466993	1.875359012346	-3.483153074803
C	0.498350462248	0.448406421566	0.534263029020
C	3.298987225479	0.448402420536	0.534388460687
C	-1.012649835874	0.441614423834	0.554198376030
TV	6.491096845930	3.571859754009	-2.507093395343
TV	0.000000000000	2.381187666473	0.845666181903
TV	0.000000000000	0.000000000000	3.774857790486

Energy = -45.430825363358 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min69

C	0.174079878847	0.412046529604	-1.312513428418
C	1.353363106825	0.251231629030	-0.286958497915
C	-1.231757452587	-0.176182901584	2.263058456802
C	-1.944743519055	-1.128966410935	1.237470633662
C	1.231787676756	2.514848469058	-1.312795192725
C	1.944686485563	3.467562126449	-0.287297261440
C	-0.174028588926	1.926667657310	2.262778870802
C	-1.353418784761	2.087326334831	1.236982170896
TV	3.298093900405	1.380222611257	-0.000371407555
TV	-0.000000000000	4.629025375724	1.787262057332
TV	0.000000000000	-0.000000000000	3.575358895254
Energy = -45.430018863052 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min70			
C	0.885003377062	0.609950919129	-1.733197802115
C	0.929746645906	-0.418100901423	-0.566809863013
C	-0.537894247488	0.609988522069	1.125606753463
C	-0.582501115013	-0.418091885648	-0.040723989799
C	3.913188409769	-1.957283879663	-2.098745242493
C	3.177307552925	0.610062578037	0.378063355343
C	0.929765863762	-1.957366927148	2.846138991189
C	1.665784788713	0.609980609839	0.369108330537
TV	4.495676086891	-0.000025338633	1.354713462897
TV	0.000000000000	3.595582322841	-0.000120656015
TV	-0.000000000000	-0.000000000000	3.412769579426
Energy = -45.429174216965 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min71			
C	0.139775067062	0.398770395446	-1.412416989193
C	1.173404055318	0.175235408392	-0.245805713201
C	-1.248684207101	-0.119485341803	2.077458556633
C	-2.119681292635	-1.692636790938	-0.043430557463
C	1.248684490383	2.458211488182	-1.127159279277
C	2.119540525854	4.031304043205	0.993614078125
C	-0.139707506322	1.940109649724	2.362610735167
C	-1.173362329893	2.163024581551	1.195854920879
TV	3.180236144398	1.620919583302	1.286146998259
TV	-0.000000000000	4.867940068650	3.145605799081
TV	0.000000000000	-0.000000000000	3.794293185023
Energy = -45.428752702406 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min72			
C	2.798151697188	-0.286382575043	0.248562923610
C	0.676342363546	-1.304932518164	-0.506850244554
C	2.048769350555	-1.308575422431	3.791262356906
C	-1.302078127136	0.330735252840	-0.596755711439
C	4.170678535947	1.758765749828	-2.546155087355
C	-0.153174780885	-0.279842309891	0.239003385278
C	5.000142598314	0.734139574498	0.999904587066
C	-1.302648990199	1.157880464404	-1.723749869960
TV	7.452048463668	3.061815999597	-2.036806305500
TV	-0.000000000000	2.048068548371	1.494666450677
TV	0.000000000000	-0.000000000000	4.292550233070
Energy = -45.426721127181 hartree			
Spin(**2) = 0.015869140625			
Geometry of 3D-min73			
C	0.175321425227	-0.728397564396	-1.940778821176

C	0.175439681775	-0.728603741159	-0.391090446147
C	-0.322862220541	0.545671702792	1.663771216690
C	-0.323030835676	0.545650056001	0.302793678674
C	3.003375412412	2.420257060529	-1.954087234235
C	3.003056504395	2.420498880466	-0.375464726603
C	1.497007928932	-1.028787041604	1.658504359552
C	1.497304737375	-1.028759650653	0.308466965363
TV	3.745568419384	0.601849795703	0.001117577864
TV	-0.000000000000	3.735843147109	-2.149062221568
TV	-0.000000000000	-0.000000000000	4.298844347918
Energy	= -45.425760426780 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min74			
C	0.760903317975	-0.278796594918	-1.544626202304
C	0.760775220802	-1.434592319810	-0.591961840324
C	-0.627239517384	-0.658376976812	1.667257339161
C	-0.627156463511	-1.055227976710	0.142953426543
C	3.314335861441	-0.657944803202	-1.830183706198
C	3.314559192112	-1.054667857611	-0.305944749052
C	1.926631526510	-0.278774720764	1.381106912242
C	1.926611905819	-1.434536635820	0.428488119480
TV	4.746099013209	-1.242840582990	-0.000054244447
TV	-0.000000000000	2.486909123882	0.000290632449
TV	0.000000000000	-0.000000000000	3.946320180061
Energy	= -45.422953367664 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min75			
C	-0.039447451217	0.500053299151	-1.716731735618
C	1.092078198710	-0.036516053784	0.859915628330
C	0.029724192214	-0.324866368345	3.028918410262
C	-1.101512392085	0.211428909856	0.452946137147
C	0.274214502738	3.032778289936	-1.633536231612
C	2.144142029131	2.286957422075	0.223353382567
C	-0.284070064498	1.852956153804	2.313533446961
C	-2.153791276784	2.598774549712	0.456928128100
TV	3.424035119531	0.645677122127	0.326153127752
TV	-0.000000000000	4.710826897863	-0.632717811744
TV	0.000000000000	-0.000000000000	3.458250711025
Energy	= -45.422634604170 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min76			
C	2.276768296203	-1.118279949360	-1.055387014076
C	0.007751905136	-1.399386294343	0.088348589354
C	1.653704359711	-0.769738958366	2.687573420209
C	-0.545742140761	0.398114502572	-2.043352415021
C	2.123622295538	0.633945853165	-2.996430326356
C	1.500632662084	-1.415896751976	0.153414539924
C	3.633116490201	-1.739162417552	1.461118013494
C	0.144230102661	1.602964769506	-1.770060256108
TV	4.315361552792	0.865058821011	1.646314273716
TV	0.000000000000	2.398326857668	0.592803388383
TV	0.000000000000	0.000000000000	5.153388843226
Energy	= -45.421988220597 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min77			
C	2.810222139422	0.054098922873	0.247865789485
C	0.686847632528	-1.210656682351	0.250751437985

C	0.686960489953	-1.210685839610	2.766376421842
C	-1.146093562641	0.054498211616	-2.494528914530
C	2.141131320752	1.318898953180	-1.742981838042
C	2.141011844790	1.318948978326	0.756157415808
C	2.810392037833	0.054083628019	2.768433333204
C	-0.279777895040	1.319122144360	-2.494698675171
TV	5.286428777983	2.528715155111	2.000840161603
TV	0.000000000000	2.529682549843	-0.000078805378
TV	0.000000000000	-0.000000000000	4.003280435631
Energy = -45.419763454261 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min78			
C	2.053810443891	0.435706352028	-2.238701867432
C	1.250152530070	-1.600604569908	-0.911432317256
C	1.785642050356	-0.960519784165	3.535461751588
C	-0.960408137669	-0.325766761136	-0.664043533728
C	2.781334323915	1.038123242730	-3.484744145244
C	1.695954236693	-0.762826669430	0.241378359205
C	3.596626843568	-0.042759314060	1.636741561936
C	-0.256771745388	0.764942684550	-0.034474670142
TV	5.966124838830	2.506182255021	-2.297747290929
TV	-0.000000000001	2.261752873610	1.092642570473
TV	-0.000000000002	-0.000000000000	5.771281223145
Energy = -45.419661070690 hartree			
Spin(**2) = 0.015869140625			
Geometry of 3D-min79			
C	0.860873333888	0.050901050352	-1.541918462644
C	0.861147341623	0.050732043785	-0.158208290961
C	-0.184908802593	0.053153440333	0.886254268332
C	-1.567498546505	0.055786449320	0.885756926153
C	4.334408187853	0.042373859498	-1.541265395878
C	4.334370364886	0.042129866011	-0.157559362692
C	3.288676282699	0.044516211947	0.887170136421
C	1.906142002100	0.048347227379	0.886777141946
TV	6.947168839597	-0.015389324442	0.001315038207
TV	-0.000000000000	3.404646564231	1.712790028494
TV	0.000000000000	-0.000000000000	3.473373815611
Energy = -45.419280458111 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min80			
C	0.028629911904	-0.529121662542	-1.558532033619
C	0.672980413195	0.038188932452	-0.317227931155
C	0.391736768808	0.636942689559	1.997620089803
C	-0.378455487654	0.419584593012	0.657656683558
C	3.026630604465	0.502159650538	-2.191767269497
C	3.176914594838	0.372717805661	-0.669296774775
C	1.883103181888	0.530257171511	1.578219783687
C	1.929650383530	0.358199490061	0.141411927265
TV	4.439758405986	1.225066188440	-1.182829780357
TV	-0.000000000000	2.614197492010	-0.374483177291
TV	0.000000000000	0.000000000000	4.561011609751
Energy = -45.418990212079 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min81			
C	1.455475601004	-1.416211522576	-1.158872537840
C	0.618258960666	-0.462343106686	-0.282086049444
C	-0.743774798454	1.046967735760	1.092240035502

C	-0.745754538209	0.172679303522	-0.511665057858
C	2.827928334476	-0.722744180491	-1.301705570886
C	2.830058125877	0.151498870180	0.301977593071
C	0.628807790705	1.740460715811	0.949537960349
C	1.466014973989	0.786662115343	0.072541639489
TV	4.808440227254	0.830380155337	0.832499510580
TV	0.000000000000	3.459351007908	0.311603793703
TV	-0.000000000000	-0.000000000000	2.946629536580
Energy	= -45.418469106897 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min82			
C	0.094426546620	0.539217165450	-1.926798847941
C	0.512344663007	0.146128409825	-0.543425285250
C	-0.094516208653	-0.519047427439	1.808919440206
C	-0.512315464670	-0.126169983185	0.425514639944
C	0.094475637287	3.011413391732	-1.224508328393
C	0.512367158147	2.618344026789	0.158888400598
C	-0.094506557012	1.953148347539	2.511235355656
C	-0.512275774746	2.346055427278	1.127846452792
TV	2.429007273049	0.187297292973	-0.680731248711
TV	-0.000000000000	4.944427153733	1.404783231687
TV	-0.000000000000	0.000000000000	4.713009481162
Energy	= -45.417873804862 hartree		
Spin(**2)	= 0.066406250000		
Geometry of 3D-min83			
C	0.002945751132	0.804722080816	-1.866277208734
C	1.348041052515	0.804024066686	-1.133840581793
C	0.237082641371	-1.778227678527	2.219458513493
C	-0.275014399600	-1.778012673415	0.894048215048
C	2.392273861810	2.095383441697	-3.177433174974
C	2.191490319037	2.095387693215	-1.592335043647
C	1.666849743461	0.804093194530	1.739364715740
C	1.028282910244	0.804264426012	0.329509436145
TV	3.811364282145	3.873347173036	-1.832759321648
TV	-0.000000000000	2.582788758996	0.000190023761
TV	0.000000000000	-0.000000000000	5.453140580068
Energy	= -45.417279274563 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min84			
C	-0.971156560542	-1.047471817350	-0.799608374333
C	0.237546374387	-0.595717660252	0.095912946633
C	-1.130411640629	0.279251343645	1.842324147151
C	-0.327196083315	0.625580897892	0.785787651647
C	4.387556612698	3.362635491491	-1.246277825550
C	3.147524385393	2.709236256846	-0.660686181126
C	1.938824293770	-1.972129099469	0.160277221178
C	1.422925252146	-0.943855710875	-0.905614593496
TV	3.634353687881	0.757098779099	-0.691421016644
TV	0.000000000000	4.229607699081	-1.716377214578
TV	0.000000000000	0.000000000000	3.396752146040
Energy	= -45.416750746020 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min85			
C	0.667319718170	-0.325993392002	-2.074220678020
C	-0.242540525187	1.995512694561	-0.961379056924
C	-0.254208339768	0.910621030672	1.715604415041
C	-0.548691250554	1.111130875986	0.241539024865

C	2.922894823140	-1.577330555332	-1.878550371436
C	3.217943640812	-1.778925879909	-0.404764053369
C	2.001246867923	-0.341018638555	1.912225301083
C	2.911185663409	-2.662483028721	0.798872324789
TV	4.581458234722	-1.854985585700	-0.267151971763
TV	0.000000000000	3.511008235217	1.371493228245
TV	0.000000000000	-0.000000000000	3.781237569020
Energy = -45.416589526807 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min86			
C	-1.046860853522	0.243697047631	-1.604852411645
C	2.909257651510	-0.081574302575	2.054703286272
C	-0.466826270596	-0.556088038768	3.202639742131
C	-3.754353097466	-2.684228130223	0.245947076526
C	0.549350604925	3.698390920046	-2.296340457200
C	3.616307226283	4.542812036770	-0.529278980958
C	-0.450701099042	1.634276070825	1.780244703331
C	-1.120027413413	2.252753967610	0.756807515269
TV	3.087098699598	1.970970674395	0.646845155424
TV	0.000000000000	5.312087127730	-1.346962767044
TV	0.000000000000	-0.000000000000	3.641754656883
Energy = -45.416522900313 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min87			
C	-0.719675862454	0.688308178481	-1.946041227894
C	1.297435440692	-2.190783248045	0.726284567996
C	-0.921396689340	-0.162850047895	3.137588116569
C	-3.461591241567	0.473913934299	-1.241958859416
C	1.297310006214	3.509801457625	-0.762442511773
C	2.293149915205	2.370044939995	1.130074061439
C	-0.444776640670	2.033603023259	1.912256738755
C	-0.247136246343	3.006743392967	0.764032218330
TV	2.540271691972	-0.636733054953	1.927634919430
TV	-0.000000000000	5.700675786189	0.000960466607
TV	0.000000000000	-0.000000000000	3.857962498031
Energy = -45.415595752030 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min88			
C	2.694165086738	-0.229014769245	1.610756630483
C	0.230953567025	-1.850064183500	-1.263891496261
C	2.636024605614	-1.640502132402	5.606396685682
C	-1.311662570001	-0.216406575506	-2.147367484166
C	3.327194441646	2.591217634646	-2.632764713968
C	0.172582806049	-0.911782408374	-0.179278234287
C	4.178153307414	1.425294522550	0.667746047919
C	-0.460329196682	0.967229801807	-1.757620474597
TV	6.841910858873	3.997615911023	-0.113878762178
TV	0.000000000000	2.349662719836	0.829577724899
TV	0.000000000000	0.000000000000	3.740643013204
Energy = -45.415113417367 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min89			
C	-3.486018589861	-1.716518069737	-0.290191142487
C	0.701635790887	0.082453326465	-0.267714257020
C	-0.346837915207	0.338787217271	2.092483990568
C	-0.326027475220	-0.308963326026	0.700322497755
C	6.348688250409	-0.968385747584	-3.017780944391

C	2.854711050352	0.672213862767	-0.954817044127
C	2.698493316692	-0.083175149819	1.405976845846
C	2.013081426681	0.282227863801	0.172008331852
TV	4.22254628610	1.913497120322	-1.473562578966
TV	-0.000000000000	3.146860058694	-0.599525756946
TV	-0.000000000000	-0.000000000000	4.818219350733
Energy = -45.412543060542 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min90			
C	1.848908931088	-0.451381929104	-1.509355763929
C	0.571734424169	0.267958981571	-1.849818465982
C	-1.905771030754	1.842216708839	0.310731988578
C	-0.704526647542	1.135558729592	0.023453281901
C	3.050040677269	1.271892708713	-0.092648993752
C	4.250860821607	1.980573896183	0.191920535131
C	0.572089253051	-2.506934764365	2.118957563242
C	1.849371345504	-1.787672604202	1.778690415243
TV	4.955698721849	-1.783060028772	2.551343870883
TV	0.000000000000	3.568961154853	-1.302722198936
TV	0.000000000000	0.000000000000	3.804512941296
Energy = -45.410260891787 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min91			
C	0.786293890101	0.612034320101	-1.537745376778
C	0.544543475761	0.218778637199	-0.088526355034
C	-0.563053323407	-1.528037508491	1.428829733022
C	-0.321058798973	-1.135013840099	-0.020365005830
C	3.296752430106	1.256543125700	-1.250042013802
C	3.777422596536	-0.155284925906	-0.899043497290
C	2.025415658846	1.358435241619	1.758447566809
C	1.544937316441	0.075900742774	1.041210171891
TV	5.099035763119	0.836524577338	0.251139940941
TV	-0.000000000000	2.694336962920	0.366302620480
TV	-0.000000000000	-0.000000000000	3.802919130231
Energy = -45.409799798224 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min92			
C	2.715810338356	-0.677006754670	-1.120060216126
C	0.567305737688	-0.910330245443	-0.456740691319
C	1.339922569248	-0.468864872277	2.057941902050
C	-1.581300250500	0.531201665709	-0.778087968291
C	2.656518561820	2.574682578686	-2.806410010978
C	1.200052247157	0.023858907448	0.661187029784
C	4.032371024882	0.003672316684	0.717130592839
C	-0.948855618138	1.465621518798	0.339753832925
TV	5.753655115216	1.343009319180	-0.041862755113
TV	0.000000000000	2.363158731705	0.833164378031
TV	-0.000000000000	0.000000000000	3.767353676864
Energy = -45.408145858884 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min93			
C	2.898236195605	-0.677187445065	-1.413832135050
C	0.793093036103	-1.495715591419	-0.655074314284
C	1.533151340820	-0.919114094524	1.860921406018
C	-1.383158617431	-0.227516501295	-0.306351418049
C	2.893425605994	1.911371323298	-2.921435909594
C	1.414393226295	-0.556007801176	0.421090628269

C	3.756915764159	1.953523264887	1.923019910135
C	-0.711295283357	0.954547734168	0.069908887024
TV	6.622190364029	4.681103174354	-0.706980634352
TV	-0.000000000000	2.458903697255	0.765279009044
TV	-0.000000000000	-0.000000000000	3.698969798611
Energy = -45.406717303048 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min94			
C	0.432478230208	-0.786772606704	-1.410821616312
C	0.977852882084	0.271416681018	-0.303780501304
C	-0.052124290158	-0.313207104830	0.763104573403
C	-0.597187013304	-1.371603714460	-0.343830919339
C	0.142748762062	1.545842652982	-0.270989844229
C	1.146068695737	3.307315446077	1.663521441909
C	0.238291942849	2.791664548976	2.603744651279
C	-0.765399193160	1.030517371115	0.669034826859
TV	3.068810345311	1.742451361967	0.369261053639
TV	-0.000000000000	5.437556737943	2.980796818400
TV	0.000000000000	-0.000000000000	3.549212223703
Energy = -45.405867622305 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min95			
C	2.562912726002	-0.982837961861	-0.667583264235
C	0.456246458951	-1.189788262651	0.090518118836
C	1.117095129084	-0.843531288140	3.569814487001
C	-0.721863248622	0.718997422025	-2.149220325138
C	2.506046001187	2.370898225737	-3.445394446596
C	1.026648547050	-0.165430875912	1.089324119254
C	3.532301352363	-0.319807510513	1.653954539857
C	0.285816730149	1.889326892855	-1.684144847756
TV	4.492874305296	0.974132634101	1.182752621119
TV	0.000000000000	2.414155091748	0.659422020781
TV	-0.000000000000	0.000000000000	4.746708585272
Energy = -45.405646869214 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min96			
C	2.555176456627	0.082286609680	-0.703652714425
C	0.443541646911	-1.113146054685	-1.204516488286
C	1.816798822370	-1.113341083933	2.151403157434
C	-1.516078506008	0.514432803198	-1.734821594288
C	3.901280300368	0.082258194559	-0.703514546423
C	-0.352466898128	0.082595180928	-0.703962220473
C	5.207692461189	-2.307716970044	1.651321116236
C	-1.516200255251	2.042275400911	-2.027374057730
TV	7.774236495545	2.392019127186	1.002662511057
TV	0.000000000000	2.391215596546	1.001429491180
TV	-0.000000000000	-0.000000000000	3.355698331830
Energy = -45.405382604943 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min97			
C	0.584787331243	1.250617096480	-3.693347498696
C	0.634457120687	-0.981779129726	1.748211566623
C	-0.765242609933	1.008505620588	0.650546175454
C	-0.704921535155	-0.373996306975	1.619853505872
C	3.209709252330	-0.331695272392	-1.784919736348
C	3.135769102652	0.519092617216	-0.467129388251
C	1.836292238372	-0.388999779627	1.302298933197

C	1.775819592675	0.493833652081	0.231333270886
TV	4.733087600259	0.752549581260	-0.860256805608
TV	-0.000000000000	3.470511968021	-2.349439589697
TV	0.000000000000	-0.000000000000	3.732775537689
Energy	=	-45.404875390999 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min98			
C	0.214090185385	0.934887432320	-3.024142926430
C	1.301076085318	0.257810783634	0.012287117563
C	-0.623617673294	-0.329598339006	1.783452082159
C	-1.576047926340	0.102493251708	0.503992494166
C	2.577902593291	1.779770650447	-2.672099889412
C	3.114822691206	1.497661662858	-1.239114342635
C	1.734635029110	0.552142640690	1.600770517625
C	0.399810687703	1.452032994521	0.291770546129
TV	4.243890070865	2.497772388032	-0.762223911876
TV	-0.000000000000	2.484981359208	0.415790456863
TV	0.000000000000	0.000000000000	4.792053064800
Energy	=	-45.401001389234 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min99			
C	0.007638249347	-1.279400104450	-2.452786909587
C	0.891479323300	0.611441268845	-0.126988965382
C	0.508063784198	0.142428968946	1.287682299684
C	-1.235601148829	-2.140589374783	-2.167640930827
C	0.032447744251	1.660157133343	-0.127059782842
C	0.865802450088	3.508169820358	2.117043755362
C	-0.225627967447	2.461281688937	2.402063513730
C	-0.503024417148	1.376716190611	1.287700774637
TV	2.861837293671	2.340078930161	0.789816811472
TV	0.000000000000	5.836959157104	4.569064724187
TV	-0.000000000000	0.000000000000	3.779975280373
Energy	=	-45.400266770574 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min100			
C	1.279689289011	-0.471752273548	-2.571311519332
C	1.605120112363	-0.521052543104	-1.060254092118
C	-0.108712707801	-0.601645460178	1.701049300660
C	-0.809571573841	-1.896443233604	1.315882696613
C	2.507696479493	1.643749989820	-2.812584539576
C	3.714921938812	1.710608720990	-1.916685723089
C	2.010308284701	0.420117391556	1.269321627087
C	1.173059592912	0.657107612299	-0.017574210869
TV	3.967990660536	4.048245137590	-1.883702507597
TV	-0.000000000000	2.658972778146	0.510771188536
TV	0.000000000000	-0.000000000000	4.838043607155
Energy	=	-45.400077989381 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min101			
C	2.835268634607	-0.423942368877	0.279942472900
C	0.695043104655	-1.597281368817	-0.242500137959
C	2.145434065260	-1.588263991957	3.839950791369
C	-2.084172524903	1.445472503780	-1.488524020321
C	4.312971393176	1.857743812215	-2.712837984988
C	0.005882802721	-0.448187250568	0.303425447922
C	5.093217965336	0.523506381156	1.240442387221
C	-1.475562443392	1.978867534371	-2.582934954282

TV	7.413595096304	2.504492887802	-1.245054662290
TV	0.000000000000	2.331937286768	1.042268828523
TV	-0.000000000000	0.000000000000	4.094180234333
Energy	= -45.399103691736 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min102			
C	1.496845817230	4.122212542851	-4.661755581734
C	0.311778522882	-2.269907757960	3.152512021210
C	1.496902665862	0.116588909684	-1.214616831115
C	0.311771551569	-2.663331143504	-0.420855040657
C	2.681930810847	6.119665730862	-5.984657186547
C	-0.934613939907	-3.210201657044	4.933905234041
C	2.681841671002	2.705133703352	-1.726262865669
C	-0.934489206764	-1.722134871859	2.736296195336
TV	4.862839860409	5.731861189768	-5.997191100525
TV	-0.000000000000	2.293072804536	1.551527819548
TV	0.000000000000	0.000000000000	4.938082179902
Energy	= -45.397154618706 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min103			
C	0.617256247588	-0.307060100204	-2.273943113744
C	-1.527862384756	-0.596546376649	-1.154826501555
C	-0.358612706622	0.595747023372	1.145868496578
C	-0.943462500921	-0.438826500877	0.222562875805
C	2.859182268710	-1.004245508897	-1.087510421864
C	3.443905879287	0.030089769857	-0.164275557143
C	1.883545126254	-0.101504214440	2.331877097659
C	4.028506389160	0.188098065422	1.213172682071
TV	4.387188805316	1.659235639170	-1.003392210306
TV	-0.000000000000	3.438075106318	-1.780820956939
TV	0.000000000000	0.000000000000	4.207729317391
Energy	= -45.396370535478 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min104			
C	3.197228118138	0.330280826446	-1.997043655144
C	-0.463318362876	-2.984272665967	-0.063640873666
C	1.719765318256	0.334419062231	1.733023213518
C	-1.358350412734	-1.067677968953	-1.429057270380
C	4.092183073754	2.242453017204	-3.363467703509
C	1.014212168526	1.413877746601	2.331499973736
C	4.092276762200	0.613848323980	0.566113321344
C	-1.358085311448	-0.494607525728	-0.029009377637
TV	6.851077428626	3.308974806571	-0.070610541819
TV	-0.000000000000	2.201197123871	1.198245765911
TV	0.000000000000	-0.000000000000	3.728030438551
Energy	= -45.395203781710 hartree		
Spin(**2)	= 0.049072265625		
Geometry of 3D-min105			
C	1.399221898179	-0.341542701866	-1.946772394957
C	0.339180609607	-0.763899159541	-0.862751249274
C	-1.789428630279	0.314212677471	0.245415891604
C	-0.725158686886	0.358824062987	-0.876383313486
C	2.547920543159	2.583269799085	0.049215586761
C	4.499004817723	3.549751556317	1.043036970008
C	1.458101951166	-2.642515813532	2.107237953980
C	1.340095377206	-0.682204735997	0.345763197445
TV	4.248694118588	2.026388388818	2.084741326396

TV	0.000000000000	3.777266938694	0.106694311585
TV	-0.000000000000	0.000000000000	3.779007927425
Energy	= -45.395198894052 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min106			
C	1.877043465412	2.107172544649	-5.148088578979
C	0.882876171488	-2.473682648399	3.258114734152
C	1.877177690045	0.525571422417	-0.545043447656
C	-1.027217896894	-2.014649544503	0.379299617407
C	3.151119733240	3.991700723998	-5.805826880785
C	-0.011502562225	-1.525817104907	4.116289634809
C	3.151017941509	2.431135896959	-1.222699277708
C	-1.027010603637	-1.036599765842	3.083699436474
TV	5.500716442670	5.684578326110	-4.387268213929
TV	-0.000000000000	1.895122681148	1.716822240197
TV	0.000000000000	0.000000000000	4.769207011762
Energy	= -45.394926361186 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min107			
C	0.671210798956	1.570951766710	-1.616224543851
C	0.671235231813	1.570630800486	-0.205102460084
C	-0.646744685536	-1.281662085567	1.766576888570
C	-0.646692666091	-1.281341488235	0.246948643817
C	2.685853882980	0.738540496411	-0.910809112877
C	3.986469725991	0.140123661624	-0.911695308265
C	1.890270497250	1.064523564626	1.759629866974
C	1.890593403299	1.064413888963	0.300502206149
TV	5.382956104749	1.085185857879	0.022098069148
TV	-0.000000000000	3.458972509920	-1.917493760740
TV	-0.000000000002	0.000000000002	3.881238568057
Energy	= -45.394879322072 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min108			
C	-1.868455481491	1.662223490033	-1.844168749739
C	2.519515202723	-2.100077470327	-0.044147010244
C	-2.356027558408	0.572770798631	2.804825724235
C	-5.608999780871	2.530465206246	-0.973212819499
C	3.456649497806	2.257443359937	-0.720512902032
C	3.456780425915	0.590162587200	1.116699652935
C	-0.283989238293	1.458456368957	1.987695715757
C	0.203787081241	2.547718768312	0.982325844194
TV	4.064269776011	-1.481788990575	1.367796040290
TV	0.000000000000	3.632021704488	0.291848365142
TV	0.000000000001	0.000000000000	3.643640498845
Energy	= -45.394748604785 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min109			
C	0.429789846053	-0.746675554937	-0.887582252411
C	-0.004448398802	0.276251633271	0.160697340278
C	-0.003546344967	0.276595699701	1.507850598990
C	-0.437895763441	-2.090288598217	-0.888639470310
C	2.884130014562	0.329614527232	-0.885303435593
C	2.449926810089	1.352538681220	0.162985456323
C	2.450715547323	1.352834569969	1.510141820000
C	2.016442562571	-1.013991823370	-0.886340911314
TV	4.908579526877	2.152702114096	0.004558964060
TV	-0.000000000000	3.389638338136	0.001017161384

TV	-0.000000000000	0.000000000000	3.444630185935
Energy	= -45.394747796300 hartree		
Spin(**2)	= 0.015380859375		
Geometry of 3D-min110			
C	0.482507114733	-0.643462916520	-2.584150364023
C	0.482311077426	-0.643775340216	-1.180139744979
C	-0.629726112834	-0.642146040034	1.266266265732
C	-0.629770305327	-0.641990786719	-0.137842062802
C	1.847548520579	1.764957581998	0.562174894926
C	1.848119516999	2.837786979954	1.649518346343
C	1.848726374683	0.427775893127	0.563054223009
C	1.848324378082	-0.644973745566	-0.524407140918
TV	3.843707101837	3.477630168976	2.443046579590
TV	-0.000000000000	3.482206912118	-0.001631473723
TV	0.000000000000	0.000000000000	4.891931581707
Energy	= -45.394202473324 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min111			
C	2.135129159767	0.406547784625	-1.870643506911
C	1.789573280486	-0.826919696490	-2.503376539703
C	1.089572826016	-3.293683373482	2.677571772606
C	-1.093406656706	0.406379903099	2.408777440699
C	2.119313201004	0.406612832302	-5.753436274700
C	2.835529123127	-2.060071973046	-0.564507943993
C	1.806254934499	-0.826841000203	1.379255285981
C	-0.385256884381	1.639810434568	2.525149098560
TV	5.403797278337	0.000154108500	-2.821320833193
TV	0.000000000000	2.466826243181	0.000026679177
TV	0.000000000000	0.000000000001	6.487604430883
Energy	= -45.392644339429 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min112			
C	0.274721597017	0.493017545398	-1.817489898697
C	0.320161637257	-0.141903283742	-0.407758512888
C	-0.565477313302	-0.593040670030	1.946007669382
C	-0.778758522759	-0.793837770801	0.445476945194
C	0.565549165795	3.020230561704	-1.212265168308
C	0.778618220061	3.220969634501	0.288077364306
C	-0.274488919199	1.934262117051	2.551195427741
C	-0.320329468223	2.569128666853	1.141399728271
TV	2.311292283644	1.087315603175	-0.007531940321
TV	0.000000000000	4.866590340297	0.953608282147
TV	-0.000000000000	-0.000000000000	4.435872971541
Energy	= -45.392618063674 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min113			
C	0.150141328325	0.408954590068	0.137139929443
C	2.487461805878	0.410337746530	1.263990416734
C	-0.085401856397	-0.730592368138	2.603574470443
C	-2.431153471182	-0.736028451929	-1.682127237178
C	1.107776440231	3.723348535560	0.097515909219
C	0.882168640008	2.334752975773	0.288528006104
C	-0.433385701356	1.751394709195	0.355690444140
C	-1.613940545240	2.516129571149	0.546492400141
TV	3.915978716800	1.736418191221	2.190749771245
TV	-0.000000000000	5.283111721559	1.094504756510
TV	-0.000000000000	-0.000000000000	3.221365461894

Energy = -45.391978258228 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min114

C	0.821784078867	0.716909197876	-1.209151483412
C	1.142117427587	-0.463787602635	-0.426341124412
C	-0.307908098166	-0.707293761346	-0.192776618343
C	-0.628170215439	0.473379445710	-0.975788050000
C	3.366990755019	2.600088131579	1.484629456289
C	4.352195844905	3.473756783508	0.848886288213
C	0.955694550584	-2.328573800451	0.834252234425
C	1.941110331923	-1.454851935825	0.198379325246
TV	4.794463127986	1.135702609487	3.085194027121
TV	0.000000000000	4.202642491583	1.265838143544
TV	-0.000000000000	-0.000000000000	4.091031071637

 Energy = -45.391697530266 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min115

C	0.041727952972	0.517102991522	-1.672509472669
C	1.022247093979	-0.165100850602	0.812576171498
C	-0.030133913504	-0.337449001559	3.140686214086
C	-1.117755487043	0.199854137441	0.734358590942
C	0.299950023667	3.202769757811	-1.899704786177
C	1.359062432238	2.017330838599	-0.180474808806
C	0.457946159397	1.889817810419	2.277534231936
C	-2.111890343084	2.726611280039	0.847441936942
TV	3.243688273905	0.613400650919	-0.350771058973
TV	-0.000000000000	4.890067469027	-0.945233157881
TV	0.000000000000	-0.000000000000	3.494085246393

 Energy = -45.389341973145 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min116

C	0.810119253864	1.729940822388	-0.193673705285
C	-0.187044046559	0.743333305200	0.501656233179
C	-0.406098351324	-1.846324509266	1.218862016385
C	-0.414873908081	-0.742557477587	0.054601182627
C	-1.361846635031	1.534398549548	1.220599011798
C	0.736105970162	1.703033511679	1.292624702782
C	0.359240902304	-1.516279477827	3.895913602138
C	-0.364352913662	-1.173587155771	2.549305063794
TV	2.472188915583	2.228031718595	1.941791396022
TV	-0.000000000000	4.537691542719	0.332322412200
TV	0.000000000000	0.000000000000	5.016981873471

 Energy = -45.388925235996 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min117

C	1.403845393202	-0.235609144422	-1.961595376618
C	0.396862882117	-0.740887492283	-0.777266360851
C	-1.577108857288	0.620148206539	0.569491837536
C	-0.536615811185	0.389826084607	-0.515708725759
C	2.736620649118	2.515279448820	0.151724690531
C	4.042234764981	3.216227833579	0.691014910393
C	1.290260637487	-2.329561111026	1.503368682960
C	1.312838221464	-1.059528140887	0.443732983886
TV	4.053942188717	1.598254658061	1.841432780936
TV	-0.000000000000	3.646905937455	0.285927365405
TV	-0.000000000000	-0.000000000000	3.702750390274

 Energy = -45.388718374143 hartree

```

Spin(**2) = 0.000000000000
Geometry of 3D-min118
C      0.636263902193      -0.400290770815      -2.451114416431
C      0.073623573520      -1.070069063724      -1.240536907313
C      -0.141495905997      -0.214397333788      0.027976407948
C      -1.204072294003      -1.254791423523      -0.317376775622
C      2.731525346207      -0.233306068217      -0.997103070291
C      2.516575507596      0.622505794712      0.271366797093
C      1.953742687258      -0.047347031870      1.481846543527
C      3.794156623982      0.807039494178      3.121497129073
TV      3.230173026571      3.271174048868      0.267956647276
TV      -0.000000000000      4.749340939651      -2.923750518088
TV      -0.000000000000      0.000000000000      3.773687590596
Energy   = -45.388631168036 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min119
C      1.929062753543      -1.653717159999      -1.991412869314
C      0.300127123155      -0.749871053988      -0.704596193498
C      -0.134962751225      1.337089346025      1.586842382529
C      -1.170438151676      1.193990308823      0.320855247916
C      1.357341426454      -0.211438684122      -1.728649351887
C      2.419019551505      0.339279778300      -0.803948599193
C      1.124594119835      0.502111703488      1.470093671474
C      1.581746908173      -0.514262992636      0.344981815725
TV      3.493671836322      0.590789286863      -0.681325364217
TV      -0.000000000000      3.386840335114      -1.478471700871
TV      -0.000000000000      -0.000000000000      4.542233822813
Energy   = -45.388333204650 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min120
C      0.751628667551      1.520206922118      -0.585914376392
C      -0.100530476508      0.717793274859      0.333575220622
C      -0.695602830580      -1.356687439964      1.289184526307
C      -0.610795723988      -0.743293479757      -0.078760378660
C      -0.756991643845      1.513343249926      1.483922999875
C      0.429058153719      0.701717985460      1.819494279171
C      0.348196920100      -1.310147786013      3.818790886863
C      -0.193712794771      -0.610975158256      2.459594949624
TV      2.480534268691      2.066214254393      2.308281521351
TV      0.000000000000      4.327297766353      0.189574646619
TV      0.000000000000      -0.000000000000      4.997187046390
Energy   = -45.388213438656 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min121
C      1.559984108898      -0.478623893758      -1.262100434306
C      0.251638611365      0.127536207819      -0.853323439475
C      -1.205285825943      0.908839753703      0.874880265342
C      -0.260496552896      1.441450166480      -0.336369485424
C      2.799598933101      1.304878244058      0.580478994077
C      3.153951821422      2.742236986674      0.373693567122
C      0.749798656555      -1.106856346131      -0.101814940516
C      1.789892604295      -1.202048870316      0.999707246262
TV      4.006533946069      -0.685713506825      2.108942957520
TV      0.000000000000      3.673450130508      0.023361768312
TV      0.000000000000      -0.000000000000      3.587014273784
Energy   = -45.386725532688 hartree
Spin(**2) = 0.000000000000

```

Geometry of 3D-min122

C	3.000327313196	-1.584759065786	-1.830076325258
C	0.803669467885	-1.392494349708	-0.713762940097
C	1.528545654308	-1.148397574653	1.690756188851
C	-1.392820691704	-0.134503105313	-0.297652415229
C	2.902157252440	2.407886197161	-2.671540530130
C	1.431410802642	-0.402557194508	0.410540840484
C	3.625281357926	2.174347315399	2.319864882650
C	-0.703809888515	1.024378666275	0.070117353196
TV	6.518894124163	4.735619537455	-0.317139810615
TV	-0.000000000000	2.372527746385	0.789552929284
TV	0.000000000000	0.000000000000	3.696410951442

Energy = -45.385981836949 hartree

Spin(**2) = 0.084228515625

Geometry of 3D-min123

C	3.198072673393	-0.079785470795	-2.069766333587
C	-0.407973328481	-1.221328833234	1.040800907492
C	1.768234517435	-0.049568795191	1.498006608820
C	-1.358476361902	0.704908797437	-0.557726182629
C	3.876216596769	3.210983254064	-3.736056103310
C	0.442545123031	-0.040949955447	1.474439934019
C	4.013861531724	0.354045373270	0.397387860656
C	-1.385849803137	1.571863268946	0.731054722119
TV	6.774769910216	1.821446187832	-1.314850130329
TV	0.000000000000	2.361373386861	0.865956624064
TV	-0.000000000000	0.000000000000	3.650555112191

Energy = -45.385451323943 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min124

C	2.270300974467	0.562695207472	-2.297765378604
C	1.535204317129	-1.094166311132	-0.514409326595
C	2.132735889771	-0.822114313903	4.717934761142
C	0.020835268303	-1.029753175819	-0.839024837940
C	1.934052769154	2.238538066823	-4.177234064157
C	1.950383567346	0.018282376210	0.460534858072
C	2.436278545812	0.849990839908	2.856951271121
C	-0.409802017649	0.366297449405	-1.299202651142
TV	3.739541848053	4.565401335398	-3.298648149183
TV	0.000000000000	2.512092198003	0.496200515289
TV	-0.000000000000	-0.000000000000	6.611516956329

Energy = -45.385223147492 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min125

C	-0.853555807395	0.481219672570	-1.790129286699
C	1.732381554221	-1.740940875582	0.153365662219
C	-1.021614496855	-0.398733281637	3.189619107817
C	-3.559256035904	-0.399242514649	-0.506738848260
C	2.307887641746	4.116249218819	-1.099738090200
C	1.227589559729	2.773143061807	0.430211454578
C	-0.853065581547	1.893166595666	2.000006198161
C	-0.060715912851	2.772900307378	1.096429837177
TV	2.873458283399	0.000464276346	1.316982485621
TV	0.000000000000	5.856862737267	0.000465226227
TV	-0.000000000000	0.000000000000	3.790192832812

Energy = -45.385179268819 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min126

C	0.307283913561	-0.873911924707	-1.746519748718
C	0.356644179649	-0.887281409711	-0.262921440195
C	0.126953822283	0.478512307682	1.664995154881
C	-0.325369539501	0.471784947367	0.259054295049
C	2.409541394348	0.074767103010	-1.083498392081
C	2.956704209503	-1.271199100067	-0.530211273791
C	1.536274906863	-0.159889585684	1.711435891354
C	1.798929758538	-0.617119858926	0.220126884651
TV	4.779348702933	0.961894800290	-0.426859535407
TV	-0.000000000000	2.701060141817	-0.021154301995
TV	0.000000000000	0.000000000000	4.063557481722
Energy = -45.385091695219 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min127			
C	-1.471614779279	0.765240381012	-1.857162120785
C	2.231598379426	-2.349948254785	0.320066154433
C	-0.661851320558	-0.280393197015	2.569204088866
C	-2.688856976313	0.248899317361	-2.434231266104
C	2.502936063682	3.521257335439	-0.267684751204
C	2.008791511955	2.247866728424	1.616584174271
C	-1.099536718088	2.187663517967	1.992391594026
C	-0.870242391738	2.999889672687	0.795114499759
TV	2.909598050226	-0.759979082600	2.277047580593
TV	-0.000000000000	5.942155718967	0.786302743255
TV	0.000000000000	0.000000000000	3.849884578065
Energy = -45.385051822220 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min128			
C	3.054726570662	0.765662052514	-1.727644017218
C	-0.436483996154	-2.626840983072	0.173808636903
C	2.223253101375	-0.364536503673	1.391202786675
C	-1.350172764220	-0.683889829289	-1.166772453574
C	4.069898322424	2.682662146187	-3.068670328945
C	0.897463852168	-0.364147958093	1.388899768262
C	4.069946157199	1.109369376657	0.826529376828
C	-1.350192027178	-0.048395847714	0.215521792507
TV	6.787863420619	3.392239594068	-0.038607029595
TV	0.000000000000	2.260936913174	1.213534999641
TV	-0.000000000000	0.000000000000	3.726064458728
Energy = -45.383792055954 hartree			
Spin(**2) = 0.015380859375			
Geometry of 3D-min129			
C	0.397082304369	-0.141951127396	-1.985691987295
C	0.668715940024	0.510934704395	-0.543563991853
C	-0.362574258939	0.987280128713	1.798235418451
C	-0.624926791426	0.711065311227	0.295337287800
C	2.835360919227	-1.730504428932	-1.577163150122
C	3.106819209878	-1.077205783915	-0.134947141888
C	1.934478846454	-0.509274725375	2.684904054765
C	1.569732275323	-0.710210355780	-0.286073656331
TV	4.491453716507	-0.452841425852	-0.271873480600
TV	0.000000000000	2.464548862825	-0.576639005696
TV	0.000000000000	-0.000000000000	4.519104249210
Energy = -45.382934878353 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min130			
C	2.806278240910	0.230116150116	-0.736107057206

C	0.659723425052	-2.570138152807	-0.732957622955
C	1.508310243499	0.058858868524	2.600495582836
C	-1.399890960885	-1.015905859637	-1.201057888248
C	2.950476622304	2.455676646674	-2.460596914240
C	1.502049805297	-0.062972256399	1.143566527263
C	3.854145875214	1.082707627067	1.213949226857
C	-0.831142021760	-0.020261185717	-0.116599160530
TV	5.586918230049	4.043283652972	0.704933726919
TV	-0.000000000000	2.519542148728	0.710624010668
TV	-0.000000000000	-0.000000000000	3.830941978055
Energy = -45.382843409326 hartree			
Spin(**2) = 0.015380859375			
Geometry of 3D-min131			
C	0.789943677918	0.340637942985	-0.967144879493
C	1.694420456868	-0.397621132987	0.162956759161
C	-0.339511948436	-0.717368202995	2.693562819297
C	-1.750218808083	0.588714039133	0.802986317051
C	-0.113257563489	2.660996026074	-2.072886645988
C	2.140921608311	1.713188037064	1.810650194396
C	0.832872254190	1.921394482202	2.528415850601
C	-2.916481704741	3.139641532829	-0.473875624561
TV	3.460870906971	-0.113750461472	0.551723575667
TV	-0.000000000000	4.519922636688	-0.174471593550
TV	-0.000000000000	0.000000000000	3.506584814254
Energy = -45.381512863893 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min132			
C	2.648347629836	-0.798073673249	-1.192902354688
C	0.525089066923	-4.358002691393	-2.501752702155
C	1.940192861934	-1.984589681375	2.155065489787
C	-1.370753575339	0.390861836817	1.128370743588
C	4.093459119762	1.574440653054	-4.103987463668
C	-0.715539660354	2.321241016197	3.240762600312
C	4.798501369796	0.386227694687	-0.751986871308
C	-0.715289597528	3.210737117689	0.754813142888
TV	7.665645704754	2.369324288902	-4.794026308697
TV	-0.000000000000	2.374621488242	0.869071026347
TV	0.000000000000	0.000000000000	3.784558194628
Energy = -45.381188294008 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min133			
C	0.744270717775	-0.197689194257	-2.411442066053
C	2.132975704092	0.038795417412	-2.955200438840
C	2.689027404274	-0.833136474108	2.178512776292
C	-0.714992713850	-2.445574382364	2.755013331571
C	1.835235390610	1.737978785008	-6.860634557644
C	2.367819410008	-0.239061460590	0.813856327727
C	2.236830902804	1.176711790344	0.688846419490
C	-1.406798024849	-1.305271129551	3.263317851041
TV	5.618171764125	0.468515320362	-1.076852647594
TV	0.000000000000	2.289930127308	0.996041154433
TV	0.000000000000	0.000000000000	6.259160837520
Energy = -45.380955229899 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min134			
C	0.858512554916	0.545466720162	-3.907127373513
C	0.858873819758	0.133424839764	-1.881431944887

C	2.850072687603	-0.882143838047	2.687932390390
C	-0.290526835159	-2.103639019050	2.427887767813
C	2.008016977323	0.339412666627	-2.894478310161
C	0.858712446999	-0.160740420804	-0.452553095412
C	0.858507250213	0.840345305259	0.507562671278
C	-1.132683794166	-0.882136119700	2.689085594312
TV	5.337621948574	0.000023236735	-0.001389094712
TV	-0.000000000000	2.443122609343	0.521594063169
TV	-0.000000000000	-0.000000000000	5.843431096264
Energy	= -45.380134985352 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min135			
C	-0.007663028097	0.728813658754	-2.846511113329
C	2.462980835518	-0.616387877985	-1.103892572876
C	1.805118063556	-1.868822344221	3.517297571063
C	-0.292996575110	-1.815478797492	0.585984123553
C	0.350085545456	0.714819750539	-1.499599076623
C	3.864964061036	-0.657953192795	-0.726936543055
C	4.523101687248	0.594696534782	-0.408321903160
C	-0.652323839122	0.741986977197	-0.475924674367
TV	6.631259191840	-0.185697400506	0.424500870544
TV	-0.000000000000	2.544374066630	0.284332175563
TV	0.000000000000	0.000000000000	4.941278430149
Energy	= -45.379931614683 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min136			
C	3.019559765329	0.592308427892	-1.498713753373
C	0.405640293763	-1.789759134041	0.840774822046
C	1.747172245283	-1.792180051121	4.191664190479
C	-1.543256305439	-0.163317987409	0.313260552440
C	4.361121094665	2.978769895945	-3.839125439834
C	-0.398353462892	-0.594788671161	1.341518059823
C	5.165224512080	1.783694174263	-0.991364759471
C	-1.543524091353	1.362980215010	0.024432774378
TV	7.853322003466	4.767544687906	-4.678293032103
TV	0.000000000000	2.389191706595	1.002878474374
TV	0.000000000000	-0.000000000000	3.348158544502
Energy	= -45.378148317780 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min137			
C	-1.293330939924	-0.743377453186	-1.489355655705
C	-0.332657411454	-0.484829313674	0.938757936598
C	-0.333477302515	-0.481764175527	3.010691772773
C	-2.438131475319	-1.708646444231	1.979991682311
C	1.515823954682	4.005893639332	-1.893300058281
C	2.649983809566	4.048801009504	-0.857879951410
C	0.371107316166	3.040522197268	1.576220593359
C	-0.588914875040	2.779296466879	0.541181711662
TV	3.239655142563	1.266880513992	-0.005839586554
TV	0.000000000000	5.981690669398	-0.409916480859
TV	-0.000000000000	-0.000000000000	3.464784458849
Energy	= -45.378121160042 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min138			
C	-0.049233188496	2.153922326791	-4.908594379555
C	2.511355804037	0.119339750090	-0.293256429436
C	-0.017625308421	1.082115564864	0.360351875534

C	-0.986020491483	0.134975967075	1.141105098723
C	2.209817087401	0.540727762470	-1.701402935593
C	1.400231905149	-2.178578549931	3.271137059584
C	1.224395066999	2.836494550028	-0.608073113209
C	-2.097064947654	0.809196943225	2.121401172468
TV	4.651436618342	3.580688940340	-3.158295237200
TV	0.000000000000	2.903593781831	1.847863337942
TV	-0.000000000000	-0.000000000000	4.389570604410
Energy = -45.377207425256 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min139			
C	0.629431547662	0.125113270901	-1.957329853611
C	0.629481752542	0.123076085100	-0.544487341368
C	-0.670114663131	0.123912822484	1.810645540961
C	-0.670065669056	0.125511273142	0.215280122953
C	3.282814781815	0.123520671393	-2.734446809465
C	3.282831587685	0.120789671092	0.232683174324
C	1.766810156859	0.125142703253	1.726090102248
C	1.766808202728	0.120443268061	0.299818724466
TV	4.794147271923	1.363118033230	0.000233097117
TV	-0.000000000000	2.731270765038	0.000503855668
TV	-0.000000000000	0.000000000000	4.527651467506
Energy = -45.376325662369 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min140			
C	1.259222057370	0.792791334195	-2.143409752857
C	0.081253042642	-0.135368601127	-0.094104269112
C	-0.915787585211	-0.801305102450	2.168664476574
C	-0.608645050888	-1.014047614290	-1.038437854845
C	-0.259860674177	1.457437289154	1.882608848124
C	0.120971926449	1.581868488843	3.273251236496
C	-1.992034553170	-0.831955542554	4.433675364803
C	-0.335214589715	0.153112641623	1.223992427505
TV	3.268165471133	1.224919047147	0.760493053746
TV	-0.000000000000	3.490087170032	-0.760802153033
TV	0.000000000000	-0.000000000000	5.946553112966
Energy = -45.376277594274 hartree			
Spin(**2) = 0.015380859375			
Geometry of 3D-min141			
C	0.328346364354	0.226205348413	-3.257745582149
C	2.301535920631	1.217413360578	-1.830071854688
C	2.588537587463	-0.992994146351	2.231587323892
C	-0.977842824940	-2.188289527658	1.717904544380
C	1.097806884651	1.431797968125	-2.793027407377
C	2.785359976169	0.916608724453	-0.477114959199
C	3.047636338203	2.031321162431	0.397129450406
C	-1.790861618877	-0.897659095071	1.798405931150
TV	5.471768169041	2.626309888628	-0.040103423559
TV	-0.000000000000	2.494255507213	0.553488941226
TV	-0.000000000000	-0.000000000000	5.889643596435
Energy = -45.375035724921 hartree			
Spin(**2) = 0.109375000000			
Geometry of 3D-min142			
C	3.416781981591	0.466712874058	-2.254707528334
C	0.547209455951	-1.129989874855	-1.031029297600
C	2.901358458058	-0.577507422228	1.770598280812
C	-0.972792594550	0.457044075519	-2.202730678717

C	4.303151146620	2.612290808247	-0.647464163775
C	1.061031555041	-0.059350229969	-0.217039330437
C	2.015060583801	-0.320579166853	0.787439070173
C	-0.459344873598	1.527598713861	-1.388423644263
TV	6.229034664054	1.893946291178	2.560485124902
TV	-0.000000000000	2.402324912046	0.624138659592
TV	0.000000000000	0.000000000000	4.941458952184
Energy = -45.369236720922 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min143			
C	2.901179271669	-1.070536229080	1.530272618206
C	0.237608937266	-1.164901105002	-1.645289911906
C	1.671476745291	-1.114985898136	1.705749602355
C	-1.488635741888	0.272328001186	-1.776654499125
C	4.315647674119	1.391631466162	-1.194700591638
C	-0.433627565969	-0.179807068752	-0.639467981715
C	4.977898787478	0.230667842944	1.730809095000
C	-0.822450935059	1.676858803039	-1.827932896891
TV	7.950864681312	2.409425580804	0.819124528541
TV	-0.000000000002	2.392034586131	0.948931324318
TV	-0.000000000002	-0.000000000003	3.487046011578
Energy = -45.368779375789 hartree			
Spin(**2) = 0.140625000000			
Geometry of 3D-min144			
C	2.447408775740	-0.878932439799	-0.595146652158
C	0.445747400956	-2.238839667947	-0.019073515889
C	1.477935082004	0.892582056041	3.621942209066
C	-0.514099127651	-0.472376816971	-2.837763348802
C	2.151905417070	2.163652553195	-3.509376505075
C	1.193267793470	-0.963570059844	-0.108444374719
C	3.455695451112	-0.190589243419	2.600689894831
C	0.159579082275	0.798741446042	-2.903469139004
TV	4.264570540113	2.131968165625	2.133847002820
TV	-0.000000000000	2.446008285545	0.423945864902
TV	-0.000000000000	0.000000000000	7.065748299738
Energy = -45.368066292223 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min145			
C	2.712181755221	0.944186345156	-1.633773308526
C	0.571429626452	-2.965421213275	2.272594849177
C	-0.465683230705	-2.965346419810	5.026319046636
C	-0.466161106859	-0.357708979594	-0.481077463995
C	4.025179510818	3.547335016397	-5.544517235044
C	1.386175122601	-1.661621541253	2.273970767377
C	4.992653740143	3.546002496748	-2.794764230528
C	-1.362774913814	0.946132762867	-0.476368570693
TV	6.354870023700	5.207552528491	-3.903428396706
TV	-0.000000000000	2.607604396953	0.000308431306
TV	0.000000000000	0.000000000000	3.913530007265
Energy = -45.367679064768 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min146			
C	1.366424631482	0.218178091841	-5.248037829703
C	1.358083969742	-1.476784023720	-1.957335960383
C	1.366334083363	-1.297702835933	6.001000381858
C	1.343450915239	-3.184309480595	1.411294182236
C	1.372283782402	1.351026636954	-4.358667817105

C	1.356202570425	-0.354236029696	-0.989685425705
C	1.348716286505	1.926232505930	0.677550482298
C	1.349804343083	-2.051512385904	2.300561550942
TV	3.293925085429	-0.125228277536	0.988797917089
TV	-0.000000000000	2.460951372771	0.331916838501
TV	-0.000000000000	-0.000000000000	9.293877779156
Energy = -45.367665688020 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min147			
C	0.612603358030	0.330351862840	-1.029437740136
C	1.488525392658	-0.646969980557	-0.206549387768
C	-0.559226047979	-0.460364501190	1.818630239469
C	-1.338593952104	0.829117433355	1.367841449722
C	-0.116344991675	2.677883311895	-2.111788968348
C	2.335115842235	1.892305230869	1.032928849627
C	-0.417040577337	1.543453189352	2.544761485326
C	-2.141457177557	2.885045239744	0.141120141972
TV	3.353514925392	-0.048594972258	0.672480316065
TV	0.000000000000	4.522639398644	0.209875158408
TV	-0.000000000000	0.000000000000	3.557967756383
Energy = -45.367174607022 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min148			
C	0.920281527414	-0.528849090944	-1.602879305068
C	0.596769977033	-0.351115445898	-0.265718460408
C	0.596153913824	-1.745183606958	1.859856750180
C	-0.028467976112	-1.437040252945	0.541962096572
C	2.678440452064	1.187365558006	-1.995818064395
C	3.746441635119	1.763763982274	-1.611191984162
C	1.545530317979	0.557243935400	1.850055576536
C	0.920935868297	0.865256043580	0.532014141089
TV	4.907518996371	3.831132647553	-1.738038743103
TV	-0.000000000000	3.907686927582	-1.696508803189
TV	-0.000000000000	0.000000000000	4.260548981242
Energy = -45.367146310055 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min149			
C	0.938695839223	-1.097184540940	0.181794903198
C	0.655738098262	-0.054401263153	-0.889300675813
C	-1.360871820351	1.271429332579	0.169264843512
C	-0.957301431037	0.223450803789	-0.894642128337
C	3.438258772945	-0.237949602820	-0.965152392761
C	3.019230761870	0.816647805745	0.069740812611
C	1.031071549177	-0.129454715859	1.153071441947
C	1.365999841175	0.943890089749	0.121225298816
TV	4.791442011957	1.945633244146	0.968428113454
TV	0.000000000000	3.452053671093	-0.012180483039
TV	-0.000000000000	0.000000000000	3.475240518667
Energy = -45.366174511364 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min150			
C	2.360453498478	-0.037972793088	-1.097966150329
C	2.164531900360	-1.279933313802	-0.229444620896
C	1.320245572826	-2.519812409012	4.638723109989
C	-0.770394718288	1.206790595979	-1.571027587967
C	1.679857880914	1.200914144631	-4.368012493478
C	1.924193026606	-1.282778677760	1.074917652985

C	1.576441272262	-0.034897946961	3.189193702380
C	-0.109040083840	2.450508840033	-1.794355971342
TV	4.557651613688	1.239225907670	-0.054788307408
TV	0.000000000000	2.484818545528	0.001372575695
TV	0.000000000000	-0.000000000000	6.839964498533
Energy = -45.365976248849 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min151			
C	0.630282639377	0.095712875392	-1.702158272316
C	0.658380757578	-0.171127639779	-0.194228849784
C	-0.011697601585	1.155696632485	3.718662537099
C	-0.767952895089	-0.234377383662	-2.203034412989
C	3.130386187958	0.445450458664	-1.725613829259
C	3.158452818284	0.178595142172	-0.217663184744
C	1.867954987837	0.210382758184	1.952508154726
C	1.920815977944	0.063816347631	0.588411705875
TV	4.568524373396	2.076766847386	0.303581318430
TV	-0.000000000000	2.723815888620	-0.721514281099
TV	-0.000000000000	-0.000000000000	4.460567299194
Energy = -45.365011359027 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min152			
C	2.947241088099	0.506767103306	-1.958957920578
C	1.285513307062	-1.046376327699	-1.082407374132
C	2.163376633792	-0.784357368262	2.874823142046
C	-1.014405135132	-1.268211317458	-0.251943982170
C	2.681661686915	2.297622423774	-3.724219779800
C	1.169158329375	-0.023823577594	0.028222415704
C	3.298791290801	0.904714769740	1.490780877043
C	-0.305001454509	-0.171023670889	0.579206200017
TV	4.721454039730	3.871494913515	0.320134377956
TV	0.000000000000	2.462652996923	0.657740524430
TV	-0.000000000000	-0.000000000000	4.938542996144
Energy = -45.363620287485 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min153			
C	0.035491455269	-0.516493874376	-2.202455918265
C	-0.635409224534	-0.516325227003	-0.803736753025
C	-0.099828574393	0.802763410738	1.333924830588
C	-0.500271899237	0.802683582658	-0.009427814634
C	3.651576848503	2.105810393288	-1.189499089466
C	2.844526240132	2.105869041422	0.188729246323
C	1.452361386471	-1.177054248549	1.849141177478
C	1.495713386589	-1.176988946521	0.476210491262
TV	3.548116480199	0.000145928110	1.002077427531
TV	-0.000000000000	3.683626347507	-2.164120256872
TV	-0.000000000000	-0.000000000000	4.329925393501
Energy = -45.360385503177 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min154			
C	3.195586749584	-2.260260384229	-1.180560468085
C	-0.015806101059	-0.682270648472	-0.749555976056
C	-0.459565581613	1.108237085504	1.926478201732
C	-1.767927516895	0.354643991422	2.184256165314
C	2.446478654664	-1.068615407593	-1.795132613455
C	2.205471956010	0.134981317495	-0.879676847081
C	0.753295738085	0.917127991889	1.067136716008

C	0.983859938296	0.155916029465	-0.060730621794
TV	3.170638518493	1.779048137889	-0.511381010354
TV	0.000000000000	3.296119862611	-1.621973915692
TV	-0.000000000000	-0.000000000000	6.194987294872
Energy	= -45.358902080625 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min155			
C	3.037687033632	0.626931971889	-4.956289693567
C	-0.296847658256	-0.907533140889	2.058645860660
C	2.285111497933	-0.689501740728	-0.565957607478
C	1.530615442523	-1.350612798289	0.604469496749
C	2.117815622655	2.720872248168	-4.751564596231
C	-0.991756956106	-0.912959073940	4.400757138512
C	4.781036939293	0.143604999447	-1.926703630530
C	-0.016657852540	0.607272097897	2.106399881541
TV	5.541176433486	3.976333485511	-3.664224572725
TV	-0.000000000000	2.220440859466	1.352406552090
TV	-0.000000000000	-0.000000000000	4.638971930942
Energy	= -45.357942850196 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min156			
C	0.601112762207	-0.237885556448	-2.224179581589
C	-0.664412677852	-0.833479354067	-1.496311810583
C	-0.347988642767	0.294164515800	0.858038246667
C	-0.689615910940	-0.921988881826	-0.001070761123
C	2.848331095487	-0.702631979947	-0.799870489667
C	3.190858748415	0.513226251714	0.059404469873
C	1.899123369509	-0.170395783914	2.282315233252
C	3.165049574651	0.424742946283	1.554600250971
TV	4.232286059588	2.617500203487	-0.511037261049
TV	0.000000000000	3.743074220459	-1.894960157101
TV	-0.000000000000	0.000000000000	4.180107551803
Energy	= -45.357754069003 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min157			
C	0.909691192407	0.510086653465	-3.036450759863
C	1.933711158075	0.295234635560	-2.069429893901
C	2.980966961049	-1.945306575091	2.151584932469
C	-0.556038192904	-1.975317413167	2.278994007751
C	1.959793026377	0.745947518373	-4.091994552575
C	1.945520633218	-0.023808349558	-0.638574405691
C	1.953724410033	1.065501815852	0.308272229213
C	-1.243000397382	-0.739584933522	2.569868086182
TV	5.691854767968	-1.195831031161	-0.461357590735
TV	0.000000000000	2.477300459005	0.552775429119
TV	-0.000000000000	0.000000000000	5.833300103952
Energy	= -45.357112389342 hartree		
Spin(**2)	= 0.058593750000		
Geometry of 3D-min158			
C	2.014564646702	-0.303295898452	-2.158330450809
C	0.957188694683	-2.333770350811	-1.530243146627
C	-1.558326882362	1.877532370802	1.085994007091
C	-0.631131574317	4.042361400343	-0.075127407444
C	2.569725801265	1.761504989306	-0.212151773037
C	3.492068763059	1.003490375793	0.516302312976
C	0.702833976067	-2.281611445490	1.403620844917
C	1.472609508430	-0.848363729275	1.019759734871

TV	3.820052264099	-0.160057948488	1.713036700550
TV	-0.000000000000	3.150378450259	-0.396497954771
TV	0.000000000000	-0.000000000000	4.476237177905
Energy	= -45.356488349349 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min159			
C	1.932302003443	-0.097556906038	-0.798302249463
C	0.489145465224	-1.527660386701	-0.202438429001
C	1.310941781323	-1.227059059655	4.409232180163
C	-0.152696328772	0.338596043926	-2.814561442102
C	1.772156791763	1.787837938804	-3.511850265306
C	1.110784176245	-0.398208638599	0.577485326189
C	2.575232011455	0.516247663502	2.350272604746
C	0.650200500153	1.547798940094	-2.402047324167
TV	4.041326541368	2.594681333954	0.008115869444
TV	0.000000000000	2.480753864553	0.537324139421
TV	0.000000000000	-0.000000000000	5.987459211173
Energy	= -45.355834101424 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min160			
C	1.270014630702	1.060161662968	-2.390642246669
C	1.193085805323	0.519604350774	-1.008893322945
C	-0.168451212383	0.785608934211	0.982982402809
C	-0.151288352659	0.667716767600	-0.473523759352
C	2.393141325176	-0.126246645933	-0.382049300494
C	3.843960225111	0.231336033624	-0.470087112239
C	1.787249636122	-0.953754017248	2.257002979406
C	1.928518493377	-0.209558787245	1.024377444641
TV	4.828478518360	-0.426702644519	1.215437512242
TV	0.000000000000	3.418000808871	-0.994254454170
TV	-0.000000000000	0.000000000000	3.862802734016
Energy	= -45.353303066359 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min161			
C	-0.154217033540	0.496777028602	-2.081545220896
C	2.747469111293	-1.200494850518	0.509100517173
C	0.130804834873	-0.669511711747	2.529525637583
C	-2.771312609772	1.027189361963	-0.061060682178
C	0.614011262271	2.559927708985	-1.069937444434
C	1.215990542147	1.568078770497	0.117678734011
C	-0.637875612045	1.830523782161	2.401008457498
C	-1.239978838886	2.821898968686	1.213360280565
TV	3.008815805201	-0.557214203220	0.596694756259
TV	-0.000000000000	4.563368838716	0.883076387214
TV	0.000000000000	0.000000000000	3.982217488598
Energy	= -45.353239710552 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min162			
C	0.536986781411	-0.205968777563	-1.616303644132
C	0.489051401803	-0.459049453387	-0.142812309468
C	-0.436617510883	-0.008274898221	1.011332792102
C	-0.726853396114	-1.402551040670	0.469792542124
C	3.264774955201	-0.122529902059	-1.566827841391
C	2.997638846442	0.327116948165	-0.121847971995
C	1.830902280928	-0.247920685188	1.776146043149
C	1.839020062078	-0.221553497662	0.372174120293
TV	4.535424900426	2.211064952610	0.601669403264

TV	0.000000000000	3.643774928669	-0.727335032904
TV	0.000000000000	0.000000000000	3.865737530933
Energy	= -45.351985897674 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min163			
C	-0.475634898703	1.252571977835	-1.125774791050
C	-0.475653734977	0.729091396162	0.509049656884
C	0.772012475696	-1.384266398909	0.812887135669
C	-0.657177666667	-0.836849965503	0.784081848183
C	0.771953245974	1.286597354842	1.259162144326
C	0.771868603295	0.694973977711	2.610873312787
C	-0.657138426558	-1.360387322327	2.419058587455
C	0.771820766473	-0.813038837848	2.390002637510
TV	2.676752868477	2.089216163188	2.577096294128
TV	-0.000000000000	4.178863896734	0.667235679382
TV	0.000000000000	-0.000000000000	4.487137154133
Energy	= -45.351697893350 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min164			
C	1.960653321336	-0.122352613810	-3.969848278127
C	2.735708983288	-0.643658658667	-1.697593310938
C	3.104943245915	0.164275673932	3.379486082375
C	0.482701948122	-1.051289745210	0.475665620203
C	1.012882236975	1.451734312321	-2.671385810334
C	2.156773066900	0.775079339371	-1.883478496758
C	1.379859424553	1.246523257905	2.185064380565
C	0.119153087846	0.322753750809	0.205379934874
TV	3.505065480941	1.390561048266	-0.176138739834
TV	-0.000000000032	2.582085515716	0.561366790671
TV	-0.000000000001	-0.000000000502	6.350168307297
Energy	= -45.351693814176 hartree		
Spin(**2)	= 0.015380859375		
Geometry of 3D-min165			
C	0.128862610717	-0.403688994805	-1.320737041045
C	0.128340118365	-0.405627253953	0.094762227424
C	0.128335688444	0.308288397691	1.329185342750
C	0.128061751663	-1.631607196577	-0.605908991923
C	0.128879383011	-0.403650200663	2.562354608752
C	0.128362440778	-0.405472953196	3.977843754701
C	0.128359121745	0.308376354036	5.212310424751
C	0.128101824056	-1.631511555277	3.277243251390
TV	3.242987658780	1.669279204533	-0.983366923892
TV	0.000000000000	3.365337471611	1.926008545644
TV	0.000000000000	-0.000000000000	7.766172870355
Energy	= -45.351187886458 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min166			
C	1.396406008738	-0.015297889783	-2.958202622311
C	2.250778313054	1.292215571962	-1.093445918308
C	-0.126460918354	-0.059631029601	1.239373734473
C	-1.248047989117	-0.071905562677	0.102518995526
C	0.126342186753	2.398558786977	-0.289134266189
C	1.247973606063	2.410619841543	0.847649330444
C	-1.396255909574	2.353800604107	3.908361494541
C	-2.250715850557	1.046208051792	2.043497577039
TV	3.444290401096	1.305759293606	0.356758133948
TV	-0.000000000000	3.906111944073	2.031464368436

```

TV          -0.000000000000      0.000000000000      3.880094853306
Energy      = -45.351061064597 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min167
C           0.063600056611      0.533317493083      -1.797793332207
C           2.383127238772      -0.795871332055      0.854893650598
C           0.312514682892      -0.305048050564      2.996568369763
C           -3.582772146396      -0.653159661537      0.657871613751
C           0.839639320581      3.025168261971      -1.625461850005
C           1.995910711507      2.807745471316      -0.573926077784
C           -0.344866764343      1.983099782932      2.069472215844
C           -1.431006350942      2.454787606175      1.028245883792
TV          3.409596207783      0.448185876701      0.006710014179
TV          0.000000000000      4.794082861318      -0.684277728859
TV          0.000000000000      0.000000000000      3.739762406522
Energy      = -45.350630289213 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min168
C           0.698185165680      0.045925131944      -1.640755467181
C           0.698484908900      0.042233834488      -0.222824865358
C           -0.010588626895      -0.021306921032      1.008393844428
C           -1.426955412306      -0.150888908005      1.009492821949
C           0.705057229443      3.481889832062      -1.219151814176
C           0.705205902027      3.479173039508      0.198727741280
C           -0.003851912891      3.417687499694      1.430118882750
C           -1.420299868003      3.287219755012      1.431154558402
TV          3.349262272852      0.303278509535      -1.942237315423
TV          -0.000000000000      6.847176150687      1.055432903126
TV          -0.000000000000      0.000000000000      3.880487182161
Energy      = -45.349968581179 hartree
Spin(**2) = 0.032226562500
Geometry of 3D-min169
C           3.220521460977      0.468537851873      -2.438248449697
C           2.478355268359      -0.863006873210      -0.652949022405
C           2.741284722458      0.587714409923      3.785985152218
C           0.016831190481      -1.358472199857      -1.479124102761
C           1.948172823913      2.331636300543      -2.199039780936
C           1.464905670861      1.450396825048      -1.017172535748
C           2.214221107967      1.280974267779      1.504804717990
C           -0.636616309461      -0.203333844401      -0.982111300436
TV          5.296447960250      0.605686575738      2.929756896250
TV          -0.000000000000      2.557322787777      0.748360236371
TV          -0.000000000000      0.000000000000      4.750277351641
Energy      = -45.349184497951 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min170
C           1.136407718274      -1.113813219438      -1.859027911616
C           2.096813807421      -2.762541407905      0.751942538502
C           2.966114257442      0.307863061540      5.326311468764
C           -1.036160758120      0.198307364364      -1.822468120141
C           1.544335270556      1.225216651622      -3.556275707013
C           2.144298380193      1.513013954167      -1.066742574193
C           1.718387875429      -0.112541642125      1.827320904918
C           -0.343287500459      1.451876587830      -1.986123662843
TV          5.490273217454      2.642714950064      0.917155531789
TV          -0.000000000000      2.518802238296      -0.281992202550
TV          -0.000000000000      -0.000000000000      5.928120694350

```

Energy = -45.348869813630 hartree
 Spin(**2) = 0.187500000000
 Geometry of 3D-min171

C	1.981342511870	0.641606156634	-3.076954939505
C	-0.003366469506	-0.700444668255	0.547978628662
C	-1.086274530519	1.666087683767	-0.431819161156
C	-0.061686584998	0.635119864793	-0.054866934373
C	2.640228895718	1.435873244422	-0.629850482044
C	4.046210898869	1.747990427549	-0.058479639536
C	0.910275008532	-1.579336379986	2.406685536739
C	1.434567067966	-0.783897068540	1.203257849080
TV	4.116755461292	-0.746351317804	2.558178528118
TV	-0.000000000000	3.226224482013	-1.697479451073
TV	-0.000000000000	-0.000000000000	4.163875594444

 Energy = -45.348630575637 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min172

C	4.160069960960	-0.363130692005	-1.612178625473
C	-0.222862796923	-2.595789754979	-0.220741841423
C	3.094228581079	-1.297094699892	3.514783774236
C	1.227798336585	0.128210634661	-0.750853821079
C	1.266739641029	1.467851035016	-4.205595862603
C	-0.115060749032	-1.376532977339	0.717973688886
C	1.916512093839	0.232204007205	0.690027771100
C	1.530988742454	1.428218669593	-1.524061828141
TV	3.572611328583	2.975704059375	1.440337433513
TV	-0.000000000000	2.523490091953	0.116479100106
TV	0.000000000000	0.000000000000	5.558768952866

 Energy = -45.348207701354 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min173

C	1.788967843465	1.410428699824	-3.938127723125
C	0.431762075288	-0.729385761759	-0.484375890175
C	-1.658206631014	0.711940821738	-0.412311732804
C	-0.330881092257	0.441534114048	-1.087642006318
C	2.906674125214	1.733742882849	-0.474738482686
C	4.282987997734	1.992557081750	0.183619555849
C	0.532447684011	-2.590253027841	2.143132343511
C	1.808787047994	-1.221204828131	3.408232466281
TV	4.582314717994	0.935443075018	2.715798484718
TV	0.000000000000	3.200874901286	-1.841986380200
TV	-0.000000000000	-0.000000000000	4.203968162044

 Energy = -45.346427601641 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min174

C	2.116783380241	-0.606525593932	0.764850460666
C	0.145739802012	-1.500163470706	-0.468567016823
C	1.667244237233	-1.532842911664	3.414253422885
C	2.282954973861	1.279780987949	-0.840519771071
C	3.552116441376	1.526680494344	-1.547024049600
C	-0.562458608936	-0.310178953509	-0.081649458024
C	4.381664930113	0.374495374324	1.748857203893
C	-1.986877885682	2.049825436633	-3.042521446662
TV	7.700021116518	3.086448005959	-1.249933911247
TV	-0.000000000000	2.361579480581	0.825022711219
TV	0.000000000000	-0.000000000001	3.790066478105

 Energy = -45.345455435456 hartree

```

Spin(**2) = 0.000000000000
Geometry of 3D-min175
C      2.437988597410      -0.104012455131      -1.278241668316
C      0.583200041902      -1.693471057712      -0.556687232593
C      1.551976024022      -1.269135855796      2.208611418755
C      -1.779274022612      -0.368380394898      -0.645786246726
C      3.366546207359      1.613050842566      -3.263391544219
C      0.611376641020      -0.850446468000      0.878591879396
C      4.600368633463      2.132386585321      1.090516367749
C      -0.838470955920      0.851101935055      -0.072566761767
TV      5.307645035084      3.329135000220      -0.381275985927
TV      -0.000000000000      2.366368729588      1.099247152441
TV      -0.000000000000      0.000000000000      4.061608078707
Energy   = -45.345439192262 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min176
C      1.196919089528      -0.134147987969      -3.046575656007
C      0.974640318532      -1.441629587882      -2.237502234756
C      -1.686730235917      1.626402559177      1.745743101293
C      -0.484797690543      1.527027548414      0.864301856689
C      2.723208451126      2.279702507814      0.357757395391
C      3.889246238081      2.100717234757      1.224594658439
C      0.831933521530      -2.137639826890      0.805962642655
C      1.575113241199      -0.902584735217      0.335542358230
TV      4.177397588436      0.288636026197      1.746199429891
TV      -0.000000000000      3.430671990079      0.844925266942
TV      -0.000000000000      -0.000000000000      4.462379534906
Energy   = -45.345401487472 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min177
C      2.404135796815      0.575239596453      -2.525278301898
C      2.847218897595      -3.080208271911      -1.328636474167
C      2.158571942436      -0.905581408889      2.454046977885
C      -0.604588382284      0.606208959733      0.255737055603
C      0.779138195071      0.369601827222      -4.249030399323
C      2.151732902108      -1.647231380837      -1.201798919399
C      0.966991614962      -0.030766925504      2.075106141812
C      -1.287360458814      1.726597966955      0.797585112609
TV      5.647485445819      -0.334902747390      0.410036184251
TV      -0.000000000000      2.222309886118      1.282708829585
TV      0.000000000000      0.000000000001      4.992017416884
Energy   = -45.344587931300 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min178
C      1.836325394891      -0.995859692252      -2.778251661351
C      0.911006379876      -1.600058790193      0.186991874737
C      3.125417593743      -1.171416385999      3.355613811987
C      -1.441808616813      -1.194205933302      -1.343631615922
C      2.273254343290      1.585451889137      -3.856027006611
C      0.368760439997      -0.275939757655      0.063131148743
C      1.872847159745      0.536247426644      1.859765748960
C      -0.827534987961      -0.068722514942      -0.712433623882
TV      5.961272650979      2.303257671500      -0.841936180541
TV      -0.000000000000      2.410644137374      0.643674091463
TV      -0.000000000000      0.000000000000      6.622030722094
Energy   = -45.343659423292 hartree
Spin(**2) = 0.000000000000

```

Geometry of 3D-min179

C	0.845763048674	-0.184574813414	-2.516808976758
C	1.770520262376	-0.780098225812	-1.458130666460
C	0.047493584036	-1.586280386882	2.824733101007
C	0.390502346198	0.120583228640	-0.208985626416
C	2.360141053681	1.886657981264	-3.348032965562
C	2.017419101197	0.179884901995	-0.314521309270
C	1.561740995355	0.484902229705	1.993443481504
C	0.637230757010	1.080561728915	0.934711934634
TV	3.820180694661	3.315496026988	-0.191973010775
TV	0.000000000000	2.435907181997	1.369861171563
TV	-0.000000000000	-0.000000000000	5.700098590653

Energy = -45.342018529956 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min180

C	1.035610453910	-2.335756008394	-0.798152919274
C	3.683758204056	-1.421592540293	-1.029759429248
C	-0.858298803393	1.782944528982	0.655330483431
C	-1.939318767536	0.844933805195	1.094345556789
C	2.325759011294	-1.616428136350	-0.463313157380
C	1.937125182213	-0.430436682229	0.431011061485
C	0.621637218907	1.895365049972	1.052489192296
C	1.472537807722	0.814849371404	0.424817815848
TV	3.281392151154	1.254399465032	-1.412857000515
TV	0.000000000000	4.694125756353	-1.875881841498
TV	-0.000000000000	0.000000000000	5.078322152309

Energy = -45.341001603115 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min181

C	0.350447228981	-0.139565484380	-2.025733104855
C	0.321693609437	-1.100023955650	-1.041130378691
C	-1.077168814727	-1.693763336309	2.705615156031
C	-1.049309965576	0.472230241074	-2.231882631962
C	3.028004853907	1.997664965260	-0.526455254403
C	3.163599294676	3.094960670609	0.673204144140
C	1.614322849571	-0.297482526759	0.829476228968
C	1.546521245093	-1.167127617419	-0.228379094728
TV	4.859155011347	2.396247600155	0.662408072804
TV	0.000000000000	3.373574795879	-0.196857658103
TV	0.000000000000	0.000000000000	3.638255581381

Energy = -45.340621688773 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min182

C	2.568238461887	0.703292327833	-3.531866122859
C	1.512206463543	-0.971800875523	-0.360192341896
C	2.158768724717	-2.018947432848	3.272959365745
C	-0.575176563345	-2.400395516117	0.210859463323
C	2.584669183478	1.466347112249	-4.779957839909
C	1.738597889899	0.393486136150	-1.026630639966
C	3.399682212876	0.158634114178	1.173299334088
C	0.076284374281	-1.045802846963	0.164775201273
TV	5.436338918136	2.560747760721	0.703186104655
TV	-0.000000000000	2.558773392528	0.275555770555
TV	-0.000000000000	-0.000000000000	5.840274057060

Energy = -45.340588136655 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min183

C	3.661399409901	0.068367456804	-1.265375067748
C	0.830835440471	-1.186477570090	-1.223121330166
C	0.707872591468	-0.438616889722	1.265604430784
C	-1.286360714344	-0.743339191779	0.058866489611
C	3.035564863322	1.956912007199	-2.790564998083
C	1.497652626896	-0.266405593570	-0.048715242620
C	3.516720909880	0.516720640495	1.166183484602
C	-0.417338045070	0.420581964283	0.565761727701
TV	6.219403842438	3.369005489956	-1.030404373359
TV	-0.000000000000	2.302396772083	1.010061642715
TV	0.000000000000	-0.000000000000	3.785323474919
Energy = -45.339165717953 hartree			
Spin(**2) = 0.140625000000			
Geometry of 3D-min184			
C	2.791872912606	-0.301669467087	0.093537176383
C	0.675134859497	-1.408226082130	-0.808051541649
C	2.211855023163	-1.353769196313	3.402856858174
C	-0.219380247033	0.799746823621	-1.714854852190
C	2.889019015886	1.568338249494	-1.866759287144
C	-0.019201788236	-0.189056681611	0.078479405293
C	3.728580040905	0.331885990890	2.120820756516
C	-0.534776239948	2.129500450900	-2.269835598476
TV	4.967523772745	2.517095370845	-0.926987410324
TV	0.000000000000	2.471444725472	0.473633339185
TV	-0.000000000000	-0.000000000000	4.231931235223
Energy = -45.339017324248 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min185			
C	3.442512634518	0.760582663494	-1.605446248257
C	2.722058848726	-0.472318474204	-1.770332521804
C	1.240871257846	-2.888437352067	3.862520815798
C	-0.519530160243	0.492738598437	-0.285704608355
C	0.928705576917	1.197305202935	-3.736609234106
C	1.063653973569	-0.955240022788	0.602716841090
C	0.966811763005	-0.168952732529	2.952455319614
C	0.301204454954	1.737140556737	-0.177572722626
TV	5.346406843218	2.755474008948	-1.096908235045
TV	0.000000000000	2.431659610669	0.496751054810
TV	-0.000000000000	-0.000000000000	6.201317702180
Energy = -45.338733582844 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min186			
C	0.847437792470	0.415285739245	-1.871409143808
C	0.848146932482	0.416261786770	-0.370266676809
C	-0.478602009312	0.976325632218	2.730342945856
C	-0.479447952461	0.976080635980	-0.377654956317
C	2.999937654965	-0.485965342000	-1.872994298606
C	3.000769876722	-0.484820688185	-0.371773421318
C	1.924591603995	-0.034564851971	1.895142799076
C	1.923788973413	-0.034453720941	0.455496600543
TV	4.805829052027	1.630586288229	-0.937809274644
TV	-0.000000000009	3.653598316588	-0.936388571736
TV	-0.000000000005	0.000000000007	4.593885891262
Energy = -45.337051787529 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min187			
C	0.826955487759	-0.509553542262	-1.857594198649

C	0.826695803032	-0.509673170973	-0.238435440365
C	-0.664354770103	-0.508528477252	1.610180365340
C	-0.664775809574	-0.508839617727	0.052746686769
C	2.959122258926	2.364326721620	-2.929779895864
C	2.958986935645	0.232989721706	0.830740094994
C	1.443664726364	2.070884371939	0.830786427535
C	1.443592177682	0.526275957211	0.831298315406
TV	4.359636764276	1.807174300997	-0.001368468338
TV	-0.000000000000	3.616788154496	-0.000990856307
TV	-0.000000000000	-0.000000000000	3.759686675683
Energy = -45.336873920880 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min188			
C	0.734155848102	0.219321515929	-2.395105651537
C	2.780997938458	1.350029817892	-1.452659914233
C	-0.566534950694	0.219030000455	2.400400261076
C	-2.760116660798	-0.586874064566	1.525307356443
C	2.781197198446	-0.911819977276	-1.452851854191
C	2.684284059265	0.219008584490	-0.514261216973
C	1.805247701939	-0.858065032559	1.764656473543
C	2.283613614868	0.219469745077	0.777532756515
TV	4.565324007983	1.883984177523	0.239486001120
TV	-0.000000000000	3.768602185800	0.000462108127
TV	0.000000000000	-0.000000000000	4.478798510816
Energy = -45.334329215071 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min189			
C	1.517798773030	0.563855239394	-2.586464895980
C	2.661022661741	1.252150577013	-0.527608164697
C	-2.141651163644	0.214029637442	0.942789167762
C	-0.728208199219	0.260434333414	0.395284467514
C	2.114256050233	2.503536905473	-1.102631550585
C	4.077111225467	1.507148874320	-0.017163805289
C	0.148728976678	-3.364385116228	2.587772416639
C	2.003363200682	0.091957163246	0.117234150472
TV	4.762297961072	1.191952913079	1.020433524485
TV	-0.000000000000	3.735606494708	-0.936955433444
TV	0.000000000000	0.000000000000	3.968946951505
Energy = -45.333931183320 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min190			
C	0.889287284288	0.440752245795	-1.832492757771
C	2.034108145127	-0.244467025913	-0.043142213971
C	-0.700565991027	-0.679075320966	3.480261753762
C	-1.511659201046	-0.009640042514	2.278313469871
C	-0.593343077668	2.470357426419	-1.930208725096
C	2.077557096742	1.873770362432	1.221078185226
C	0.663219276676	1.787260729407	1.640173381954
C	-3.005884350179	4.205013952690	-1.072752370246
TV	3.735165860738	0.287791364119	-0.908074048483
TV	-0.000000000000	4.691929759000	-1.415574771912
TV	0.000000000000	0.000000000000	3.828771116015
Energy = -45.331808433062 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min191			
C	2.732388860122	0.252323478089	-1.161951343431
C	1.354871405511	-2.231432200593	-1.735205703399

C	1.425141413426	-2.433733267924	1.812986708321
C	-0.802081234342	1.057781783915	0.111436475517
C	1.696317139062	0.679620955792	-2.128317282938
C	0.705446289338	-1.341924775898	-0.651661010253
C	0.980883000852	-1.929026747458	0.672999785566
C	-1.484695968027	2.256622277435	0.494769698015
TV	5.655610018804	0.164804952337	-0.371255462069
TV	0.000000000000	2.289566264674	1.012617483962
TV	0.000000000000	0.000000000001	6.185901418543
Energy = -45.331242567223 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min192			
C	0.900232215224	-1.524726952513	-0.996772530522
C	0.535442417114	-0.397946872556	-0.233172539222
C	-1.819919873034	0.303816710662	0.862374837239
C	-0.844738094590	-0.024167149328	-0.204726889527
C	3.889808676848	-0.419263573626	-0.520855196725
C	2.914622494266	-0.091598668998	0.546170667754
C	1.169009464755	1.406921515505	1.339109954648
C	1.534353006583	0.280844379160	0.574640300301
TV	5.759427332504	3.493110581287	0.056253712449
TV	0.000000000000	4.042676598363	-0.680569324515
TV	-0.000000000000	0.000000000000	3.524178367192
Energy = -45.331133789272 hartree			
Spin(**2) = 0.015869140625			
Geometry of 3D-min193			
C	0.031667370531	-0.645938188128	-0.919414904255
C	1.461451277868	-0.985564232909	-0.711981290615
C	-0.625854750951	-0.006065970669	1.567095198057
C	-0.755976470962	-1.020491890480	0.388987172333
C	0.631036297986	2.875497161042	-0.903018940455
C	1.191579199039	2.404077970755	0.387766176559
C	0.057467231287	2.485895089625	1.473707955189
C	-0.991353565308	1.331475975907	1.439014912245
TV	3.573830505578	0.543853028743	-0.758206671595
TV	0.000000000000	4.818920422801	0.591737163478
TV	-0.000000000000	0.000000000000	3.693899851781
Energy = -45.330658547226 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min194			
C	0.750932282378	0.130978113864	-3.775239679908
C	2.146269692045	-0.346327231663	-1.502838042109
C	2.107642339930	-1.435678211324	3.668922798713
C	-0.151795239332	-2.072961131743	0.588718395879
C	1.619161284990	1.323339652367	-3.332512394625
C	1.832674429029	-0.647766810189	-0.073182619024
C	2.600403629252	1.569600647182	1.604685674398
C	0.385542959078	-0.707016233906	0.206626031110
TV	4.255404942032	3.659018369345	0.936588531485
TV	-0.000000000000	2.462019230868	0.518321542159
TV	0.000000000000	0.000000000000	6.105338688063
Energy = -45.328186421300 hartree			
Spin(**2) = 0.066406250000			
Geometry of 3D-min195			
C	0.539461214532	0.869256816297	-1.491067579374
C	1.072692442847	0.234458819612	1.100653214771
C	0.087449448439	0.046529777771	3.686902257891

C	-1.381914143004	0.465656208499	0.145109683579
C	0.240189946831	2.844781557593	-1.260900422981
C	1.360311137462	1.981585165855	-0.756067557033
C	-0.701266980890	1.739845232552	2.114358370589
C	-1.674746268930	1.878552516552	0.937548370930
TV	3.212942552860	1.092353297901	0.422649005940
TV	0.000000000000	4.158098347764	-0.406292328715
TV	0.000000000000	-0.000000000000	3.878209024008
Energy = -45.328045267209 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min196			
C	1.092823137021	0.501518781509	-1.415414371030
C	0.299630536545	-0.340380159064	-0.406505234132
C	0.190599331992	0.424463950038	0.945059818864
C	-1.223656146028	-2.739026345109	0.149737705058
C	3.315650452254	1.511714008299	-1.893451007561
C	2.522443791855	0.669831148577	-0.884551161481
C	2.413399926582	1.434668826154	0.467001088051
C	0.999199420388	-1.728829596579	-0.328326085698
TV	4.445669552909	2.020387099677	-0.956095627228
TV	0.000000000000	3.365487682317	1.467720705315
TV	0.000000000000	0.000000000000	3.663773647982
Energy = -45.326291002259 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min197			
C	0.468603501265	-1.421885987802	-1.498395883962
C	0.601202289498	-0.195882399026	-0.714102749493
C	-0.655110365753	0.665433947184	1.010233919005
C	-0.765673749540	0.335584456650	-0.344341289133
C	3.779159530450	0.646029901641	-0.971371192394
C	3.039566694135	0.214086253385	0.183236196998
C	0.803238468419	0.841992218899	1.290537841013
C	1.590187503134	0.271940806180	0.259441986004
TV	4.709384334399	2.599684339960	0.673264617167
TV	0.000000000000	2.932853403995	-0.978862537708
TV	0.000000000000	-0.000000000000	5.028839567697
Energy = -45.325003747511 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min198			
C	0.598798946713	-1.221444135114	-2.041243751232
C	0.485000305410	-0.670557548071	-0.685642589847
C	0.803264447878	1.003798784183	0.926338785248
C	-0.254777113737	0.354875345090	-0.114742366543
C	2.042171450933	0.768364067626	0.028644315927
C	2.635385381749	-1.964471257264	0.306220425126
C	1.053313060456	-0.346929566321	1.558810058887
C	1.803806165864	-0.707973211169	0.254076493578
TV	4.319152984121	1.110705661678	-0.960060096154
TV	0.000000000000	3.642858578248	-1.122696923040
TV	0.000000000000	-0.000000000000	4.560879169025
Energy = -45.322386829313 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min199			
C	0.696421360069	-2.018874689812	-3.367217476785
C	0.745196650004	-0.156194669614	-1.457343872754
C	-0.301188850559	-1.160339520096	2.759928272373
C	-1.318521165292	1.239001943681	2.890979010636

C	2.997700425627	1.576955575516	-1.607583387748
C	2.858129168350	0.886881719211	-0.367869034996
C	1.587723507662	-0.922760786150	0.841885399697
C	1.528550562978	0.278329954483	-0.125503930153
TV	4.924951446059	-0.180195966830	-2.168530963135
TV	0.000000000000	3.143979917587	0.812254967671
TV	-0.000000000000	0.000000000000	3.519810551458
Energy = -45.320675597802 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min200			
C	1.113039222498	-2.449863511733	-0.171682058411
C	3.832745650066	-1.965744605701	-0.186926210053
C	-0.871438276311	1.639697076717	0.080017449189
C	-2.073488942107	1.607860181312	0.951719150559
C	2.315453178050	-1.663829838008	0.205632090515
C	2.044616939274	-0.207817310744	0.261420895081
C	0.645831975894	1.846948921443	0.530283507420
C	1.272050559807	0.726628474997	-0.303696220337
TV	3.186795065262	1.599788241410	-0.966808297210
TV	-0.000000000000	4.074230392248	-2.463288109479
TV	0.000000000000	-0.000000000000	4.601749340038
Energy = -45.320241919222 hartree			
Spin(**2) = 0.000000500000			
Geometry of 3D-min201			
C	1.658864099003	0.062652808376	-1.848357779155
C	0.695847039736	-0.473930724835	-0.528498726012
C	-1.564385368075	0.899613646336	0.105353058108
C	-0.074189360977	0.789422321671	0.000905708985
C	2.098744698459	1.739472463000	-0.470159594045
C	4.915118731042	1.680163185239	1.373260060935
C	0.774282484892	-2.381584939665	1.254484830305
C	1.566232559366	-1.053839984675	0.650008016331
TV	4.379981261617	-0.093995900061	2.352674950539
TV	0.000000000000	3.683786372252	-0.023230170700
TV	0.000000000000	0.000000000000	3.596963557440
Energy = -45.318305892197 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min202			
C	0.957212898001	0.283528032369	-1.735158194903
C	0.475948897032	-2.543794774666	-1.275116251910
C	2.685393570891	-1.735204964011	0.590102950841
C	-1.152228492156	0.800019170470	1.140837474584
C	3.823447833631	0.900490999097	-3.873801275752
C	0.241604941056	-1.524833823339	-0.139128696709
C	1.342798289286	-1.839957403368	0.952479458480
C	-1.765907031760	1.969984266827	1.754841862770
TV	6.905817198178	-0.915549808836	-1.488849537538
TV	0.000000000000	2.486955823882	0.719134230808
TV	-0.000000000000	0.000000000001	4.670367941752
Energy = -45.317152441677 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min203			
C	0.867140747734	-0.372849254412	-2.370095738944
C	0.727573884264	-0.065734653056	-0.968996652884
C	-0.534162980011	2.318185252767	1.944290165175
C	-1.405007737270	1.086500293828	2.140406519737
C	3.003486121821	-1.314578009842	-1.980522804358

C	2.878978878169	-1.116052374364	-0.449523976953
C	1.655400048657	0.769121616233	1.105457234813
C	1.953728735810	0.289432434015	-0.287114801932
TV	5.358714917196	0.243690407057	-1.722985800234
TV	-0.000000000000	2.489290141138	-0.387465251197
TV	0.000000000000	0.000000000000	4.071139051950
Energy = -45.316690980621 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min204			
C	2.012402572941	-0.719374090980	-3.199153906733
C	2.647402219170	-0.940037941714	-0.017703423409
C	2.016374328876	-2.168756385857	2.949951142694
C	-0.102786279047	0.907888793922	0.424835632831
C	1.380881909965	0.654481606492	-5.421076114596
C	2.017298055468	0.108820982570	-0.860369468003
C	2.010437194687	-0.394463171753	1.209355313359
C	-0.741532729809	2.180562572778	0.715093930779
TV	4.872633343293	1.829257936037	0.408660391470
TV	0.000000000000	2.602803288011	0.597970498562
TV	-0.000000000000	-0.000000000000	5.788707239378
Energy = -45.316623876385 hartree			
Spin(**2) = 0.015869140625			
Geometry of 3D-min205			
C	2.791737241648	-0.193891759709	-1.500471955122
C	1.410793855018	-1.756097244398	-0.150976185109
C	1.993098030950	-1.509024542118	4.341363272315
C	-0.054149942672	-0.068151270678	-2.146258764541
C	2.290299967157	0.952476669013	-4.278851063873
C	0.879635432085	-0.615248119253	0.623316044156
C	1.256649249885	1.390965001943	2.414247003632
C	0.752315416777	1.250264280242	-2.079689542541
TV	4.180454593512	2.480711141357	0.895850580191
TV	0.000000000000	2.563405066015	0.482531147561
TV	0.000000000000	0.000000000000	5.905544580874
Energy = -45.314977838146 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min206			
C	-0.268836337830	0.660618347657	-2.384816889143
C	0.222967807830	-0.206742863581	-1.181535317980
C	-0.620094979339	1.281280707541	1.540989792162
C	-1.156384668583	-0.344821850489	-0.476933397947
C	0.287382432655	2.252027946692	-0.719602360134
C	0.567915970552	1.756940910999	0.693677193382
C	-0.895320077239	1.766817279938	3.753730082477
C	-1.247761340341	2.388174777718	2.430308914878
TV	2.206676656110	1.250370822470	-0.000253124704
TV	-0.000000000000	5.143499941641	3.536240442034
TV	0.000000000000	0.000000000000	5.320083802974
Energy = -45.314597152068 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min207			
C	0.540991732416	0.611118583573	-1.930601719329
C	2.690690246069	-1.913707093872	1.206075722969
C	0.381827934522	-0.273010634263	3.346019457239
C	-1.981176527465	0.707593394998	-1.151609141044
C	0.009971879435	2.510984505308	-0.983737478759
C	2.262818389959	2.618438065512	1.923668890010

C	-0.835141298857	1.530557631509	2.174259968569
C	-1.575280958387	2.146981147088	1.014945902092
TV	2.933062480883	-0.350147973103	1.688632856527
TV	-0.000000000000	5.523524165766	-0.076351557011
TV	-0.000000000000	0.000000000000	3.943065736713
Energy	= -45.314539455655 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min208			
C	0.441097402038	-0.154051572072	-2.158481286267
C	1.829884304601	0.085662324366	-1.679631442055
C	-0.859697718550	-0.037391804451	1.960349837177
C	-2.248344398822	-0.276702871784	1.480879488673
C	3.201568903186	2.077453833832	-0.957568390284
C	2.482669843438	1.344247648510	0.210558687986
C	1.497459089868	-0.884434373587	0.935542537688
C	2.216466619998	-0.151217782902	-0.232671135373
TV	5.117610101935	1.384106959184	0.176535341598
TV	0.000000000000	3.459382735021	-0.784817948583
TV	-0.000000000000	-0.000000000000	3.813244100451
Energy	= -45.313591103022 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min209			
C	1.207822926678	0.301696415413	-0.981447596644
C	0.880208133619	0.502952726721	0.476338277183
C	-0.256775857899	-1.463879097191	1.396093636815
C	0.045792792421	-0.775102463715	0.241511568137
C	3.324945466514	0.506552202788	-2.451336184840
C	4.173811177972	-0.757939930724	-1.963456679483
C	1.917124716564	0.552713973688	1.625810122938
C	-0.316843640257	1.444447295535	0.964767606239
TV	4.303251255253	-0.324297650650	-0.747077328692
TV	-0.000000000000	4.315561694764	-0.744983214353
TV	-0.000000000000	-0.000000000000	3.761890081828
Energy	= -45.312783242992 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min210			
C	0.850166862133	-0.010954961544	-1.543649702278
C	0.697954112758	-0.532721232706	-0.136513620439
C	0.231047818888	0.463904635271	1.031619820806
C	-1.265536776954	-2.065204630204	0.137247760387
C	0.850314156686	2.503391345878	-0.609704746357
C	0.697824564188	1.981613181114	0.797387346217
C	0.231046217815	2.978200208150	1.965601306142
C	-1.265514016734	0.449075399186	1.071346062599
TV	3.243278895943	1.809852615665	-1.021752877336
TV	0.000000000000	5.028618730313	1.868026675224
TV	-0.000000000000	0.000000000000	3.853335859900
Energy	= -45.312725546579 hartree		
Spin(**2)	= 0.015869140625		
Geometry of 3D-min211			
C	0.389963138698	0.561509322189	-0.824705898880
C	0.444100555932	-0.968011026502	-0.677811577401
C	-0.514313488796	0.717294206420	4.247429123142
C	-2.065110428923	0.350345357344	-0.021252905960
C	1.662743071619	3.843616558408	-2.302010765754
C	0.006803481401	2.241406740755	0.341421326329
C	-1.701313466777	2.739656745989	1.918775927293

C	-1.140527926746	3.253684733406	0.585041729209
TV	2.278586915500	-0.856102986805	0.907742163819
TV	0.000000000000	5.812623097987	-1.394029107183
TV	-0.000000000000	-0.000000000000	3.930348432636
Energy	= -45.311541520636 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min212			
C	2.633096491787	-0.283613818813	-2.675337369633
C	0.986508272442	-2.048623544809	-0.219163291118
C	1.316075943458	-2.245024389392	4.073599343052
C	0.017550836675	-0.407388581138	-2.018815762685
C	2.238681330870	1.120616857825	-3.180206940831
C	1.332363315366	-0.907820095538	0.636977496644
C	2.126159587852	-1.114197742676	1.770443021304
C	0.459630573278	0.723537620086	-1.089743172888
TV	3.832916239673	2.482339109160	0.708509454616
TV	0.000000000000	2.526553347048	0.489292825276
TV	0.000000000001	0.000000000000	6.848096121299
Energy	= -45.311443179488 hartree		
Spin(**2)	= 0.244384765625		
Geometry of 3D-min213			
C	-0.076974803774	-0.148277193344	-1.029355712047
C	1.049310057672	0.176401975816	0.053303916496
C	0.285591942099	-0.730878863396	1.069016162424
C	-0.705978181028	-1.179378164021	-0.113068165887
C	0.030192585721	1.261367180820	-0.479879333401
C	1.070434449032	2.950518664811	0.849064689807
C	0.009516381278	2.308630739975	1.811693345292
C	-0.812212950499	1.659681434730	0.705406750381
TV	3.269578367595	1.362818835541	0.086153037310
TV	-0.000000000000	4.789953347165	2.477555421457
TV	-0.000000000000	-0.000000000000	3.469161006842
Energy	= -45.310247320268 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min214			
C	1.936043609313	-0.821502172368	-3.099056881627
C	1.276192728215	-1.268929320634	-0.883291227286
C	0.896478222639	-0.786723193593	2.397078181571
C	-1.321338487482	0.306148454443	-1.395774715798
C	3.375829094856	1.591504796073	-1.681775210821
C	1.484873600562	-0.363514135494	0.188434730679
C	3.929736548020	1.100932975263	4.122024269940
C	-0.584664524931	1.671659371281	-1.261156695437
TV	5.463920124307	1.986945010223	3.070562244806
TV	0.000000000000	2.367327772283	1.130104668604
TV	-0.000000000000	0.000000000000	4.579899372771
Energy	= -45.309532693231 hartree		
Spin(**2)	= 0.097412109375		
Geometry of 3D-min215			
C	0.264621499503	-0.212521837629	-1.869176324181
C	0.660725310351	-0.579106079252	-0.663226397653
C	-0.132887462211	0.151033845479	1.608520871906
C	-0.378186646557	-0.908923154951	0.470861859428
C	2.832231996813	-0.003776564360	-2.643701222420
C	3.228337428557	-0.370222787782	-1.437686140156
C	2.434721021705	0.359871532686	0.834018299844
C	2.189394366931	-0.700043293573	-0.303597798611

TV	5.135243665740	0.417836799652	-1.548854844694
TV	0.000000000000	2.571600140500	0.774250598117
TV	0.000000000000	-0.000000000000	4.680006785416
Energy	=	-45.305751409970 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min216			
C	1.669300263036	-1.242641090517	-1.256475573358
C	0.706107281559	-1.242929769208	-0.211067341797
C	-0.350990893771	0.637379808924	1.257241196983
C	-0.126870338348	-0.871675984948	1.006954870969
C	3.006151206373	-0.775780436151	-1.288794549664
C	3.712816502414	-0.119234054560	-0.250179267542
C	0.932918877308	1.490702191319	1.278452442607
C	0.148755178766	1.618936936814	0.204758371147
TV	4.319716878538	1.511884495372	-0.007992941099
TV	0.000000000000	3.273067595593	-2.041182301669
TV	-0.000000000000	-0.000000000000	5.713516059731
Energy	=	-45.305112780501 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min217			
C	0.955364690940	0.421431393928	-1.492869711277
C	1.025609794870	-0.506380550197	-0.183251944351
C	-0.600274780152	-0.031094767218	1.671227281809
C	-0.403738956390	-0.595470151688	0.301677641833
C	2.906322242687	-1.058965985491	-1.650482028426
C	3.598902899061	0.126076329931	-1.075111550466
C	1.678403511944	-0.558573996630	4.805728495325
C	1.498223342111	1.802481832158	-1.485406988415
TV	4.672582012915	1.142582453775	-0.239107935369
TV	0.000000000000	3.350911634893	-0.290639266948
TV	0.000000000000	0.000000000000	3.611204754675
Energy	=	-45.304266554194 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 3D-min218			
C	0.396922582946	-1.636987412006	-2.122148256044
C	-0.153774559420	-0.515460081872	-1.411943005797
C	1.207152662702	-0.963735636687	0.200918758703
C	-0.413248573208	-0.918329128066	0.035665533469
C	2.188994901758	-0.637384770958	-0.970127892714
C	3.382960572583	-0.923297580626	0.055459162969
C	1.933851306639	-1.618091013651	2.544068877253
C	2.254652367860	-1.217496036248	1.109590542861
TV	4.647894564830	-1.148518784590	-0.612262946227
TV	0.000000000000	2.448883554990	0.682001584689
TV	0.000000000000	0.000000000000	4.730527336273
Energy	=	-45.304074980053 hartree	
Spin(**2)	=	0.097412109375	
Geometry of 3D-min219			
C	2.805385266095	-1.996330704611	-4.835164042282
C	-0.036948042075	1.899557373091	2.753234726931
C	0.171490963659	0.641908131264	2.163725738698
C	-0.992732870210	0.026260894980	1.564255322771
C	2.575254748314	-0.126535711434	-2.195897061831
C	2.452814890732	-0.626139710592	-0.618080479854
C	1.306962685471	-0.084066391336	1.513648369269
C	1.111453929171	-0.588212580459	0.172918267650
TV	4.108578178815	0.698068429101	-1.928298126555

TV	0.000000000000	3.227885792657	-1.363493040930
TV	0.000000000000	-0.000000000000	4.610287006270
Energy	= -45.302881325792 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min220			
C	2.151019128692	-0.065873404575	-0.113951247384
C	0.413078217859	-1.951346021173	0.701686990766
C	1.393795886233	-1.386050538511	3.840539047388
C	1.152611829204	-0.235452588557	-1.224815070620
C	3.631018513798	2.305217345702	-3.288683526968
C	-0.452473454227	-0.756066624445	1.222814003907
C	4.325656524774	1.167342617211	0.285641313700
C	-1.781523959755	1.536211367656	-1.853588119005
TV	7.526845131410	4.268157916259	0.166348584094
TV	-0.000000000000	2.298289457440	1.136213904288
TV	0.000000000000	0.000000000000	4.192881448213
Energy	= -45.301927019770 hartree		
Spin(**2)	= 0.312500000000		
Geometry of 3D-min221			
C	0.710414141370	-0.050287654960	-2.600835559607
C	2.265307666039	0.268811221639	-2.230853789919
C	3.490987205929	-0.743273746523	1.622414864533
C	-0.224825726916	-2.914416292034	1.462250567962
C	0.669597916936	1.463380266191	-2.972182840974
C	2.580772889022	0.503294726083	-0.774781078510
C	2.158448526512	1.353304696767	0.479292126986
C	-1.045969791367	-1.703836618141	1.942968439922
TV	5.882776412987	1.105204906629	-0.449523134680
TV	0.000000000000	2.422593737535	0.962686686924
TV	-0.000000000000	0.000000000000	3.797277883039
Energy	= -45.301909269855 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min222			
C	1.987739705565	-0.367699806850	-1.595240618424
C	1.586933433263	0.303651833645	-0.200296959841
C	-0.734791865506	0.681850093813	1.139131834354
C	0.222039627569	1.116826358945	-0.042749623984
C	2.947318722408	1.186602535235	-0.244844247685
C	2.859149952174	2.278950573969	-1.266830319324
C	0.377461534877	-1.612071408116	0.749339215412
C	1.330257099326	-0.648966413891	0.942502695845
TV	3.734987962641	0.084995859773	0.987106819075
TV	-0.000000000000	3.964397780826	0.055295426379
TV	0.000000000000	0.000000000000	3.872115395557
Energy	= -45.299967620185 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min223			
C	0.633818889548	-0.180061503331	-1.481894369557
C	0.391222045013	-0.480200198270	-0.065179404473
C	0.132856463573	0.297151135196	1.190656266192
C	-0.652273211103	-1.762401845642	-0.138312741035
C	3.069049495513	0.840375424842	-2.103550497626
C	2.826250651891	0.540438109666	-0.686816398347
C	2.568006151510	1.317742850880	0.569103479762
C	1.782843517230	-0.741902495662	-0.760228210635
TV	4.870179026903	2.041146059417	-1.243386536985
TV	0.000000000000	3.337084179743	1.343358450657

TV	0.000000000000	0.000000000000	3.856542529569
Energy	= -45.299796699155 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min224			
C	0.683996078134	-0.447264089761	-1.955313409411
C	0.466179650715	-1.669770688921	0.038514838441
C	-0.569805557095	0.281387563975	1.478250523624
C	-0.559959557564	-0.345128722626	0.087699343326
C	4.159979184789	5.246156057936	-1.180424954355
C	3.012791612106	2.919878895308	-0.235732972604
C	1.495251697946	-0.579837015013	0.544230762935
C	0.723377033133	-3.138274454698	0.310081405815
TV	4.336431797972	3.475300449232	1.004795380176
TV	0.000000000000	3.430754067110	-0.797795745570
TV	-0.000000000000	-0.000000000000	3.879750188568
Energy	= -45.298805055837 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min225			
C	0.967950318888	0.328752610853	-1.080991623227
C	2.183265061459	-0.104538549825	-0.075562018241
C	-0.433010719825	-0.272569570899	1.895623383392
C	-1.458803075306	0.511039739065	1.047868357181
C	-0.781453577512	3.138330753829	-2.254413336013
C	1.720006616224	2.324938958262	1.333146586662
C	0.752646242056	1.800618981531	2.418317489154
C	-3.103909569192	2.118555762657	0.466354488113
TV	3.563025824438	0.288776483959	0.073206992988
TV	-0.000000000000	4.635429908476	0.093846434692
TV	0.000000000000	-0.000000000000	3.224827531534
Energy	= -45.298483866889 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min226			
C	1.636441496866	-0.840787682277	-2.843927190266
C	1.685559276663	-1.267353006936	-1.423510448230
C	1.722077023536	-0.721677616623	0.905900221714
C	0.227323370990	-0.593317647616	0.458676406177
C	2.322751681449	1.258472163923	-3.278778981870
C	2.412386826968	-0.233439236617	-0.397896714460
C	2.900724184254	-0.162724784178	3.154695691656
C	2.88489363378	0.982501351024	0.052750605908
TV	3.671716036024	3.178337713022	-0.508829745424
TV	0.000000000000	2.415854786355	0.895195043100
TV	-0.000000000000	-0.000000000000	6.354423952024
Energy	= -45.297173496826 hartree		
Spin(**2)	= 0.187500000000		
Geometry of 3D-min227			
C	0.426604104096	-0.512151817677	-0.914059747606
C	0.075805504584	-0.464885170823	0.506622432525
C	0.042658224030	0.229205489260	1.690342691675
C	-0.349834907324	-1.685289275594	-0.222179625570
C	2.494269969056	0.548046833184	-1.718534570931
C	2.845589994457	0.501126275341	-0.298144171584
C	2.461675347791	1.242395834418	0.955305043774
C	2.068858568265	-0.672289822436	-0.988862715846
TV	4.838114775075	2.025780047025	-0.002245159805
TV	-0.000000000000	3.352307858747	1.928423688802
TV	0.000000000000	0.000000000000	3.857497358677

Energy = -45.294662894375 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min228

C	0.124201810575	-0.849372766232	-1.372869454426
C	0.739490692598	0.375721735226	-0.344715138976
C	0.571063271802	0.160122862907	1.155419358323
C	-1.143306955028	-1.560095605573	-0.910382884494
C	0.070312009280	1.822392054380	-0.209429806147
C	0.841858254065	2.856886995028	0.843111427778
C	-0.233088766503	2.331622273441	1.940770518027
C	-0.629352299024	1.202928042640	1.118109734704
TV	2.965917407133	1.913157968988	-0.490579976373
TV	-0.000000000000	5.121490786749	2.416819247873
TV	-0.000000000000	0.000000000000	3.563027573022

 Energy = -45.294071561265 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min229

C	0.504097648865	0.435885784557	-2.035324685161
C	0.499759031159	0.389860833944	-0.611792250357
C	-0.650095952948	0.866735314375	1.612384512646
C	-0.774497517820	0.203761008183	0.249548547121
C	2.893729132809	-0.201720892964	-3.524939208213
C	3.799976093919	-1.298737315970	1.229743964251
C	1.587181045113	0.143497407310	1.595054778356
C	1.630536032674	0.232678521211	0.221952815667
TV	5.061619673798	-0.075872308734	1.316577221828
TV	-0.000000000000	3.270704329169	2.021418750631
TV	0.000000000000	0.000000000000	4.478004459620

 Energy = -45.293650120205 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min230

C	0.899634423926	0.531359426356	-1.168706797403
C	1.108714574855	-0.408853758583	-0.127513234667
C	-0.417977742871	-0.551758179821	0.272338621999
C	-0.530675889914	0.602494969155	-0.773309634739
C	3.425682939704	2.398310726812	0.846006759428
C	4.177820194271	3.450153981389	0.019649631813
C	1.033603321382	-2.322585095688	1.009072894104
C	1.947012853911	-1.389495611206	0.484551787450
TV	4.618884169301	1.815258552526	2.985936954088
TV	0.000000000000	3.730954796104	0.239920450032
TV	-0.000000000000	0.000000000000	3.538424693032

 Energy = -45.293527965507 hartree
 Spin(**2) = 0.000000000000
 Geometry of 3D-min231

C	0.514238020592	0.387660571816	-2.067354966767
C	0.762027068275	0.272936339283	-0.674376270426
C	-0.466968180965	1.194890751986	1.734254225407
C	-0.251500540588	0.271757056372	0.498217666107
C	3.469889872502	-1.927366022121	-0.578564095452
C	3.184503640934	-0.683843657867	-0.181565477690
C	0.941768146614	-0.252323886665	1.311508771642
C	1.778906783568	-0.313486363717	0.134491109812
TV	4.586089495082	0.061004791237	-0.532835262766
TV	0.000000000000	4.316413592408	-2.519042077086
TV	-0.000000000000	-0.000000000000	4.586247838981

 Energy = -45.285705030139 hartree

```

Spin(**2) = 0.000000000000
Geometry of 3D-min232
C      0.816190896705      0.235620992165      -1.670903133140
C      1.427967887500      -0.546284859546      -0.691870358541
C      -1.440087867041      -1.018614268310      3.053247250632
C      -1.751748442034      0.068944156215      1.985740455331
C      -0.807862927584      3.562481489133      -2.078584723845
C      2.954075536453      1.922630921064      0.345025371581
C      3.069633345103      0.605888281308      4.111062223834
C      -4.581641252686      5.202028850678      -0.919310135516
TV      3.519578312971      -0.371747740622      -1.239510805726
TV      -0.000000000000      7.136291621432      -1.666011083039
TV      0.000000000000      -0.000000000000      3.525444696719
Energy   = -45.285322065604 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min233
C      0.514620347407      -0.118810358386      -1.822287446687
C      0.514805608212      0.018331820384      -0.321561782952
C      -0.536236883747      0.195568836304      1.993664834832
C      -0.536043332259      -0.295924579132      0.596857469632
C      3.395629301371      -0.466364814901      -1.700485294525
C      3.395670663252      0.366799509670      -0.444643589774
C      1.955182433638      -0.295708354020      2.963841762990
C      1.955184607203      0.195612044874      -0.373874757493
TV      4.982252758887      1.483455081663      -0.522681070573
TV      0.000000000000      2.966117854002      -1.043704927492
TV      0.000000000000      0.000000000000      4.734289245687
Energy   = -45.284715150788 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min234
C      1.165021821646      0.074956972092      -1.770256207704
C      0.735767703925      0.602444375330      -0.456992504176
C      0.141031163367      0.455502569307      1.821579592698
C      0.064475060375      -0.413269741526      0.583539071175
C      2.253862212314      -0.029067175400      -2.626908149922
C      4.148572661182      -0.306100780787      -1.042322069373
C      -0.599828101071      1.578055733238      2.444904840222
C      1.357615620681      0.390842456995      0.873554857384
TV      4.165585582282      1.506013217056      -1.166420690667
TV      0.000000000000      3.652138842470      -1.101548052751
TV      -0.000000000000      -0.000000000000      4.683666615078
Energy   = -45.284318515510 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min235
C      0.131347276878      -1.815213823745      -1.406511871619
C      1.163408681304      -0.912372952190      0.232377735938
C      -0.486428104732      -1.092747723749      2.256142941094
C      -0.003677714726      -1.249669924361      0.875631756549
C      2.687133127721      0.504036500298      -1.697858710657
C      3.500557764359      1.926524873648      -1.502499068587
C      1.556450711015      -1.816170938934      3.714941249855
C      2.294771712251      2.717389055265      -1.972436578228
TV      4.303736914090      3.928766977063      -1.301350024195
TV      0.000000000000      3.201909477477      -1.369898748918
TV      -0.000000000000      0.000000000000      4.674396363589
Energy   = -45.282439376413 hartree
Spin(**2) = 0.000000000000

```

Geometry of 3D-min236

C	0.927256426851	-0.695152559353	-1.224574532971
C	0.395341967054	0.598185584910	-1.700800541270
C	0.395122978117	0.459535492392	0.759140211657
C	-0.673954464582	0.527835860268	-0.471055297036
C	1.459698166067	-0.538181207355	0.144441047798
C	2.529087650769	0.529465107650	-0.469753751981
C	0.927927273516	1.752614289326	0.283441285273
C	1.459746708653	1.596261734487	-1.085995933417
TV	4.575359444488	0.002228320379	0.002069078924
TV	-0.000000000000	3.601140897865	-1.813832503962
TV	-0.000000000000	-0.000000000000	4.032335632571

Energy = -45.282083459368 hartree

Spin(**2) = 0.000013000169

Geometry of 3D-min237

C	2.468354074589	-0.181541002746	-0.970957237130
C	0.216343367260	-1.039788349960	-2.389011436907
C	1.594111964023	-1.267647992981	3.244033846237
C	-1.696791481798	-0.457070909158	-0.735053043438
C	3.527769088574	0.458357834651	-2.046311380823
C	0.516187683733	-1.468433731702	-0.569038310570
C	4.546061848120	1.476102210522	3.743057393662
C	-0.294654413986	-0.361206800986	-1.098743584586
TV	5.002051919909	1.667107855788	2.279262443694
TV	-0.000000000000	2.160189181260	1.411853613298
TV	-0.000000000000	-0.000000000006	4.936075815536

Energy = -45.281986882188 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min238

C	2.041484001797	-0.332729491010	-0.948367778413
C	1.215359219698	-1.467835207387	1.095969373002
C	1.704070251292	-0.479011161366	4.301898821688
C	-0.292080989934	0.595557077785	-3.484400768003
C	2.174302196641	0.768732291979	-3.254011986030
C	1.435768364056	-0.237267375574	0.319321839116
C	0.978598992721	1.078355167911	2.350523159358
C	0.349485267663	1.916733657311	-3.211221269040
TV	3.992015492598	2.678018306281	-0.008760943600
TV	0.000000000000	2.568089218383	-0.184892719390
TV	-0.000000000000	-0.000000000000	6.674541465115

Energy = -45.279173649188 hartree

Spin(**2) = 0.084228515625

Geometry of 3D-min239

C	3.050603135571	0.591173817313	-4.372829583923
C	0.899635816346	-2.665194351004	3.724210665914
C	2.344821299192	-0.797837909280	0.514320909066
C	1.001224215299	0.273121765200	-1.312729355666
C	2.390469803770	2.774365509947	-5.619680822681
C	0.081451207811	-1.730429388740	4.621359476560
C	2.757075709329	1.343543209918	-0.661494752309
C	-1.230245801932	0.345273385151	1.057781651812
TV	5.744062533504	4.501825675180	-2.731982006734
TV	0.000000000000	2.175833275863	1.267727394546
TV	0.000000000000	0.000000000000	5.003701857771

Energy = -45.277744431864 hartree

Spin(**2) = 0.312500000000

Geometry of 3D-min240

C	0.710607153650	-1.593681485246	-0.151306121815
C	1.110828649421	-0.121946912471	0.035100613042
C	-0.982807544866	1.021594649547	1.105057453063
C	-0.139474334978	0.816584672476	-0.040467959647
C	3.008468615400	-0.922337319955	-2.443498576858
C	4.279867652635	2.064292925211	-2.601992488409
C	1.583156091448	-2.826688668933	3.448913134028
C	1.900523420786	-0.031099859707	1.402892990104
TV	4.897710328671	0.757542929128	-1.206936605920
TV	-0.000000000000	3.437807195002	-0.822914746701
TV	-0.000000000000	0.000000000000	3.884301013199
Energy = -45.276133452465 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min241			
C	4.132431506986	0.334108568895	-4.352418213258
C	0.313854250775	-1.860739231158	2.472444942004
C	1.612541025496	0.563180088328	-1.372381948407
C	-0.946741421788	1.000672025386	-1.010222217432
C	2.952570229196	2.534834800831	-4.763751990146
C	-0.217649704402	-1.213215435985	3.762091327071
C	3.752232857373	1.350298853868	-0.315174115270
C	-1.214480684144	0.104464745769	1.349251351457
TV	6.104282294678	3.023794138777	-2.932038429386
TV	-0.000000000000	2.004328618494	1.685447605949
TV	-0.000000000000	0.000000000000	5.079480382632
Energy = -45.272851702542 hartree			
Spin(**2) = 0.187500000000			
Geometry of 3D-min242			
C	0.641731304162	-0.742608897631	-1.691196603032
C	0.826230966042	-0.800152391785	-0.154490462575
C	-0.488598127167	-0.419798070304	2.051382441592
C	-0.485303356096	-0.833926046243	0.647652350566
C	3.311591312976	-0.185321628748	-1.795148583607
C	3.338122558948	0.726827783230	-0.615009996596
C	1.936941312746	-0.138923812327	2.630155065099
C	1.762847482459	0.655678130056	-0.573556757092
TV	4.875569121922	2.315270945042	-0.722773700364
TV	-0.000000000000	2.774713619428	-0.720721070402
TV	0.000000000000	-0.000000000000	4.513577781301
Energy = -45.270399457992 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min243			
C	-0.194754022167	-1.301580412066	-1.600910968744
C	0.980308996813	0.843211231320	0.536970428989
C	-0.177212490964	-0.083977588172	0.708875612466
C	-0.818665015257	-1.123967370946	-0.123136462543
C	0.289701075325	1.923745089205	-0.267131515686
C	0.788110867144	3.089808502336	0.741322149456
C	0.267737309288	1.909854478861	1.557675278891
C	-0.889015971149	1.359324767960	0.621380401591
TV	3.232092911772	1.743411332734	0.434899428359
TV	0.000000000000	5.572897429129	2.422814187226
TV	-0.000000000000	-0.000000000000	3.265989048780
Energy = -45.270390895403 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min244			
C	2.610518100299	0.006044452543	-1.807366373846

C	0.836631968210	-1.883813607007	-0.031690034339
C	1.327054847231	-0.183692586753	1.555257914373
C	-1.153712539965	-0.286268786277	0.245120035363
C	2.846772288228	2.359179302759	-3.862257461313
C	1.478362278932	-0.525766940170	0.148584609714
C	3.686214243324	0.896682183429	0.188318248668
C	-0.222266426931	0.111525026306	1.443263765971
TV	4.926960850905	3.537410787502	-1.966011983970
TV	-0.000000000000	2.747554647194	0.608047327033
TV	-0.000000000000	0.000000000000	4.050927951089
Energy = -45.268816702061 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min245			
C	0.988397000317	-0.246581500896	-1.891101520571
C	0.059259082362	0.303960994033	0.493828015257
C	-1.303334418533	2.105054867935	1.819673088943
C	-0.869349232147	1.218448154325	1.039378985534
C	3.484630519776	-0.963086692764	-3.021206198286
C	4.768195706270	-0.592550266251	-2.476336993012
C	2.151143551970	-0.511067164773	2.170331798556
C	0.967318228799	-0.123431120815	1.501401435736
TV	4.816997032293	-0.394119769061	-1.593053761101
TV	0.000000000000	3.641845008894	-0.553489405130
TV	-0.000000000000	-0.000000000000	4.830653751423
Energy = -45.268656217834 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min246			
C	0.822348227652	0.633437443050	-2.604731220830
C	0.573456056646	0.141393222947	-1.254485650927
C	0.834849578191	0.221640659827	0.840872266054
C	-0.207480474021	0.578093228444	-0.198954888165
C	1.674905982293	-0.523311732471	-0.345945518637
C	2.860752788416	0.415126923347	-0.027871862299
C	1.663361340759	1.753819022907	2.103687787701
C	2.090216283048	1.165864400289	0.843017688255
TV	4.460729126110	3.126509528319	-1.983128302423
TV	-0.000000000000	3.684535480893	-2.013201785640
TV	0.000000000000	-0.000000000000	4.938492058984
Energy = -45.267769677536 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min247			
C	1.806370170469	-0.229600295403	0.815979156112
C	-0.249861647846	-1.206261096998	-0.010512311966
C	1.805148740475	-0.852034322055	2.134348557282
C	-0.251161571655	0.125149233744	-2.829105342966
C	4.008544740804	0.575929908550	-3.783856081751
C	0.441523897261	0.021045339171	0.284950923544
C	3.139749066271	1.694208677631	2.531986813495
C	0.440150407859	1.132754922481	-2.068105478583
TV	5.386102817144	2.233249362949	1.058634255576
TV	0.000000000000	2.235482944366	1.055430994682
TV	-0.000000000000	-0.000000000000	5.788913544279
Energy = -45.266950682466 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min248			
C	0.461391621829	0.771465023660	-1.133079202507
C	0.448892444484	0.522305097407	0.462418819211

C	-0.329734914612	-1.092277913148	2.226775880179
C	-0.025504165262	-0.821351877914	0.934511792911
C	2.770979315420	1.200155842874	-2.975073047959
C	4.068570811153	1.408296794537	-3.432712140084
C	1.569458235688	0.849725634797	2.860449523889
C	1.538142839946	0.747862002798	1.486534554792
TV	4.699412617729	1.586208385827	-1.734721721122
TV	0.000000000000	3.010895926697	-1.700472488674
TV	-0.000000000000	0.000000000000	5.033734930467
Energy	= -45.265920856618 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min249			
C	0.419090122723	0.388229188164	-2.126296205547
C	1.574375579631	-0.205655924689	-1.753661926307
C	-0.851855008199	0.737334788817	2.563309096271
C	-1.880286643346	-0.468137961040	2.542246811168
C	3.267578533540	-1.824563816824	-1.774682793621
C	2.827554682849	-1.556975316906	-0.400087818244
C	2.575741758417	-0.914549634669	2.144936758812
C	1.812950680417	-0.632344402820	-0.360728935079
TV	4.749497933518	-0.073322753402	-1.822647772178
TV	0.000000000000	3.811691838004	-1.906950271595
TV	-0.000000000000	0.000000000000	4.741939290170
Energy	= -45.265864630177 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min250			
C	1.143826692147	-1.416444688701	-0.619962583444
C	0.976905021994	-0.057773761203	-0.108871678635
C	-0.545018143739	1.470395603663	1.361489012856
C	-0.641456247214	0.238688440047	0.332446298025
C	2.501209036650	-1.840445238308	-0.959403501673
C	3.156314846742	-0.726131040433	-0.145161154237
C	0.270504405950	2.295976064067	2.371298694475
C	2.351511106720	0.529940240087	-0.099147264362
TV	3.925505344444	1.586960621772	-0.759901663461
TV	-0.000000000000	4.717867118225	-0.475553062021
TV	0.000000000000	0.000000000000	3.271940849308
Energy	= -45.264370623824 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min251			
C	0.725126486795	-0.095910399538	-2.205045354720
C	1.861143402062	0.870498735030	-1.562727051899
C	-0.610621659935	-0.095212083037	2.364189379572
C	-1.802466662137	-0.700054752634	1.616644023904
C	2.472879913071	-1.371301736857	-1.431243294325
C	2.418132601867	-0.155327397685	-0.598379740303
C	1.861843135219	-1.062017059930	1.724299740526
C	2.418854361602	-0.035857513345	0.759973147947
TV	4.275806310145	1.879892165880	-0.023370388452
TV	0.000000000000	3.761135731275	-0.051807646316
TV	0.000000000000	0.000000000000	4.570493184132
Energy	= -45.264144174590 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min252			
C	2.375129005714	1.216613079397	-3.476876941223
C	2.392397793955	-0.057642686173	0.046733333685
C	2.368814297581	-1.331234344706	4.950412239339

C	-0.758173212252	-0.077150498704	-0.512188122529
C	2.383744401887	2.490066523756	-5.619556287655
C	2.358626144810	1.216051704651	-0.715877083030
C	2.379117254253	-0.057290427669	2.807783691927
C	-0.540597473946	1.196572053505	-0.552329134164
TV	6.047100257408	0.006942343720	0.373847992892
TV	-0.000000000000	2.547566980453	-0.000419354240
TV	0.000000000000	0.000000000000	7.052117557570
Energy = -45.261317711840 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min253			
C	1.992514085380	2.663013476171	-3.876267389652
C	1.197693547643	-1.864267783476	3.625903489456
C	1.955094412724	-0.899255763221	-0.191428926014
C	-1.314939740801	-0.956084267194	-0.797406059146
C	3.235926552876	5.044598884572	-4.194451481085
C	-0.254155988567	-1.920053545560	3.806043641627
C	3.235966721156	1.214562668937	-1.177882130758
C	-1.315672151361	-0.681766973948	0.640500862488
TV	5.709401050637	3.924434117242	-2.616327195287
TV	0.000000000000	2.194503599738	1.656685830953
TV	-0.000000000000	-0.000000000000	4.796515355499
Energy = -45.258118206868 hartree			
Spin(**2) = 0.049072812500			
Geometry of 3D-min254			
C	1.476882544289	0.533636562715	-1.488516531517
C	0.504578386863	-0.251254150563	-0.591204711894
C	-1.798328250133	0.793002783793	0.493987841486
C	-0.363783490403	0.944376637342	0.067619696050
C	2.212028968101	1.538709109511	-0.567152758887
C	4.750405728849	2.153588945050	0.653258304509
C	0.545643841967	-2.237644506178	1.110914798960
C	1.232141393325	-1.384075109003	0.049122108667
TV	4.789797466196	0.008354832990	1.612138412356
TV	0.000000000000	3.746939948888	0.099582745515
TV	0.000000000000	-0.000000000000	3.448892101541
Energy = -45.258058268747 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min255			
C	1.550747961206	1.642321472994	-3.379209161147
C	-0.332773795872	-1.757170729061	2.050103452019
C	2.731956238914	-0.043475246118	0.703073638168
C	1.147496381209	0.663230827763	-2.517370074646
C	3.583910218233	3.020905767327	-6.233851037094
C	-2.123854858017	-1.650256561417	4.524195800093
C	2.286674057232	2.241931770798	-0.440481704312
C	-1.063882414075	-0.406702402708	2.436575822918
TV	4.884102215848	4.692046957819	-3.682563850250
TV	0.000000000000	2.308662801561	1.419263968045
TV	0.000000000000	0.000000000000	5.785175088575
Energy = -45.257510667313 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min256			
C	3.104553886886	0.150179978705	-1.696906369990
C	1.444156707042	-1.359763645937	-0.366918275857
C	2.583338364097	-1.250120737240	3.510950398748
C	-0.899111854817	0.041552798006	-1.412030105831

C	3.966622257449	1.797525139605	-3.615305750452
C	0.795006578340	-0.093951686958	0.223719059002
C	3.263121537363	0.367330301022	1.611464370027
C	-2.922944011858	1.259130754125	0.465912990735
TV	4.709155984836	1.886594089450	1.099314034157
TV	-0.000000000000	2.645525102264	0.360460072606
TV	0.000000000000	0.000000000000	4.826494315550
Energy = -45.256405174641 hartree			
Spin(**2) = 0.000003999984			
Geometry of 3D-min257			
C	0.805676168233	1.057918439326	-1.702269890426
C	0.826514602223	0.025423975796	0.241255477604
C	-0.617310881762	-1.518289359274	1.757366268713
C	-0.205990326054	-1.171127475257	0.305447122956
C	3.303955681690	0.482560115558	-2.479852579272
C	3.881339648399	-0.893609941815	-2.030733800918
C	1.312602992832	2.367638920207	2.886930490757
C	1.784465359846	0.352841118375	1.454622133574
TV	5.054566410738	0.048034182396	-1.120363645063
TV	-0.000000000000	2.696672322423	0.081518117152
TV	0.000000000000	0.000000000000	3.991136391677
Energy = -45.247985871508 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min258			
C	-1.187734683868	-1.800636813926	-2.851341928048
C	0.752883415104	1.153805719335	-0.504514852670
C	0.159731035250	-0.097245122764	2.769070685487
C	-1.342172228450	-0.249008037350	-0.030216131366
C	1.312257666489	3.956723269521	-0.431115918939
C	2.099094737063	2.855530942676	0.427833106703
C	-0.400475919680	2.090873813852	2.839527101182
C	-1.342779578453	2.246439691617	1.644573532315
TV	3.597338256761	1.553802634832	0.002872905097
TV	-0.000000000000	4.992026052012	0.002735760927
TV	-0.000000000001	0.000000000000	3.273665963452
Energy = -45.244819661409 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min259			
C	0.519792839327	-0.353947274459	-3.010113210131
C	1.360018753318	-0.034439352964	-0.567889293100
C	-0.033122116680	0.737280252336	1.309586631072
C	-3.524361568637	-0.031230718623	1.931305610744
C	3.500239190328	2.177164025503	-2.032696635117
C	2.420119095986	1.258570865023	0.829581811316
C	1.694855049706	-1.370071899391	0.941193607612
C	2.623562802412	-0.379760495521	0.158009775151
TV	4.843487119253	1.116160117326	0.054538417637
TV	-0.000000000000	3.528291674677	-1.373354428514
TV	0.000000000000	-0.000000000000	3.496545704580
Energy = -45.244766742406 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min260			
C	1.499468747973	-1.376870930526	-1.019124703668
C	0.581242004706	-0.526487761503	-0.308283822074
C	-1.250845694028	0.703204862216	0.795487161358
C	-0.929936062234	-0.374826547847	-0.319983964881
C	2.963738556057	-1.190015192130	-0.791173123233

C	2.695922663856	0.573044018428	0.999489541624
C	1.463561709512	1.209411839884	1.620791223686
C	1.269570156972	0.372983474913	0.535110321570
TV	4.543701365403	2.211256918054	0.712097706507
TV	0.000000000000	3.609398040432	-0.073096961801
TV	0.000000000000	0.000000000000	3.704384506524
Energy = -45.243375450367 hartree			
Spin(**2) = 0.102539062500			
Geometry of 3D-min261			
C	3.584409294779	0.115464249928	-1.246374646201
C	0.907474339973	-1.264573257620	-1.157782519089
C	0.726523361402	-0.760225877368	1.148693250666
C	-0.679361478477	-0.557693482995	0.595029544770
C	3.105302871688	2.023597436872	-2.774758235260
C	1.530704734259	-0.318132128036	-0.060746864002
C	3.435775542218	0.563239027708	1.213766247963
C	-0.600284581000	0.902870310257	0.289468259684
TV	7.241196339064	3.089785937870	-0.921738002878
TV	-0.000000000000	2.377985622017	0.871318993884
TV	0.000000000000	0.000000000000	3.683566299190
Energy = -45.242765117866 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min262			
C	2.515183614629	0.650578666257	-2.475510132160
C	2.290569434536	-0.754676746836	-0.386455406338
C	2.858947382344	-0.655128548364	2.345764950774
C	-0.740237675446	-1.413722542397	-0.672542225066
C	2.209123084998	1.678986868891	-4.392972837596
C	2.344273213477	0.575456878787	-0.998752907131
C	1.344422230398	1.063856054986	2.056970040931
C	-0.739517885311	-0.037286218741	-0.617389292687
TV	6.078410450544	2.626269613143	0.824496711409
TV	0.000000000000	2.617469005116	0.108371669233
TV	0.000000000000	-0.000000000000	5.555630210865
Energy = -45.231481059205 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min263			
C	2.111807786410	0.768024920083	-2.625267872202
C	0.521607207748	-0.446122403140	-0.646293263797
C	-0.552574272317	0.936579467192	1.706970072740
C	-1.556955318079	-2.535952217180	0.751733602984
C	3.065862788514	0.740259692953	-1.493224491151
C	2.689984168088	0.649595852705	-0.137489741501
C	0.830899825930	0.749700861344	1.507766302039
C	1.226382263718	0.434883756893	0.097773403266
TV	4.744346054993	3.246535062103	0.460816630193
TV	0.000000000000	3.502988699376	-0.132757296452
TV	0.000000000000	0.000000000000	4.788608860179
Energy = -45.231422297062 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min264			
C	1.328517220223	-0.059628060805	-3.368575156743
C	1.324678706285	-0.529373805626	-0.740377874465
C	1.310635276757	0.402784613717	1.558926134078
C	-1.901309861141	-1.067564396953	-1.625050387615
C	1.337754528423	-0.286265944017	-2.107538738885
C	1.319128170877	0.646833393552	0.191840083497

C	1.322067868858	0.173866521812	2.819523275532
C	-1.901362964871	0.315265125337	-1.379303894742
TV	6.455650052212	0.906527798677	2.341731655580
TV	-0.000000000001	2.601479876397	0.462408795869
TV	0.000000000004	-0.000000000000	7.487318029391
Energy = -45.231248472837 hartree			
Spin(**2) = 0.140625000000			
Geometry of 3D-min265			
C	0.993166449334	1.492945093193	-1.543787936410
C	0.993119947902	1.492892647449	-0.239905639332
C	-0.947783359023	-1.489585525744	1.754127221722
C	-0.947872199787	-1.489626477669	0.450233175677
C	0.993141821332	1.492966728902	1.063968073367
C	0.993109603600	1.492928224189	2.367861161555
C	-0.947849216162	-1.489630060057	4.361924282455
C	-0.947860957070	-1.489631633220	3.058034995124
TV	3.235333982507	-0.000324160360	0.661083290412
TV	-0.000000000002	5.965753893999	-0.000767436168
TV	-0.000000000000	0.000000000002	5.215558128144
Energy = -45.228233927130 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min266			
C	1.163882680956	0.489876962587	-3.246059812476
C	0.016474869294	0.043676941002	-0.000228042132
C	-0.022596273806	0.022255424793	3.246341398064
C	-1.169860082896	-0.424371763445	-0.000330625817
C	3.593743680898	1.448215189471	-3.245888810353
C	2.446332367120	1.002003990770	-0.000056333666
C	2.407268710442	0.980574218748	3.246522928455
C	1.259995563794	0.533985698222	-0.000160315638
TV	4.859681197486	1.916592953997	0.000344747357
TV	-0.000000000000	3.548697495058	0.016046322078
TV	-0.000000000001	-0.000000000000	6.492693509965
Energy = -45.223229332915 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min267			
C	0.998876487753	-0.746460678014	-1.599940925772
C	0.595368610582	0.084330006556	-0.488320270043
C	-0.081514763527	-1.481595904341	1.698763552707
C	-0.412163777802	-0.373016950916	0.622166186618
C	3.239038061157	0.002886720574	-2.287741243564
C	3.666801804959	-0.804999852073	-1.164994918335
C	1.858955921297	0.018539357611	1.711355764011
C	0.809522150040	0.649016102487	0.858138176592
TV	4.506183271504	-1.124061598851	-0.569220617046
TV	-0.000000000000	3.301163475995	-0.036174722059
TV	0.000000000000	0.000000000000	4.205764214597
Energy = -45.212009401796 hartree			
Spin(**2) = 0.000000000000			
Geometry of 3D-min268			
C	0.430880087353	1.029870027946	0.298477499025
C	-0.050028707907	0.839289477556	1.740108784205
C	0.145634660880	-1.660935429877	0.689834079011
C	0.581416548825	-2.116557370913	-0.810763164512
C	1.040531711608	1.241514540104	2.617665271752
C	0.781641768929	2.166062564792	3.652802530215
C	-0.332355416066	-2.057387393493	2.205064185414

C	0.205083864148	-0.249882233570	0.711608103090
TV	2.417481938459	-0.186497087718	0.763792397579
TV	-0.000000000000	7.065189344670	-1.399614611553
TV	-0.000000000000	-0.000000000000	4.087880086253
Energy	= -45.197136883490 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min269			
C	3.463934387906	-0.583573857573	-3.221799096937
C	1.495713667236	-2.215187650612	-1.370506422598
C	3.463923683968	-1.893173482342	4.344873519284
C	-1.361898005863	1.495109536287	0.688297285503
C	1.500270239671	0.190990692324	-5.087713534678
C	1.495737285006	-0.905676883920	-1.318344367272
C	1.500450129761	-1.118603550335	2.478858541145
C	-1.362251931183	2.804653926086	0.740148633348
TV	4.820272627981	0.752483209563	0.015472132983
TV	-0.000000000002	2.619111480968	0.104305670903
TV	0.000000000005	-0.000000000001	7.618604893349
Energy	= -45.192217400672 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min270			
C	3.475283675316	1.192927410451	-2.078260715865
C	1.797766961507	-1.054745514316	0.112054031980
C	2.892541133021	-2.527153132820	1.437692726664
C	-1.049573916444	1.303267745657	1.358717165490
C	3.258461086379	1.174098623558	-3.593635318548
C	1.078884031304	-2.303604823493	-0.416209175055
C	1.453145155569	-2.214828290292	1.056520195304
C	-0.416663602764	2.642250213499	1.695108747424
TV	5.627092025453	0.035909225041	-0.557812538524
TV	0.000000000000	2.481038215854	1.032193774090
TV	0.000000000000	-0.000000000000	5.077437842301
Energy	= -45.185992251702 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min271			
C	1.837919224782	-0.189308501787	-1.714770731932
C	1.498855384775	0.925207415500	-0.794993976204
C	-0.648872375956	1.397448128703	0.978173805556
C	0.300811046973	1.702683173760	-0.202983962892
C	3.061116035711	1.147371304814	-0.588559694101
C	2.403233344720	1.934553570112	-1.594795161049
C	0.854273793853	-2.566785932364	1.601272002996
C	1.268771754805	-1.412025391980	1.797669693972
TV	3.700697823983	-0.813174952977	0.822105964838
TV	-0.000000000000	5.626876883058	-1.495568306686
TV	0.000000000000	-0.000000000000	3.877132939478
Energy	= -45.176283452114 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 3D-min272			
C	0.811584902730	0.620768139040	-3.551688966214
C	0.759914476174	0.190051341792	-1.535112657184
C	3.487379140338	-1.442775122847	0.280255763559
C	-0.376007055235	-1.975381087583	2.762465245749
C	1.838781509734	0.401543117700	-2.523379024506
C	0.752785257367	-0.115340648034	-0.104137282199
C	0.827472393013	0.927932653022	0.855303570778
C	-1.232425516623	-0.776808258899	2.993171049824

TV	6.060641613511	-0.674911759370	-2.671638294786
TV	0.000000000000	2.387000190524	0.508999088203
TV	0.000000000000	0.000000000000	5.845932019144
Energy	=	-45.170410545258 hartree	
Spin(**2)	=	0.312500000000	
Geometry of 3D-min273			
C	0.382117895944	2.590797650962	-1.302452895429
C	0.387508648866	1.695550457565	-0.056235199321
C	-0.421449264062	-1.698192278339	1.302312367234
C	-0.416140346100	-2.593282461256	0.056041651170
C	2.007881642387	2.600431338947	-1.182892200211
C	2.013272503441	1.705218299273	0.063331157253
C	1.204302690031	-1.688576912191	1.182832779878
C	1.209637725004	-2.583649251340	-0.063475507696
TV	3.251523888738	0.019294871870	-0.000101312035
TV	0.000000000000	8.574046608458	0.004635209481
TV	0.000000000000	-0.000000000000	2.492545319727
Energy	=	-45.067395327039 hartree	
Spin(**2)	=	0.000000000000	

(ii) 2D

Geometry of 2D-min0

C	0.794607238981	-1.159235688860	-1.202580713854
C	0.077310880258	-2.401335677432	-1.202677110858
C	1.668979505105	2.513084207947	2.248482297837
C	0.951771324254	-1.213352661082	2.248424800309
C	1.298571278352	2.422682209350	-4.661104981301
C	2.015609308792	1.180534829466	-4.661090565340
C	2.548688265657	3.493892138629	5.714393783097
C	1.831595877732	-0.232522811396	5.714317334529
TV	2.151417439927	1.242046296272	-0.000000000000
TV	-0.000000000001	2.484306514885	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.570633400409 hartree	
Spin(**2)	=	0.000000000000	

Geometry of 2D-min1

C	0.231083829933	-1.017328070195	-1.157871700331
C	-0.486413755634	-2.259443709729	-1.157951253228
C	1.195012709564	3.023194911362	2.3058957711387
C	0.477514791269	-0.702687894817	2.306068505673
C	0.818034301526	2.590587319824	-4.605447802647
C	1.535508749540	1.348710243100	-4.605389952810
C	2.536883481894	3.329547850241	5.765083061546
C	1.819509401650	-0.396355835405	5.765099855205
TV	2.151773691282	1.242554143876	0.000000000000
TV	-0.000000000001	2.483952359776	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.570613408786 hartree	
Spin(**2)	=	0.000000000000	

Geometry of 2D-min2

C	1.657896646263	-1.772785039980	-1.351181365506
C	0.223545565683	-1.773006365099	-1.351272078237
C	1.044635204865	2.008089314197	2.107507642156
C	1.761948721378	-1.718510807678	2.107461686699
C	2.662055518176	2.066979910605	-5.027273807855
C	1.944999460342	0.824663671204	-5.027260039805
C	2.156328803334	3.921836409887	5.599819715127

C	2.873443182455	0.195331858110	5.599851406296
TV	2.151512226910	1.242371888710	0.000000000000
TV	-0.000000000001	2.484426761957	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.570207475934 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min3			
C	0.997871549326	0.203372854869	-1.713922812573
C	-0.433496324018	0.202006948431	-1.713670495789
C	-0.642005033614	0.418569112389	1.713672638095
C	0.077627511385	-0.832257977764	1.713919294241
C	0.997872736866	2.691387522843	-1.713930791689
C	-0.433498335043	2.690029262581	-1.713676768677
C	-0.642008032141	2.906575762798	1.713678665688
C	0.077635927255	1.655761891900	1.713930270710
TV	2.150997839334	1.238573056381	-0.000000000000
TV	-0.000000000000	4.976033373043	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.565357816800 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min4			
C	0.611914782031	0.408449699927	-0.052493253764
C	-0.633210118704	-0.309029969989	-0.052407089042
C	0.612020797451	1.843786728711	-0.052372629488
C	-0.633126888877	-1.744368796799	-0.052401562648
C	3.102289981432	0.408735503208	-0.052400210921
C	1.857126449963	-0.308673214131	-0.052381866885
C	3.102383067002	1.844067350816	-0.052474689234
C	1.857199350555	-1.744019771977	-0.052439470772
TV	4.980603844039	0.000569303420	0.000000000000
TV	-0.000000000000	4.305133333682	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.558217867315 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min5			
C	-0.983606969299	-0.173405473891	0.165824112192
C	-0.118642191995	-1.283991246983	0.165850109535
C	-0.240044043696	1.028973565524	0.165840560404
C	-2.328276560487	-0.602093601772	0.165826030228
C	3.776959342616	1.147050497340	0.165792312086
C	1.225883119825	-0.854867143748	0.165810728991
C	2.333672323164	1.526590499372	0.165846658645
C	5.842744157894	-0.505154233532	0.165870714793
TV	4.639508219811	-1.154822538653	0.000000000000
TV	0.000000000000	4.788126548050	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.489961577496 hartree		
Spin(**2)	= 0.066406812500		
Geometry of 2D-min6			
C	0.594308771001	0.389309299177	0.312436825388
C	-0.728046890655	-0.116339044903	0.312196771215
C	0.594259243727	1.803387254218	0.312544563069
C	-0.728008802889	-1.560662453971	0.312295792170
C	4.193309865306	1.096446749893	0.312378511015
C	1.916479193376	-0.116143858087	0.312440890726
C	2.799148912982	1.096877249394	0.312559691653
C	1.916503821542	-1.560425668977	0.312535690650

TV	5.803664682944	-0.000277457943	0.000000000000
TV	0.000000000000	3.869906441793	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.456726128394 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min7			
C	-1.313613549241	-1.796060008645	1.105355313771
C	-2.018318987860	-3.065629851790	1.107543558782
C	0.833398810785	2.012158200471	1.096402558059
C	0.128160588648	-1.797089458572	1.098394135623
C	4.071210119142	3.849957542928	-2.251385586288
C	3.884142883319	2.573437248793	-2.238182791195
C	2.980295891695	3.280656155841	1.103171714477
C	2.275288473721	-0.528641464010	1.099120834602
TV	6.440314565248	3.805572379457	0.000000000000
TV	-0.000000000001	2.539681067472	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.452599916131 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min8			
C	-1.799196788251	-1.251009911327	0.977436753758
C	-2.504469531789	-2.520679827410	0.981325812162
C	0.348424334730	2.557882979077	0.974470664519
C	-0.357175987685	-1.251090642898	0.973619276065
C	2.986376634112	1.238145342108	-2.386912251126
C	3.172254817505	2.508803084277	-2.347968688660
C	1.790361834639	5.097104130331	0.980283206669
C	2.495479011851	1.288124306885	0.983191698407
TV	6.441789592659	3.808783480314	0.000000000000
TV	-0.000000000001	2.539320492066	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.452592897013 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min9			
C	-1.586557786291	-1.661090776183	0.525650186224
C	-2.292081578362	-2.930676569648	0.525892476178
C	0.560500613844	2.147930265606	0.532902725394
C	-0.144729044248	-1.660977018938	0.529799252017
C	1.318412495596	4.347701491351	-2.715989561290
C	1.322494254068	3.082665668126	-2.907620149898
C	2.707850787865	3.417364591052	0.530645732874
C	2.002655066598	-0.391243736473	0.533522398574
TV	6.441731644832	3.808805048472	0.000000000001
TV	-0.000000000001	2.539171473544	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.452583599438 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min10			
C	-1.717924398546	-1.207259295868	0.976605395692
C	-2.423010907626	-2.476937878355	0.981066787543
C	0.428913049717	2.601616719829	0.977380392087
C	-0.276287307217	-1.207301904141	0.974867693746
C	2.849500239679	1.106285831786	-2.468542500594
C	2.824952214672	2.378309960234	-2.278871317432
C	1.870624063747	5.140817798895	0.985357162919
C	2.575287370682	1.331748228660	0.987582857835
TV	6.439791140336	3.808527023870	0.000000000000

TV	-0.000000000001	2.539260072879	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.452538177294 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min11			
C	-1.800847190639	-1.287576267145	1.168280665526
C	-2.506357353769	-2.557211265554	1.172588368896
C	0.346634584095	2.521328040214	1.172465225121
C	-0.358936694201	-1.287592072403	1.168314384696
C	2.165696110511	0.849816899354	-2.191853764762
C	2.354810127928	2.120577060935	-2.190575323016
C	1.788456303643	5.060480072661	1.182173953922
C	2.493299338584	1.251442025134	1.182286105745
TV	6.441593864936	3.808458279634	0.000000000000
TV	-0.000000000001	2.539451708284	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.452511019556 hartree		
Spin(**2)	= 0.000000500000		
Geometry of 2D-min12			
C	-1.709082803123	-1.452970510008	0.767648003987
C	-2.412697034970	-2.729184581726	0.769241210703
C	0.436140381063	2.375718828253	0.771436544552
C	-0.267117713027	-1.453114550345	0.768693936446
C	3.084237336497	4.423545375688	-2.468132844057
C	3.087698728413	3.075775171995	-2.467524802387
C	2.580989093720	3.652558001346	0.775050540748
C	1.877847350789	-0.176419991395	0.775921661736
TV	6.436626976994	3.829173417539	-0.000000000000
TV	-0.000000000001	2.552498037297	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.451538706374 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min13			
C	-0.730516991234	0.085551076315	0.485736438951
C	0.832544443278	-1.871414861604	0.485777385767
C	-0.125420462269	1.462381215352	0.485648199193
C	-1.918655818052	-0.661847555979	0.485776573029
C	3.710594081910	1.046067897248	0.485868958545
C	0.580337058361	-0.490650614334	0.485754121279
C	2.373593677352	1.633752902552	0.485892041043
C	5.273599712925	-0.910939937352	0.485719383573
TV	4.088283351128	-1.797205810297	0.000000000000
TV	-0.000000000000	5.546903217989	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.451243756430 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min14			
C	-1.833569165883	-0.772701639121	1.346782881104
C	-2.536960646259	-2.049035302780	1.350520790504
C	0.311431557243	3.056444637498	1.350888608488
C	-0.391918112784	-0.772589762051	1.347077446037
C	2.171274624003	0.460372645163	-2.030980193471
C	2.173065454938	1.808845060743	-2.030584658283
C	2.455781942673	4.331808538274	1.359384599090
C	1.753029066433	0.503045748619	1.359464138262
TV	6.434344004130	3.828054292867	0.000000000000
TV	-0.000000000001	2.552808362877	0.000000000000

TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.450868141757 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min15			
C	-1.730718612344	-0.477637124430	1.326230794634
C	-2.436568280724	-1.745269365259	1.330737352509
C	0.416895394782	3.325520030188	1.330419549145
C	-0.289021632510	-0.477046268422	1.325895123790
C	1.755246945019	-0.356129955098	-2.017295798228
C	1.962646511985	0.911679074753	-1.924940970486
C	2.564427825364	4.593860916524	1.341047281063
C	1.859226568805	0.791212618072	1.340460279324
TV	6.442451975548	3.804809521644	-0.000000000000
TV	-0.000000000001	2.534904307676	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.449220266052 hartree		
Spin(**2)	= 0.312500000000		
Geometry of 2D-min16			
C	-1.746602857685	-1.544072010089	0.737455608672
C	-2.453098396448	-2.806719057534	0.738857950370
C	0.401773999708	2.243815343978	0.734045196934
C	-0.304960309797	-1.544761830054	0.733431803819
C	3.345149990493	4.705131797095	-2.392883352324
C	3.043190827124	3.439654363089	-2.337144076294
C	2.549508810163	3.505756908903	0.739067298530
C	1.843053275805	-0.282897771568	0.739503822020
TV	6.447354892684	3.785898851406	-0.000000000000
TV	-0.000000000001	2.525996571117	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.447948482763 hartree		
Spin(**2)	= 0.312500000000		
Geometry of 2D-min17			
C	-1.423045475876	-1.439756041457	1.103894681505
C	-2.130821899506	-2.696156611773	1.104922573137
C	0.726889242315	2.329255880826	1.088836010920
C	0.018262217950	-1.440315728124	1.092654538403
C	3.650870307107	3.956723564638	-2.012520135002
C	4.053493097339	2.701334816129	-2.060899281841
C	2.876306293714	3.585066037829	1.094421854110
C	2.167693544984	-0.184209164048	1.090595943126
TV	6.450623926204	3.767219907267	-0.000000000000
TV	-0.000000000001	2.513037610963	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.444558983870 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min18			
C	-1.427264228052	-0.946384254128	1.073717841715
C	-2.136016441754	-2.203020287025	1.080608458261
C	0.722359849816	2.822965017748	1.079494916421
C	0.013481477786	-0.946675102572	1.073090868727
C	1.976606069543	0.878299223200	-2.105545306308
C	2.381639550007	2.135392192865	-2.102944122723
C	2.164751780816	5.335776660274	1.096725137348
C	2.872309761658	1.565759046714	1.096855516520
TV	6.449768766236	3.768280989164	0.000000000000
TV	-0.000000000001	2.513233011050	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.444297218551 hartree
 Spin(**2) = 0.000000000000
 Geometry of 2D-min19

C	2.319910455984	-1.910400697617	-0.379145596685
C	1.588175089361	-3.177780971274	-0.869602916530
C	3.051147940137	1.891674367434	1.690331819217
C	2.319444744753	-1.910498813377	1.199728841887
C	1.587302650985	1.891491464033	-2.524672780658
C	0.855402050251	0.624037583743	-2.883423694146
C	3.783327282788	3.158701487692	3.705469522531
C	0.856097044906	0.624155717448	3.346026179171
TV	2.195335849506	1.267157731581	-0.000000000000
TV	-0.000000000000	2.534920092907	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.428870888180 hartree
 Spin(**2) = 0.058594187500
 Geometry of 2D-min20

C	-0.558849846292	-2.312131362928	-0.247042468906
C	-1.289004821021	-3.577550385745	-0.737060780620
C	-0.559451143757	2.750073233473	1.335892811468
C	0.170792797904	-1.045140688338	1.825949419243
C	0.902734490334	2.745633212751	-2.394946153176
C	0.172393059579	1.480564491401	-2.753196005556
C	2.361206931465	2.751020214545	3.527520321511
C	1.630815234911	-1.043986414442	3.886817136828
TV	2.191044375870	1.264629247985	-0.000000000000
TV	-0.000000000002	2.530276088703	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.426794625796 hartree
 Spin(**2) = 0.000000000000
 Geometry of 2D-min21

C	1.354921388852	-1.393149540183	-0.733136632012
C	0.623800016801	-2.658629708339	-0.239773540881
C	0.623864990410	2.403200076981	1.366266949479
C	1.354977060055	-1.393257166073	1.859692725193
C	1.355288842607	1.138026814094	-2.385987878927
C	-0.106447184380	1.138144089676	-2.746133360677
C	1.355847558353	3.668614225891	3.512277837239
C	2.086793250776	-0.127803083399	3.872295713740
TV	2.192635011493	1.265289440486	-0.000000000000
TV	-0.000000000001	2.531107637556	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.426294026727 hartree
 Spin(**2) = 0.058593750000
 Geometry of 2D-min22

C	-0.578820689181	-1.372833567053	-0.580531226716
C	-1.308162782263	-2.635944337047	-0.087194685509
C	-1.308087796266	2.419227758134	1.522553719631
C	-0.578703810633	-1.371179991896	2.017268428849
C	1.609336469849	2.416056591527	-2.238562388214
C	2.338770696246	1.152554015994	-2.598843815288
C	1.609956735689	2.420989976744	3.714419009040
C	0.880634368680	-1.369292891268	4.076561120886
TV	2.188280003300	1.263540742195	-0.000000000000
TV	-0.000000000002	2.526879395758	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.423610592282 hartree

```

Spin(**2) = 0.000000000000
Geometry of 2D-min23
C      0.122759868406      0.709137822613      -0.677046650975
C      0.122699437115      -0.672405797368      -0.677049716527
C      1.168116704651      1.754708955499      -0.677167315284
C      -0.922757319718      -1.717797587265      -0.676937463107
C      0.122772051538      4.181493884414      -0.676991501485
C      0.122736122047      2.799954151101      -0.677086826875
C      1.168087711512      5.227125757932      -0.677023652625
C      -0.922759927360      1.754626714372      -0.676948191737
TV      3.474589921437      0.000121168480      0.000000000000
TV      0.000000000000      6.944845015640      0.000000000000
TV      0.000000000000      0.000000000000      20.000000000000
Energy   = -45.410265117958 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min24
C      0.498487988306      0.928584496722      -0.740442318314
C      -0.400085549330      -0.209507506816      -0.740357326167
C      1.833786061711      0.362930157575      -0.740347916546
C      -1.853943153489      -2.023734291956      -0.740561303523
C      -0.519151395415      4.846251949177      -0.740686598550
C      -0.170054873684      3.493072815989      -0.740783691140
C      0.380034549808      5.984047484809      -0.740452882725
C      0.147543288200      2.281427003395      -0.740643674219
TV      3.602688942403      0.922911931578      -0.000000000000
TV      0.000000000000      7.436184219595      0.000000000000
TV      0.000000000000      0.000000000000      20.000000000000
Energy   = -45.396007489068 hartree
Spin(**2) = 0.312500000000
Geometry of 2D-min25
C      -0.842644365971      -0.897945106798      -0.280439192593
C      -0.990179990267      -2.152234408875      -0.948046682165
C      0.146766010597      2.865746328626      1.617313342311
C      -0.588842881003      -0.896693801552      1.271291543165
C      2.999315598857      2.862161635812      -2.387295453919
C      2.849823146006      1.607851295752      -3.001075361658
C      2.270451553503      4.119153981635      1.638969900665
C      1.560656065088      0.356686743152      1.682947089925
TV      4.336236638547      2.506971830610      0.000000000000
TV      0.000000000000      2.508330780222      0.000000000000
TV      0.000000000000      0.000000000000      20.000000000000
Energy   = -45.385276544236 hartree
Spin(**2) = 0.312500000000
Geometry of 2D-min26
C      0.517324181603      -0.160674310264      0.280503527866
C      -0.304241574796      -1.338844335547      0.280539121422
C      -0.304170331952      1.017501579466      0.280572012585
C      -3.059455191810      0.575157798971      0.280448270910
C      4.131008634540      0.551272129639      0.280544442846
C      1.961461153181      -0.160164115709      0.280469744053
C      2.812626305213      1.054198448510      0.280486937972
C      4.131152656573      -0.871531331489      0.280530949590
TV      5.872312570356      -1.949387794277      -0.000000000000
TV      0.000000000000      3.900104483597      0.000000000000
TV      0.000000000000      0.000000000000      20.000000000000
Energy   = -45.382580468030 hartree
Spin(**2) = 0.000000000000

```

Geometry of 2D-min27

C	-0.279462459033	1.342939957506	-0.052328429637
C	-0.599249966820	-0.073543221033	-0.052401003336
C	0.519513302272	2.515077511861	-0.052351148049
C	-0.465724521012	-1.470396251020	-0.052343346155
C	3.068278701418	0.173266339339	-0.052403347161
C	2.748484977494	-1.243204764988	-0.052259831547
C	2.935052303891	1.570149508780	-0.052301500408
C	1.949707759847	-2.415340836659	-0.052402032231
TV	4.801831903178	-1.502639360479	-0.000000000000
TV	0.000000000000	5.065492967532	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.382340678797 hartree

Spin(**2) = 0.066406250000

Geometry of 2D-min28

C	2.791478476918	-1.199960147017	-0.499082593540
C	1.710232142985	-3.167026446882	-1.223560255951
C	3.483688684371	2.661883207763	1.421457500280
C	0.555282808673	-0.062200612235	1.049079812510
C	1.343532925023	1.372380706900	-2.664837465446
C	2.070792194880	0.091817968437	-2.655975654250
C	2.130371546904	2.700082670435	4.557107306168
C	0.661610071916	0.027952961248	4.557780442681
TV	2.198088558872	1.395366966493	-0.000000000000
TV	-0.000000000001	2.603597964143	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.363830934516 hartree

Spin(**2) = 0.628906250000

Geometry of 2D-min29

C	-0.055783249780	-0.276490703477	-1.063928666588
C	-0.728140001838	-1.530237595220	-1.245990737614
C	1.286983088520	3.485751078651	0.552340781382
C	1.285743395867	-0.275506840174	-0.284475539639
C	3.299027255936	0.977539873535	-1.246745600928
C	2.626589953285	-0.276067768855	-1.065126239989
C	1.292141016112	4.740881868191	2.630680043910
C	1.290628662752	0.979715412690	1.972365224313
TV	5.481324228622	0.000482632390	-0.000000000000
TV	-0.000000000000	2.507282328807	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.363279621403 hartree

Spin(**2) = 2.000000000000

Geometry of 2D-min30

C	-0.745843175196	0.581072205834	-0.668946372257
C	-0.746664812081	-0.659072281070	-0.668925816108
C	1.866911089050	2.821945862118	-0.668925802727
C	-0.746920899992	-2.080694375576	-0.668975980293
C	0.418173385672	4.305617912045	-0.668941221860
C	0.418957798904	2.820987112512	-0.668892542601
C	1.866110177021	4.306468542771	-0.668962626849
C	-0.745632377053	2.002624829251	-0.668945577560
TV	3.777646294628	0.001685903204	-0.000000000000
TV	0.000000000000	7.203454696617	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.360871806765 hartree

Spin(**2) = 0.058593750000

Geometry of 2D-min31

C	1.313907544745	-2.955148363324	3.513846717752
C	-0.159358621241	-1.703214039170	2.010988959557
C	1.125082524770	5.634445128254	-1.541356807018
C	-0.646849435933	-0.451709576857	1.505045647620
C	3.090184536047	0.628233820577	0.463314536546
C	1.575552800943	1.879758831347	-1.090391689608
C	2.602222393066	1.879763397113	-0.042141530040
C	0.864818391927	-4.206511189958	3.061571662517
TV	4.740993090231	-1.422998992922	-0.000000000000
TV	0.000000000000	2.503098860476	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.357426412176 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min32			
C	-1.759409316638	-1.107674700610	0.332771792708
C	-2.453238205105	-2.404453937801	0.333895458235
C	0.382181844300	2.782654365867	0.333406351194
C	-0.311735213135	-1.107900945756	0.332295811037
C	3.200580031259	0.790261164469	-2.917504598807
C	3.200748893267	2.164197105540	-2.917245023703
C	1.112222135661	4.683927869435	3.583133805183
C	1.111405056514	0.870253572080	3.582926020270
TV	4.283027187446	2.592805521838	-0.000000000000
TV	-0.000000000001	2.593817264486	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.350995834576 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min33			
C	-1.204453108208	-1.404880990310	0.485243288729
C	-1.898598959851	-2.701651718123	0.485265276130
C	0.936342919439	2.485853006858	0.485702392035
C	0.242141699960	-1.404627867460	0.485724040705
C	1.664451630386	0.587950180115	-2.802409837237
C	1.662737504013	1.807416558791	-2.802354338663
C	1.701663629665	5.773984269327	3.763019619644
C	1.701743431690	1.806076906672	3.763274101805
TV	4.283529981166	2.594046635964	0.000000000000
TV	-0.000000000001	2.593695390738	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.350811279553 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min34			
C	2.363318761079	-0.399563638819	-0.625572231733
C	1.382006510500	-1.457815476887	-0.625641254093
C	-0.797676504732	1.845016435165	-0.625784762769
C	0.080024062030	-1.951850114187	-0.625753619006
C	-0.279130738147	3.832148729651	-0.626121800518
C	-1.596490391308	3.123679438464	-0.625984769244
C	2.691224752849	5.353408871295	-0.625493460793
C	-2.990078201267	3.482743245627	-0.626026991484
TV	3.514959723352	-0.908976573348	-0.000000000000
TV	-0.000000000000	7.150210069054	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.348480748710 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min35			
C	0.389627769977	-0.008400387939	0.478493531898

C	-0.929007645986	-0.588333812535	0.478089239417
C	0.389495461966	1.515744589527	0.478373090742
C	-0.929174491175	-1.986665376195	0.478112915434
C	3.877194014310	2.100087680287	0.477537979195
C	1.235608377375	-1.287404047685	0.478808294848
C	3.877063958505	3.489242867215	0.477743261617
C	2.641036310794	-1.287686393210	0.478136251292
TV	6.035648152994	2.041101506284	-0.000000000000
TV	-0.000000000000	4.082129145069	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.342367097139 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min36			
C	1.985779480498	2.058695070475	-0.770478305800
C	-2.609131047347	-0.592870836799	-0.770311586521
C	1.276118799945	0.831266549689	-0.770557370208
C	-1.374785816348	-1.305191379797	-0.770512667894
C	-0.666793017166	4.196756919680	-0.770523117620
C	-0.666269200577	2.771905860985	-0.770302417994
C	0.042952378907	5.424109689130	-0.770577800130
C	0.568037333556	2.059503987274	-0.770511991145
TV	3.885939579301	-0.000722175598	0.000000000000
TV	-0.000000000000	6.730151359849	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.341110381066 hartree		
Spin(**2)	= 0.058593750000		
Geometry of 2D-min37			
C	-0.057835505493	0.136228908623	0.933758801377
C	-1.416095804946	-2.344431352866	0.374881608980
C	1.413592521944	2.612769835736	0.490853811744
C	-2.093444781924	-1.099975880684	0.226652049339
C	4.241540466814	0.116260471018	0.075749849208
C	2.107438299237	1.365026767369	0.289243046660
C	3.529853790859	1.363917785862	0.083038239871
C	0.636753324032	-2.682421018535	2.095735721183
TV	7.769531666498	-1.278752874926	0.000000000000
TV	0.000000000000	2.495548016250	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.337490831507 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min38			
C	-0.891880003179	-0.023219719568	1.012511354420
C	1.071780172133	-1.983887538637	-0.303420225893
C	-0.086603226574	1.144028366438	0.668296763438
C	-3.746304335157	-0.377097205724	1.156014617347
C	3.382361249689	1.859482471864	0.308205467278
C	1.375934073766	-0.715260317360	0.544194603767
C	1.933871406950	1.899486021300	-0.160227084126
C	4.844996446532	0.000176623618	0.183619741374
TV	3.716452947880	-0.731812526544	-0.000000000000
TV	-0.000000000000	4.969252556307	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.335402258105 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min39			
C	-2.165513445045	-0.528258377089	0.098369152837
C	-1.478969876229	0.679337263717	0.393583701453

C	1.569644127343	1.884637256770	-0.443294342194
C	0.980883388059	-1.737965782430	0.028616146860
C	4.029883538430	4.299781288366	-0.811803639006
C	4.716719920814	3.092261089872	-0.517323824537
C	-0.149023042738	0.678395763324	0.944350721526
C	2.698874328555	-0.530644648568	-1.359817682976
TV	8.175567002463	3.620896782298	0.000000000000
TV	-0.000000000001	2.415120712636	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.328605694151 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min40			
C	0.358302979945	0.243134219727	0.478640567935
C	-1.120889368836	0.242910616042	0.478675228749
C	1.082133027847	1.454117656181	0.477963913160
C	-1.844808339330	-0.968234144978	0.478386520945
C	4.956694940860	1.455021363933	0.478172362013
C	1.081778915778	-0.968115236239	0.477915780193
C	3.716283884357	2.167990578448	0.477934860920
C	2.322347715124	-1.680239933667	0.477605330530
TV	6.801765627158	0.001066974180	0.000000000000
TV	-0.000000000000	3.847733900509	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.328297734953 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min41			
C	2.263993373651	1.984152419643	0.893988656648
C	-0.953440943160	-2.236368284931	-0.110375848341
C	-0.264319518277	1.606600135741	-0.148508301345
C	-2.400940024357	-2.230873216108	-0.037360923292
C	4.629810806665	0.104504610753	-0.013995826076
C	1.906527368011	0.325411093301	-0.618491547842
C	3.189112974709	-0.016494516706	0.025339103654
C	1.207096351984	-0.937723388803	-0.280076523898
TV	7.720810465839	-1.509291421038	-0.000000000000
TV	-0.000000000000	2.563029417643	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.320675193560 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min42			
C	0.660653708938	0.543613066187	-0.676310395009
C	-0.424553261494	-0.475980066859	-0.676240461773
C	0.283972276607	1.890443854084	-0.674178778120
C	-0.048595287328	-1.822989522628	-0.674255416515
C	3.199635981225	1.252708409112	-0.677928370848
C	2.114465600989	0.233083010319	-0.677936842900
C	2.822953271720	2.599531441369	-0.679697796871
C	2.490470726048	-1.113886351502	-0.679703256565
TV	5.077984113146	1.418091669615	0.000000000000
TV	0.000000000000	4.916721884596	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.308426502322 hartree			
Spin(**2) = 0.066406250000			
Geometry of 2D-min43			
C	3.559712977086	-0.647642427213	-1.039370237975
C	-1.788313384683	0.646225479152	-0.310165608687
C	-0.491685483322	0.646373545254	0.679710151141

C	0.022342085804	-0.647443745965	1.280252304923
C	4.938082225925	-0.647531391152	-1.264844860807
C	0.491183235511	0.646332850419	-0.664139832955
C	1.788067244310	0.646346851026	0.325451869968
C	1.400619060441	-0.647467754721	1.054693366369
TV	4.960726095923	-0.000003106777	0.000000000000
TV	-0.000000000000	2.587585595889	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.303887742331 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min44			
C	-1.828704672919	0.813483271101	0.989300427581
C	1.383874568189	-1.036641933901	0.990864947695
C	-0.782512262254	1.909727270695	0.988840746397
C	0.003024965304	-1.036559471027	0.991190275506
C	3.214910577032	0.822171145486	0.989359871765
C	0.691140215927	0.160641656304	0.990837955279
C	2.165999453979	1.911102879781	0.988888338255
C	5.113481754039	-0.989483005987	0.989101612144
TV	4.419191425819	-2.539702298986	0.000000000000
TV	-0.000000000000	5.096951560552	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.299087106774 hartree			
Spin(**2) = 0.058593750000			
Geometry of 2D-min45			
C	-3.545274263322	-3.973347216051	0.076864662298
C	-0.972040137675	-1.207459276514	0.077564146515
C	2.266327065940	4.278505211627	0.074646305768
C	-3.376850596108	-0.839213263857	0.077201210262
C	4.081171643011	2.141899137651	0.076820957778
C	0.242742128811	-0.541696850602	0.079243239916
C	3.827992683995	0.747989753511	0.075571456310
C	6.740733098727	-0.714603358331	0.075116386230
TV	4.333717290908	-0.917197379024	0.000000000000
TV	0.000000000000	5.594626435395	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.298753680305 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min46			
C	0.142544322437	0.601889236138	-0.568886063035
C	0.143696063019	-0.762235578772	-0.568483921526
C	1.190312528273	1.653935318232	-0.569080421922
C	0.142007514289	-2.036109953090	-0.568445065917
C	0.137882057536	4.066531148474	-0.56888878359
C	0.138634496796	2.701698224475	-0.569167007094
C	0.140221464381	5.340526425907	-0.568529374426
C	-0.909276475641	1.649865528833	-0.569104510252
TV	3.484963905430	0.007547000819	0.000000000000
TV	0.000000000000	8.708401743423	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.293821188232 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min47			
C	3.901129880048	2.111056624859	-0.684014477925
C	-2.216818117127	-2.250281098343	0.845351776720
C	0.468294612197	1.285974643399	0.239342330270
C	-0.970001255623	-2.651744527386	0.177752162760

C	2.657762208896	0.518987104533	0.739164956908
C	1.337202407675	0.105759092742	0.413785421430
C	2.727423268760	1.966643108560	0.447836004897
C	1.301580999941	-1.335265534156	0.282276186917
TV	5.775026837435	1.631085440108	-0.000000000000
TV	0.000000000000	3.756360848865	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.292272168165 hartree			
Spin(**2) = 0.058593750000			
Geometry of 2D-min48			
C	0.517817523413	0.522934239801	0.626010848619
C	-2.162137080012	-1.569494392782	-0.872762807467
C	0.556472513709	1.943471112173	0.634738800984
C	-0.321768721400	-0.635917851021	0.556667222368
C	4.207986647381	0.953772916651	0.217774181621
C	1.932330221531	0.083139078728	0.670251788040
C	2.818870927452	1.222082748715	0.664232060338
C	1.959899203929	-1.337215502237	0.684959992526
TV	5.934092423823	1.831151309610	0.000000000000
TV	0.000000000000	3.715476425954	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.291266707108 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min49			
C	-0.368455141451	-1.021901614346	1.281839775737
C	-1.053710855034	-2.297636184595	1.352069121658
C	1.874772036066	2.843361798629	0.969961149252
C	1.073366549595	-1.003783883295	0.969802052092
C	1.471887683553	2.201398963806	-1.664194827669
C	1.473329554370	-0.359317283108	-0.355760061393
C	4.002003476646	4.137010033961	1.351879514184
C	3.316656853482	0.302194079212	1.281545313842
TV	6.504929403653	3.874764064124	-0.000000000000
TV	-0.000000000001	2.559117204143	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.287753877539 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min50			
C	1.048415088498	1.056157952817	-0.778187631794
C	0.186497200923	-0.079580110148	-0.778176304568
C	2.502459810388	1.056175497926	-0.778175190077
C	-1.216492723509	-0.079552833921	-0.778147946093
C	-0.514981517438	3.460477789034	-0.778233474706
C	-1.216585013050	2.192106736363	-0.778169148580
C	-0.515015927827	4.835078035955	-0.778193630462
C	0.186433992563	2.192028606839	-0.778151844635
TV	4.580999960069	0.000030124901	-0.000000000000
TV	0.000000000000	6.183097828640	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.286673558142 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min51			
C	0.630724469469	1.508551172919	-0.840714071435
C	-0.025092895356	0.235093519397	-0.836338950069
C	2.033879988610	1.247420307412	-0.571100814206
C	-1.226565443989	-1.580862853764	-0.103545928878
C	0.123866514679	4.043631619344	-0.152418943611

C	-0.068979788853	2.752361475621	-0.819176597036
C	0.963432690354	5.237458725672	-0.571080340314
C	-1.211491914016	3.317179574506	-1.458611942933
TV	3.384118794980	1.480984300502	0.000000000000
TV	0.000000000000	6.149485456692	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.280981531378 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min52			
C	0.763320411979	1.028651165594	-0.778197872156
C	-0.073323824338	-0.175964406301	-0.778161116355
C	2.180655134545	1.029496109971	-0.778223323306
C	-1.412976132476	0.298120236229	-0.778283858136
C	0.245054810718	3.606847882223	-0.778067435366
C	-1.413895036321	1.757403109122	-0.778304487579
C	0.246449089493	4.855715935546	-0.777972058996
C	-0.074553543047	2.232621642486	-0.778225019018
TV	4.799006698371	0.002548882758	-0.000000000000
TV	0.000000000000	6.406151666827	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.277237622163 hartree			
Spin(**2) = 0.066406250000			
Geometry of 2D-min53			
C	0.549074601188	-0.372564583559	-0.183644571629
C	0.668790202700	-1.778065842664	0.114552790453
C	-0.238880154358	0.805484323329	0.112334394831
C	-2.793548683321	0.322770648218	-0.537453927155
C	3.307673789283	0.887847862713	0.756901232147
C	1.828856617234	0.061688786017	-0.654668787488
C	2.135172763775	1.454526324098	-0.128232135770
C	3.944831371382	-0.207858925392	0.144223991285
TV	5.622495284788	-1.230394908096	0.000000000000
TV	0.000000000000	3.678733344248	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.275599448275 hartree			
Spin(**2) = 0.312500000000			
Geometry of 2D-min54			
C	1.159252293585	-0.597173271122	-1.697512023977
C	-0.104005395550	0.196782007021	-1.698083558181
C	-0.530047752792	1.038305237375	1.482798113930
C	-0.528164832876	-0.162836557907	1.915365889242
C	1.159226895205	2.598124890289	-1.697576793283
C	-0.104044729899	1.804280484853	-1.697959781081
C	-0.525296002386	3.439841656219	1.478059088735
C	-0.526920475267	2.239715532953	1.914909064628
TV	2.527280011163	-0.000139627363	0.000000000000
TV	0.000000000000	4.802829499705	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.272020874195 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min55			
C	1.039331134720	-0.007757200888	-1.971292832077
C	-0.161687031589	0.000098888922	-1.538531037490
C	0.170036896152	0.631524184309	1.754813607814
C	-0.622750251357	-0.632061973580	1.754929366789
C	3.441724547207	0.008039197905	-1.970925606334
C	2.240554846065	0.000156635449	-1.538719894744

C	1.779594948595	0.631596329074	1.754911426279
C	2.572377530075	-0.631989426577	1.754814969779
TV	4.804696707947	-0.000035827048	-0.000000000000
TV	-0.000000000000	2.527592425014	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.271244728817 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min56			
C	-1.026104552542	0.643684869083	0.698467143855
C	0.447722411284	-1.482129830127	-0.635283316343
C	-0.118023871303	1.604059501865	0.188283669231
C	-1.585443766388	-0.477164453199	0.699216467496
C	3.828971638736	0.821192000341	-0.125618306344
C	1.007281648208	-0.361435835590	-0.635088310903
C	2.491084745420	1.482199322670	0.188000393405
C	5.509990869475	-1.176492163116	-0.125656775806
TV	4.289845531547	-2.119892356927	-0.000000000000
TV	0.000000000000	5.383153152049	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.268846175005 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min57			
C	1.384150002792	1.292863910404	-0.036296838838
C	-1.236954902591	-1.868658131613	-0.035838995129
C	0.146415896092	2.000995879932	-0.035979261229
C	-2.493447520284	-1.870373419673	-0.035864092198
C	4.771689868874	0.073429696992	-0.036116487318
C	2.101333851430	0.065408457342	-0.036690266311
C	3.519640725617	0.068045470671	-0.036417842681
C	1.385012467288	-1.162503011170	-0.036277426767
TV	8.625104270865	-1.922965739920	-0.000000000000
TV	0.000000000000	3.870222121082	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.263926251195 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min58			
C	-0.653415080519	-0.938327126415	0.788867214081
C	-1.347063534083	0.285754304874	0.978033718607
C	1.703651893473	1.499668014624	1.577875979702
C	0.807384249992	-0.939930189454	0.362870484183
C	1.497647260214	2.897082584012	-1.724657302598
C	1.105589343337	0.277517647012	-0.453542161173
C	3.848992284183	2.735841653452	1.308071134566
C	3.129206789713	-0.937079388543	1.410433998284
TV	6.600556568814	0.000165841378	0.000000000000
TV	0.000000000001	2.449165584953	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.260094070143 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min59			
C	5.309019923481	1.102093923819	1.179968919670
C	-2.423854233614	-0.527360562013	-0.430545341972
C	-0.216090922094	1.838970092831	0.089617568444
C	-1.611370926900	-1.692696292190	-0.386459755466
C	3.491589126451	0.883649780761	-0.406513218948
C	1.994207261692	-0.560848248117	-0.387969071277
C	2.007551049726	0.885697853095	-0.364181211448

C	1.198478474459	-1.731009579524	-0.283361147697
TV	5.924333536391	-0.034045783478	-0.000000000000
TV	-0.000000000000	3.775277443238	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.259639003466 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min60			
C	-0.731790744994	0.288406888174	0.506046804000
C	0.572657432289	-2.164815055179	0.441687652130
C	0.120337419649	1.439086421958	0.369861732431
C	-1.870814869493	-0.584931569794	0.531134732759
C	3.768880445378	1.428869576804	0.206213282703
C	-0.457577770131	-1.089944321218	0.493943607145
C	2.528872664783	1.544710755538	-0.384590467955
C	5.298021988102	-0.283551474153	-0.063235234178
TV	3.921550401849	-1.435546768507	0.000000000000
TV	-0.000000000000	6.278228369654	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.258816149718 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min61			
C	0.554718949782	0.167845809157	0.392848477450
C	-0.418410162051	-0.976227946736	0.392830607628
C	0.504938143308	1.562234930768	0.392815693315
C	-1.720528034194	-0.626301819846	-0.323610563141
C	4.151122197857	1.243416588112	1.109326068942
C	1.927628674304	-0.301475885602	0.392801290256
C	2.850606904979	0.888343097128	0.392811966544
C	1.876628532964	-1.696422157967	0.392793869323
TV	5.871527528293	-1.860101779808	0.000000000000
TV	0.000000000000	3.729723568825	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.258220369943 hartree		
Spin(**2)	= 0.066406250000		
Geometry of 2D-min62			
C	-2.608354799570	-0.441196084822	-0.166940295494
C	-1.163975538906	-0.316550883105	0.092683601134
C	2.934364671366	2.129194247493	-1.030154559338
C	-0.262651806488	-0.872648773770	0.982976454655
C	0.660790768339	3.464057560468	-0.849722239103
C	1.546976578867	2.329885299028	-1.025294788442
C	-0.006276580255	5.890574879121	-0.661998511157
C	0.309117965936	1.463514318356	-1.048591863501
TV	3.496117122958	-0.522526060352	0.000000000000
TV	0.000000000000	5.730253563770	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.256588333190 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min63			
C	-0.960471149023	-3.279288014340	1.050006933397
C	-2.335850883186	-3.278625485415	1.042725377648
C	1.183383539920	3.102855468263	1.044347944166
C	-0.193761373141	-2.002674766819	1.050728462798
C	3.006392414501	3.094828558720	-1.952827654963
C	3.121742979407	1.818120052927	-1.822834433913
C	3.330260484036	4.378750022103	1.020204447880
C	2.567716980956	0.548923043621	1.031144368677

TV	7.052455218860	5.103255462754	0.000000000000
TV	-0.000000000001	2.553486597781	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.256318189029 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min64			
C	0.684269338213	0.732000296584	-0.721561353674
C	0.167573033491	-0.592643064405	-0.721519624931
C	2.154184123458	0.731811889623	-0.721561007675
C	-1.243789815994	-0.592653024104	-0.721525555114
C	-0.537714021361	4.242414906284	-0.721559950666
C	-0.537922711412	2.987250594710	-0.721614998651
C	-0.537949890027	5.623207534569	-0.721542596393
C	-0.538084848093	1.588920247145	-0.721579544262
TV	3.914770623799	-0.000206075421	0.000000000000
TV	0.000000000000	7.448077297712	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.254149244892 hartree		
Spin(**2)	= 0.222656250000		
Geometry of 2D-min65			
C	-1.754584567266	-1.045799740209	0.908904655526
C	-0.373201404547	-0.738016061017	0.908438784541
C	-3.007556497078	1.397798415001	0.908213850582
C	2.199483101264	-0.173057061870	0.907991741001
C	3.683076523315	2.104087076516	0.908874397019
C	0.847540843905	-0.467687851907	0.907976245776
C	4.073414035082	3.291724318223	0.908735720976
C	3.555001037627	-0.603811552580	0.908292409614
TV	6.266018922688	-0.610451403578	0.000000000000
TV	0.000000000000	6.293700250201	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.251324656356 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min66			
C	1.099014278395	-1.100988868571	0.746952261216
C	-0.182122882872	-0.268432752896	0.746880034284
C	0.642773289817	0.930458139042	0.747094786707
C	-1.522622176525	-0.587346036323	0.746918895079
C	4.014158015176	1.704287330473	0.746791352475
C	1.392719311086	2.217789649220	0.746899870790
C	2.673782305515	1.385141773619	0.746702894582
C	1.849027209897	-4.469263327246	0.747043140420
TV	6.752258199959	-2.015527826015	0.000000000000
TV	0.000000000000	4.655470958049	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.248585179217 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min67			
C	0.034932496102	1.313327093313	0.207073007442
C	0.034919165347	-0.075827213376	0.206641500252
C	1.262847541943	1.399212099896	-0.811171443439
C	-1.017532430366	-0.872439511371	-0.543013415094
C	0.210565996455	3.585178101885	-1.560957580253
C	0.210600572765	2.196040153848	-1.560723311003
C	1.262793656834	4.381606873654	-0.811020350770
C	-1.017472350910	2.109746303442	-0.543079725766
TV	3.584095814542	-0.000328131694	-0.000000000000

TV	0.000000000001	4.543973232939	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.243911990259 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min68			
C	-1.068348462248	2.034123838050	-1.535667397069
C	-0.035744965969	1.028533407560	-1.114952541410
C	-1.017296676231	3.503953079616	-1.452578627918
C	-0.023705586176	-0.502467180018	-1.452024676219
C	2.827770889494	-0.223258784094	1.181192497650
C	2.245720773364	-1.193461056236	0.380049838978
C	5.622085736485	-1.973189266885	2.386778576310
C	1.290230029749	-1.797736352135	1.182060319879
TV	2.513097933381	-2.449856178322	-0.000000000000
TV	0.000000000000	5.022564770085	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.240845995522 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min69			
C	0.442860618749	0.480644493187	-0.511795685879
C	-1.793266278641	-0.658837550104	0.152048570927
C	0.483702617163	1.926298913739	-0.535946639565
C	-0.393221107240	-0.705971362155	-0.485173057020
C	2.961439504432	0.060548235255	0.423350521740
C	1.791317441904	-0.044054947150	-0.422429177463
C	3.382451974040	1.193797850851	1.069630060353
C	1.842716042964	-1.419778931970	-0.542040419910
TV	5.070771674190	-0.822934118213	0.000000000000
TV	-0.000000000000	3.854556632424	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.239049983358 hartree		
Spin(**2)	= 0.187500000000		
Geometry of 2D-min70			
C	1.347007087348	1.654485469919	-0.205706100837
C	0.876951336352	0.287464414101	-0.212746359045
C	2.773715167696	2.090656749644	-0.630825619151
C	-0.940688496051	-0.906836152006	-1.512366434694
C	-1.300210701069	1.674985837528	-0.864920325300
C	-0.674042091789	2.930604893433	-0.938939900495
C	-1.307526131103	4.237436776491	-0.920034573107
C	0.752286896646	2.862577888915	-0.704472845716
TV	3.336746344150	1.805228754926	-0.000000000000
TV	-0.000000000000	6.373842623380	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.236948951941 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min71			
C	1.143353702731	0.468443298861	-0.385878957896
C	-0.905690688118	-1.983253938657	0.222612970501
C	0.562784949731	1.614715697759	0.186073546351
C	-1.708900420613	-0.835999156095	0.219125782450
C	3.974835947545	1.280345668708	0.551493818745
C	2.308987703944	-0.110103707204	0.464688960401
C	2.648939104469	1.286313989001	1.065870817648
C	1.702394907242	-1.459049237353	0.818630472127
TV	5.591678293149	-3.052902869729	-0.000000000000
TV	0.000000000000	3.762707277194	0.000000000000

TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.236160311799 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min72			
C	-0.715002321931	1.127471883789	-0.463607130912
C	0.200363539944	-0.095810105679	-0.463596822581
C	0.462428414942	1.970484518129	-0.464148963395
C	-0.120689601985	-1.369094081909	-1.295436617335
C	0.772162562353	3.432945563448	-0.464726522772
C	2.200740284783	3.703580993506	-0.465077707748
C	-0.120906915752	4.398239499313	0.366591451830
C	-2.124077048970	1.256518961072	-0.463664662962
TV	3.522480557018	-0.384950604833	-0.000000000000
TV	-0.000000000000	5.768037355652	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.231893570183 hartree		
Spin(**2)	= 1.312502500001		
Geometry of 2D-min73			
C	-0.914055022039	-0.255189731799	0.083365258362
C	1.198953080378	-1.962807211800	0.084752154308
C	-0.298297246603	1.140743033877	0.081407577196
C	-2.285597233687	-0.426052497250	0.084697492703
C	3.549100381616	0.212770139599	0.080910350816
C	0.399951036865	-0.835465085992	0.083449384358
C	2.387543190674	0.731904583952	0.080952494323
C	5.662040658659	-1.495232887796	0.081332624847
TV	4.646146959539	-2.055755940899	-0.000000000000
TV	0.000000000000	6.113639176004	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.229097131617 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min74			
C	-0.910277837687	-1.014873229657	0.216239508436
C	-2.298375222052	-3.657470448452	0.221921101087
C	1.691334524306	1.629283475292	0.216866343661
C	0.371538225787	-1.014473554281	0.215646278856
C	3.736201426344	0.976825714214	-3.039425490034
C	3.736941243762	-0.259873628988	-3.039444172482
C	4.361424476433	1.629706283424	0.223232638079
C	2.972790279679	-1.012935217395	0.224178398979
TV	7.372493242951	3.965577463452	0.000000000000
TV	-0.000000000001	2.642891149598	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.227398982860 hartree		
Spin(**2)	= 0.140625000000		
Geometry of 2D-min75			
C	-1.344128764022	-0.297377170313	0.407903253012
C	-0.521754768195	-1.221524345960	0.407898985578
C	0.246354767492	1.279668994951	0.411002485014
C	-3.588534175356	-2.078756320778	0.411258376505
C	3.656180549105	0.547803056790	0.409987712276
C	0.901982419303	-1.286637150557	0.410045839819
C	2.345190441314	1.113166599117	0.411203450439
C	6.127945355091	-0.402677920850	0.411024860241
TV	4.898208319178	-0.576425966722	-0.000000000000
TV	-0.000000000000	4.933359895947	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.226821210245 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min76

C	-0.746160414338	-0.364793946755	0.697690586119
C	0.985126959707	-1.910970061936	0.273670936915
C	0.289420156996	0.649470404485	1.215525845006
C	-1.252943361215	-1.699362849406	1.215312051558
C	3.245229532993	1.984233937694	0.697848687759
C	0.478347501382	-0.576246106966	-0.243937491468
C	2.020763271016	1.772530036403	-0.243816642401
C	4.976292055737	0.438038708699	0.273879127882
TV	3.462514731630	0.000166070225	0.000000000000
TV	-0.000000000000	4.697755445003	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.221952037229 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min77

C	1.810991743095	-0.352174884139	-1.548626344913
C	0.533304109321	-0.614906741686	-1.548546284355
C	-0.361815437132	2.572608744623	1.528671740647
C	-1.639511161186	-0.948991805106	1.528626591603
C	4.366337273141	0.173252806702	-1.548631961785
C	3.088661570302	-0.089502937589	-1.548492623554
C	2.193559361728	3.097935313072	1.528793406722
C	0.915863008039	-0.423644536139	1.528688250538
TV	5.110739098345	1.050721859639	0.000000000000
TV	0.000000000000	3.258900462329	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.221689794170 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min78

C	3.139446959407	-0.906811297921	-1.452783490246
C	-3.252561498678	1.059397779111	-1.452801888549
C	0.583843077831	1.818841952634	1.628157656165
C	-0.694526472290	-1.704117350275	1.627958323712
C	5.696129599484	-0.387400681956	-1.452445827275
C	-0.695769792380	1.578206162276	-1.453019872033
C	3.140509238236	2.338047325574	1.627996390332
C	1.862252287835	-1.185136060629	1.627950456539
TV	5.113427909952	1.038368236958	-0.000000000000
TV	-0.000000000000	3.263507059496	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.221687478963 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min79

C	-0.781788899641	-1.426660448351	-0.306481817488
C	0.505259070930	-1.594447689628	-0.834548812783
C	-0.381055955660	1.161772525631	0.460304464216
C	-1.038240641063	-0.020569486932	-0.073879625067
C	2.173232239853	0.442207984112	0.026294001947
C	1.658575347931	-0.903932908635	-0.628313700855
C	2.105277576440	1.931649991228	-0.134994064099
C	4.810717148486	-0.262557794033	0.530767017111
TV	3.796864764269	-1.605468538153	-0.000000000000
TV	-0.000000000000	6.014168690180	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.218914523205 hartree

Spin(**2) = 0.140625000000

Geometry of 2D-min80

C	0.821423714962	0.836196775376	0.541405340458
C	0.821477421923	-0.468413344751	0.541465821167
C	0.821491537389	2.140872873396	0.541455397584
C	0.821420921032	-1.773087708463	0.541400020614
C	2.701521730702	-0.794320337809	-1.895442103762
C	2.701619269108	-2.098934486463	-1.895548715783
C	2.701624001416	0.510365982686	-1.895541505176
C	2.701500183616	-3.403621100679	-1.895445573758
TV	3.761939762044	-1.968963299404	0.000000000015
TV	0.000000000001	5.218623510078	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.218578708032 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min81

C	-0.727580149191	-0.716838619875	-0.194751064572
C	-0.082950877570	-1.440133684886	-1.139446546239
C	-0.321848607722	0.701327553385	0.094089358657
C	-2.183101547256	-0.956508685576	0.094206297134
C	3.145459227279	0.796051566660	0.172958492555
C	2.078022411479	-0.154502559940	0.172818783908
C	2.194184092798	1.928794643093	0.202679390070
C	5.817352906509	0.369070944567	0.202536018988
TV	4.755137765133	-0.551855275220	0.000000000000
TV	0.000000000000	4.786197534987	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.218393712017 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min82

C	0.716691753370	1.328435836115	-0.324783450379
C	-1.232817316491	-0.534005872695	-1.427852463915
C	0.980629665467	0.110115080804	-1.134951397774
C	-2.504205066749	-1.900864450065	-0.455141664046
C	-1.093299927571	4.473576236122	-0.592072424221
C	0.219574882343	3.941184517915	-0.246086985883
C	-0.224648094249	6.368682612585	-2.034110585410
C	0.480814769228	2.543778263524	-0.191085684432
TV	3.736756221900	0.601096146898	-0.000000000000
TV	0.000000000000	6.200706635727	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.217044203941 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min83

C	0.107960149700	1.053916292372	0.238646767856
C	-1.350653028422	1.055793895784	0.276037265711
C	0.884275974392	2.166699841312	0.698770911484
C	0.901008850197	-0.180297124249	0.076708801806
C	2.191003367132	0.090172036143	-0.382952300291
C	2.487936784116	-0.595658088407	2.272084435502
C	2.612398540984	0.616057643609	1.700750791286
C	1.991150367762	-1.744331361018	1.720079676976
TV	4.656503318415	-0.628828823098	0.000000000000
TV	-0.000000000000	3.710910176548	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.216455222788 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min84

C	0.535031319666	0.285907582943	0.168506215254
C	0.164062810947	-1.008037294575	0.947573016077
C	0.989271690458	1.734887265348	0.554494144385
C	-1.162433037033	-1.338197527337	0.966966729203
C	2.407730430483	1.784705285550	0.868734996949
C	2.048424263455	-0.174579805854	-0.219019338084
C	2.960263289807	1.076049318782	-0.385790852490
C	1.943355064763	-1.693818961264	-0.657369904059
TV	3.976042737811	0.587864596688	-0.000000000000
TV	0.000000000000	3.937977420991	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.211726285130 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min85

C	0.675075892268	0.052427582721	-0.055008744413
C	-0.675918787209	0.051994298972	-0.055045185897
C	0.637232936876	3.324776548479	-0.049823630648
C	-0.628597228038	-3.221730284849	-0.049827866951
C	3.291823570073	0.052560917503	-0.054988323033
C	1.940804461526	0.052140364009	-0.055034122531
C	3.254062621529	3.324882725483	-0.049819246800
C	1.988225057430	-3.221573339734	-0.049823652453
TV	5.233615225243	0.000303459679	-0.000000000000
TV	0.000000000000	6.547454691726	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.210699987215 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min86

C	-0.847804481711	-1.402542024925	0.592007320205
C	0.506850512169	-1.616603138333	0.821728779206
C	0.653593946992	1.492453770222	-0.699378281515
C	-1.479729610392	-0.126006122169	0.596825711133
C	4.174312478517	1.470242997749	0.423620608735
C	1.571540503092	-0.715919897702	0.597096467275
C	-0.428552700061	0.898726732643	0.710852120680
C	5.412202689186	-0.308228554918	0.307231645992
TV	4.465559101084	-0.862256235866	0.000000000000
TV	0.000000000000	5.129013275521	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.210618991741 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min87

C	-1.184473757212	2.114086435815	-0.370180846408
C	0.677765506864	0.077638780811	0.302823775568
C	0.369831232481	2.813909372855	-0.572076181960
C	-0.030464597807	-0.818128082489	-0.537280869895
C	2.039402224903	0.153742274297	0.060677236874
C	3.566539827760	-3.143899754499	1.186020448286
C	2.594606555612	1.487791195076	-0.048565819814
C	1.843393105452	-2.286191978051	-0.440208381156
TV	3.945673418312	-3.079547848148	0.000000000000
TV	-0.000000000000	5.024195363738	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.207501731719 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min88

C	0.879025892239	-0.026384057263	-0.337090914971
C	-0.003102611234	-1.235954156245	-0.517240880106
C	0.915559087416	1.420853899203	-0.532163569397
C	-3.661023235001	-0.169270406511	-0.533126482420
C	4.582275462495	0.746293906018	-0.513564348350
C	2.329988751717	-0.485704010317	-0.337449791268
C	3.212251169332	0.723594261029	-0.517176142888
C	1.604474969484	-0.259429666390	1.038060561447
TV	5.955389174061	-1.763535976714	-0.000000000000
TV	-0.000000000000	3.774117452333	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.207075035508 hartree			
Spin(**2) = 0.750000000000			
Geometry of 2D-min89			
C	0.101453215806	-0.296535124925	-0.121575400708
C	-1.268442892249	-0.331633616937	-0.108788858130
C	3.099697279013	0.508663120169	1.467509497060
C	-3.566189103981	0.354036999094	-0.067746546242
C	3.818522794684	0.475746071268	0.088012028208
C	1.470485083630	-0.273606632445	-0.093158186548
C	2.358913143783	0.923171129820	0.117625162970
C	3.776189075106	-0.968095297779	-0.131691156486
TV	5.962628596650	-1.745858205887	-0.000000000000
TV	0.000000000000	3.764763149169	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.207002455625 hartree			
Spin(**2) = 0.515625000000			
Geometry of 2D-min90			
C	0.104270477873	-0.081822885784	1.119876620384
C	-0.787129802821	-1.216632253429	1.174170041188
C	0.104700610623	1.326003052135	1.118457118804
C	1.079070812367	0.622929205188	-0.434203896112
C	3.826659766602	0.619270353039	1.222852773839
C	1.506604920887	1.702380984954	0.732868196684
C	2.477642065823	0.622359515645	1.156336717635
C	1.505893976394	-4.134881446526	0.733311421396
TV	6.003645551916	-1.838446189353	-0.000000000000
TV	-0.000000000000	3.677440870042	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.205295303288 hartree			
Spin(**2) = 0.750000000000			
Geometry of 2D-min91			
C	-0.834276040169	-0.596090796493	0.214306371041
C	0.025395955553	-1.614116654658	0.212905154748
C	-0.404837807670	0.821618636623	0.214613642437
C	-2.302352551600	-0.780921155694	0.214627161129
C	3.146595726049	0.709521458382	0.214735954020
C	2.018524086826	-0.238810705107	0.214824470762
C	2.147820793601	1.865089244436	0.214722516153
C	5.842652960290	0.117266508769	0.214755743500
TV	4.799992919504	-0.810840097980	-0.000000000000
TV	-0.000000000000	4.863595011779	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.203372910255 hartree			
Spin(**2) = 0.066406250000			
Geometry of 2D-min92			
C	0.864655751395	2.553924766371	-0.713525146529

C	-0.277691348132	-0.296590897563	-1.710928817370
C	1.535153352112	1.503198788134	-1.410520239453
C	-2.395430250588	-1.647265061912	-1.710627884844
C	0.375833412780	4.583469246627	0.391172546062
C	-0.768121920162	3.854550140671	0.392836115689
C	1.433029038901	3.837434776474	-0.276013050324
C	-0.538984189383	2.581509918598	-0.275450480752
TV	3.164929945602	2.014996446376	-0.000000000000
TV	-0.000000000000	7.100414418073	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.202034022730 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min93			
C	-2.027379121001	0.369699706111	1.447087932859
C	-1.277650180686	-0.368194370163	0.037118581369
C	0.940707558434	2.296050405831	0.138052958817
C	-0.433977757951	-1.541821383828	0.129838880249
C	4.646875489960	1.110002760433	0.122727804212
C	3.172405506828	-0.355979299002	0.122976121291
C	3.159157916503	1.115109140628	0.037626100283
C	2.315523632558	-1.557200033212	0.130354685369
TV	5.937719663675	0.007159487922	0.000000000000
TV	-0.000000000000	3.845930915402	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.201117164253 hartree		
Spin(**2)	= 0.750000000000		
Geometry of 2D-min94			
C	0.048123385801	0.603780682011	-0.509359584925
C	-0.433188073994	-0.782593112004	-0.612487081773
C	1.243869051290	1.361718841403	-0.511369096450
C	-1.402913700552	-3.851875563880	-0.848459323760
C	-0.362668416026	5.924139309682	-0.849691965251
C	0.952024193165	2.770772926199	-0.355400593270
C	0.354185154079	7.126639386212	-0.778113026550
C	-1.107173399324	1.500333366819	-0.353509283895
TV	3.144650877941	2.062945488077	-0.000000000001
TV	-0.000000000000	9.096938972631	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.200759078999 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min95			
C	0.597479579474	0.982923053672	-1.413147526281
C	0.605550453879	-0.319687672907	-1.457778462663
C	0.589306143750	2.285378885690	-1.457149575565
C	0.599126632663	-1.561269382219	-0.836859013343
C	2.282353140123	0.350117996231	1.306522329739
C	1.415980242320	-0.622593148298	1.350351156796
C	3.149039434345	1.322706244609	1.352134131365
C	0.601876111909	-1.561078290925	0.730784950140
TV	3.359612850978	-1.265889147817	0.000000000000
TV	-0.000000000000	5.088661347704	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.195220113102 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min96			
C	-1.083497667595	-0.765392252902	0.552883890813
C	0.054435768557	-1.171415753119	-0.158246355233

C	-0.591561575847	-0.205697899990	1.879296422532
C	-2.399172016206	-0.863667469646	0.126876372930
C	3.242342859185	-0.124051796398	2.651161098038
C	1.238333381022	-0.935759989303	0.553969061039
C	1.978398923877	-0.033193572434	2.651993608377
C	5.759899266189	-0.670312622330	1.879863265585
TV	4.925688481845	-0.358889827925	-0.000000000000
TV	0.000000000000	3.683736023179	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.190603407829 hartree		
Spin(**2)	= 2.000000000000		
Geometry of 2D-min97			
C	-0.394538234106	-0.333583288041	1.225906359429
C	0.424531665765	-1.569412818472	0.720392234622
C	0.313109647095	0.974812531906	1.219750723997
C	-1.567646030909	-0.911671443552	1.899435951708
C	4.647399381232	4.854156463653	-0.760336769207
C	0.565032311122	-3.737176001486	2.019596280027
C	2.221787008944	1.896992378072	-0.299797673620
C	3.321155169984	-0.262811788581	-0.233257565840
TV	2.459446673708	-1.525530125545	-0.000000000000
TV	-0.000000000000	5.762637231693	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.190062641767 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min98			
C	0.851418482768	0.945827497286	-0.591362384880
C	0.427899823117	-0.350464113501	-0.276730072474
C	2.349632222722	0.502946889483	-0.561420700028
C	-1.280069722114	-2.439727761695	-0.092574092002
C	-0.450394831656	4.724670566585	-0.929313204586
C	-0.126282447701	3.367498781303	-0.995595480109
C	-0.506036695080	5.891592609173	-1.696581146282
C	0.261326235968	2.189031409390	-0.846435077980
TV	3.145466045540	1.601132196726	-0.000000000000
TV	0.000000000000	8.061814837966	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.188935246507 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min99			
C	-0.525186236964	0.310468604430	-0.662167909889
C	-0.324440014989	-0.993763202395	-0.662328187067
C	2.067715518664	2.520906277581	-0.661915140138
C	-0.103203056020	-2.204249051874	0.110598535575
C	-0.267834141213	3.791948045010	-0.662029308529
C	0.705745958621	2.619137365360	-0.661951643428
C	-0.103323225183	5.066055248409	-1.435291398060
C	-0.428278881538	1.653157347358	-0.661972726947
TV	3.477026818162	-0.254016836900	-0.000000000000
TV	0.000000000000	7.270420526592	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.183476688095 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min100			
C	-1.955542423458	1.587701547089	-1.031187690061
C	2.508805257369	-3.810466894243	1.744638841314
C	-0.552617014544	1.356241675210	-0.207242195772

C	-1.527954483911	0.764905145073	0.920250645120
C	3.232175968670	0.760707730496	0.524318636176
C	0.841962344803	-0.688498356720	0.188908025241
C	1.898215332734	1.391902922523	0.887958536494
C	4.492029545445	-1.088197889101	-0.174771521580
TV	3.592656816159	-1.874267583641	-0.000000000000
TV	0.000000000000	4.052128993773	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.177904500824 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min101			
C	-0.587589563701	-0.231286445790	-0.294684980848
C	0.163521994473	-1.455419210982	-0.373270303071
C	0.168640664225	1.173682478200	-0.175279171039
C	-1.997486524543	-0.041845806909	-0.150662235801
C	2.206310316768	0.346549508566	0.247209385826
C	1.619925985831	-1.659420259437	-0.541579973412
C	1.539977378842	1.251431898192	-0.696928029659
C	5.938675635369	-0.056229988452	1.024342770971
TV	4.754465059820	-0.886901956986	0.000000000000
TV	0.000000000000	4.341994702457	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.176331777453 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min102			
C	0.013338588254	-0.034570332503	1.037814371221
C	-0.310463872642	-1.479914790871	0.821629782816
C	0.649215439361	1.054820937407	0.307131694443
C	-1.668814539749	-1.512675605432	0.279168107736
C	4.636000055128	1.456148646229	0.081130219266
C	2.032073280468	1.242200304530	0.082526201906
C	3.273422658045	1.359709015226	-0.003058492575
C	-0.262969298328	-2.618342658051	1.963571243561
TV	7.534303921631	-0.594753528117	0.000000000000
TV	-0.000000000000	3.588250714737	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.174954744146 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min103			
C	-0.297826058478	-0.157635598294	0.682046298466
C	0.573698809992	-0.924146822236	-0.037047200360
C	-0.319772709098	1.229938435906	0.461098542903
C	-2.463369001641	-1.760116740611	0.623756686874
C	3.483526086683	1.572904152242	-0.182763536350
C	1.735634623625	-0.065571434090	-0.091049329549
C	1.891554420088	1.444208434772	-0.214323540567
C	4.028763410670	0.356309214342	-1.017563044549
TV	3.251656970208	-1.813434127741	-0.000000000000
TV	-0.000000000000	5.767729375881	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.173341155546 hartree			
Spin(**2) = 0.058593750000			
Geometry of 2D-min104			
C	-0.127914321794	1.077293595434	0.071136430486
C	0.246597057817	-0.318010307096	-0.387075613699
C	0.042057272768	0.443300808105	1.261007576104
C	-2.128835149556	-1.672220870069	-0.618086909485

C	-1.132410973142	4.841321620115	-0.786541877301
C	-0.774434515467	3.494023422331	-0.775852795898
C	-0.761137513013	6.201145731054	-0.618721328801
C	-0.459516227849	2.321216701106	-0.484221429285
TV	3.742779130604	0.993574592842	0.000000000000
TV	-0.000000000000	7.510934903629	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.173051644500 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min105			
C	-0.740023452230	1.785143034431	0.474169546269
C	-0.888103725187	0.281963447684	0.570757310807
C	0.745623929474	1.877293028604	0.037269670980
C	-1.607164955601	-0.862685536957	-0.102032342953
C	0.889654701678	5.728797532451	-0.724435044326
C	-0.047772118375	-0.473671237019	-0.250884013315
C	1.230262647914	4.424227623882	-1.023978995305
C	-1.818497170102	2.689210438696	0.318303929042
TV	3.918360857192	-0.206550184851	0.000000000000
TV	-0.000000000000	4.979932222649	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.172877893774 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min106			
C	0.620684976823	0.128089815392	-0.903293760389
C	0.565731644344	-1.259242559733	-0.714369602882
C	1.767575445802	1.129821716667	-1.069919189237
C	-0.833281879137	2.367059596279	-0.139565377590
C	0.092191223745	3.231937410878	-0.790017087779
C	0.665942198281	2.138139468331	-1.589259308323
C	0.398982504257	4.588630495730	-0.613543979722
C	-0.312647319235	1.055227164290	-1.464628488982
TV	3.458282139059	-0.355495202201	0.000000000000
TV	0.000000000000	7.082347596492	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.168421084739 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min107			
C	0.470902640732	0.544829593266	0.728490326904
C	-0.617829489201	-0.485780623844	0.680599413447
C	-0.618674582466	1.571542108439	0.664887421675
C	-1.614937306612	0.538906479719	0.523833026962
C	2.984288754747	-0.086529993632	-1.473923782663
C	1.785367568137	0.507272992372	0.538848212556
C	2.973573392398	0.292825202207	-0.062735526595
C	2.996087557756	-1.161148523909	-2.215138188696
TV	5.947977331532	-3.633416178600	0.000000000000
TV	0.000000000000	3.439573269725	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.166548523767 hartree			
Spin(**2) = 0.312500000000			
Geometry of 2D-min108			
C	0.880058463895	0.516322963488	0.174210803872
C	-0.584574162927	-0.967539948933	-1.092428224648
C	0.590499585304	1.772775639913	0.620382840247
C	-0.815863041934	-2.066747046476	-0.119623276292
C	3.726022971778	1.808010830418	-0.087077252935

C	2.209246079905	-0.018513780171	0.699059067685
C	2.760876867914	1.400323805211	1.106087942082
C	1.791687350446	-1.412182936703	1.198776835887
TV	4.321822989761	1.650717716888	0.000000000000
TV	0.000000000000	3.824157648321	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.163530891119 hartree			
Spin(**2) = 0.000000999999			
Geometry of 2D-min109			
C	0.308239314197	0.617560059264	-1.147424618170
C	-0.849958701761	-0.398259759960	-1.147738926960
C	1.198516221330	-0.404519707637	-0.331733533267
C	-2.123364557447	-0.390141210948	-1.963552236851
C	0.361379007373	4.600275333054	-1.148390032817
C	0.343867911771	3.307356980433	-1.147575739330
C	0.301119242235	5.997233769139	-1.148315674097
C	0.367282619834	2.014573568208	-1.147099618714
TV	3.321819619242	-0.013664724720	-0.000000000000
TV	0.000000000000	7.418222681386	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.162516720476 hartree			
Spin(**2) = 0.140625000000			
Geometry of 2D-min110			
C	-2.431070681225	3.134266308699	-1.182397113795
C	3.160464355985	-4.537492876723	1.895274107252
C	-0.553285511161	1.382892544345	0.515966878553
C	-1.852204944579	0.708671249163	0.324881091533
C	3.290664182299	0.634662715126	0.546411264648
C	0.761565836531	-0.824238452916	0.389464408134
C	2.015428210071	1.382898077659	0.168126259540
C	4.545513079178	-1.607363685022	0.195146381077
TV	3.829560671128	-2.245777362874	0.000000000000
TV	0.000000000000	4.388663811075	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.161623161060 hartree			
Spin(**2) = 0.066405687500			
Geometry of 2D-min111			
C	0.557259467858	-0.225808220701	-0.758514636655
C	-0.052700025470	-1.480358850026	-0.250249334514
C	-0.350226506500	0.814477721891	-0.859678354218
C	-1.620929787443	-0.018563199531	0.853837619601
C	3.622781691045	0.857696401123	1.328000023261
C	1.989999907952	-0.008194047338	-0.257733652067
C	2.491706349955	1.288662338506	0.420213890628
C	3.247814735156	-0.560996280349	1.768219451207
TV	3.895738015836	-0.958681579570	0.000000000000
TV	-0.000000000000	3.628843088297	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.158098571712 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min112			
C	0.839476094602	0.147911934024	0.495032650606
C	-0.385367947807	-0.251244262679	0.922228621416
C	1.712155220414	1.376026274337	0.674439791716
C	-1.611478411876	-0.626001361363	0.894056690607
C	3.193060231743	1.105512624151	0.520273293640
C	1.615295371578	-0.408808784296	-0.595743089021

C	2.514364153961	0.865459713808	-0.810596316697
C	1.779275304873	-1.782598390801	-0.587843040661
TV	6.043152779646	-1.873092437270	-0.000000000000
TV	0.000000000000	3.965976185232	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.154453848878 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min113			
C	0.141519099312	0.297534151429	0.318106328812
C	0.142180629179	-0.521607401855	-0.938128376371
C	1.243923193402	1.357785865081	0.256533438830
C	0.141051180808	0.714262799350	-1.536011055687
C	0.139621687599	3.380559844138	-1.109750424509
C	0.139920315110	2.013919751537	-0.612109688782
C	0.141446593885	4.618346989239	-1.185384066065
C	-0.963640728206	1.355298351273	0.256158601232
TV	3.554611903309	0.003878295226	0.000000000000
TV	-0.000000000000	6.523001190701	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.133523243955 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min114			
C	0.890106999910	-0.040198996897	0.362510435939
C	-0.142272158753	-1.063553955738	-0.045700550903
C	0.176705115408	1.085098444409	-0.276266900227
C	-0.132120475889	0.066413018329	-1.150031880411
C	3.465831288794	0.839829873424	0.362534048882
C	2.433474424042	-0.183527193799	-0.045677642787
C	2.752505232441	1.965159592316	-0.276269682463
C	2.443702984079	0.946473238155	-1.150047360446
TV	5.151474106636	1.760111086623	-0.000000000000
TV	-0.000000000000	3.577826811061	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.130707952995 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min115			
C	-0.547885448301	1.092978806796	0.374702650991
C	-0.759120920813	-0.237315784507	0.903813402920
C	0.690939455680	0.980939728064	-0.563298669958
C	-0.329736479703	-0.194794921038	-0.563104116575
C	1.051398022174	3.453792471399	-1.477070975342
C	0.246903192426	2.383060764877	-1.061834393103
C	1.902073343161	4.379529899802	-1.458859989344
C	-0.954626485825	2.357116688269	-0.309424730114
TV	3.013836130548	-1.871849787800	-0.000000000000
TV	-0.000000000000	7.237767112715	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.123337511852 hartree			
Spin(**2) = 0.000000000000			
Geometry of 2D-min116			
C	-0.447944386502	1.228730542297	0.905172699535
C	-0.715735674009	-0.107695948349	1.122059676207
C	0.756478123318	1.526674255134	-0.021955061046
C	-1.523729756360	-0.905429830262	0.308945869042
C	0.309530626259	5.157513752364	-1.428063159767
C	-0.378144843586	1.904256385792	-1.093380979282
C	1.223470518975	4.583442627101	-0.624291740256

C	-1.459944750510	2.062786547697	0.130682756755
TV	3.525342316604	0.243911129295	0.000000000000
TV	-0.000000000000	4.468671513725	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.112367329028 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min117			
C	0.624363103945	-0.463287320254	-0.741608423815
C	0.897887361256	-1.725785145349	-1.586511659577
C	0.551955729992	0.838398461575	-0.741378514522
C	-0.063106983795	-2.653845058082	-0.740571718968
C	0.265491831220	3.419949044466	-0.740400931826
C	0.392497356363	2.161572309990	-0.740851065301
C	2.102118390717	5.421299523199	-0.740479150280
C	-2.724604866453	5.409099907055	0.104505054510
TV	3.622248386425	0.340750081186	0.000000000000
TV	0.000000000000	7.475051183389	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.110808496896 hartree		
Spin(**2)	= 1.312500000000		
Geometry of 2D-min118			
C	0.326803778268	0.723164307417	-0.117685417362
C	0.311374336373	-0.673336823539	-0.112546906051
C	1.085908623664	-0.027441339938	-2.674198415447
C	0.191033426301	-1.942829841167	0.332152061954
C	0.154831565363	4.592527101916	0.462347609418
C	0.164500587279	3.265135523119	0.463084307605
C	0.678064037615	7.828720520005	-1.401082500008
C	0.200555997600	1.994168870790	0.327544488797
TV	3.388799790831	1.452321689193	0.000000000000
TV	-0.000000000000	7.807273372153	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.089269984926 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min119			
C	0.100156016909	0.636016683725	-0.228354764327
C	0.100177462210	-0.602914001227	-1.125688611003
C	0.100175328120	1.875095537981	-1.125709263515
C	0.100160640443	-1.841974353950	-0.228365701526
C	1.735831242607	0.635345569911	-0.228362106993
C	1.735831433800	-0.603598567353	-1.125718280987
C	1.735827919735	1.874405674004	-1.125694029008
C	1.735815025627	-1.842676716744	-0.228358561272
TV	3.271317914581	-0.000104767692	-0.000000000000
TV	0.000000000000	4.956018242823	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.067428805658 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 2D-min120			
C	0.697443145126	-1.680146781476	1.009396095004
C	-0.565517427688	-1.228650756775	0.890247087682
C	1.389955169133	1.071393794461	-0.218159526465
C	-1.738698523487	-0.668744324236	0.909494165488
C	4.024626028744	1.079117426122	0.881795500288
C	1.922649009681	2.523300480319	0.138504591908
C	2.820734238192	1.678847590128	1.008230820602
C	1.415537710773	-2.963471521251	1.355774501039

TV	6.947146436433	-2.970718015806	0.000000000000
TV	0.000000000000	4.191641763917	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.027487159149 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 2D-min121			
C	0.669587700790	-0.050698647903	-0.567390036457
C	-0.838979396389	0.058180030492	-0.567388222501
C	-0.258818277950	0.738915474970	0.576374603717
C	0.089273123227	-0.731452635010	0.576331416025
C	3.577491771086	0.409178093017	-0.567399550126
C	2.068938253690	0.518067241300	-0.567401025045
C	2.649079834569	1.198760138396	0.576414484479
C	2.997177063129	-0.271603605427	0.576286379003
TV	5.815739542565	0.919712926046	0.000000000000
TV	0.000000000000	2.941527428595	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.016896412926 hartree	
Spin(**2)	=	0.000000000000	

(iii) 1D

Geometry of 1D-min0

C	2.891042989071	0.701818141079	-3.557332854326
C	0.387262348708	0.267467337245	-0.783810798590
C	0.387018232677	0.043712112914	0.646788250093
C	-0.866300652734	-0.292085959162	2.791448988908
C	1.638947029935	0.603093424701	-2.928347984056
C	1.639552118269	0.376061393800	-1.478507642723
C	1.639161608760	-0.064953730528	1.341534396204
C	0.385792713988	-0.390878468077	3.420635038419
TV	2.504591976667	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.350787612999 hartree	
Spin(**2)	=	0.000000000000	

Geometry of 1D-min1

C	0.696065406265	1.277849340382	-0.197517829562
C	0.695909299923	-1.024321818143	-1.076326653755
C	0.696102447199	-1.520798291445	0.223743594402
C	-0.614411031468	0.088951908237	1.412064622337
C	2.006540997280	0.967818848688	-0.889573647457
C	2.006429707850	-0.332221621613	-1.386179064328
C	2.006641209303	-1.211237259137	0.915950214730
C	0.696027727364	0.781183260863	1.102562725369
TV	2.620936152757	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.245668827661 hartree	
Spin(**2)	=	0.000000000000	

Geometry of 1D-min2

C	0.732257185204	1.340938147373	-0.222283374576
C	0.732329113148	-1.040883450610	-1.147922703322
C	0.732313608343	-1.581584841856	0.243783441354
C	-0.519165162437	0.112413591032	1.471839863226
C	1.983589784802	1.038485037695	-0.909898322687
C	1.983601161926	-0.353263607628	-1.450449438480
C	1.983675208404	-1.279174687674	0.931311594050

C	0.732108108876	0.799940363300	1.169177828394
TV	2.502749085648	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.243958698629 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min3			
C	0.070055521701	0.366029145703	-1.692367261759
C	0.069875948129	0.502698243374	-0.225777380314
C	-0.295674096334	-2.841926025277	-0.462129656172
C	0.068383952029	0.727556112339	2.547981868389
C	1.346660826606	0.304834722876	-2.309497218093
C	1.347499652557	0.561172544518	0.461863007685
C	0.987888559283	-2.931094959269	-0.339875894430
C	1.346499607503	0.679032613513	1.929709634017
TV	2.555935378103	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.242730904260 hartree		
Spin(**2)	= 2.812500000000		
Geometry of 1D-min4			
C	1.501808094029	1.002566011488	-2.287803747039
C	-0.377912219453	-0.777409588864	0.483541248656
C	-0.377801265770	-1.835752051220	-0.543245581143
C	-0.377812252804	1.231244118940	2.404767858796
C	2.857563502014	1.003142765899	-2.288705696362
C	0.904881799865	-0.281241916661	0.961520518014
C	0.905029751327	-2.277858818931	-0.973338063655
C	0.904942649229	0.784206511156	1.978958200534
TV	2.565599475123	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.242250370314 hartree		
Spin(**2)	= 2.812500000000		
Geometry of 1D-min5			
C	0.160366410908	0.395104963947	-2.378918713492
C	0.160383973477	0.531437800355	0.401270275839
C	-0.464410858984	-2.921247740017	-0.188068855944
C	0.160380678622	0.583292807650	1.873377795275
C	1.438588513894	0.428275066694	-1.759387413282
C	1.438620015913	0.502682725085	-0.288245648274
C	0.813967289757	-2.914886943494	-0.307323277890
C	1.438651424640	0.603753695095	2.493509459034
TV	2.556496724004	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.239232590668 hartree		
Spin(**2)	= 4.812500000000		
Geometry of 1D-min6			
C	2.899525732260	0.181374039383	-1.481323127134
C	0.562594993007	-0.225555718739	-0.455401982023
C	-2.566533103379	-1.091743235326	1.727062421719
C	-0.229606691941	-0.684844674496	0.701453220257
C	4.160794789080	0.181348938803	-1.481402258429
C	2.012873551905	-0.225600043760	-0.455441986208
C	0.656989893465	-1.091836882951	1.727264304246
C	2.805025690594	-0.684883628082	0.701431335695

TV	4.484762034603	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.232865148379 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min7			
C	0.747692308829	0.017707230694	0.362231297585
C	0.747460245448	-1.125127745090	-2.295684304123
C	-1.706967419454	-1.683287024047	-3.596382028095
C	-0.479386382758	0.877579395635	2.349380273011
C	1.974622013330	-0.270343969582	-0.306213646185
C	1.974424366131	-0.833574892099	-1.616727052442
C	4.427341406574	1.443649160532	3.646414355670
C	0.747595338938	0.583604341704	1.671519139497
TV	2.453806078632	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.224610298398 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min8			
C	1.203727853780	-0.345696092056	-0.780221070858
C	-0.071953203113	-0.847034279313	-4.045795206581
C	-0.069573081668	-0.023357982039	1.305245752279
C	-1.342763491090	0.296792613670	3.371604839205
C	1.202150231203	-0.536419786395	-2.026342805517
C	1.202255005807	-0.751516455853	-3.425327696568
C	1.204559359446	-0.130126365601	0.615790845717
C	-0.068648572902	0.201557268316	2.756191217284
TV	2.548614710538	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.220903138490 hartree		
Spin(**2)	= 2.812500000000		
Geometry of 1D-min9			
C	2.014502455142	0.363690234162	-1.514861844970
C	0.665715178294	0.363871730923	-1.514700015642
C	-3.256737166416	-0.369352860366	1.515965440908
C	0.708586503188	-0.369184059289	1.516155191167
C	4.631029053233	0.363703831968	-1.514901722644
C	3.282248845614	0.363877940430	-1.514710662768
C	-0.640216837357	-0.369350107830	1.515966460277
C	3.325109793041	-0.369188788458	1.516156305673
TV	5.233074008551	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.206679465961 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min10			
C	2.967806621789	0.791159912630	-3.697308382301
C	-0.992541980087	0.442568192320	-1.654646109434
C	0.326736007353	0.094617346445	0.416809522257
C	-0.349198937001	-0.453269388562	2.974171352829
C	1.647739324574	0.690055333806	-3.106860061539
C	0.327509090690	0.326883527149	-0.969979122698
C	2.963419930278	-0.112923991372	1.695216041638
C	0.995714125243	-0.195435679886	3.017698886052
TV	2.640202911540	0.000000000000	0.000000000000

TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.200839523234 hartree	
Spin(**2)	=	0.750000000000	
Geometry of 1D-min11			
C	0.182397458429	0.752145346653	-0.404459905391
C	1.395022348972	1.106929996001	-1.005208255924
C	-2.332272323406	-0.354549627089	1.470991793520
C	1.397444278823	-0.376964174445	1.509403221007
C	2.698203888872	1.083153873010	-0.965364978150
C	4.001157152786	1.105909042917	-1.003302178653
C	0.183726711557	-0.023664301549	0.910062569588
C	4.003537392387	-0.377892623106	1.510664443489
TV	5.032675336679	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.185124086058 hartree	
Spin(**2)	=	2.000000000000	
Geometry of 1D-min12			
C	0.941429922627	1.201221460350	-1.111333375043
C	-0.316824560072	-1.331928521705	0.270449237723
C	-0.317100994599	-2.792355983211	0.049778864408
C	-0.316424086386	1.429481724045	1.111241534357
C	2.199073411438	1.294550080469	-1.654335731166
C	0.940886533725	-0.651015296486	0.361399261747
C	0.940506158807	-3.415518574005	-0.035726512106
C	0.941170068593	0.871084049546	0.580939424844
TV	2.515330879387	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.184533561434 hartree	
Spin(**2)	=	2.000000000000	
Geometry of 1D-min13			
C	0.928610906378	-0.610202343133	-1.857046128303
C	0.268679196364	1.792536211045	-0.573355528482
C	-0.367626803066	0.504101245135	1.829050851818
C	0.361346802215	-1.899327797162	0.543073595098
C	2.239457257742	-0.610181164839	-1.856951531521
C	1.579521398260	1.792680126202	-0.573334698795
C	0.943221120101	0.504073785378	1.829068600520
C	1.672192896881	-1.899268231905	0.542983134406
TV	2.621687565394	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	=	-45.181246482862 hartree	
Spin(**2)	=	0.000000000000	
Geometry of 1D-min14			
C	1.038443369110	1.858203220305	-0.248359213547
C	1.041159459873	-0.358039377626	-1.866186096205
C	1.038718183898	-1.974272283441	0.349391208100
C	-0.264474023761	0.241086565106	1.966950212530
C	1.047217043800	0.242076150412	1.966536164249
C	2.352848257228	-0.356809659784	-1.866104365233
C	2.350396890311	-1.974126493815	0.350276696261
C	-0.273228700271	1.857904505113	-0.249642055089
TV	2.623367432226	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000

TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.180840072268 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min15			
C	0.871132850028	1.653253161140	2.905759443448
C	0.871057921488	-0.678838000255	-1.633354267087
C	0.871187628068	-0.508250490509	-0.225405971967
C	-2.822535241048	-0.250774779508	1.921390583560
C	4.564680934213	-0.955135457858	-3.762642837956
C	2.102274160372	-0.779431638565	-2.366944337545
C	2.102450000271	-0.406527576919	0.512001721667
C	-0.360098938344	0.992431542024	2.631929094826
TV	2.462516195205	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.173015997672 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min16			
C	0.391396751783	-0.214581510452	-1.489682295363
C	-0.356513235432	-0.777450005448	1.168203642083
C	-0.262249152198	-2.927783543508	-1.603880188199
C	-0.373602946776	1.962600044578	1.314899176590
C	1.703522204430	-0.214628528059	-1.489905676281
C	0.955594442179	-0.777458055246	1.168055740899
C	1.049886001916	-2.927662573792	-1.603895580642
C	0.938572829256	1.962552986791	1.314822129884
TV	2.624266931608	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.172666034015 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min17			
C	1.253667705717	2.592780571816	-0.910794309517
C	0.378559320455	-0.987411249491	-0.990879170575
C	0.259153146251	-2.824702892814	1.043132384175
C	-0.301893531170	0.739888161178	1.100126515841
C	2.565931855924	2.592730897726	-0.910817241139
C	1.690812201295	-0.987899494275	-0.990669152367
C	1.571463473946	-2.824567745756	1.043067165845
C	1.010371873058	0.739884354024	1.100378251873
TV	2.624546641243	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.172645674899 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min18			
C	0.734744221165	0.901239477887	-0.859519313526
C	0.703990355184	-1.223075875505	-2.596678894881
C	0.561538794237	-1.157758303158	0.938836988024
C	-0.715158488103	1.002956563775	2.626461107067
C	2.047337152537	0.901011975264	-0.858494661314
C	2.016673525978	-1.223312750231	-2.596626214512
C	1.874197177652	-1.158406613386	0.937066183927
C	0.597536309321	1.001725308497	2.626003308482
TV	2.625254368597	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.172538624165 hartree
 Spin(**2) = 0.000000000000
 Geometry of 1D-min19

C	1.073290245835	1.192692380957	-0.400801948956
C	0.291250802696	-1.225422989291	-2.611194552707
C	0.787910302774	-1.325566777374	0.658263264203
C	-1.029998092714	0.854835955770	2.318668299683
C	2.388090169613	1.216137789811	-0.391521838289
C	1.683132742029	-1.224946067187	-2.611503078683
C	2.100877770475	-1.334597540849	0.680612664232
C	0.274757716950	0.857956391167	2.318333839462
TV	2.627457383660	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.172134492029 hartree
 Spin(**2) = 0.000000000000
 Geometry of 1D-min20

C	1.152811984108	-0.599319454522	-2.701777277562
C	-0.017913920082	1.310598285706	-0.054200454593
C	1.224080613841	0.469441489335	2.576074357885
C	-0.709001204335	-1.361691645102	0.540936684356
C	2.388476845363	-0.598841758771	-2.701456278595
C	1.292921336004	1.317959107753	-0.045960628796
C	2.527755951497	0.465416355258	2.577150608977
C	0.605180075954	-1.353902634072	0.525564047566
TV	2.627879843477	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.172112148450 hartree
 Spin(**2) = 0.000000000000
 Geometry of 1D-min21

C	1.682822518705	2.673246889256	0.366184580120
C	0.372927938480	-0.278077700711	-1.421657002044
C	1.679372838298	-2.556755696425	0.061158451636
C	-0.938280191380	-0.158324018222	1.357713319588
C	0.369087072979	0.053572294850	1.348948858171
C	1.680327676784	-0.284671472838	-1.418752583689
C	2.986760351967	-2.649742343739	-0.042853246947
C	0.375591012533	2.527210289497	0.429405696628
TV	2.614783956253	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.171536397047 hartree
 Spin(**2) = 0.312500000000
 Geometry of 1D-min22

C	2.797631542086	0.939777649894	-2.833493241772
C	0.206828897941	-1.070923955049	-0.942653961454
C	0.183222759450	1.032944516031	0.852213808295
C	0.227938089203	-1.002405590825	2.722298182379
C	1.539779496106	0.939496938667	-2.833181103257
C	1.493778876175	-1.070563287694	-0.943070984196
C	1.527490858751	1.032953739078	0.851951277556
C	1.485606933601	-1.002340070106	2.722190525764
TV	2.631040962338	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

 Energy = -45.171229466830 hartree

```

Spin(**2) = 0.000000000000
Geometry of 1D-min23
C      0.705759238083      -0.877156734125      -3.726513230358
C      0.384125587184      2.306174674685      1.033027946507
C     -1.771304004581      0.043929161696     -0.497259002910
C     -1.461577180313     -0.132416502479      2.242539339072
C      4.565972087603     -0.877096085505     -3.726647889425
C      1.696490848351      2.305196458223      1.033431182541
C     -0.455915680792      0.046640733433     -0.495595920726
C     -0.149392969312     -0.134266131139      2.242736946077
TV      2.628084478367      0.000000000000      0.000000000000
TV      0.000000000000     20.000000000000      0.000000000000
TV      0.000000000000      0.000000000000     20.000000000000
Energy   = -45.170358103996 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min24
C      2.403754295022      0.531318105509     -2.924862671548
C     -1.482493356310      1.632217727083      0.657507452478
C     -0.178124998489     -0.967394433609     -0.362987577591
C     -1.477084939989     -1.594307415755      2.544451642917
C      3.795746166092      0.531445038515     -2.924717924670
C     -0.226869887292      1.632259085241      0.657411775095
C      1.101467986970     -0.967234794289     -0.363066068115
C     -0.232942124242     -1.594391239369      2.544468330891
TV      2.636395974925      0.000000000000      0.000000000000
TV      0.000000000000     20.000000000000      0.000000000000
TV      0.000000000000      0.000000000000     20.000000000000
Energy   = -45.166048328941 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min25
C      1.120529897718     -0.518268532226     -1.287547559313
C     -0.121210133347     -0.434915244977     -0.682813804028
C     -2.664557005542     -0.219031032028      0.884812800871
C      1.120150498955     -0.134357686786      1.501126235760
C      3.631634580077     -0.514349941565     -1.262764955642
C      2.362184493873     -0.435098474376     -0.682840884514
C     -0.117406142011     -0.219464588773      0.884988612044
C      3.631207953289     -0.143497302387      1.433958709950
TV      5.022258996992      0.000000000000      0.000000000000
TV      0.000000000000     20.000000000000      0.000000000000
TV      0.000000000000      0.000000000000     20.000000000000
Energy   = -45.152935661480 hartree
Spin(**2) = 2.000000000000
Geometry of 1D-min26
C      0.580354657881      1.287385246463     -0.289418661559
C      0.854801970859     -1.111954517134     -1.349882601899
C      1.172339833209     -1.718068135386     -0.048261791246
C      0.160773567115     -0.188292945400      1.356310953418
C      1.852567473877      0.965586355609     -0.960963075583
C      2.051115447027     -0.392262180327     -1.537650667513
C      1.369255253875     -0.897807073310      1.101268136943
C      0.378171741287      1.244257487658      1.203687938550
TV      2.467553018319      0.000000000000      0.000000000000
TV      0.000000000000     20.000000000000      0.000000000000
TV      0.000000000000      0.000000000000     20.000000000000
Energy   = -45.137873994488 hartree
Spin(**2) = 0.000000000000

```

Geometry of 1D-min27

C	1.024547441574	1.257344882011	-2.095586653232
C	-0.762857371643	-0.549576044265	-2.083090736203
C	1.101540960136	0.082628509425	0.408897535366
C	-0.196517779607	-0.239194450431	2.538927416702
C	1.240387149888	0.310334224975	-1.022881098679
C	0.543962555535	-0.107676229070	-2.488509828847
C	2.410097691582	-0.013120951977	1.080971972219
C	1.110809460090	-0.331447783120	3.134693626499
TV	2.613659675798	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.137533144660 hartree

Spin(**2) = 1.312500000000

Geometry of 1D-min28

C	0.666624422606	1.488740836960	-2.013513957345
C	-1.655336958994	-1.459652373999	0.490462783821
C	-0.938235940528	-2.634641958535	0.125892150248
C	0.434050260208	1.046742573378	1.243982315112
C	1.950230312556	1.488515544478	-2.011355890451
C	3.948378648032	-0.137836513093	0.904502446232
C	0.428165503486	-2.634017531634	0.124238306045
C	1.863878390009	1.041609841549	1.254682706563
TV	2.800280285988	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.133607987859 hartree

Spin(**2) = 0.312500000000

Geometry of 1D-min29

C	2.695715958980	-0.611300837541	-2.641530535274
C	0.104263254903	0.151199641963	0.090179728178
C	1.003977766966	-1.332197138912	0.547812756629
C	-2.276346765199	-0.258546204981	2.865808781439
C	1.403981898686	-0.512444594210	-2.052593837183
C	0.444110031910	-0.404346142701	1.414193647117
C	1.382072178487	-0.246062569387	-0.567690138110
C	-0.979436827661	-0.197508139645	3.458483918680
TV	2.592852185276	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.117984350454 hartree

Spin(**2) = 2.812500000000

Geometry of 1D-min30

C	0.048938920536	-0.258119427390	-1.554227988412
C	0.048940791191	1.066395080820	-1.154242140988
C	0.049068562445	0.264906867786	1.502796988519
C	0.049082897737	-1.059516668570	1.102561435882
C	1.489729433947	-0.509470819779	-1.021776080962
C	1.489710816810	0.981546457600	-0.571482252824
C	1.489841967826	0.516360733802	0.970334496258
C	1.489838594783	-0.974666606843	0.519856475758
TV	2.881537246498	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.112260204796 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min31

C	0.604007075609	0.000292197549	0.259123700270
C	-1.159842251268	0.528986610894	-1.557871364979
C	1.054615654074	-0.390838110118	1.604182461856
C	-0.703773896970	0.143033916630	-0.230458742847
C	2.984188816361	-0.063935724662	0.480199843153
C	2.492580479331	0.563834564464	-1.678135913518
C	2.368031515884	-0.425065481069	1.724711105235
C	1.863232057151	0.203170681317	-0.439214682405
TV	4.959934960967	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.083608643834 hartree			
Spin(**2) = 0.312499250000			
Geometry of 1D-min32			
C	-0.135124607231	-0.080338482951	0.323207141737
C	-0.811765223234	0.232889271671	-0.968060673807
C	3.607140541236	-0.352596635323	1.445456661486
C	-2.182980473091	0.232924429945	-0.968073503810
C	2.894943075418	-0.080442756975	0.323312950164
C	2.069651877019	0.189855721311	-0.798028073640
C	4.907526348266	-0.352655977635	1.445648904436
C	0.690157186321	0.189831202626	-0.798121708489
TV	5.754449870098	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.077255938017 hartree			
Spin(**2) = 0.000000000000			
Geometry of 1D-min33			
C	0.497499652126	-0.184147007945	-2.166702375324
C	0.497450030733	1.008248551227	-1.231296377716
C	-0.533504568127	0.962172838710	2.407459844449
C	-0.433987254797	-1.651031130878	1.045268396920
C	1.878593257067	-0.193153691871	-2.157624672704
C	1.878678257541	1.000641150766	-1.221471745822
C	0.943938977356	0.962196449428	2.407498739046
C	0.850772073557	-1.651268372448	1.045283702174
TV	2.761891836041	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.073377416088 hartree			
Spin(**2) = 0.000000000000			
Geometry of 1D-min34			
C	1.104887492701	-0.413528119593	-3.297444289058
C	0.064699370805	0.696807926248	0.005846350164
C	0.180364030767	0.351144271297	3.478613392411
C	0.064712649276	-0.809173540449	0.174940997927
C	2.598508523357	-0.413546205434	-3.297392821449
C	1.447694372422	0.697460956679	0.001874103959
C	1.674013298676	0.351146866569	3.478694143143
C	1.447720585379	-0.810652409710	0.171199182151
TV	2.765897067529	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.070419574563 hartree			
Spin(**2) = 0.000000000000			
Geometry of 1D-min35			
C	0.413691926892	-1.468410597573	-2.426184329733

C	0.295938105411	2.160434200743	-0.724297492080
C	-0.395529585890	0.059283502779	2.139743251135
C	-0.395693461995	-0.890212566739	0.959871973756
C	1.907700376053	-1.468352243273	-2.426270746640
C	1.789615279335	2.160425286031	-0.724311879758
C	0.987180742466	0.072740168470	2.127794433283
C	0.987076715341	-0.878749105713	0.943682284833
TV	2.765863608602	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.070316419256 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min36			
C	0.185678609261	0.821520094097	-4.054247027619
C	0.064250896298	-0.128762220200	-0.845739391604
C	0.064447618160	-0.501448853940	0.626508784061
C	-0.738038640294	-1.277882724655	3.855333177618
C	1.679648941816	0.821525329871	-4.054226921570
C	1.447596141864	-0.126898180911	-0.852472471363
C	1.447597956326	-0.499152500039	0.617604278219
C	0.755903678437	-1.277933086929	3.855455393868
TV	2.765865470295	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.069336315221 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min37			
C	-0.981375191357	-0.100884076537	-1.006759595567
C	0.203907372411	-0.239304105843	-0.423319682827
C	-3.752151783490	-0.733829873600	1.716507207684
C	1.319569207998	-0.386567930937	0.210288949269
C	5.277234750712	0.115984594045	-1.930882731420
C	4.815368205471	-0.182402723959	-0.642387416224
C	2.505645722911	-0.519964751020	0.793271826777
C	4.025541634575	-0.432320433359	0.429134405981
TV	7.315584944861	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.068908222536 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min38			
C	1.201026917415	-0.409164865346	-3.283387435444
C	-0.062323890481	0.695991880457	-0.006130423568
C	0.401313064811	0.346705867757	3.472317479444
C	-0.062391231012	-0.810427237899	0.158867786144
C	2.580339657023	-0.409156380460	-3.283284815957
C	1.317182717230	0.698660989024	0.010236076554
C	1.889600159267	0.346714926001	3.472280529827
C	1.317132620004	-0.809665433936	0.175431862249
TV	2.758650470461	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.063199511587 hartree		
Spin(**2)	= 0.750000000000		
Geometry of 1D-min39			
C	1.437719931215	0.366180433782	-2.400163245443
C	-1.677479266679	1.287953945757	1.859344651152

C	-0.275793526200	-0.667015729693	-1.095491069209
C	-0.598756047496	-1.413221960474	2.085196824341
C	0.134222952860	-0.411837675518	-2.537210778911
C	-0.373151163353	1.255714520149	1.916643498126
C	1.027436439499	0.108171333076	-0.956793838847
C	0.704162569789	-1.455887230463	2.077043080242
TV	2.606962120495	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.062256928595 hartree		
Spin(**2)	= 0.312500000000		
Geometry of 1D-min40			
C	0.544681175496	1.885932709240	1.480530813575
C	0.722432042000	-0.732453948619	-1.597825707395
C	0.707137025683	-0.646191039945	-0.078039803805
C	-0.543292251270	-0.170075618277	1.879268345788
C	0.746733312430	0.484604363753	2.129603364257
C	2.029968142546	-0.760709822490	-2.174966019716
C	1.999242047354	-0.979679353055	0.633550039604
C	0.232307681831	0.653097472573	0.661203295662
TV	2.621737226984	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.061135817466 hartree		
Spin(**2)	= 2.000000000000		
Geometry of 1D-min41			
C	0.438551457086	-0.265839977312	-2.179363319890
C	0.438524860304	1.036221653870	-1.394471045463
C	-0.430182328500	0.265381198478	2.180116896483
C	-0.430184352268	-1.035779564667	1.393743218405
C	1.887946678787	-0.265834499879	-2.179368710010
C	1.887917668897	1.036244695574	-1.394511916189
C	1.019215447070	0.265382507116	2.180115711386
C	1.019212208496	-1.035776013170	1.393739165259
TV	2.898789726788	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.048768499464 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min42			
C	1.024752983902	-0.075459496274	-2.733769117617
C	1.024717050710	0.491587637373	-1.322403480692
C	-1.009130726637	0.306488084612	2.065543607653
C	-1.009147869477	-1.194172934840	1.822818704397
C	2.474176637159	-0.075476770843	-2.733785535961
C	2.474144007656	0.491538593573	-1.322360873932
C	0.440300919689	0.306508804869	2.065616907665
C	0.440283686527	-1.194155626504	1.822881049602
TV	2.898855787103	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy	= -45.048338385567 hartree		
Spin(**2)	= 0.000000000000		
Geometry of 1D-min43			
C	2.119255712971	1.493139488708	-2.152811072129
C	0.327097180029	-1.188924520775	0.773707801756
C	-2.430990786612	-3.506864800780	-0.210439447774

C	-1.804198274833	1.447353239639	0.954048644364
C	3.371705077569	1.493971991672	-2.150678382368
C	2.878251135780	0.119778086432	0.919441893467
C	-1.023312173093	-3.612758257374	-0.256147102832
C	2.198115816766	1.409276620132	1.084947165410
TV	2.683783061699	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.045217818108 hartree			
Spin(**2) = 0.000000000000			
Geometry of 1D-min44			
C	1.141409085045	-0.089291191744	-0.026055189104
C	0.024575792770	0.339261707575	-0.836855946565
C	0.024661525591	-0.161882597264	0.888553512671
C	-1.092057439292	-0.089352755819	-0.025939977475
C	4.757595539625	-0.089096953740	-0.026058102978
C	3.641155499372	0.340423956702	-0.837034239000
C	3.641291003722	-0.160927791436	0.889253201559
C	2.524945417835	-0.089134374268	-0.025863259113
TV	7.233195624983	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.043942470135 hartree			
Spin(**2) = 1.312500000000			
Geometry of 1D-min45			
C	1.717985303690	-0.058311615794	-2.697227352965
C	-0.534092192949	1.586063614256	1.910680662052
C	0.777021641421	-0.356863883439	-1.014670974953
C	-1.878360099768	-1.179473991679	1.583309810229
C	1.146284035159	-1.249955191107	-2.171481797121
C	0.862315889098	1.586599215514	1.911164429138
C	2.084821679555	0.166716743885	-1.254392614481
C	-0.494393419563	-1.191703247467	1.642764114458
TV	2.662215926306	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.031346755185 hartree			
Spin(**2) = 0.000000000000			
Geometry of 1D-min46			
C	0.050028847026	-0.172127380411	-0.697254342777
C	1.581190332177	1.135318617100	-1.440217068840
C	0.050065242435	0.069616876851	0.906294342510
C	0.050004763585	-1.237697073091	1.649251788574
C	1.581153984726	-0.172076009828	-0.697146109863
C	3.112327743638	1.135350393497	-1.440142851749
C	1.581181768988	0.069561319363	0.906216127143
C	1.581144970757	-1.237698703480	1.649353464324
TV	3.062232743499	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -45.020105766712 hartree			
Spin(**2) = 0.000000000000			
Geometry of 1D-min47			
C	0.575290462216	1.842237266073	0.627802388458
C	1.342275705841	1.216747988658	1.677577817118
C	-2.243749095189	-0.487030207735	0.175335166181
C	1.636143624624	0.218354212225	0.596418030365

C	3.099748658669	-1.912748667655	-0.187619710147
C	3.866427234996	-1.288031117710	-1.238029890633
C	0.280536806182	0.416503064293	0.263832892073
C	4.160501468892	-0.288817806317	-0.157549207127
TV	5.048730560828	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -44.983490924777 hartree			
Spin(**2) = 0.000000000000			
Geometry of 1D-min48			
C	-0.026941410595	-0.013917459464	-0.607089237520
C	1.258730098631	0.665918990341	-0.175020107225
C	-2.170017139804	-0.794563997768	0.622220065217
C	1.687170189738	-0.114895941606	1.054337809994
C	2.544548365520	-0.013847034279	-0.607053952345
C	3.830235682204	0.665869384442	-0.174973451484
C	0.401449120933	-0.794650647095	0.622180467798
C	4.258713039021	-0.114886376228	1.054369798562
TV	5.143007614367	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000
Energy = -44.945851879637 hartree			
Spin(**2) = 0.000000000000			

S5. Primitive lattice of 3D-min10, 3D-min12, and 3D-min13

(i) 3D-min10

C	1.250950276601	3.270843977735	2.832280962946
C	1.250825723173	2.511724973444	5.310415652655
C	0.001354814204	4.045870867698	3.102057891869
C	1.250862398251	1.949943009581	3.907906053659
C	0.001333550039	2.424151712098	0.794161598300
C	0.001210527711	2.796934896068	5.945908429379
C	1.250933928561	2.709298298849	1.429740061031
C	0.001267865449	1.174900546518	3.638046518164
TV	2.499224040018	0.000000000000	0.000000000000
TV	0.000030949010	4.115314703300	0.000000000000
TV	-0.000048640214	0.958254132540	6.492354517796

(ii) 3D-min12

C	3.606079713321	0.878697180841	6.094636497566
C	3.606438206722	-0.236048286936	7.248407229588
C	2.345589090485	1.738863241087	6.094755242897
C	2.345346252297	2.853988862186	4.941029283803
C	2.345644352010	2.850649777299	2.009481654887
C	3.605657320068	2.853854030597	4.133030638564
C	3.605914978791	2.851792517737	2.757958312723
C	2.345730174310	2.848828648194	0.634322546979
TV	2.520604640221	0.000000000000	0.000000000000
TV	1.259643447297	3.089747409611	0.000000000000
TV	1.260069396348	0.005258234985	7.422033107613

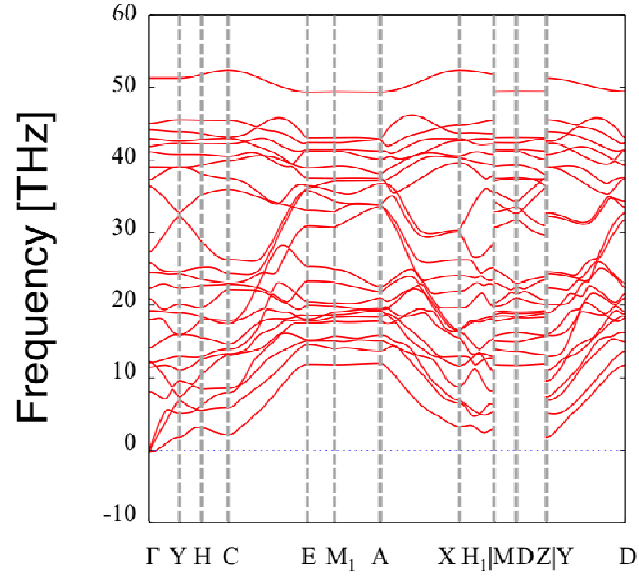
(iii) 3D-min13

C	2.216469437277	2.445974962274	4.952644826501
C	3.470135930818	2.348804909729	5.631818701658
C	2.216912616819	2.621215209839	3.451454307489
C	2.217644108191	1.283280268100	2.586440092207
C	3.470552096590	3.321207530547	2.896200777500
C	2.216999906055	3.603728289169	0.814237851500
C	3.471272259753	1.410665257136	1.679153656691

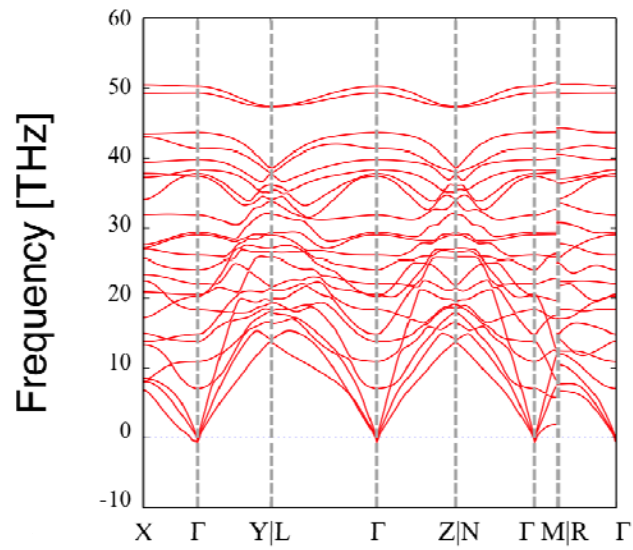
C	3.470818671036	2.903607568159	1.369307102559
TV	2.507324625909	0.000000000000	0.000000000000
TV	1.253188423812	3.530916143473	0.000000000000
TV	2.506440011809	2.100736841762	6.318499246203

S6. Phonon dispersion curve of 3D-min10, 3D-min12, and 3D-min13

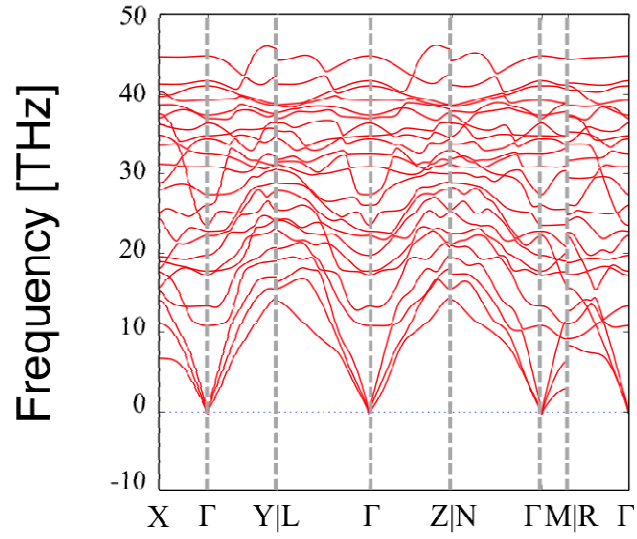
(i) 3D-min10



(ii) 3D-min12



(iii) 3D-min13



S7. Symmetry k-points of 3D-min10, 3D-min12, and 3D-min13

(i) Symmetry k-points of 3D-min10 ($P2/m$). The coordinates of symmetry k-points are given in fractions of the primitive reciprocal lattice vectors b_1 , b_2 , b_3 .

$\times b_1$	$\times b_2$	$\times b_3$	
0.00000000	0.00000000	0.00000000	Γ
0.00000000	0.00000000	0.50000000	Y
0.00000000	0.23113863	0.55672762	H
0.00000000	0.50000000	0.50000000	C
0.50000000	0.50000000	0.50000000	E
0.50000000	0.23113863	0.55672762	M_1
0.50000000	0.50000000	0.00000000	A
0.00000000	0.50000000	0.00000000	X
0.00000000	0.76886137	0.44327238	H_1
0.50000000	0.23113863	0.55672762	M
0.50000000	0.00000000	0.50000000	D
0.50000000	0.00000000	0.00000000	Z
0.00000000	0.00000000	0.50000000	Y
0.50000000	0.00000000	0.50000000	D

(ii) Symmetry k-points of 3D-min12 and 3D-min13 (*P1*). The coordinates of symmetry k-points are given in fractions of the primitive reciprocal lattice vectors b_1 , b_2 , b_3 .

$\times b_1$	$\times b_2$	$\times b_3$	
0.00000000	-0.50000000	0.00000000	X
0.00000000	0.00000000	0.00000000	Γ
0.50000000	0.00000000	0.00000000	Y
0.50000000	-0.50000000	0.00000000	L
0.00000000	0.00000000	0.00000000	Γ
-0.50000000	0.00000000	0.50000000	Z
-0.50000000	-0.50000000	0.50000000	N
0.00000000	0.00000000	0.00000000	Γ
0.00000000	0.00000000	0.50000000	M
0.00000000	-0.50000000	0.50000000	R
0.00000000	0.00000000	0.00000000	Γ