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Supporting Information

## Predicting dopant activity of chemical compounds against ammonia borane with key descriptors: electronegativity and crystal structure

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## I. EXPERIMENTAL METHOD

Detailed descriptions of materials used in experiments are as follows: Ammonia borane (Sigma Aldrich, 97 %), CuCl<sub>2</sub> (Sigma Aldrich, 99.995 %), Nb (Kojundo Chemical Lab., 99.99 %), NbF5 (Sigma Aldrich, 98 %), NbO (Kojundo Chemical Lab., 99.99 %), Nb2O5 (Kojundo Chemical Lab., 99.99 %), TiH2 (Sigma Aldrich, 98 %. All of the samples are handled in a glovebox filled with purified Ar atmosphere in order to prevent oxidation. Each of the above materials is mixed with ammonia borane using a planetary ball-mill apparatus (Fritsch Pulverisette 7) with 20 stainless steel balls (7 mm in diameter) and 300 mg samples (ball : powder ratio = 70 : 1, by mass). The milling process is performed under 0.1MPa Ar atmosphere. The total milling process time and additive amount is collected in Table 1. Please note that some mixtures are prepared by hand-mixing in a glovebox where the milling time of 5 min indicates the hand mixing. Hydrogen desorption temperature of ammonia borane is analyzed by thermal mass spectrometry measurements (TDMS, ULVAC, BGM-102) combined with thermogravimetry and differential thermal analysis (TG-DTA, Bruker, 2000SA).

## II. EXPERIMENTAL DATA SET

The experimental data is collected in Table 1. Sample numbers 18, 33,48,49,50,51,52,53, and 54 are experimentally performed where other samples are acquired from previous work as well as other researchers work.

## III. EXPERIMENTAL RESULT



FIG. 1: The difference in electronegativity of chemical compounds and corresponding desorption temperature of ammonia borane in experiment. Data is classified by the phases of dopants. Dash line indicates the  $H_2$  desorption temperature of ammonia borane without dopants

The difference in electronegativity of chemical compounds, which are classified by the phase of the dopant, and the corresponding desorption temperature of ammonia borane is shown in Figure 1. Please note that dispersion of metal chlorides is due to various experimental conditions of metal chlorides data sampled as seen in Table 1. However, the fundamental correlation of electronegativity and desorption temperature are the same in principle.

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Nn.   additive protect   Space (mont)   and (mont)   meture (mont)   formation point   formation (more protect)   formation protection   formation   for			<b>A</b> .	Tab	le 1		1	1			1		1	1	1		
No.   additive   Stractur re   Time re   Time re   Time re   Time re   Time re   Callence re   Time re   Time reTime re   Time			Crystal					Formati				Electron	Electron		Desorptio	heating	
e   r	No.	additive	Structur	milling Time	amount (mol%)	melting point	Formation enthalpy	on	χ p of cation	χpof anion	χp difference	affinity of	affinity of	cation valence	n temperatu	rate (°C	Note
IKCI   cubic   660   10   770   436   83   0.62   3.6   2.1   11.1   5   88.5     3/KCI2   memocli   60   10   874   421   175   0.65   3.61   2.111   16   3   Ref.5     4/LCI   cubic   60   10   672   779   108   1   3.16   2.18   0.62   3.61   2   116   3   Ref.5     5/CACI2   phombod   60   10   772   7795   108   1   3.16   2.16   0.02   3.61   2   114   3   Ref.5     5/CACI2   phombod   60   10   422   -315   140   1.54   3.16   1.26   0.08   3.61   3   106   3   3.61   3   101   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61   3.61			e			ľ		entropy	1			cation	anion		re	min-1)	
2 Nact   ubic   60   10   801   -411   72   0.035   3.16   2.21   0.05   3.61   1   111   3   Ref.5     3 SrC12   monceli   60   10   605   -408   59   0.95   3.16   2.21   0.05   3.61   2   116   3   Ref.5     5 G(C12   orthorh   60   10   774   -404   90   1.31   3.16   1.82   0.62   3.61   2   116   3   Ref.5     9 MAC13   moncoli   60   10   425   -3.15   140   1.84   3.16   1.62   0.08   3.61   3   101   3.61   1.17   S   Ref.5     9 MAC12   moncoli   60   10   322   561   13   1.15   0.63   3.61   3   101   3.8   3.61   1.31   0.61   3.61   3   101   3.8   1.61   1.26   1.24   3.61   3.61 <td></td> <td>1 KCI</td> <td>cubic</td> <td>60</td> <td>10</td> <td>770</td> <td>-436</td> <td>83</td> <td>0.82</td> <td>316</td> <td>2 34</td> <td>0.5</td> <td>3.61</td> <td>1</td> <td>114</td> <td>3</td> <td>Ref 5</td>		1 KCI	cubic	60	10	770	-436	83	0.82	316	2 34	0.5	3.61	1	114	3	Ref 5
3   Sinciz   monochi   660   10   874   -829   115   0.058   3.16   2.218   0.052   3.61   2   116   3   Ref.5     GLACLZ   whomho   60   10   772   -795   108   1   3.16   2.18   0.02   3.61   2   116   3   Ref.5     SMCI2   whombo   60   10   774   -795   108   1.185   0.02   3.61   3   106   3   Ref.5     BMCI2   whombo   60   10   425   -315   140   1.54   3.16   1.61   0.08   3.61   3   111   3.61   3   111   3   Ref.5   112   111   1.65   3.16   1.53   0.53   3.61   3   111   3   Ref.5   112   1.56   3.16   1.55   0.67   3.61   2   108   1.61   1.53   0.61   2   108   1.61   1.56   <		2NaCl	cubic	60	10	801	-411	72	0.93	3.16	2.23	0.55	3.61	i	115	3	Ref.5
4   LiCi   cubic   660   10   605   3-408   59   0.88   3.16   2.16   0.02   3.61   1   11   116   3   Ref.5     6   MgC12   rhombol   60   10   774   -641   90   1.31   3.16   1.82   0.83   3.61   2   114   3   Ref.5     7TiCl3   rhombol   60   10   654   -4481   118   1.55   0.43   3.61   3   101   3   Ref.5     10VC13   monech   60   10   300   -581   131   1.66   3.16   1.51   0.67   3.61   2   103   Ref.5     112CrCl2   orthorh   60   10   773   -313   103   1.88   3.16   1.28   3.61   2   108   Ref.5     135crCl2   rhombol   60   10   7735   -331   103   1.61   1.28   3.61   2   108		3 SrCl2	monocli	60	10	874	-829	115	0.95	3.16	5 2.21	0.05	3.61	2	116	3	Ref.5
SCaCL2   orthorhe   60   10   772   -776   108   1   3.16   2.11   3.61   2   1116   3   Ref.5     7/TICL3   thombol   60   10   425   -315   140   1.54   3.61   1.60   3.61   3   106   3   Ref.5     9/AIC3   monocli   60   10   192   -704   111   1.63   3.16   1.53   3.61   3   111   3   Ref.5     10/VC13   hexagon   60   10   275   4.415   110   1.65   3.16   1.51   0.73   3.61   2   104   3   Ref.5     12/C/C12   orthorh   60   10   725   -313   109   1.68   3.16   1.25   3.61   2   108   3.61   2   108   3.61   1.26   1.24   3.61   2   108   3.61   1.25   3.61   1.21   3.61   1.23   3.61   1.23		4 LiCl	cubic	60	10	605	-408	59	0.98	3.16	2.18	0.62	3.61	1	116	3	Ref.5
6MgCl2   hombol   60   10   774   -641   90   1.31   3.16   1.82   0.0   3.61   2   114   3   Ref.5     8/MCl2   hombol   60   10   654   -481   118   1.55   3.61   0.0   3.61   2   1177   3   Ref.5     9/AICl3   monocli   60   10   300   -581   131   1.63   3.16   1.51   0.63   3.61   3   101   3   Ref.5     112/Crcl2   orthorh   60   10   273   -313   103   1.88   3.16   1.28   3.61   2   103   3   Ref.5     13/Fccl2   rhombol   60   10   735   -313   103   1.88   3.16   1.28   3.61   2   108   3.61   2   108   3.61   1.24   3.61   2   108   3.61   1.24   3.61   2   108   3.61   1.24   3.61		5 CaCl2	orthorho	60	10	772	-795	108	1	3.16	2.16	0.02	3.61	2	116	3	Ref.5
ThCl3   hombol   60   10   425   -315   140   1.54   3.16   1.61   0   3.61   2   106   3   Ref.5     9AlCl3   monocli   60   10   192   -704   111   1.61   3.16   1.53   0.63   3.61   3   101   3   Ref.5     10VCl3   hexagon   60   10   227   -415   110   1.66   3.16   1.53   0.63   3.61   2   103   3   Ref.5     12CrCl2   orthork   60   10   677   -342   118   1.83   3.16   1.33   0.15   3.61   2   108   3   Ref.5     16CuCl2   monocit   5   1498   -220   108   1.9   3.16   1.26   1.24   3.61   2   13   Ref.5     16CuCl2   monocit   5   498   -220   108   1.9   3.16   1.26   1.24   3.61   2 <td></td> <td>6 MgCl2</td> <td>rhombo</td> <td>60</td> <td>10</td> <td>714</td> <td>-641</td> <td>90</td> <td>1.31</td> <td>3.16</td> <td>1.85</td> <td>0</td> <td>3.61</td> <td>2</td> <td>114</td> <td>3</td> <td>Ref.5</td>		6 MgCl2	rhombo	60	10	714	-641	90	1.31	3.16	1.85	0	3.61	2	114	3	Ref.5
BMnCl2   monocli   60   10   654   4481   118   1.55   3.16   1.61   0   3.61   2   117   3   Ref.5     10/VCl3   monocli   60   10   300   -581   131   1.63   3.16   1.53   0.53   3.61   2   103   3   Ref.5     12/CrC12   orthork   60   10   820   -395   115   1.66   3.16   1.5   0.67   3.61   2   104   3   Ref.5     13/Foci2   thombol   60   10   773   -313   109   1.88   3.16   1.26   0.24   3.61   2   108   3   Ref.5     14/CoC12   monocli   5   1   498   -220   108   1.9   3.16   1.26   1.24   3.61   2   103   3   Ref.5     17/CuC12   monocli   5   1   498   -220   108   1.9   3.16   1.22 <td></td> <td>7 TiCl3</td> <td>rhombo</td> <td>60</td> <td>10</td> <td>425</td> <td>-315</td> <td>140</td> <td>1.54</td> <td>3.16</td> <td>1.62</td> <td>0.08</td> <td>3.61</td> <td>3</td> <td>106</td> <td>3</td> <td>Ref.5</td>		7 TiCl3	rhombo	60	10	425	-315	140	1.54	3.16	1.62	0.08	3.61	3	106	3	Ref.5
9AICI3   menocili   60   10   132   -7.04   111   1.61   3.16   1.55   0.43   3.61   3   101   3   Ref.5     112LnC12   orthorh   60   10   2275   -415   110   1.66   3.16   1.51   0   3.61   2   103   3   Ref.5     13Fc12   orthorh   60   10   627   -342   118   1.33   1.61   1.26   0.67   3.61   2   108   3   Ref.5     14Cc212   monocit   5   1498   -220   108   1.9   3.16   1.26   1.24   3.61   2   108   3   Ref.5     13Cc212   monocit   5   1498   -220   108   1.9   3.16   1.26   1.24   3.61   2   3   Ref.5     13Cc122   monocit   5   2498   -220   108   1.9   3.16   1.26   1.24   3.61   2		8 MnCl2	rhombo	60	10	654	-481	118	1.55	3.16	5 1.61	C	3.61	2	117	3	Ref.5
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		9 AICI3	monocli	60	10	192	-704	111	1.61	3.16	5 1.55	0.43	3.61	3	101	3	Ref.5
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12CrC12 prithering 60 10 677 -345 118 1.6 1.5 0.67 3.61 2 78 Ref.5   14CoC12 membol 60 10 735 -313 109 1.88 3.16 1.23 0.06 3.61 2 78 Ref.5   15CuC12 menociti 5 5 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 108 Ref.5   17CuC12 menociti 5 20 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 75 Ref.5   19CuC12 menociti 60 10 498 -220 108 1.9 3.16 1.22 1.3 3.61 1 109 3.8 75 Ref.5   20NIC12 memociti 60 10 1547 -127 96 139 3.16 1.23 1.3 3.61 1 109 3 Ref.5   22AgeC1 cubic 60 10 1547		11 ZnCl2	orthorho	60	10	275	-415	110	1.65	3.16	5 1.51	C	3.61	2	103	3	Ref.5
13]#cU2 rhombol 60 10 677 -342 118 1.43 3.16 1.13 0.15 3.61 2 78 3 Ref.5   15CuC12 monoclit 5 1 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 108 3 Ref.5   17CuC12 monoclit 5 10 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 75 3 Ref.5   18CuC12 monoclit 5 20 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 75 3 Ref.5   20NiC12 monoclit 60 10 498 -220 108 1.9 3.16 1.23 1.3 3.61 1 109 3 Ref.5   21AgC1 cubic 60 2 1547 -127 96 1.33 3.16 1.23 1.3 3.61 1 105 3 Ref.5   22AgC1 cubic <td></td> <td>12 CrCl2</td> <td>orthorho</td> <td>60</td> <td>10</td> <td>820</td> <td>-395</td> <td>115</td> <td>1.66</td> <td>3.16</td> <td>1.5</td> <td>0.67</td> <td>3.61</td> <td>2</td> <td>104</td> <td>3</td> <td>Ref.5</td>		12 CrCl2	orthorho	60	10	820	-395	115	1.66	3.16	1.5	0.67	3.61	2	104	3	Ref.5
1 ACoCl2 rhombol 60 10 735 -313 109 1.88 3.16 1.28 0.66 3.61 2 81 3 Ref.5   1 GCuCl2 monoclii 5 5 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 103 3 Ref.5   1 GCuCl2 monoclii 5 20 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 63 3   1 GCuCl2 monoclii 60 10 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 763 8 7.7   2 NGCL2 momooli 60 10 1049 -227 96 1.39 3.16 1.23 1.3 3.61 1 106 3 8 7.5 23 8 7.67 -342 118 1.83 3.16 1.23 1.3 3.61 1 7.9 8 1.86 1.33 3.61 2 86 1 8 1.6<		13 FeCl2	rhombo	60	10	677	-342	118	1.83	3.16	1.33	0.15	3.61	2	78	3	Ref.5
IbCuCL2   monoclii   5   1   498   -220   108   1.9   3.16   1.26   1.24   3.61   2   108   3   Ref.5     11CuCl2   monoclii   5   10   498   -220   108   1.9   3.16   1.26   1.24   3.61   2   75   3   Ref.5     13CuCl2   monoclii   60   10   498   -220   108   1.9   3.16   1.26   1.24   3.61   2   75   3   Ref.5     20NIC12   monoclii   60   10   1547   -127   96   1.93   3.16   1.23   1.3   3.61   1   109   3   Ref.5     23AgC1   cubic   60   20   1547   -127   96   1.93   3.16   1.23   1.3   3.61   1   73   3   Ref.5     23AgC1   cubic   60   20   1547   -127   96   1.93   3.16   1.23		14/CoCl2	rhombo	60	10	735	-313	109	1.88	3.16	1.28	0.66	3.61	2	81	3	Ref.5
Incluct2   monoclii   5   9   498   -220   108   1.9   3.16   1.26   1.24   3.61   2   103   3   Ref.5     118   CuC12   monoclii   5   20   498   -220   108   1.9   3.16   1.26   1.24   3.61   2   69   3     19   CuC12   monoclii   60   10   498   -220   108   1.9   3.16   1.25   1.16   3.61   1   109   3   Ref.5     22/AgC1   cubic   60   10   1547   -127   96   1.33   3.16   1.23   1.3   3.61   1   105   3   Ref.5     22/AgC1   cubic   60   20   1547   -127   96   1.33   3.16   1.23   1.3   3.61   1   73   3   Ref.5     22/AgC1   cubic   60   20   1547   -127   96   1.33   3.16 <t< td=""><td></td><td>15CuCl2</td><td>monocli</td><td>5</td><td></td><td>498</td><td>-220</td><td>108</td><td>1.9</td><td>3.16</td><td>1.26</td><td>1.24</td><td>3.61</td><td></td><td>108</td><td>3</td><td>Ref.5</td></t<>		15CuCl2	monocli	5		498	-220	108	1.9	3.16	1.26	1.24	3.61		108	3	Ref.5
11 12 13 10 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 75 3 Ref.5   19 CuCl2 monocli 60 10 498 -220 108 1.9 3.16 1.26 1.24 3.61 2 75 3 Ref.5   20 Nici2 rhombol 60 10 1001 -316 107 1.91 3.16 1.23 1.3 3.61 1 109 3 Ref.5   22 AgC1 cubic 60 10 1547 -127 96 1.33 3.16 1.23 1.3 3.61 1 105 3 Ref.5   23 AgC1 cubic 60 100 1547 -127 96 1.33 3.16 1.23 1.3 3.61 1 173 3 Ref.5   24 PeC12 rhombol 5 5.6 1001 -91 1.91 3.16 1.23 1.36 3.61 2 93 1 Ref.1 <			monocii	1 5	5	498	-220	108	1.9	3.16	1.26	1.24	3.61		103	3	Ref.5
Instructize   International   5   2.20   498   -2.20   108   1.9   3.16   1.24   3.61   2   99   3     19   Cucize   rhombol   60   10   1001   -316   1.24   3.61   2   81   3   Ref.5     21AgC1   cubic   60   2   1547   -127   96   1.93   3.16   1.23   1.3   3.61   1   105   3   Ref.5     23AgC1   cubic   60   20   1547   -127   96   1.93   3.16   1.23   1.33   3.61   1   105   3   Ref.1     23AgC1   cubic   5.6   1001   -316   107   1.91   3.16   1.25   1.16   3.61   2   98   1   Ref.1     25NiC12   primbol   5   2.6   1735   -313   109   1.88   3.16   1.28   0.66   3.61   2   93   5   Ref.3 <td></td> <td>17/CuCl2</td> <td>monocli</td> <td></td> <td></td> <td>498</td> <td>-220</td> <td>108</td> <td>1.9</td> <td>3.16</td> <td>1.26</td> <td>1.24</td> <td>3.61</td> <td></td> <td>/5</td> <td>3</td> <td>Ref.5</td>		17/CuCl2	monocli			498	-220	108	1.9	3.16	1.26	1.24	3.61		/5	3	Ref.5
19-UCL2   Intoncin   00   10   438   -220   108   1.9   3.16   1.26   1.24   3.01   2   75   3   Ref.5     221AgC1   cubic   60   10   1001   -316   1.23   3.361   1   109   3   Ref.5     22AgC1   cubic   60   10   1547   -127   96   1.93   3.16   1.23   1.3   3.61   1   173   3   Ref.5     24FeC12   rhombol   5   5.7   677   -342   118   1.83   3.16   1.23   1.31   3.61   2   80   1   Ref.1     25[NIC12   rhombol   5   5.6   1001   -316   107   1.91   3.16   1.25   1.16   3.61   2   80   1   Ref.1     26[C12   rhombol   5   2.6   735   -313   109   1.88   3.16   1.33   0.15   3.61   3   100		18/CuCl2	monocii		20	498	-220	108	1.9	3.10	1.20	1.24	3.01		69	3	Defe
220/RCL2 rh0/RD0 60 10 100 -500 100 1.20 1.20 1.20 1.20 3.61 1 109 3 Ref.5   22AgC1 cubic 60 10 1547 -127 96 1.93 3.16 1.23 1.3 3.61 1 105 3 Ref.5   23AgC1 cubic 60 20 1547 -127 96 1.93 3.16 1.23 1.33 3.61 1 105 3 Ref.5   24FeC12 rhombol 5 5.6 1001 -316 107 1.91 3.16 1.23 1.16 3.61 2 80 1 Ref.1   25NiC12 rhombol 5 5.4 275 -415 110 1.65 3.16 1.23 3.61 2 93 1 Ref.1   26/C12 orthomc 5 2.6 735 -313 109 1.88 3.16 1.23 0.66 3.61 2 92 1 Ref.2   20AC13 momoclii		1900012	monocii	60	10	498	-220	108	1.9	3.10	1.20	1.24	3.01		/5	3	Ref.5
22 PQC1 Cubic 60 12 1547 -127 96 1.93 3.16 1.23 1.3 3.61 1 105 3 Ref.5   23AgC1 cubic 60 20 1547 -127 96 1.93 3.16 1.23 1.3 3.61 1 73 Ref.5   24FeC12 rhombol 5 5.6 1001 -316 107 1.91 3.16 1.25 1.16 3.61 2 86 1 Ref.1   26DC12 orthorhc 5 2.8 581 -123 120 2.28 3.16 0.88 2.13 3.61 2 94 1 Ref.1   29FeC13 rhombol 5 2.1 306 -339 142 1.88 3.16 1.33 0.15 3.61 3 100 1 Ref.2   31MgC12 rhombol 5 2.1 306 -33 1.61 1.35 0.43 3.61 3 100 1 Ref.3   33Nb cubic 60 10 166 <td></td> <td>20 101012</td> <td>cubic</td> <td>60</td> <td></td> <td>1547</td> <td>-310</td> <td></td> <td>1.91</td> <td>2 16</td> <td>1.20</td> <td>1.10</td> <td>2.01</td> <td>1</td> <td>100</td> <td>2</td> <td>Rel.5</td>		20 101012	cubic	60		1547	-310		1.91	2 16	1.20	1.10	2.01	1	100	2	Rel.5
22/26/Cl Cubic 60 10 1547 -127 90 1.93 3.16 1.25 1.3 3.61 1 73 3 Ref.5   224FeC12 rhombot 5 5.7 677 -342 118 1.83 3.16 1.33 3.61 2 80 1 Ref.1   25NiC12 rhombot 5 5.4 275 -415 110 1.66 3.16 1.51 0 3.61 2 93 1 Ref.1   26ZnC12 orthorhc 5 2.8 581 -123 120 2.28 3.16 0.58 2.13 3.61 2 94 1 Ref.2   29FeC13 rhombot 5 2.1 306 -399 142 1.88 3.16 1.28 0.66 3.61 2 92 1 Ref.3   30AIC13 monoclit 5 2.5 192 -704 111 1.61 3.56 0 3.61 3 100 1 Ref.3   31MgC12 rhombot 120 33		221AgCI	cubic	60	10	1547	-127	06	1.55	216	1.23	1.3	2.01		105	2	Ref.5
22/PEC12 rhombol 5 5.7 677 -342 118 1.83 3.16 1.33 0.15 3.61 2 86 1 Ref.1   225/NC12 rhombol 5 5.6 1001 -316 107 1.91 3.16 1.25 1.16 3.61 2 86 1 Ref.1   26ZnC12 orthorhc 5 2.8 581 -123 120 2.28 3.16 0.88 2.13 3.61 2 94 1 Ref.1   28CoCl2 rhombol 5 2.6 735 -373 109 1.88 3.16 1.33 0.15 3.61 3 100 1 Ref.2   29FeCl3 rhombol 5 2.5 192 -704 111 1.61 3.16 1.85 0.3.61 2 93 5 Ref.3   31MgCl2 rhombol 120 33 772 -795 108 1 3.16 1.85 0.3.61 2 111 5 Ref.3   34Th hexagon 60		23 AgCI	cubic	60	20	1547	-127	90	1.55	3.10	1.23	1.3	3.01		73	3	Ref 5
25/NC12 rhombol 5 5.6 1001 -316 105 5.16 1.35 5.16 1.36 1.25 5.16 2.61 1 Ref.1   25/NC12 orthomb 5 5.6 1001 -316 107 1.91 1.65 3.16 1.25 1.16 3.61 2 93 1 Ref.1   27/PC12 orthomb 5 2.6 735 -313 109 1.88 3.16 1.28 0.66 3.61 2 92 1 Ref.2   29/FeC13 rhombol 5 2.5 192 -704 111 1.61 3.16 1.33 0.15 3.61 3 100 1 Ref.2   31MgC12 rhombol 120 33 774 -641 90 1.31 3.16 1.25 0.43 3.61 2 93 5 Ref.3   32CaCl2 rhombol 120 33 772 -795 108 1 3.16 2.16 0.02 3.61 2 1115 3 Ref.3 33		24 FoC12	rhombo		57	677	-342	118	1.33	3.16	1.23	0.15	3.01		80	1	Ref 1
26/R012 orthorh 5 5.4 275 -415 110 1.65 3.16 1.51 0 3.61 2 93 1 Ref.1   27PrC12 orthorh 5 2.8 581 -123 120 2.28 3.16 0.88 2.13 3.61 2 94 1 Ref.1   28CoCl2 rhombol 5 2.6 735 -313 109 1.88 3.16 1.23 0.15 3.61 2 92 1 Ref.2   29FeCI3 rhombol 5 2.5 192 -704 111 1.61 3.16 1.55 0.43 3.61 2 93 5 Ref.3   31MgC12 rhombol 120 33 772 -795 108 1 3.16 2.16 0.02 3.61 2 93 5 Ref.3   33Nb cubic 60 10 1668 0 31 1.54 - - 0.02 3.61 2 93 1 Ref.3   34Ti hexagon <td< td=""><td></td><td>25 NiCl2</td><td>rhombo</td><td></td><td>5 56</td><td>1001</td><td>-342</td><td>107</td><td>1.03</td><td>3.10</td><td>1.33</td><td>1 16</td><td>3.01</td><td></td><td>86</td><td>  1</td><td>Ref 1</td></td<>		25 NiCl2	rhombo		5 56	1001	-342	107	1.03	3.10	1.33	1 16	3.01		86	1	Ref 1
27 PRC12 orthoring 5 2.8 5.81 -1.23 1.103 1.103 0.816 2.13 3.61 2 94 1 Ref.1   28 CoCl2 rhombol 5 2.6 735 -313 100 1.88 3.16 1.28 0.66 3.61 2 92 1 Ref.2   29 FeCl3 rhombol 5 2.5 192 -704 111 1.61 3.16 1.33 0.15 3.61 3 100 1 Ref.2   31 MgCl2 rhombol 120 33 772 -795 108 1 3.16 1.85 0 3.61 2 93 5 Ref.3   32 CaCl2 orthoring 60 10 1668 0 31 1.54 - - 0.02 3.61 2 111 5 Ref.3   33 Nb cubic 60 10 1907 0 24 1.66 - - 0.67 - 0 116 3 Ref.5   36 Cr cubic 60		267nCl2	orthorho	5	5 54	275	-415	110	1.51	3.10	1.23	1.10	3.01		93	1	Ref 1
28 CoC12 rhombol 5 2.6 735 -313 109 1.88 3.16 1.23 0.15 3.61 2 92 1 Ref.2   29 FeCI3 rhombol 5 2.1 306 -399 142 1.83 3.16 1.33 0.15 3.61 3 100 1 Ref.2   30 AlC13 monocli 5 2.5 192 -704 111 1.61 3.16 1.85 0 3.61 2 93 5 Ref.3   32 CaC12 orthorhd 120 33 772 -795 108 1 3.16 1.85 0 3.61 2 2 111 5 Ref.3   33 Nb cubic 60 10 1668 0 31 1.54 - - 0.02 3.61 2 1115 3 Ref.5   34 Ti hexagon 60 10 1910 0 29 1.63 - - 0.53 - 0 116 <t< td=""><td></td><td>27 PtCI2</td><td>orthorho</td><td>5</td><td>28</td><td>581</td><td>-123</td><td>120</td><td>2.28</td><td>3.16</td><td>0.88</td><td>213</td><td>3.61</td><td>2</td><td>94</td><td>1</td><td>Ref 1</td></t<>		27 PtCI2	orthorho	5	28	581	-123	120	2.28	3.16	0.88	213	3.61	2	94	1	Ref 1
229 FeC13 ihombol 5 2.1 306 3.39 142 1.83 3.16 1.33 0.15 3.61 3 100 1 Ref.2   30 AlC13 monocli 5 2.5 192 -704 111 1.61 3.16 1.55 0.43 3.61 3 100 1 Ref.2   31 MgCl2 inhomol 120 33 772 -795 108 1 3.16 2.16 0.02 3.61 2 111 5 Ref.3   33 Nb cubic 60 2 2477 0 36 1.6 - - 0.92 - 0 120 3   33 Nb cubic 60 10 1910 0 29 1.63 - - 0.08 - 0 116 3 Ref.5   36 Cr cubic 60 10 1246 0 32 1.55 - - 0 - 115 3 Ref.5   39 Co hexagon 60 10 1455 0		28 CoCl2	rhombo	5	2.0	735	-313	109	1.88	3.16	1 28	0.66	3.61	2	92	1	Ref 2
30 AICI3 monocli 5 192 -704 111 1.61 3.16 1.55 0.43 3.61 3 100 1 Ref.2   31 MgCl2 rhombol 120 33 714 -641 90 1.31 3.16 1.85 0 3.61 2 93 5 Ref.3   32 CaCl2 orthorhc 120 33 772 -795 108 1 3.16 2.16 0.02 3.61 2 111 5 Ref.3   33 Nb cubic 60 2 2477 0 36 1.6 - - 0.92 - 0 115 3 Ref.5   35V cubic 60 10 1907 0 24 1.66 - - 0.53 - 0 115 3 Ref.5   36 Cr cubic 60 10 1246 0 32 1.55 - 0 - 116 3 Ref.5   39 Co hexagon 60 10 1495 0 30		29 FeCI3	rhombo	5	21	306	-390	142	1.83	3 16	1 33	0.15	3.61	3	100	l i	Ref 2
31 MgCl2 rhombol 120 33 714 -641 90 1.31 3.16 1.85 0 3.61 2 93 5 Ref.3   32 CaCl2 orthorhc 120 33 772 -795 108 1 3.16 2.16 0.02 3.61 2 111 5 Ref.3   33 Nb cubic 60 2 2477 0 36 1.6 - 0.92 - 0 120 3   34 Ti hexagon 60 10 1668 0 31 1.54 - - 0.08 - 0 116 3 Ref.5   35V cubic 60 10 1907 0 24 1.66 - - 0.67 - 0 116 3 Ref.5   36 Cr cubic 60 10 1538 0 27 1.83 - - 0.15 - 0 116 3 Ref.5   39 Co hexagon 60 10 1495 0 30		30 AICI3	monocli	5	2.5	192	-704	111	1.61	3.16	1.55	0.43	3.61	3	100	l i	Ref.2
32 CaCl2 orthorfic 120 33 772 -795 108 1 3.16 2.16 0.02 3.61 2 111 5 Ref.3   33 Nb cubic 60 2 2477 0 36 1.6 - - 0.02 - 0 120 3   34 Ti hexagon 60 10 1668 0 31 1.54 - - 0.08 - 0 115 3 Ref.5   35 V cubic 60 10 1910 0 29 1.63 - - 0.53 - 0 116 3 Ref.5   36 Cr cubic 60 10 1246 0 32 1.55 - - 0 116 3 Ref.5   38 Fe cubic 60 10 1495 0 30 1.91 - - 1.16 - 0 116 3 Ref.5   40 Ni cubic 60		31 MgCl2	rhombo	120	33	714	-641	90	1.31	3.16	1.85	0	3.61	2	93	5	Ref.3
33 Nb   cubic   60   2   2477   0   36   1.6   -   0.92   -   0   120   3     34 Ti   hexagon   60   10   1668   0   31   1.54   -   -   0.08   -   0   115   3   Ref.5     35 V   cubic   60   10   1907   0   24   1.66   -   -   0.67   -   0   115   3   Ref.5     37 Mn   cubic   60   10   1246   0   32   1.55   -   0   -   0   115   3   Ref.5     38 Fe   cubic   60   10   1495   0   30   1.88   -   -   0.66   -   0   116   3   Ref.5     39 Co   hexagon   60   10   1455   0   30   1.81   -   -   0.66   -   0   116   3   Ref.4		32CaCl2	orthorho	120	33	772	-795	108	1	3.16	2.16	0.02	3.61	2	111	5	Ref.3
34 Ti   hexagon   60   10   1668   0   31   1.54   -   -   0.08   -   0   115   3   Ref.5     35V   cubic   60   10   1910   0   29   1.63   -   -   0.53   -   0   115   3   Ref.5     36 Cr   cubic   60   10   1907   0   24   1.66   -   -   0.67   -   0   116   3   Ref.5     37 Mn   cubic   60   10   1246   0   32   1.55   -   -   0.67   -   0   116   3   Ref.5     38 Fe   cubic   60   10   1495   0   30   1.88   -   -   0.66   -   0   116   3   Ref.5     40Ni   cubic   60   10   1455   0   33   1.91   -   -   1.24   -   0   116		33 Nb	cubic	60	2	2477	- c	36	1.6			0.92	-	0	120	3	
35   v   cubic   60   10   1910   0   29   1.63   -   0.53   -   0   116   3   Ref.5     36   Cr   cubic   60   10   1907   0   24   1.66   -   -   0.67   -   0   116   3   Ref.5     37   Mn   cubic   60   10   1246   0   32   1.55   -   -   0   116   3   Ref.5     38   Fe   cubic   60   10   1538   0   27   1.83   -   -   0.15   -   0   116   3   Ref.5     39   Co   hexagon   60   10   1495   0   30   1.91   -   -   1.16   -   0   116   3   Ref.5     41   Cu   cubic   60   10   425   0   30   1.91   -   -   1.24   -		34 Ti	hexagor	60	10	1668	c	31	1.54			0.08	-	0	115	3	Ref.5
36   Cr   cubic   60   10   1907   0   24   1.66   -   -   0.67   -   0   115   3   Ref.5     37/Mn   cubic   60   10   1246   0   32   1.55   -   -   0   -   0   115   3   Ref.5     38/Fe   cubic   60   10   1538   0   27   1.83   -   -   0.66   -   0   115   3   Ref.5     39/Co   hexagon   60   10   1495   0   30   1.88   -   -   0.66   -   0   116   3   Ref.5     40/Ni   cubic   60   10   1455   0   33   1.9   -   -   1.16   -   0   116   3   Ref.5     42/Zn   hexagon   60   10   420   0   42   1.65   -   -   0   -   0 <t< td=""><td></td><td>35V</td><td>cubic</td><td>60</td><td>10</td><td>1910</td><td>c</td><td>29</td><td>1.63</td><td>-</td><td></td><td>0.53</td><td>-</td><td>0</td><td>116</td><td>3</td><td>Ref.5</td></t<>		35V	cubic	60	10	1910	c	29	1.63	-		0.53	-	0	116	3	Ref.5
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		36Cr	cubic	60	10	1907	c (	24	1.66	-		0.67	· -	0	115	3	Ref.5
38   Fe   cubic   60   10   1538   0   27   1.83   -   -   0.15   -   0   115   3   Ref.5     39/Co   hexagon   60   10   1495   0   30   1.88   -   -   0.66   -   0   116   3   Ref.5     40/Ni   cubic   60   10   1455   0   30   1.91   -   -   1.66   -   0   116   3   Ref.5     41/Cu   cubic   60   10   1455   0   33   1.9   -   -   1.24   -   0   116   3   Ref.5     42/Zn   hexagon   60   10   420   0   42   1.65   -   0   -   0   114   3   Ref.4     44/LiH   cubic   30   50   800   -56   40   0.93   2.2   1.22   0.62   0.75   1   90 </td <td></td> <td>37 Mn</td> <td>cubic</td> <td>60</td> <td>10</td> <td>1246</td> <td>c</td> <td>32</td> <td>1.55</td> <td>-</td> <td></td> <td>0</td> <td>-</td> <td>0</td> <td>116</td> <td>3</td> <td>Ref.5</td>		37 Mn	cubic	60	10	1246	c	32	1.55	-		0	-	0	116	3	Ref.5
39[Co   hexagon   60   10   1495   0   30   1.88   -   -   0.66   -   0   116   3   Ref.5     40 Ni   cubic   60   10   1455   0   30   1.91   -   -   1.16   -   0   116   3   Ref.5     41 Cu   cubic   60   10   1085   0   33   1.9   -   -   1.16   -   0   116   3   Ref.5     42 Zn   hexagon   60   10   420   0   42   1.65   -   0   -   0   114   3   Ref.4     44 LiH   cubic   30   50   800   -56   40   0.93   2.2   1.27   0.55   0.75   1   90   2   Ref.4     44 LiH   cubic   30   50   816   -182   41   1   2.2   0.2   0.75   2   92   2 <t< td=""><td></td><td>38 Fe</td><td>cubic</td><td>60</td><td>10</td><td>1538</td><td>c c</td><td>27</td><td>1.83</td><td>-</td><td></td><td>0.15</td><td>-</td><td>0</td><td>115</td><td>3</td><td>Ref.5</td></t<>		38 Fe	cubic	60	10	1538	c c	27	1.83	-		0.15	-	0	115	3	Ref.5
40 Ni cubic 60 10 1455 0 30 1.91 - - 1.16 - 0 116 3 Ref.5   41 Cu cubic 60 10 1085 0 33 1.9 - - 1.24 - 0 116 3 Ref.5   42Zn hexagon 60 10 420 0 42 1.65 - - 0 114 3 Ref.5   43 NaH cubic 30 50 800 -56 40 0.93 2.2 1.27 0.55 0.75 1 90 2 Ref.4   44LiH cubic 30 50 692 -91 171 0.98 2.2 1.22 0.62 0.75 1 90 2 Ref.4   46 MgH2 tetragon 30 50 816 -182 41 1 2.2 0.62 0.75 2 92 2 Ref.4   46 MgH2 tetragon 30 50 150 -111 30 1.		39 Co	hexagor	60	10	1495	c c	30	1.88	-		0.66	; -	0	116	3	Ref.5
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		40 Ni	cubic	60	10	1455	c c	30	1.91	·		1.16	; -	0	116	3	Ref.5
42Zn   hexagon   60   10   420   0   42   1.65   -   -   0   -   0   114   3   Ref.5     43 NaH   cubic   30   50   800   -56   40   0.93   2.2   1.27   0.55   0.75   1   90   2   Ref.4     44 LiH   cubic   30   50   692   -91   171   0.98   2.2   1.22   0.62   0.75   1   90   2   Ref.4     45 CaH2   orthorhc   30   50   816   -182   41   1   2.2   1.22   0.02   0.75   2   93   2   Ref.4     46 MgH2   tetragon   30   50   285   -75   31   1.31   2.2   0.89   0   0.75   2   92   2   Ref.4     47 AlH3   rhombol   30   50   150   -111   30   1.61   2.2   0.66   0.08   0		41 Cu	cubic	60	10	1085	C	33	1.9	-		1.24		0	116	3	Ref.5
43 NaH cubic 30 50 800 -56 40 0.93 2.2 1.27 0.55 0.75 1 90 2 Ref.4   44 <lih< td=""> cubic 30 50 692 -91 171 0.98 2.2 1.22 0.62 0.75 1 90 2 Ref.4   45[CaH2 orthorhc 30 50 816 -182 41 1 2.2 1.20 0.62 0.75 2 93 2 Ref.4   46[MgH2 tetragon 30 50 285 -75 31 1.31 2.2 0.89 0 0.75 2 92 2 Ref.4   47AlH3 rhombol 30 50 150 -11 30 1.61 2.2 0.59 0.43 0.75 3 110 2 Ref.4   48<tih2< td=""> cubic 30 50 350 -120 30 1.54 2.2 0.66 0.08 0.75 2 106 2   49 NbF5 monoclii 60</tih2<></lih<>		42 Zn	hexagor	60	10	420	C C	42	1.65	-	-  -	C		0	114	3	Ref.5
44[LiH cubic 30 50 692 -91 171 0.98 2.2 1.22 0.62 0.75 1 90 2 Ref.4   45 CaH2 orthorhc 30 50 816 -182 41 1 2.2 1.2 0.02 0.75 2 93 2 Ref.4   46 MgH2 tetragon 30 50 285 -75 31 1.31 2.2 0.89 0 0.75 2 92 2 Ref.4   47 AIH3 rhombol 30 50 150 -111 30 1.61 2.2 0.59 0.43 0.75 3 110 2 Ref.4   48 TiH2 cubic 30 50 350 -120 30 1.54 2.2 0.66 0.08 0.75 2 106 2   49 NbF5 monocli 60 2 73 -1814 160 1.6 3.98 2.38 0.92 3.4 5 106 3 5 50		43 NaH	cubic	30	50	800	-56	6 40	0.93	2.2	2 1.27	0.55	0.75	1	90	2	Ref.4
45[CaH2 orthorhor 30 50 816 -182 41 1 2.2 1.2 0.02 0.75 2 93 2 Ref.4   46 MgH2 tetragon 30 50 285 -75 31 1.31 2.2 0.89 0 0.75 2 92 2 Ref.4   47 AH3 rhombol 30 50 150 -111 30 1.61 2.2 0.59 0.43 0.75 3 110 2 Ref.4   48 TiH2 cubic 30 50 150 -120 30 1.54 2.2 0.66 0.08 0.75 2 106 2   49 NbF5 monoclii 60 2 73 -1814 160 1.6 3.98 2.38 0.92 3.4 5 106 3   50 NbD cubic 60 2 1940 -406 48 1.64 3.44 1.84 0.92 1.46 5 118 3   51 Nb2O5		44 LiH	cubic	30	50	692	-91	171	0.98	2.2	2 1.22	0.62	0.75	1	90	2	Ref.4
46 MgH2   Itetragon   30   50   285   -75   31   1.31   2.2   0.89   0   0.75   2   92   2   Ref.4     47 AlH3   rhombol   30   50   150   -11   30   1.61   2.2   0.59   0.43   0.75   3   110   2   Ref.4     48 <tih2< td="">   cubic   30   50   350   -120   30   1.54   2.2   0.66   0.08   0.75   2   106   2     49<nbf5< td="">   monocli   60   2   73   -1814   160   1.6   3.98   2.38   0.92   3.4   5   106   3     50<nbo< td="">   cubic   60   2   1940   -406   48   1.6   3.44   1.84   0.92   1.46   2   118   3     51<nb2o5< td="">   monocli   60   1   1520   -1900   137   1.6   3.44   1.84   0.92   1.46   5   118</nb2o5<></nbo<></nbf5<></tih2<>		45CaH2	orthorho	30	50	816	-182	41	1	2.2	1.2	0.02	0.75	2	93	2	Ref.4
47/AIH3   rhombol   30   50   150   -11   30   1.61   2.2   0.59   0.43   0.75   3   110   2   Ref.4     48 <tih2< td="">   cubic   30   50   350   -120   30   1.54   2.2   0.66   0.08   0.75   2   106   2     49<nbf5< td="">   monoclii   60   2   73   -1814   160   1.66   3.98   2.38   0.92   3.4   5   106   3     50<nbo< td="">   cubic   60   2   1940   -406   48   1.6   3.44   1.84   0.92   1.46   2   118   3     51<nb2o5< td="">   monoclii   60   1   1520   -1900   137   1.6   3.44   1.84   0.92   1.46   5   118   3</nb2o5<></nbo<></nbf5<></tih2<>		46MgH2	tetragon	30	50	285	-75	31	1.31	2.2	0.89	0	0.75	2	92	2	Ref.4
48 1H2   (cubic   30   50   350   -120   30   1.54   2.2   0.66   0.08   0.75   2   106   2     49 NbF5   monoclii   60   2   73   -1814   160   1.6   3.98   2.38   0.92   3.4   5   106   3     50 NbO   cubic   60   2   1940   -406   48   1.6   3.44   1.84   0.92   1.46   2   118   3     51 Nb2O5   monoclii   60   1   1520   -1900   137   1.6   3.44   1.84   0.92   1.46   5   118   3		47 AIH3	rhombo	30	50	150	-11	30	1.61	2.2	0.59	0.43	0.75	3	110	2	Ref.4
49 NPF-5   Imonociii   60   2   7.3   -1.814   160   1.6   3.88   2.38   0.92   3.4   5   106   3     50 NbO   cubic   60   2   1940   -406   48   1.6   3.44   1.84   0.92   1.46   2   118   3     51 Nb2O5   monoclii   60   1   1520   -1900   137   1.6   3.44   1.84   0.92   1.46   2   118   3		48 TiH2	cubic	30	50	350	-120	30	1.54	2.2	0.66	0.08	0.75	2	106	2	
50 000   cubic   60 2  1940 -406 48 1.6 3.44 1.84 0.92 1.46 2  118 3  51 Nb2O5   monocli 60 1  1520 -1900 137 1.6 3.44 1.84 0.92 1.46 5  118 3		49NbF5	monocli	60		73	-1814	160	1.6	3.98	2.38	0.92	3.4	5	106	3	
ן 118 3 וויס וויסט 184 גער 137 1.6 גער 1900 137 1.6 1.84 גער 1.86 5 1.86 18 3		50 NBO	cubic	60	/ <sup>2</sup>	1940	-406	48	1.6	3.44	1.84	0.92	1.46	2	118	3	
		51100205	monocli	60	1 1	1520	-1900	137	1.6	3.44	1.84	0.92	1.46	9 5	118	3	Defe
		52 AB	1	60											114	3	Ket.5

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