

Supplementary Information for
Participation of Transition Metal Atoms in Noncovalent Bonds
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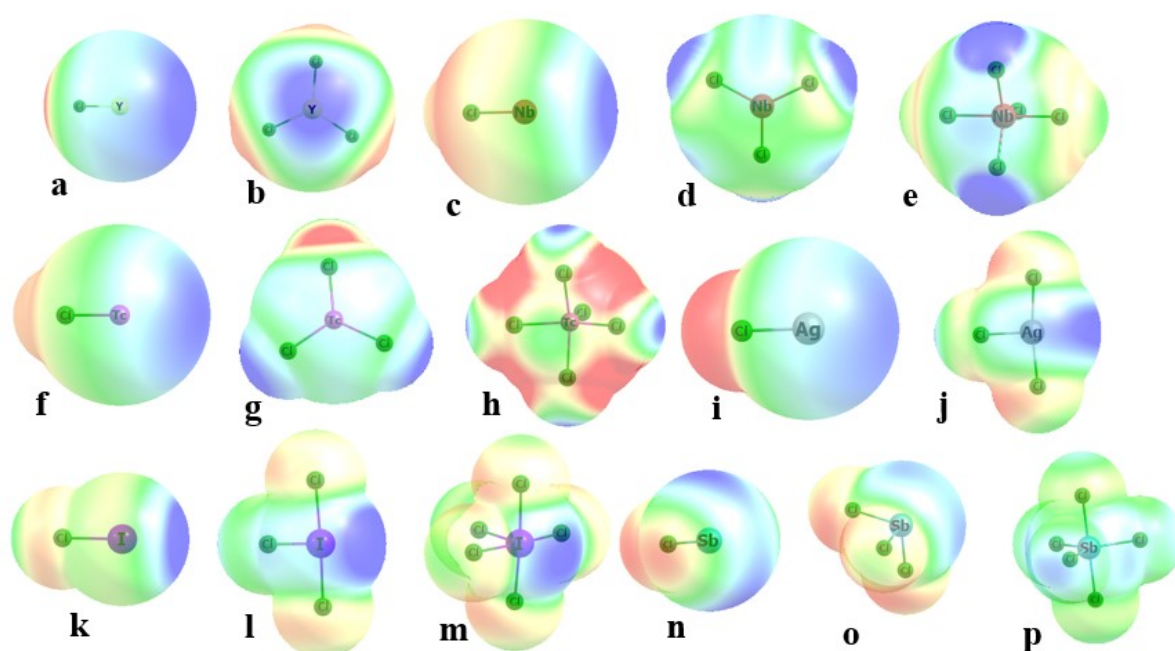


Fig S1. Molecular electrostatic potential surrounding a) YCl, b) YCl₃, c) NbCl, d) NbCl₃, e) NbCl₅, f) TaCl, g) TaCl₃, h) TaCl₅, i) AgCl, j) AgCl₃, k) ICl, l) ICl₃, m) ICl₅, n) SbCl, o) SbCl₃, p) SbCl₅, on a surface corresponding to 1.5 x vdW radius. Red and blue regions respectively indicate negative and positive MEP.

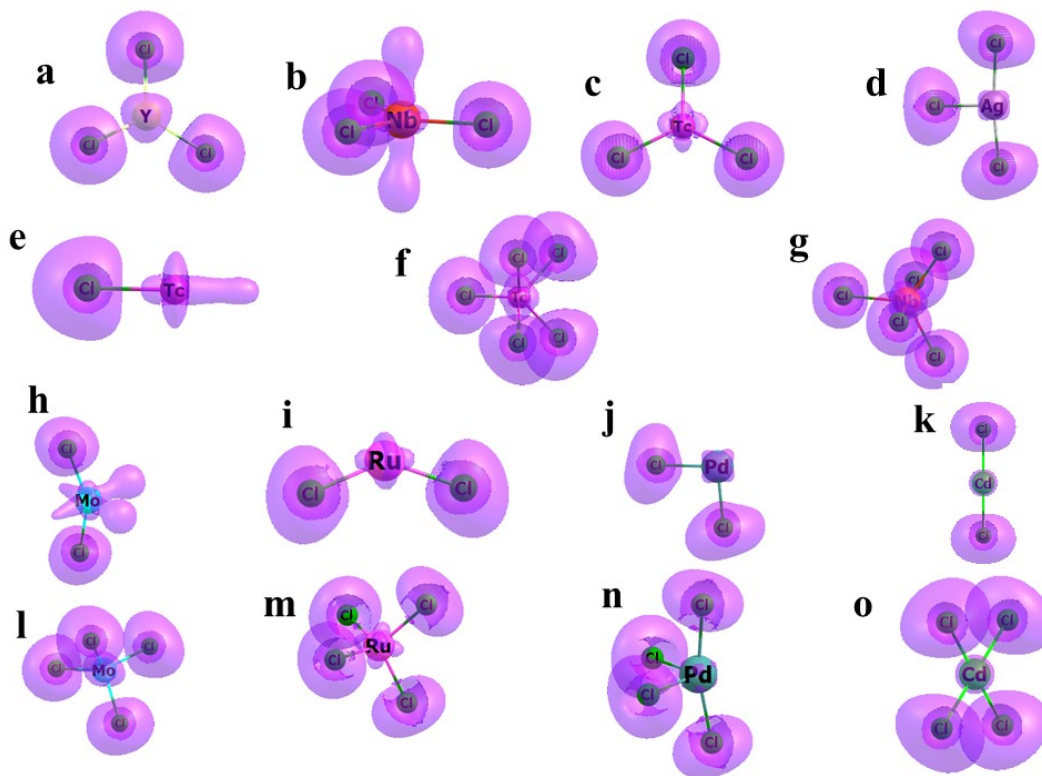


Fig S2. ELF diagram of a) YCl_3 , b) NbCl_3 , c) TcCl_3 , d) AgCl_3 , e) TcCl_2 , f) TcCl_5 , g) NbCl_5 h) MoCl_2 , i) RuCl_2 , j) PdCl_2 , k) CdCl_2 , l) MoCl_4 , m) RuCl_4 , n) PdCl_4 , o) CdCl_4 . Contour shown is 0.8 au.

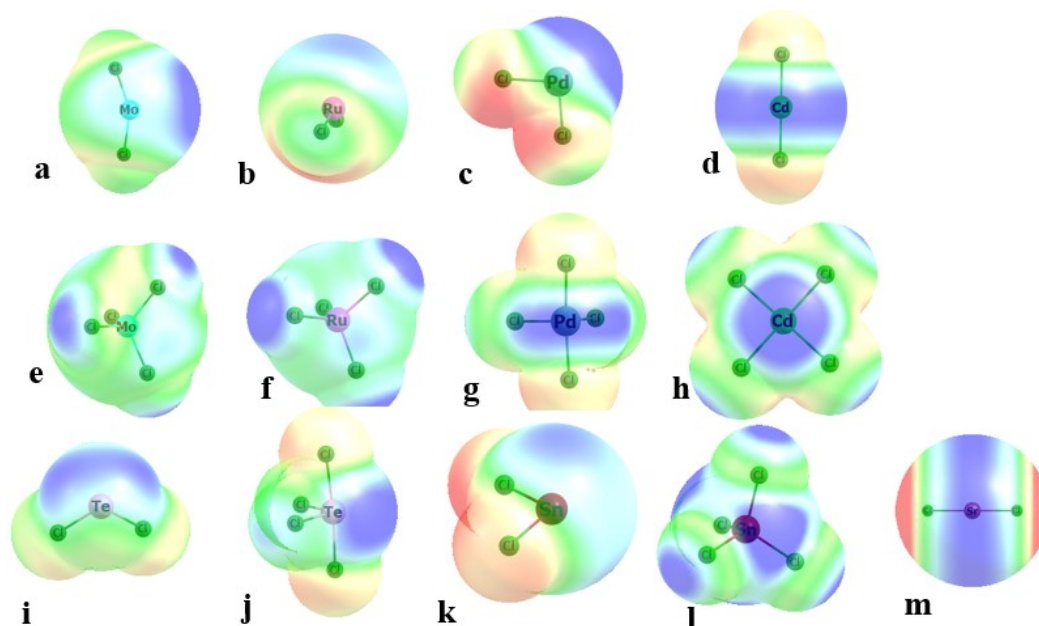


Fig S3. Molecular electrostatic potential surrounding a) MoCl_2 , b) RuCl_2 , c) PdCl_2 , d) CdCl_2 , e) MoCl_4 , f) RuCl_4 , g) PdCl_4 , h) CdCl_4 , i) TeCl_2 , j) TeCl_4 , k) SnCl_2 , l) SnCl_4 , m) SrCl_2 on a surface corresponding to $1.5 \times \text{vdW radius}$. Red and blue regions respectively indicate negative and positive MEP.

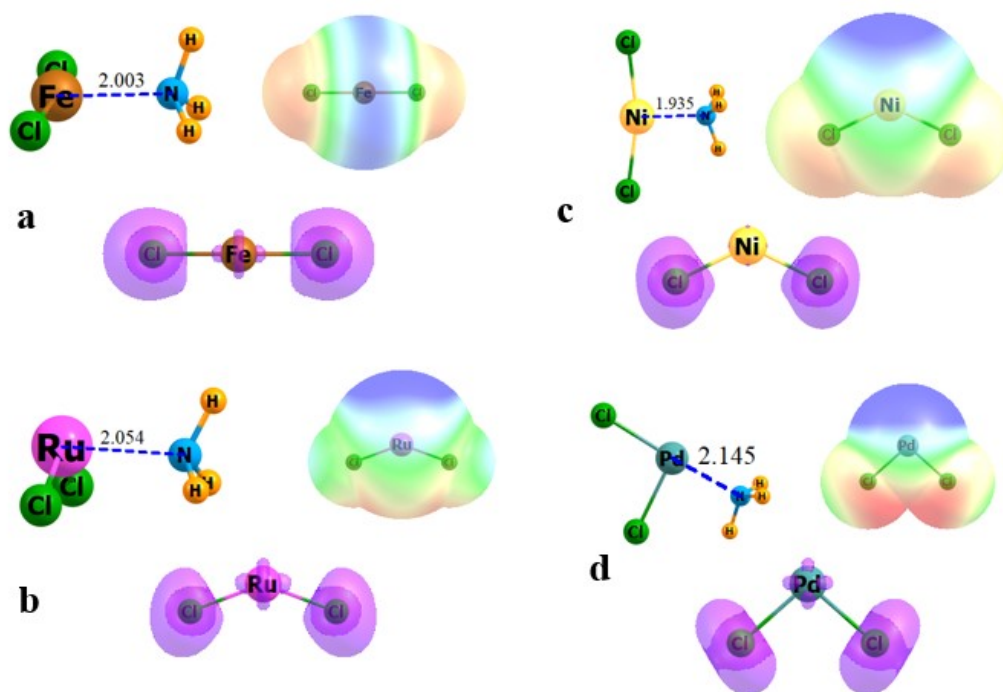


Fig S4. Optimized geometry, MEP, and ELF of complexes of NH_3 with a) FeCl_2 , b) RuCl_2 , c) NiCl_2 , d) PdCl_2 . Distances in Å.

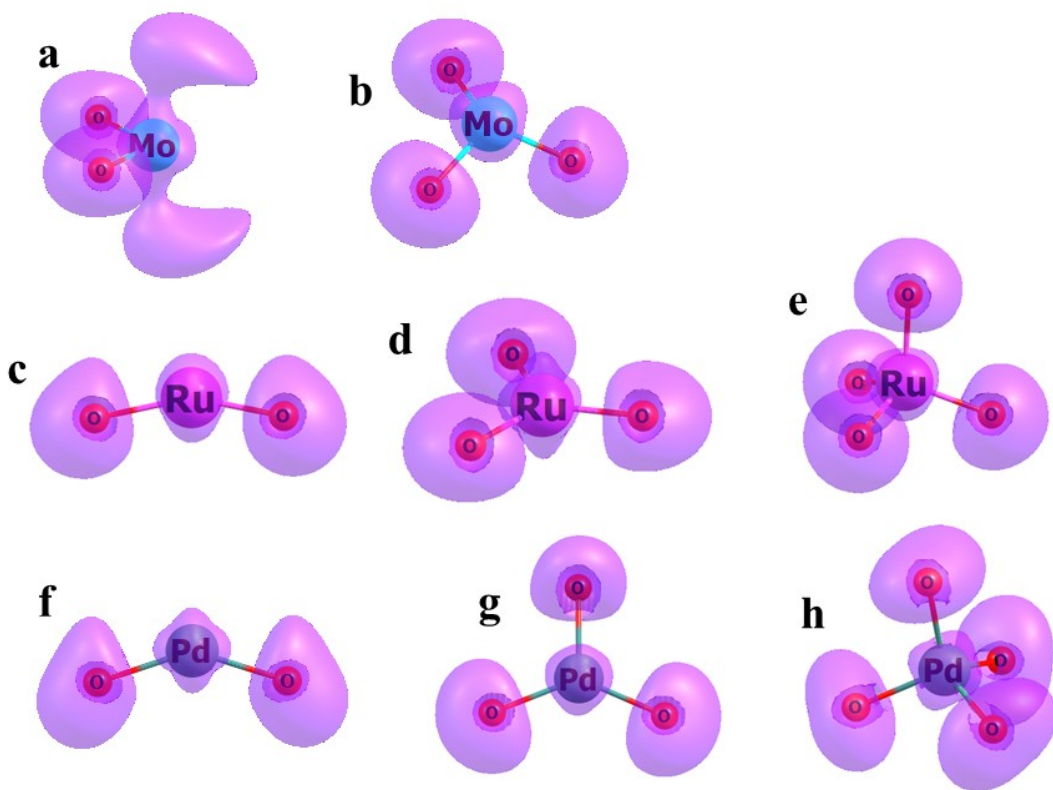


Fig S5. ELF diagram of a) MoO_2 , b) MoO_3 , c) RuO_2 , d) RuO_3 , e) RuO_4 , f) PdO_2 , g) PdO_3 , h) PdO_4 . Contour shown is 0.8 au.

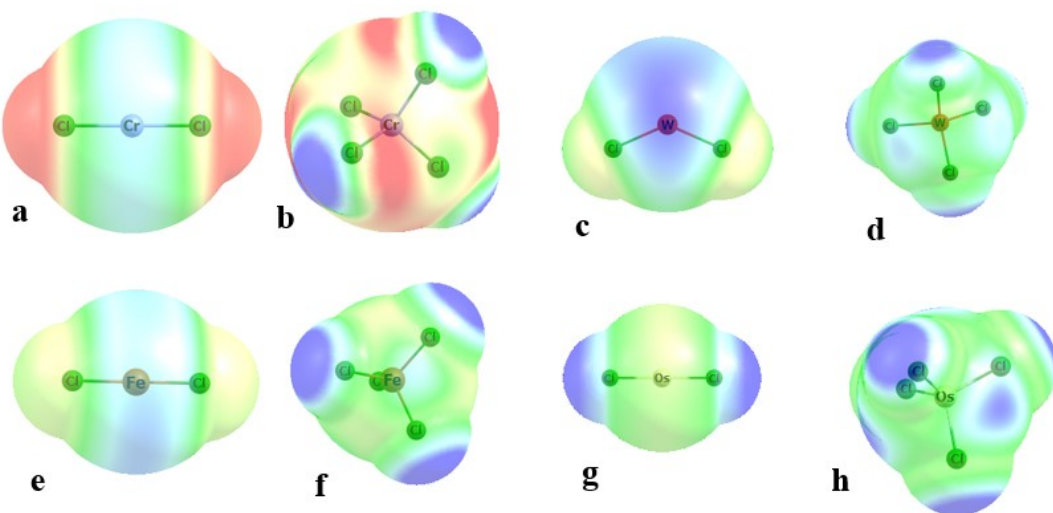


Fig S6. Molecular electrostatic potential surrounding a) CrCl_2 , b) CrCl_4 , c) WCl_2 , d) WCl_4 , e) FeCl_2 , f) FeCl_4 , g) OsCl_2 , h) OsCl_4 , on a surface corresponding to 1.5 x vdW radius. Red and blue regions respectively indicate negative and positive MEP.

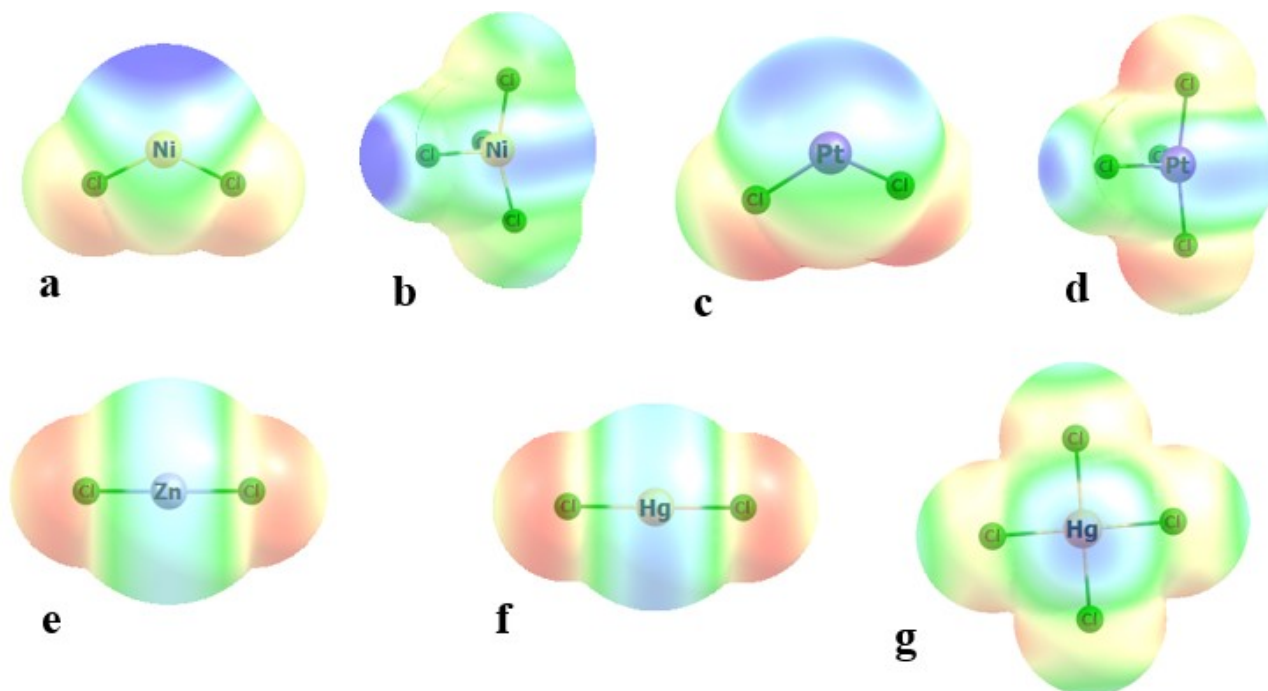


Fig S7. Molecular electrostatic potential surrounding a) NiCl_2 , b) NiCl_4 , c) PtCl_2 , d) PtCl_4 , e) ZnCl_2 , f) HgCl_2 , h) HgCl_4 , on a surface corresponding to $1.5 \times \text{vdW}$ radius. Red and blue regions respectively indicate negative and positive MEP.

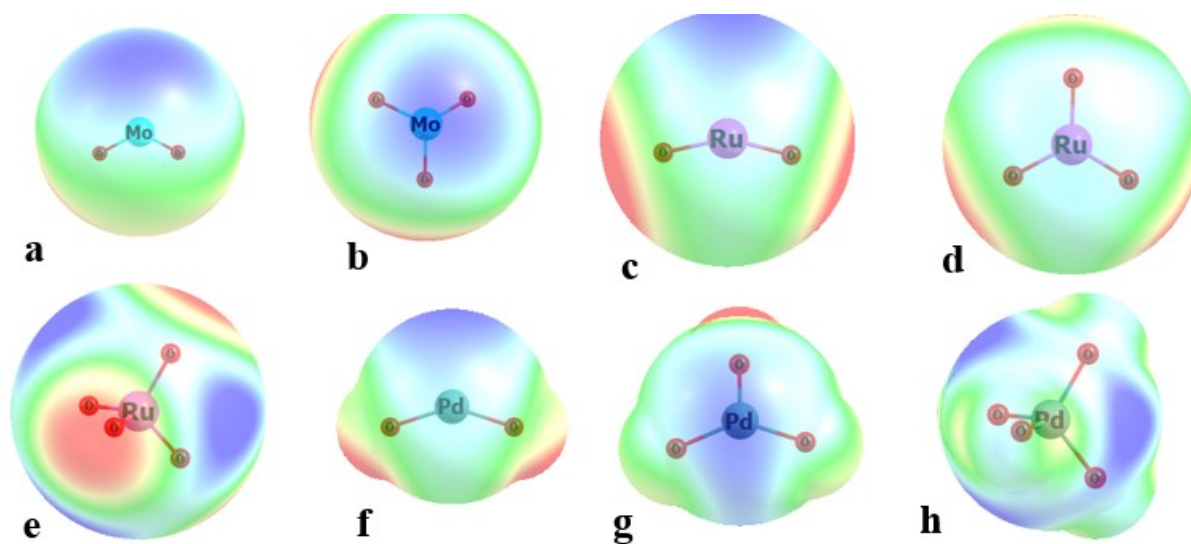


Fig S8. Molecular electrostatic potential surrounding a) MoO_2 , b) MoO_3 , c) RuO_2 , d) RuO_3 , e) RuO_4 , f) PdO_2 , g) PdO_3 , h) PdO_4 on a surface corresponding to $1.5 \times \text{vdW}$ radius. Red and blue regions respectively indicate negative and positive MEP.

Table S1. T1 tests of single-configuration wavefunction of ACl_n

A	n	2S+1	T1 ^b
I	1	1	0.0084
	3	1	0.0123
	5	1	0.0143
Te	2	1	0.0110
	4	1	0.0129
Sb	1	1	0.0141
	3	1	0.0125
	5	1	0.0110
Sn	2	1	0.0140
	4	1	0.0108
0 Sr	2	1	0.0057
1 Y	1	1	0.0130
	3	1	0.0095
3 Nb	1	1	0.0242
		3	0.2225
		5	0.0274
	3	1	0.0233
		3	0.0203
	5	1	0.0207
4Mo	2	1	0.0268
		3	0.0334
		5	0.0210
	4	1	0.0317
		3	0.0131
5 Tc	1	1	0.0391
		3	0.0363
	3	1	0.0399
		3	0.0273
		5	0.0316
	5	1	0.0267
		3	0.0308
		5	0.0257
6 Ru	2	1	0.0355
		3	0.0317
	4	1	0.0277
8 Pd	2	1	0.0322
		3	0.0398
	4	1	0.0213
9 Ag	1	1	0.0157
	3	1	0.0171
10 Cd	2	1	0.0114
	4	1	0.0101
		3	0.0131

Table S2. T1 tests of single-configuration wavefunction of singlet MO_n

M	n	T1
4 Mo	2	0.0847
	3	0.0327
6 Ru	2	0.0357
	3	0.0313
	3	0.0313
8 Pd	4	0.0310
	2	0.0405
	3	0.0580
	4	0.0521

Table S3. Comparison of interaction energies ($-E_{\text{int}}$, kcal/mol) of complexes between ACl_n and NH₃

Group	A	n	M06-2X	CCSD	M06-2X
			def2-TZVP	def2-TZVP	aug-cc-pVTZ
3	Y	1	25.12	17.25	25.03
		3	38.60	30.84	37.94
5	Nb	1	42.88	36.68	42.96
		3	34.45	29.52	34.24
		5	35.07	30.27	35.22
6	Mo	2	37.52	32.20	38.23
		4	32.47	28.59	32.54
8	Ru	2	55.37	54.09	52.88
		4	31.77	29.32	32.11
10	Pd	2	37.72	34.90	38.43
		4	40.18	36.92	41.58
11	Ag	1	28.90	25.48	28.99
		3	39.58	36.61	41.18
12	Cd	2	22.76	19.34	22.97
		4	23.38	18.38	23.59

Table S4. Comparison of interaction energies ($-E_{\text{int}}$, kcal/mol) of complexes between ACl_n and NH_3 , all with the def2-tZVP basis set

Group	A	n	M06-2X	CCSD
17	I	1	12.91	9.48
		3	20.24	15.78
		5	18.44	14.92
16	Te	2	13.22	9.37
		4	21.03	15.70
15	Sb	1	31.28	27.42
		3	13.21	9.10
		5	36.32	31.36
14	Sn	2	24.67	21.23
		4	26.93	22.27
2	Sr	2	24.78	16.45

Coordinates of Complexes with NH_3

ICl

53	-0.000299000	-0.000395000	0.163323000
17	0.000494000	0.000239000	-2.212003000
7	0.000701000	0.001508000	2.788700000
1	-0.718863000	-0.616981000	3.143698000
1	-0.175410000	0.935008000	3.140767000
1	0.896823000	-0.311690000	3.142552000

ICl_3

53	-0.000758000	-0.050077000	0.002052000
17	-2.466588000	-0.294050000	0.000641000
17	0.003731000	2.307787000	-0.003648000
17	2.470903000	-0.303789000	0.000609000
7	-0.010649000	-2.540198000	-0.005681000
1	-0.307597000	-2.902508000	0.893910000
1	0.934555000	-2.854009000	-0.203556000
1	-0.649024000	-2.877132000	-0.718614000

ICl_5

53	0.001712000	-0.000069000	0.051265000
17	0.067653000	-0.003270000	-2.262695000
17	2.427538000	-0.323075000	0.194975000
17	-0.326843000	-2.426657000	0.120075000
17	-2.424932000	0.322449000	0.059160000
17	0.318659000	2.427729000	0.131714000
7	-0.109805000	0.005018000	2.614554000
1	0.821693000	-0.127184000	2.994701000

1	-0.714414000	-0.749855000	2.921468000
1	-0.484664000	0.893568000	2.929983000

TeCl₂

52	0.000706000	-0.474588000	-0.000035000
17	-0.700376000	1.767520000	-0.000010000
17	2.315834000	0.072453000	0.000062000
7	-2.642444000	-0.667181000	0.000087000
1	-2.974363000	-0.168607000	0.818564000
1	-3.053556000	-1.593830000	-0.000074000
1	-2.974481000	-0.168272000	-0.818139000

TeCl₄

52	0.000094000	0.030571000	-0.381912000
17	-2.447349000	-0.235738000	-0.283666000
17	-0.000205000	-0.454373000	1.884464000
17	0.000533000	2.337691000	0.076031000
17	2.447182000	-0.236741000	-0.283571000
7	-0.000640000	-2.454384000	-0.389164000
1	-0.832075000	-2.763491000	0.106334000
1	0.828260000	-2.765320000	0.109396000
1	0.000655000	-2.864462000	-1.317537000

SbCl

51	-0.474036000	-0.435133000	-0.000001000
17	1.877168000	0.148189000	0.000000000
7	-0.778614000	1.862543000	-0.000002000
1	-1.238148000	2.226478000	-0.827583000
1	0.189363000	2.181997000	-0.000688000
1	-1.236925000	2.226288000	0.828331000

SbCl₃

51	0.057154000	-0.000003000	-0.532843000
17	-0.463177000	-1.790846000	0.912214000
17	2.366269000	-0.000241000	0.060122000
17	-0.462687000	1.791034000	0.912134000
7	-2.633146000	0.000191000	-0.505214000
1	-3.068301000	-0.821837000	-0.909993000
1	-3.068744000	0.824471000	-0.904914000
1	-2.832683000	-0.002914000	0.490418000

SbCl₅

51	0.001360000	-0.000313000	0.010140000
17	0.057663000	-0.013217000	2.324487000
17	2.294117000	-0.470377000	-0.299774000
17	0.471165000	2.298923000	-0.240652000

17	-2.301874000	0.471668000	-0.186161000
17	-0.471360000	-2.298719000	-0.243567000
7	-0.087240000	0.020537000	-2.253324000
1	0.840919000	-0.159022000	-2.631721000
1	-0.413690000	0.932338000	-2.566568000
1	-0.730989000	-0.701869000	-2.569266000

SnCl₂

50	-0.002361000	0.238330000	-0.643734000
17	1.822115000	-0.856449000	0.530450000
17	-1.831921000	-0.837717000	0.542445000
7	0.027297000	1.645542000	1.298572000
1	-0.701736000	1.242952000	1.884567000
1	-0.127247000	2.645198000	1.221709000
1	0.922658000	1.477370000	1.751232000

SnCl₄

50	0.021321000	-0.000007000	-0.000019000
17	-0.322481000	2.069032000	-1.029375000
17	-0.335740000	-0.143037000	2.304552000
17	2.357646000	-0.001822000	0.006637000
17	-0.325374000	-1.925388000	-1.277386000
7	-2.336504000	0.002023000	-0.007139000
1	-2.690726000	0.796866000	0.518195000
1	-2.691517000	-0.850800000	0.416814000
1	-2.687116000	0.060761000	-0.959382000

SrCl₂

38	0.000122000	-0.331401000	-0.428597000
17	-2.488187000	-0.323116000	0.476251000
17	2.488394000	-0.322613000	0.476256000
7	-0.000765000	2.255541000	-0.035415000
1	-0.825610000	2.400765000	0.542243000
1	0.000099000	2.980212000	-0.744385000
1	0.822738000	2.400848000	0.544130000

YCl

39	-0.000624000	-0.001514000	0.239840000
17	0.000751000	0.010260000	-2.200294000
7	0.000952000	-0.011105000	2.694665000
1	-0.199117000	0.918259000	3.066724000
1	0.908051000	-0.304088000	3.060270000
1	-0.704029000	-0.651804000	3.061610000

YCl₃

39	0.000580000	-0.001356000	-0.173112000
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17	1.988332000	-1.462752000	-0.328884000
17	0.279242000	2.449658000	-0.329655000
17	-2.263682000	-0.982604000	-0.334860000
7	-0.008031000	-0.002400000	2.254394000
1	-0.885217000	-0.370809000	2.613688000
1	0.107133000	0.941121000	2.616329000
1	0.745515000	-0.573765000	2.628375000

NbCl

41	0.222658000	0.038758000	0.000013000
17	-2.058347000	-0.046722000	-0.000011000
7	2.481014000	-0.073633000	0.000019000
1	2.804269000	-0.563958000	0.833399000
1	2.888690000	0.861956000	-0.007980000
1	2.802860000	-0.577392000	-0.825887000

NbCl₃

41	-0.000006000	0.033632000	0.000697000
17	0.000513000	2.286561000	0.331050000
17	-2.190925000	-0.551600000	-0.468708000
17	2.190652000	-0.552420000	-0.468740000
7	-0.000363000	-2.048844000	0.982541000
1	0.824373000	-2.176032000	1.561327000
1	-0.000170000	-2.788247000	0.280258000
1	-0.825507000	-2.175904000	1.560786000

NbCl₅

41	-0.003503000	-0.003933000	0.075197000
17	-0.047298000	-0.054146000	2.333193000
17	-0.892164000	2.132249000	-0.244680000
17	0.886234000	-2.128644000	-0.312509000
17	2.136293000	0.888082000	-0.209704000
17	-2.124779000	-0.886739000	-0.345667000
7	0.080735000	0.094585000	-2.277100000
1	0.749698000	-0.580381000	-2.637291000
1	0.367686000	1.022514000	-2.575420000
1	-0.829787000	-0.106608000	-2.681428000

MoCl₂

42	0.076807000	-0.041419000	-0.000426000
17	-2.079950000	-0.800469000	0.000383000
17	2.330581000	-0.325755000	0.000439000
7	-0.707119000	1.986621000	0.000260000
1	0.031408000	2.684382000	0.001475000
1	-1.284382000	2.146160000	0.824727000
1	-1.283813000	2.148530000	-0.824125000

MoCl₄

42	0.018916000	0.042832000	-0.000110000
17	-0.862221000	-0.975950000	-1.811056000
17	0.857579000	2.134103000	-0.001340000
17	2.051327000	-1.001036000	0.000815000
17	-0.862642000	-0.972551000	1.812640000
7	-1.994760000	1.157092000	-0.001267000
1	-2.754332000	0.481657000	-0.000876000
1	-2.102530000	1.740331000	-0.826032000
1	-2.103034000	1.741811000	0.822393000

TcCl

43	0.220487000	0.325298000	0.000158000
17	-1.893164000	-0.397659000	-0.000059000
7	2.185096000	-0.655654000	0.000790000
1	2.174249000	-1.272542000	0.807852000
1	3.054760000	-0.128418000	0.014120000
1	2.178162000	-1.237067000	-0.833309000

TcCl₃

43	-0.000189000	0.000166000	-0.172936000
17	-2.024549000	0.958993000	-0.250075000
17	0.181157000	-2.232443000	-0.250208000
17	1.843217000	1.272747000	-0.250820000
7	0.001046000	0.000454000	1.912885000
1	-0.859661000	0.410019000	2.272062000
1	0.786351000	0.541378000	2.270901000
1	0.077061000	-0.949774000	2.271870000

TcCl₅

43	0.002496000	0.005426000	0.136474000
17	0.072721000	0.150149000	2.290101000
17	-1.383897000	1.751966000	-0.377761000
17	1.298886000	-1.832346000	-0.276414000
17	1.802460000	1.303770000	-0.425648000
17	-1.787740000	-1.366671000	-0.232841000
7	-0.015170000	-0.035223000	-2.146212000
1	0.795095000	-0.546161000	-2.485642000
1	0.025488000	0.921211000	-2.486226000
1	-0.863010000	-0.478557000	-2.489471000

RuCl₂

44	-0.000012000	-0.145154000	-0.362244000
17	-2.093355000	-0.384645000	0.416476000
17	2.093439000	-0.384578000	0.416462000

7	-0.000124000	1.845540000	0.144592000
1	0.829151000	2.030535000	0.706483000
1	-0.829522000	2.031004000	0.706118000
1	0.000337000	2.483246000	-0.645974000

RuCl₄

44	0.016003000	0.000289000	-0.000021000
17	0.272075000	-1.054640000	1.904581000
17	0.278910000	2.176068000	-0.039611000
17	-2.234939000	0.003643000	-0.000307000
17	0.272626000	-1.123323000	-1.864863000
7	2.222308000	-0.003863000	0.000413000
1	2.574301000	-0.956487000	0.017550000
1	2.578871000	0.485338000	0.816053000
1	2.579097000	0.455741000	-0.832144000

PdCl₂

46	0.041912000	-0.424534000	0.000235000
17	0.715718000	1.724033000	-0.000018000
17	-2.142862000	-0.021115000	-0.000306000
7	2.126381000	-0.931461000	-0.000496000
1	2.581258000	-0.020057000	-0.002355000
1	2.433286000	-1.441896000	-0.822250000
1	2.434274000	-1.438859000	0.822779000

PdCl₄

46	-0.000261000	-0.068391000	-0.245680000
17	-2.281761000	-0.149749000	-0.440348000
17	0.000767000	-0.308739000	1.952284000
17	0.009187000	2.155295000	-0.112930000
17	2.281111000	-0.166888000	-0.442643000
7	-0.013559000	-2.185984000	-0.490228000
1	-0.107017000	-2.597484000	0.434818000
1	0.863269000	-2.492103000	-0.903434000
1	-0.807496000	-2.471190000	-1.056694000

AgCl

47	-0.000132000	0.001307000	0.216280000
17	0.000242000	-0.012300000	-2.111619000
7	0.000203000	0.014143000	2.462697000
1	0.446899000	0.848792000	2.826374000
1	0.497881000	-0.786897000	2.835669000
1	-0.944116000	-0.013206000	2.831434000

AgCl₃

47	-0.000008000	-0.118842000	0.001006000
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17	-2.306974000	-0.208719000	-0.005541000
17	0.000611000	2.139023000	0.003997000
17	2.306919000	-0.209831000	-0.005541000
7	-0.000825000	-2.265921000	0.004137000
1	-0.006521000	-2.599335000	0.963211000
1	0.841063000	-2.601131000	-0.454895000
1	-0.837831000	-2.600569000	-0.464105000

CdCl₂

48	0.000000000	0.116456000	0.000000000
17	-2.346961000	0.247553000	0.000000000
17	2.232016000	0.833454000	0.000000000
7	0.191653000	-2.287957000	0.000000000
1	-0.748077000	-2.672642000	0.000000000
1	0.680282000	-2.639335000	0.816734000
1	0.680282000	-2.639335000	-0.816734000

CdCl₄

48	-0.002015000	-0.001390000	-0.078829000
17	1.621114000	-1.741645000	-0.308656000
17	-1.746492000	-1.621059000	-0.297484000
17	1.740631000	1.619095000	-0.309955000
17	-1.621250000	1.743153000	-0.303384000
7	0.018809000	0.007204000	2.343115000
1	-0.642676000	-0.667914000	2.712723000
1	-0.230581000	0.922088000	2.704570000
1	0.940284000	-0.230128000	2.695838000

CrCl₂

24	0.072093000	-0.096240000	-0.000286000
17	-2.086301000	-0.676392000	0.000161000
17	2.252788000	-0.387024000	0.000175000
7	-0.421682000	1.933996000	0.000111000
1	0.377132000	2.561217000	-0.000325000
1	-0.992548000	2.144419000	0.815645000
1	-0.993317000	2.144225000	-0.814942000

CrCl₄

24	-0.011630000	0.039905000	-0.031972000
17	-0.642861000	-1.370730000	-1.512938000
17	0.442865000	2.103865000	-0.348368000
17	2.059227000	-0.593220000	0.053966000
17	-0.567780000	-0.646874000	1.929874000
7	-2.066252000	0.733827000	-0.128705000
1	-2.696230000	-0.047081000	0.030362000
1	-2.278205000	1.139818000	-1.035179000

1	-2.237333000	1.431063000	0.590028000
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WCl₂

74	-0.087663000	0.024198000	-0.000113000
17	1.977006000	-0.982181000	0.000157000
17	-2.311908000	-0.258432000	0.000213000
7	1.155328000	1.839431000	0.000180000
1	0.581522000	2.677900000	0.000359000
1	1.755831000	1.873125000	-0.823519000
1	1.755747000	1.872710000	0.823956000

WCl₄

74	0.000764000	0.000168000	-0.067252000
17	0.132954000	-2.090318000	-0.938805000
17	0.626547000	-0.000963000	2.134061000
17	-2.285385000	-0.007409000	0.253106000
17	0.119540000	2.093101000	-0.934790000
7	2.274461000	0.007895000	-0.369775000
1	2.575409000	0.010623000	-1.339737000
1	2.679949000	-0.806306000	0.085536000
1	2.674739000	0.822979000	0.088538000

FeCl₂

26	0.000001000	-0.187871000	0.043752000
17	2.163601000	-0.421838000	-0.029504000
17	-2.163598000	-0.421843000	-0.029504000
7	-0.000006000	1.814806000	-0.011543000
1	-0.829998000	2.155486000	-0.488773000
1	0.830220000	2.155502000	-0.488356000
1	-0.000257000	2.212610000	0.923517000

FeCl₄

26	-0.004866000	0.000126000	-0.000169000
17	0.279789000	-0.634750000	2.009414000
17	0.281341000	2.057889000	-0.456199000
17	-2.113585000	0.003231000	0.002301000
17	0.274361000	-1.424860000	-1.554025000
7	2.082105000	-0.002739000	-0.002011000
1	2.425198000	-0.936164000	0.204005000
1	2.428054000	0.641876000	0.702589000
1	2.426134000	0.284530000	-0.913475000

OsCl₂

76	0.000002000	-0.155588000	-0.148471000
17	-2.205332000	-0.234757000	0.318285000
17	2.205334000	-0.234746000	0.318285000

7	-0.000019000	1.873022000	0.034168000
1	0.829774000	2.174821000	0.545220000
1	-0.829829000	2.174800000	0.545204000
1	-0.000016000	2.345450000	-0.867493000

OsCl₄

76	-0.012480000	0.000221000	-0.000052000
17	-0.279777000	-1.187985000	-1.853493000
17	-0.281383000	2.199351000	-0.100931000
17	2.264268000	0.001150000	-0.000323000
17	-0.279052000	-1.012945000	1.954637000
7	-2.217418000	-0.000824000	0.000573000
1	-2.578529000	-0.950241000	0.035080000
1	-2.580078000	0.443399000	-0.838592000
1	-2.579952000	0.503130000	0.805322000

NiCl₂

28	0.003426000	-0.159450000	-0.000123000
17	2.140668000	-0.413887000	0.000095000
17	-2.131622000	-0.428745000	0.000095000
7	-0.020813000	1.775132000	-0.000033000
1	0.929356000	2.134806000	-0.008359000
1	-0.509161000	2.114596000	0.823568000
1	-0.524200000	2.114025000	-0.814773000

NiCl₄

28	-0.001116000	-0.084317000	-0.231586000
17	-2.153709000	-0.172315000	-0.531088000
17	0.007759000	-0.286250000	1.893730000
17	-0.002026000	2.036789000	-0.147844000
17	2.150721000	-0.170593000	-0.539213000
7	-0.001552000	-2.056901000	-0.486473000
1	-0.838810000	-2.442871000	-0.059054000
1	0.835834000	-2.442571000	-0.058913000
1	-0.001616000	-2.285110000	-1.477276000

PtCl₂

78	-0.000996000	-0.284252000	-0.000001000
17	0.955754000	1.723304000	-0.000002000
17	-2.179224000	0.185137000	0.000002000
7	1.983270000	-0.999105000	-0.000010000
1	2.585152000	-0.175519000	-0.001137000
1	2.204086000	-1.552339000	-0.822693000
1	2.204554000	-1.550239000	0.823963000

PtCl₄

78	0.000090000	-0.029260000	-0.191273000
17	-2.287776000	-0.096343000	-0.396801000
17	-0.000971000	-0.572530000	1.954039000
17	-0.000083000	2.192311000	0.092245000
17	2.288138000	-0.096231000	-0.395795000
7	0.000438000	-2.096748000	-0.623535000
1	-0.000625000	-2.608084000	0.257389000
1	0.839595000	-2.347336000	-1.141952000
1	-0.837306000	-2.347604000	-1.144079000

ZnCl₂

30	0.000000000	0.033677000	0.000000000
17	-2.149038000	0.364093000	0.000000000
17	2.004040000	0.870402000	0.000000000
7	0.234566000	-2.092019000	0.000000000
1	-0.676527000	-2.540837000	0.000000000
1	0.749768000	-2.405874000	0.816760000
1	0.749768000	-2.405874000	-0.816760000

ZnCl₄

30	-0.005072000	0.000168000	0.062930000
17	-0.009357000	-2.247259000	-0.369961000
17	-2.253105000	0.013016000	-0.359107000
17	2.243034000	-0.010872000	-0.373408000
17	0.014572000	2.248394000	-0.365953000
7	0.021879000	-0.005646000	2.199993000
1	-0.922144000	-0.040190000	2.572619000
1	0.473245000	0.831806000	2.555124000
1	0.530452000	-0.812882000	2.547708000

MoO₂

42	0.135639000	-0.001000000	0.000026000
8	1.009832000	1.442372000	-0.000047000
8	1.036618000	-1.428190000	-0.000047000
7	-2.097923000	-0.010894000	-0.000022000
1	-2.443863000	0.475626000	0.826490000
1	-2.495435000	-0.947129000	-0.000453000
1	-2.443696000	0.476308000	-0.826205000

MoO₃

42	0.175114000	0.000041000	-0.000132000
8	0.585274000	-1.162426000	-1.168827000
8	0.587089000	1.594454000	-0.418641000
8	0.579663000	-0.434260000	1.591524000
7	-2.027719000	0.001394000	-0.002999000
1	-2.393428000	-0.904514000	0.281613000

1	-2.393810000	0.210075000	-0.929194000
1	-2.389733000	0.700797000	0.641652000

RuO₂

44	0.212446000	0.007560000	0.000026000
8	0.815152000	-1.535813000	-0.000054000
8	0.610164000	1.617667000	-0.000054000
7	-1.967305000	-0.099830000	-0.000007000
1	-2.326916000	-0.570191000	-0.823629000
1	-2.324871000	0.851197000	-0.000389000
1	-2.327233000	-0.569654000	0.823784000

RuO₃

44	-0.430042000	0.000815000	-0.008672000
8	-0.374063000	1.496176000	-0.714382000
8	-0.516832000	-0.133450000	1.638128000
8	-0.373374000	-1.361701000	-0.945726000
7	2.792436000	-0.004266000	0.058800000
1	3.179206000	0.748176000	0.615739000
1	3.138058000	0.110274000	-0.886601000
1	3.171698000	-0.872625000	0.416691000

RuO₄

44	-0.315502000	0.000018000	0.000012000
8	0.140752000	-0.512708000	1.507347000
8	0.145327000	-1.048641000	-1.196343000
8	0.142624000	1.561380000	-0.308523000
8	-1.968162000	-0.000315000	-0.002584000
7	2.510541000	0.000782000	0.000500000
1	2.869136000	-0.946954000	0.029230000
1	2.880935000	0.497786000	0.802622000
1	2.873914000	0.445162000	-0.835050000

PdO₂

46	-0.159218000	-0.192662000	-0.160164000
8	0.962478000	-1.404026000	0.407850000
8	-1.575597000	0.653611000	0.408880000
7	1.161973000	1.413505000	0.058987000
1	1.935421000	1.027253000	0.594766000
1	0.648881000	2.095032000	0.612152000
1	1.510860000	1.848968000	-0.786108000

PdO₃

46	-0.002526000	0.001473000	-0.238241000
8	-1.723190000	-0.335981000	-0.284128000
8	1.149491000	-1.318789000	-0.319855000

8	0.564479000	1.660395000	-0.295521000
7	0.018108000	-0.010741000	1.731371000
1	0.664566000	-0.751580000	2.000314000
1	-0.940710000	-0.200355000	2.020823000
1	0.339342000	0.914332000	2.014365000

PdO₄

46	-0.167326000	0.048079000	-0.000193000
8	-0.019774000	-0.890092000	-1.474271000
8	-0.022285000	-0.880756000	1.480105000
8	-1.919707000	-0.020439000	-0.001075000
8	0.233232000	1.724019000	-0.004870000
7	2.054733000	-0.154441000	0.001026000
1	2.259352000	-1.147919000	0.031169000
1	2.445238000	0.303762000	0.817244000
1	2.437568000	0.251764000	-0.845836000