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Supporting Information: Combustion Reactions Between Transition-Metal Chlorides and Sodium Amide and Their Ignition Temperature

Shinji Noguchi,[a] Jin Odahara,[a] Hayato Sakai,[b] Nataly Carolina Rosero-Navarro [b], Akira Miura*[b] and Kiyoharu Tadanaga[b]

[a] Graduate School of Chemical Science and Engineering, Hokkaido University, Kita-13, Nishi-8, Kita-ku,Sapporo, Hokkaido 060-8628.

[b] Faculty of Engineering, Hokkaido University, Kita-13, Nishi-8, Kita-ku, Sapporo, Hokkaido 060-8628.

Corresponding Author: amiura@eng.hokudai.ac.jp

Table S1. Synthesized nitrides and their lattice constants.

Products	Lattice constant *a* / Å	*b* / Å	*c* / Å
WN (our work)	4.1589(15)	=*a*	=*a*
WN (ICSD#30381)	4.13(1)	=*a*	=*a*
Mo_2N (from $MoCl_5$)	4.180(2)	=*a*	=*a*
Mo_2N (ICSD#251625)	4.1922(2)	=*a*	=*a*
NbN (from $NbCl_5$)	4.361(8)	=*a*	=*a*
NbN (ICSD#982)	4.394(3)	=*a*	=*a*
Ta_3N_5 (our work)	3.894(9)	10.21(4)	10.24(6)
Ta_3N_5 (ICSD#16253)	3.893	10.264	10.264
WN (from WCl_4)	4.147(4)	=*a*	=*a*
WN (ICSD#30381)	4.13(1)	=*a*	=*a*
Mo_2N (from $MoCl_3$)	4.182(6)	=*a*	=*a*
Mo_2N (ICSD#251625)	4.1922(2)	=*a*	=*a*
VN (our work)	4.130(3)	=*a*	=*a*
VN (ICSD#644864)	4.13470(2)	=*a*	=*a*
CrN (our work)	4.119(14)	=*a*	=*a*
CrN (ICSD#37412)	4.144(1)	=*a*	=*a*
Fe_3N (our work)	4.76(2)	=*a*	4.43(2)
Fe_3N (ICSD#255834)	4.7383(5)	=*a*	4.3867(5)
MnN_x (our work)	4.218(4)	=*a*	4.142(4)
MnN_x (ICSD#290804)	4.2193(1)	=*a*	4.1287(1)
Cu_3N (our work)	3.8009(6)	=*a*	=*a*
Cu_3N (ICSD#40057)	3.819(1)	=*a*	=*a*
W (from WCl_6)	3.16689(5)	=*a*	=*a*
W (from WCl_4)	3.1656(4)	=*a*	=*a*
W (ICSD#43421)	3.16475(20)	=*a*	=*a*
Cu (from $CuCl_2$)	3.6152(8)	=*a*	=*a*
Cu (ICSD#43493)	3.61505(10)	=*a*	=*a*
Cr (from $CrCl_3$)	2.898(5)	=*a*	=*a*
Cr (ICSD#44731)	2.88494(7)	=*a*	=*a*

Table S2. Oxygen and nitrogen content in the products dried overnight at 393 K. N_{theo} is the theoretical nitrogen ratio of the composition in the products column.

Products	N_{exp} / wt%	O_{exp} / wt%	N_{theo} / wt%
WN (from WCl_6)	5.4	9	7.8
Mo_2N (from $MoCl_5$)	5.2	22	6.8
NbN (from $NbCl_5$)	3.6	22	13.1
Ta_3N_5 (from $TaCl_5$)	1.0	17	11.4
WN (from WCl_4)	4.5	9	7.8
Mo_2N (from$MoCl_3$)	4.3	22	6.8
VN (from VCl_3)	8.7	19	21.6
CrN (from $CrCl_3$)	3.8	22	21.2
Fe_3N (from $FeCl_2$)	1.2	28	7.7
Mn_3N_2 (from $MnCl_2$)	10.3	18	14.5
Cu_3N (from $CuCl_2$)	0.4	14	6.8

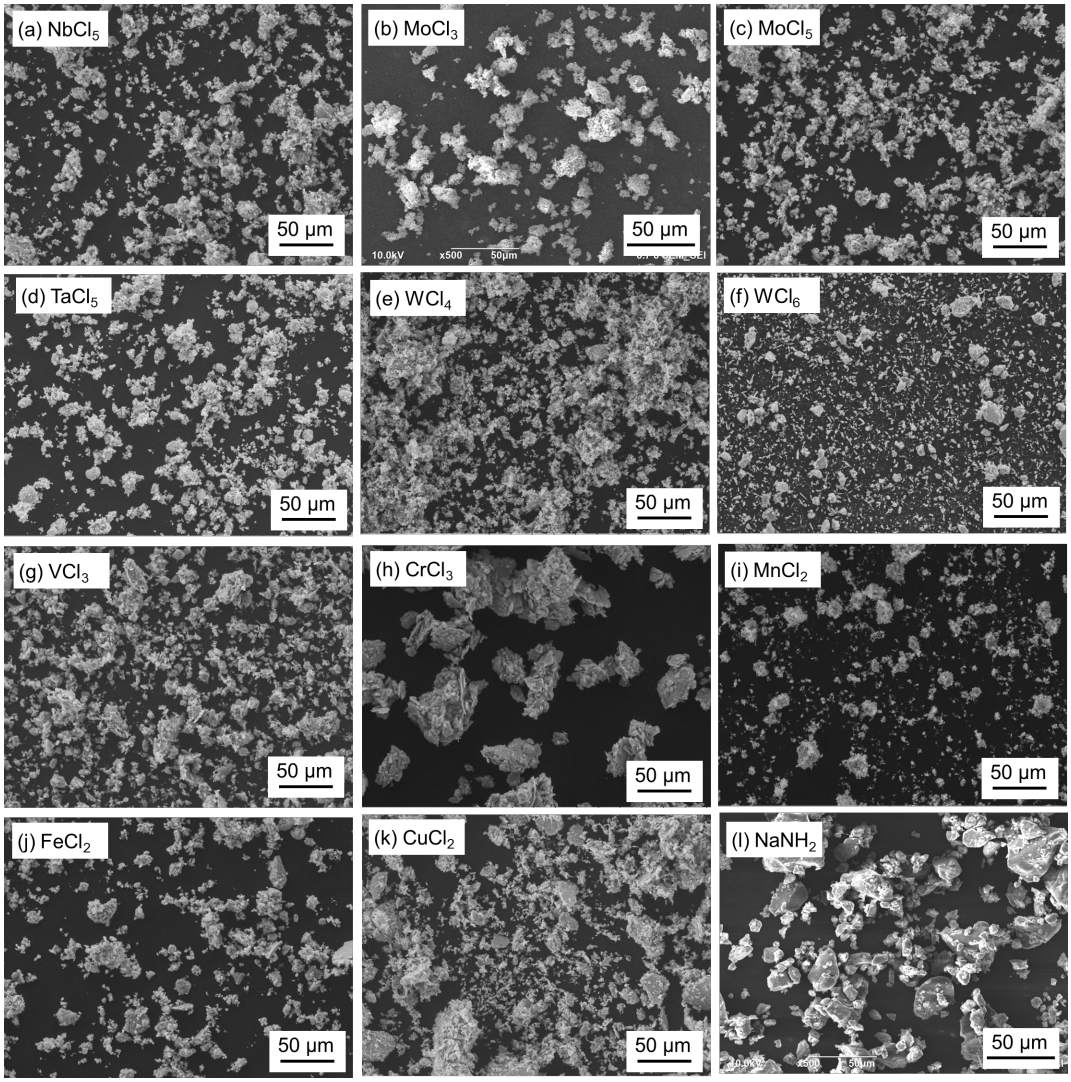


Figure S1. SEM images of some of the metal chlorides and sodium amide: (a) $NbCl_5$, (b) $MoCl_3$, (c) $MoCl_5$, (d) $TaCl_5$, (e) WCl_4, (f) WCl_6, (g) VCl_3, (h) $CrCl_3$, (i) $MnCl_2$, (j) $FeCl_2$, (k) $CuCl_2$ (l) $NaNH_2$.

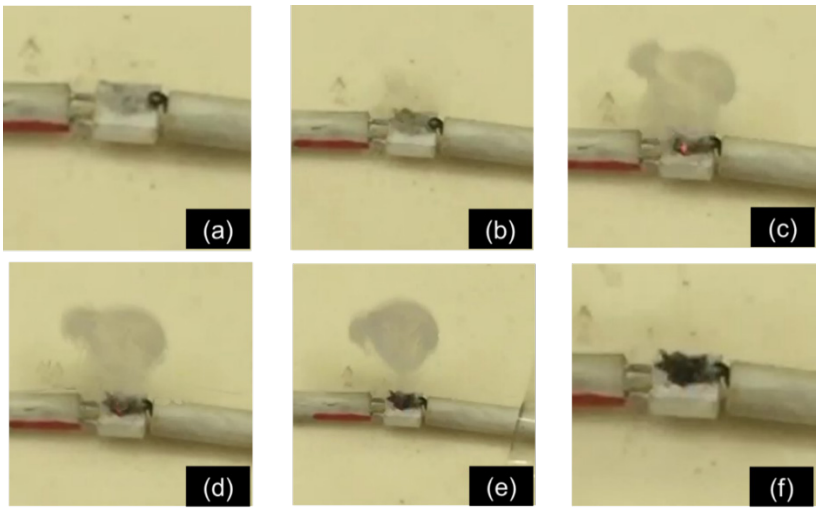


Figure S2. Photos of measuring ignition temperatures above room temperature using a microheater.

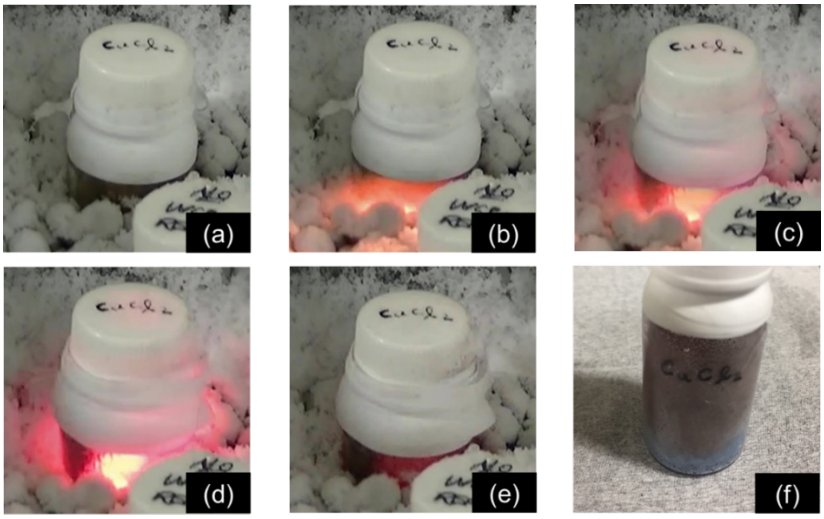


Figure S3. Photos of measuring ignition temperature below room temperature.

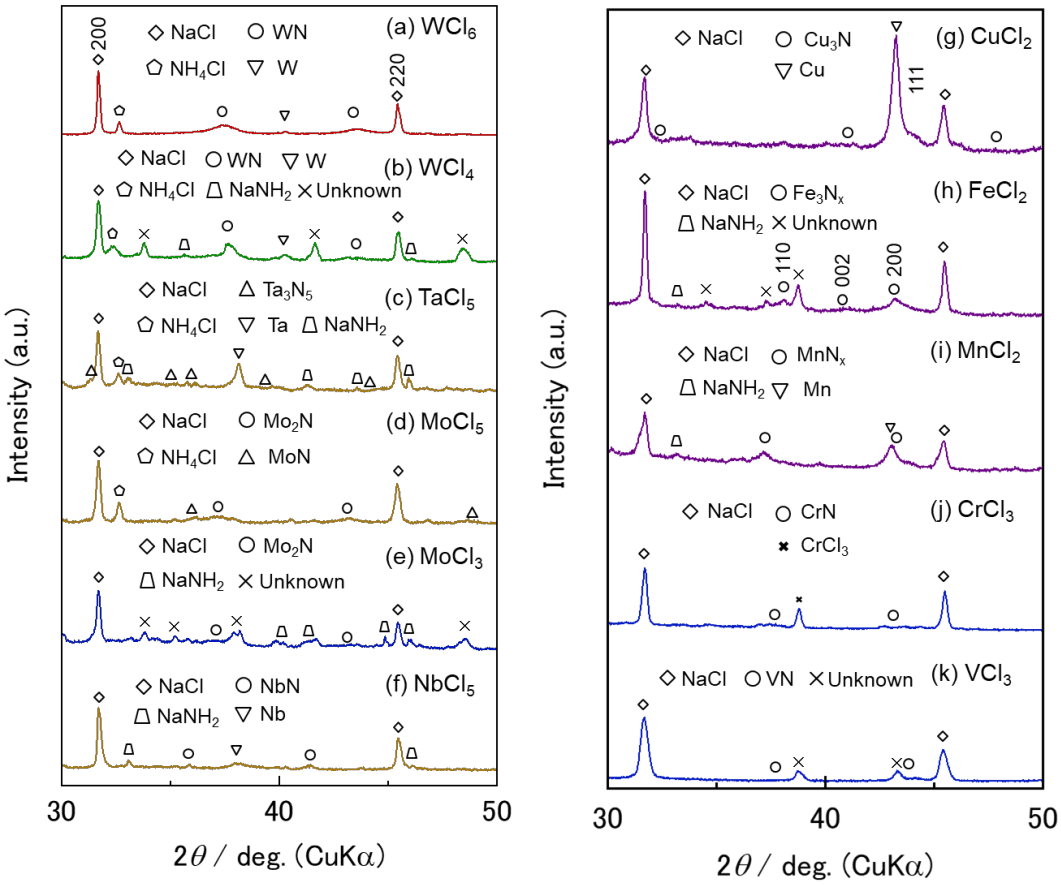


Figure S4. (a) XRD patterns of products using $NaNH_2$ and (a) WCl_6, (b) WCl_4, (c) $TaCl_5$, (d) $MoCl_5$, (e) $MoCl_3$, (f) $NbCl_5$, (g) $CuCl_2$, (h) $FeCl_2$, (i) $MnCl_2$, (j) $CrCl_3$, (k) VCl_3, and $NaNH_2$ before washing without expose to air.

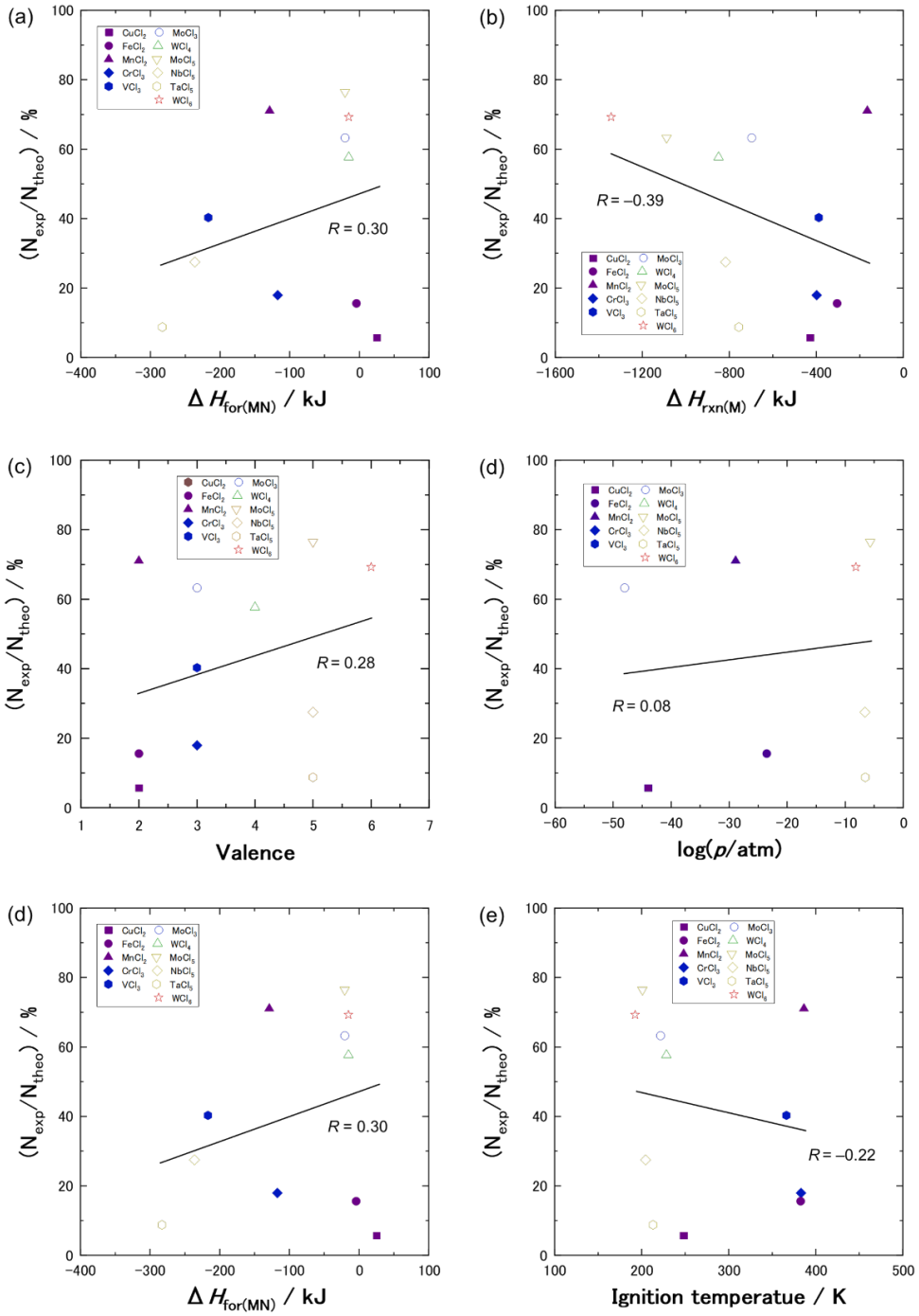


Figure S5. The relationship between the nitrogen content of the product and various parameters (a)the reaction enthalpy to form metal nitride, (b)the reaction enthalpy to form metal, (c)the valence of the metal chloride, (d)the vapor pressure of the metal chloride, (e)the formation enthalpy of metal nitride, and (f)the ignition temperature.