Electronic Supporting Information for

Thermal properties of binary chlorides relevant to molten salt nuclear chemistry

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DEFINITIONS, EQUATIONS, DATA PROCESSING, AND REPORTING

Significant Figures: All values are presented with the same number of significant figures as taken from the original report/reference text.

Temperature: For consistency and better use of thermodynamic equations, all temperatures are presented in absolute units (K). If needed, the temperature was converted using the absolute conversion T(K) = T (°C) + 273.15, with preservation of the number of significant figures.

Variance: Indicated with a "±" followed by the value. If no value is given, no variance was given in the original report/reference text.

Data Averaging: When a property measurement for a single compound has three or more reports, an [ϕ]average value was calculated along with the standard deviation, indicated with a "±." The average values are presented at the bottom of the table below a solid line and are italicized.

Phase change and thermodynamic measurements: Please note, in some cases phase change temperatures or thermodynamic phase change values are reported under reduced or increased pressure, or increased temperature. These are noted with a superscript letter and explained in the table footer.

dec = Decomposes [¶]Estimated Value ~ = Approximate Value > = Occurs at a Higher Temperature

Vapor Pressure Expressions: [§]Vapor pressure coefficients A–D, as needed, come from **Eq. 1**.

$$\boldsymbol{logP_{mmHg} = -\frac{A}{T} + B - Clog(T) + 10^{-3}DT} \quad \textbf{(1)}$$

[%]Many expressions with multiple phases were originally designated as "A and B" in the primary literature.

[&]When multiple solid, liquid, gas phases have been characterized or computed the phases are represented as X_n (S, L, G; respectively) where n = phase number 1, 2, 3…

[‖]Different crystal modifications are indicated by α/β.

Vapor Pressure Expressions: For uniformity, all vapor pressure expressions were presented in units of mmHg. Values originally presented in bar or atm were converted to mmHg using **Eq. 2** or **3**, respectively. Values that have been converted are marked with the symbols given. Conversion to pascals can be achieved using **Eq. 4**.

$$^{\dagger}\ logP_{mmHg} = logP_{bar} + \log(750.062) = -\frac{A}{T} + B - Clog(T) \quad \textbf{(2)}$$

$$^{\ddagger}\ logP_{mmHg} = logP_{atm} + \log(760) = -\frac{A}{T} + B - Clog(T) \quad \textbf{(3)}$$

$$logP_{Pa} = logP_{mmHg} + \log(133.322) = -\frac{A}{T} + B - Clog(T) \quad \textbf{(4)}$$

Thermodynamic calculations: Where possible, thermodynamic calculations were performed to fill in gaps using fundamental **Eqs. 5-7**. All calculations were performed with T = 298 K. Values that have been converted are marked with the symbols given. When desired the isobaric heat capacity may be calculated using **Eq. 8**.

$$^{\Delta}\ \Delta G = \Delta H - T\Delta S \quad \textbf{(5)}$$

$$^{*}\ \Delta S^{\circ}_{f} = S^{\circ}_{molecule} - S^{\circ}_{elements} \quad \textbf{(6)}$$

$$^{\Diamond}\ \Delta X_{sub} = \Delta X_{fus} + \Delta X_{vap}\ (X = H, S) \quad \textbf{(7)}$$

$$C_p = \frac{\partial H}{\partial T}\ at\ constant\ P \quad \textbf{(8)}$$

SOLVENT ELEMENT DATA

ALKALI (A) METAL ELEMENTS

Table S1. Melting (T_M) and Boiling (T_B) Phase Change Temperatures.

Compound	T_M (K)	T_B (K)	Ref
LiCl	883	1656	[1, 2]
NaCl	1075.33	1738	[1]
KCl	1044	1773	[1, 3]
RbCl	997	1663	[1]
CsCl	919	1570	[1]
FrCl[φ]	850	1496	[4]
FrCl[φ]	863	1548	[4]

[φ]These values were given in the same research publication, please see ref. [4] for more detail.

Table S2a. Experimental Solid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	D	T range (K)	Ref
NaCl	12,440	14.31	0.90	–0.46	298-1075	[5]
KCl	12,230	20.34	3.0		298-1044	[5]
RbCl[†]	10,920	14.533	2.32		700-996	[6]
RbCl	11,670	20.157	3.0		298-997	[5]
CsCl	10,800	19.99	3.02		700-919	[5]

Table S2b. Experimental Liquid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	T range (K)	Ref
LiCl	10,760	22.30	4.02	883-1656	[5]
NaCl	11,530	20.77	3.48	1075-1738	[5]
KCl	10,710	18.91	3.0	1044-1773	[5]
KCl[‡]	11,101	20.83	3.52	1189-1418	[7]
RbCl[†]	10,004	15.892	3.08	996-1679	[6]
RbCl	10,300	18.77	3.0	997-1663	[5]
CsCl[‡]	10,052	20.51	3.52	1102-1387	[7]
CsCl	9815	20.38	3.52	919-1570	[5]

Table S3. Computed Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
LiCl (G_1)	11,620	16.416	2.79	700-883	[6]
LiCl (G_2)	10,101	11.073	1.56	883-1633	[6]
$(LiCl)_2$ (G_1)	12,523	23.031	4.68	700-883	[6]
$(LiCl)_2$ (G_2)	9525	12.653	2.31	883-1633	[6]
$(LiCl)_2$ (G_3)	5312	4.617	0.37	1633-2000	[6]
$(LiCl)_3$ (G_1)	10,248	11.131	2.64	900-1633	[6]
NaCl (G_1)	11,972	17.865	3.26	700-1074	[6]
NaCl (G_2)	10,661	17.766	3.63	1074-1757	[6]
$(NaCl)_2$ (G_1)	13,231	26.333	5.69	700-1074	[6]
$(NaCl)_2$ (G_2)	10,638	26.344	6.49	1074-1757	[6]
$(NaCl)_2$ (G_3)	8739	21.075	4.87		[6]
KCl (G_1)	12,151	17.254	2.99	700-1045	[6]
KCl (G_2)	11,326	20.148	4.21	1045-1714	[6]
$(KCl)_2$ (G_1)	14,592	26.312	5.40	800-1045	[6]
$(KCl)_2$ (G_2)	12,877	31.525	7.67	1045-1714	[6]
$(KCl)_2$ (G_3)	4,849	4.185	0.32	1714-2000	[6]
CsCl (G_1)	10,796	17.327	3.12	700-918	[6]
CsCl (G_2)	10,522	22.717	5.04	918-1569	[6]
$(CsCl)_2$ (G_1)	12,271	25.545	5.41	700-918	[6]
$(CsCl)_2$ (G_2)	11,754	36.567	9.32	918-1569	[6]
$(CsCl)_2$ (G_3)	4610	4.252	0.33	1569-2000	[6]

Table S4a. Crystalline Phase Thermodynamic Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
LiCl	–408.6	59.3	–384.4	48.0	[1, 6]
NaCl	–411.2	72.1	–384.1	50.5	[1]
NaCl	–411.2	72.1	–384.1$^{\Delta, *}$	66.9	[6]
KCl	–436.5	82.6	–408.5	51.3	[1]
KCl	–436.5	82.6	–408.5$^{\Delta, *}$	51.6	[6]
RbCl	–435.4	95.9	–407.8	52.4	[1]
RbCl	–435.1	95.2	–407.3$^{\Delta, *}$	51.4	[6]
CsCl	–443.0	101.2	–414.5	52.5	[1]
FrCl$^{\varphi}$	–181.6				[4]
FrCl$^{\varphi}$	–439.3				[4]

$^{\varphi}$These values were given in the same research publication, please see ref. [4] for more detail.

Table S4b. Gas Phase Thermodynamic Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	$\Delta G_f^{o\,\Delta, *}$	C_p	Ref
LiCl	–195.4	212.9	–216.9	33.3	[6]
$(LiCl)_2$	–593.5	288.8	–595.7	72.2	[6]
$(LiCl)_3$	–962.3	335.8	–936.6	102.0	[6]
NaCl	–191.7	229.8	–211.7	35.8	[6]
$(NaCl)_2$	–586.7	325.4	–586.6	119.8	[6]
KCl	–214.6	239.1	–233.3	36.5	[6]
$(KCl)_2$	–615.4	350.4	–614.8	80.9	[6]
RbCl	–233.1	241.3	–248.9	36.5	[6]

Table S5. Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap), and Sublimation (sub).

Cmpd	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
LiCl	19.8	23.4	114.1[a]		212.5[◊]		[1, 8, 9]
LiCl	19.5	22.1					[6]
NaCl	28.16	26.2, 28.0	223.0	277.32 ± 2.8[a]	221.84 ± 2.0[a]	305.3[◊]	[1, 8, 10-12]
NaCl	28.3	26.3					[6]
KCl	26.28	25.9	187.7	267.53± 1.6[a]	214.01 ± 1.0[a]		[1, 8, 12]
KCl	26.2	25.0					[6]
RbCl	24.4	18.4, 24.47					[1, 8, 10]
RbCl	23.7	23.8	148.5	88.5	172.2[◊]	112.3[◊]	[6]
CsCl	20.4	14.6					[1, 8]
CsCl	20.3	22.1					[6]
FrCl					181.6		[4]

[a]Value recorded at 800 K.

ALKALINE EARTH (Ae) METAL ELEMENTS

Table S6. Melting (T_M) and Boiling (T_B) Phase Change Temperatures.

Compound	T_M (K)	T_B (K)	Ref
$BeCl_2$	688	755	[1]
$MgCl_2$	987	1685	[1]
$CaCl_2$	1048	2208	[1]
$SrCl_2$	1147	1523	[1]
$BaCl_2$	1234	1833	[1]
$RaCl_2$	~1173		[13]

Table S7a. Experimental Solid Phase Vapor Pressure Coefficients.[§, %, &]

Compound	A	B	C	T range (K)	Ref
$BeCl_2$	7870	27.15	5.03	298-688	[5]
Be_2Cl_4	8970	37.0	7.65	298-688	[5]
$MgCl_2$[‡]	12,820	9.168±0.048		802-985	[14]
$CaCl_2$[†]	17,494	17.772	2.72	1000-1045	[6]
$SrCl_2$ (S_1)[†]	20,129	30.576	6.38	990	[6]
$SrCl_2$ (S_2)[†]	21,693	43.420	10.14	990-1146	[6]
$BaCl_2$ (S_1)[†]	19,689	23.239	4.12	1000-1198	[6]
$BaCl_2$ (S_2)[†]	20,773	35.811	7.91	1198-1235	[6]

Table S7b. Experimental Liquid Phase Vapor Pressure Coefficients.[§, %, &]

Compound	A	B	C	T range (K)	Ref
$BeCl_2$	7220	26.28	5.03	688-755	[5]
$MgCl_2$[‡]	11,735	20.27	4.076	1208-1413	[7]
$MgCl_2$	10,840	25.53	5.03	987-1685	[5]
$CaCl_2$[†]	17,032	23.760	4.85	1045-2279	[6]
$CaCl_2$	13,570	9.22		1110-1281	[5]
$SrCl_2$[†]	18,381	25.141	5.11	1146-2000	[6]
$BaCl_2$[†]	18,956	28.682	6.08	1235-2000	[6]

Table S8. Computed Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
$BeCl_2$ (G_1)	7404	15.399	2.10	400-688	[6]
$BeCl_2$ (G_2)	8277	32.246	7.59	688-760	[6]
$(BeCl_2)_2$ (G_1)	9334	21.283	3.10	500-688	[6]
$(BeCl_2)_2$ (G_2)	11,028	53.192	13.83	688-760	[6]
$(BeCl_2)_2$ (G_3)	2721	4.791	0.57	760-2000	[6]
$MgCl_2$ (G_1)	13,605	17.819	2.68	800-980	[6]
$MgCl_2$ (G_2)	11,955	19.216	3.71	980-1634	[6]
$MgCl_2$ (G_3)	12,347	3.765	0.18	1634-2000	[6]
$(MgCl_2)_2$ (G_1)	18,276	25.918	4.42	900-980	[6]
$(MgCl_2)_2$ (G_2)	14,943	28.441	6.40	980-1634	[6]
$(MgCl_2)_2$ (G_3)	4476	4.959	0.50	1634-2000	[6]

Table S9a. Crystalline Phase Thermodynamic Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$BeCl_2$	–490.4	75.8	–445.6	62.4	[1]
$BeCl_2$	–496.2	75.8	–449.5[Δ, *]	62.4	[6]
$MgCl_2$	–641.3	89.6	–591.8	71.4	[1]
$MgCl_2$	–644.3	89.5	–594.7[Δ, *]	71.3	[6]
$CaCl_2$	–795.4	108.4	–748.8	72.9	[1]
$CaCl_2$	–795.4	108.4	–748.8[Δ, *]	72.6	[6]
$SrCl_2$	–828.9	114.9	–781.1	75.6	[1]
$SrCl_2$	–828.9	114.9	–780.2[Δ, *]	75.6	[6]
$BaCl_2$	–855.0	123.7	–806.7	75.1	[1]
$BaCl_2$	–858.6	123.7	–810.3[Δ, *]	75.2	[6]

Table S9b. Gas Phase Thermodynamic Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$BeCl_2$	–360.2	252.0	–366.0[Δ, *]	51.6	[6]
$(BeCl_2)_2$	–823.2	381.5	–798.2[Δ, *]	115.4	[6]
$MgCl_2$	–392.5	277.0	–398.8[Δ, *]	57.1	[6]
$(MgCl_2)_2$	–954.4	418.9	–926.8[Δ, *]	123.6	[6]
$CaCl_2$	–470.5	290.3	–478.1[Δ, *]	59.4	[6]
$SrCl_2$	–473.2	316.3	–484.6[Δ, *]	55.7	[6]
$BaCl_2$	–498.7	325.7	–510.7[Δ, *]	56.2	[6]

Table S10. Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap), and Sublimation (sub).

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
$BeCl_2$	8.66						[1]
$BeCl_2$	8.58	12.5					[6]
$MgCl_2$	43.1		190[◊]		233.1[a]		[1, 9]
$MgCl_2$	39.9	40.8					[6]
$CaCl_2$	28.05	24.3					[1, 8]
$CaCl_2$	27.3	26.1		102.9		129.0[◊]	[6]
$SrCl_2$	16.22	15.1					[1, 8]
$SrCl_2$	16.5	14.4		109.7		124.1[◊]	[6]
$BaCl_2$	15.85	18.4					[1, 8]
$BaCl_2$	16.0	12.9					[6]

[a]Value recorded at 800 K.

FUEL ELEMENT DATA

ACTINIDE (An) METAL ELEMENTS

Table S11. Melting (T_M), Boiling (T_B), Sublimation (T_{sub}), Triple Point Temperature (T_{TP}), and Triple Point Pressure (P_{TP}) Phase Change Data.

Compound	T_M (K)	T_B (K)	T_{sub} (K)	T_{TP} (K)	P_{TP} (mmHg)	Ref
			Trivalent Actinides			
$AcCl_3$			1223			[15]
UCl_3	1108	1930	1123			[1, 16]
$NpCl_3$	1073		1023-1073			[17, 18]
$PuCl_3$	1033±5	2063	1073			[1, 19, 20]
$AmCl_3$	988, 773[a]	1453[a]	1023, 1123			[1, 19, 21, 22]
$CmCl_3$	968±10					[23]
$BkCl_3$	876					[23]
$CfCl_3$	818					[24]
$EsCl_3$	>723					[25]
			Tetravalent Actinides			
$ThCl_4$	1043	1194	1088			[1, 26]
$PaCl_4$	950, 773[a]		673			[27]
UCl_4	863±5	1062	873, 673[a]	863±1	18.4	[1, 28-31]
$NpCl_4$	803	1120	773	811		[17, 19, 32]
$PuCl_4$	856[b]	1110[b]				[33]
			Pentavalent Actinides			
$PaCl_5$	579	693[c]	~473			[1, 34, 35]
UCl_5	560	800				[1, 19]
			Hexavalent Actinides			
UCl_6	450.65±2.5	550	348-373[a]			[1, 3, 19, 36]

[a]Under reduced pressure, ca. 10^{-4} mmHg [b]Extrapolated from **An**Cl_4 (**An** = Th, U, Np) thermodynamic data [c]Extrapolated from vapor pressure data.

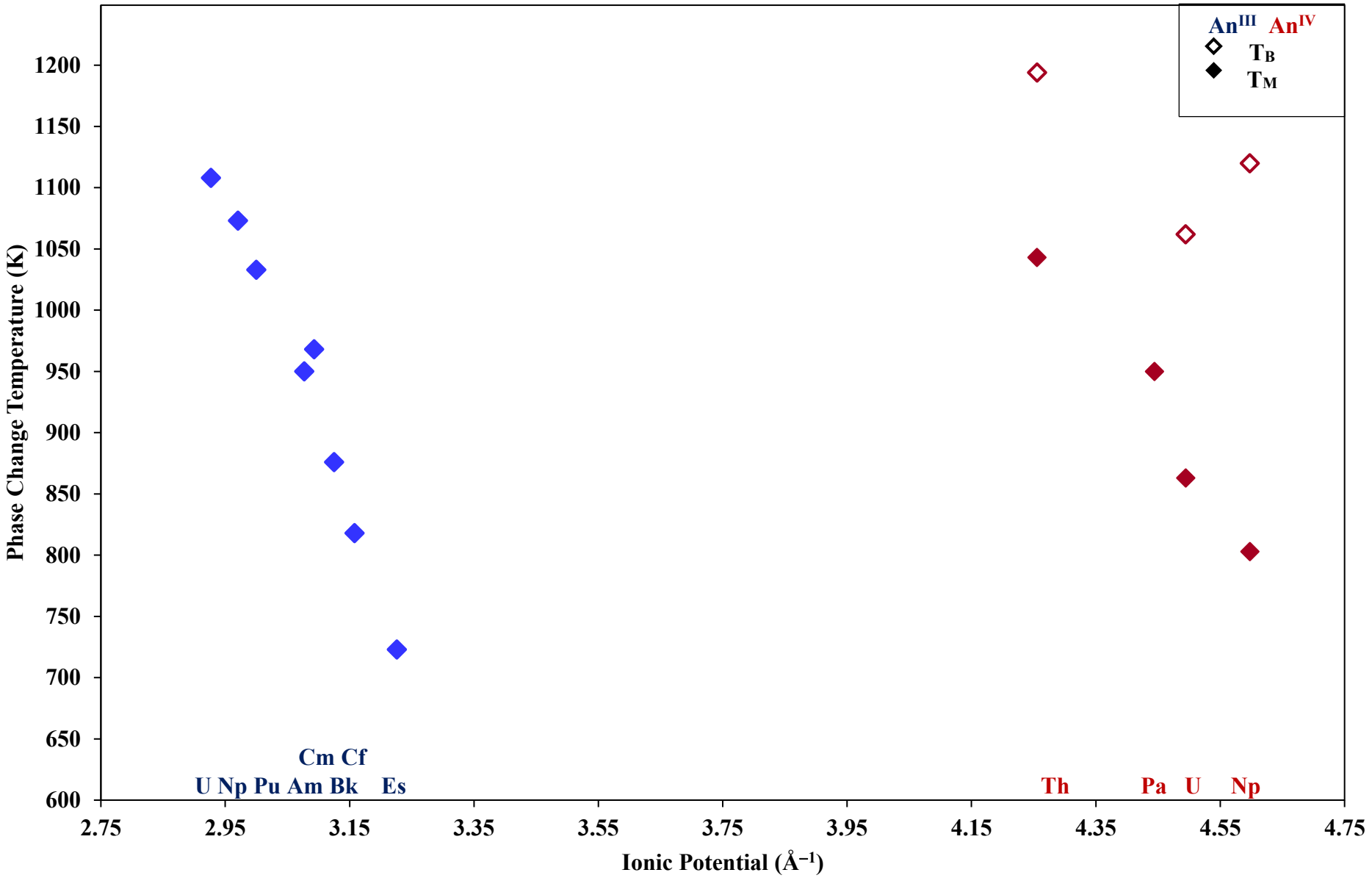

Figure S1. Graphical depiction of melting (T_M, solid diamonds) and boiling points (T_B, empty diamonds) in Kelvin of actinide chlorides, **An**Cl_x (x = 3, 4) in Kelvin by ionic potential (IP, $Å^{-1}$) using 6-coordinate Shannon ionic radii (CN_6).

Table S12a. Experimental Trivalent Actinides (An^{III}) Solid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	T range (K)	Ref
UCl_3	12,000	10.0			[18]
UCl_3	11,149	8.90		590-790	[18]
UCl_3	11,552	8.97		>790	[18]
UCl_3[†]	15,543	23.436	4.31	800-1114	[6]
$PuCl_3$[†]	18,270	29.725	5.34	700-1033	[6]
$PuCl_3$	15,910±120	12.726±0.126		850–1033	[37]
$PuCl_3$	18,270	32.60	5.34	298-1033	[5]

Table S12b. Experimental Trivalent Actinides (An^{III}) Liquid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	T range (K)	Ref
UCl_3[†]	13,506	24.778	5.35	1114-1851	[6]
$PuCl_3$[†]	15,490	28.883	6.45	1033-2065	[6]
$PuCl_3$	12,356±32	10.237±0.033		1033–1100	[37]
$PuCl_3$	12,590	9.509			[18]
$PuCl_3$	15,490	31.76	6.45	1033-2063	[5]

Table S12c. Experimental Tetravalent Actinide (An^{IV}) Solid Phase Vapor Pressure Coefficients.[§, ‖]

Compound	A	B	C	T range (K)	Ref
$ThCl_4$	12,910	14.30			[18]
$ThCl_4$	12,900	14.30		974-1043	[5]
$ThCl_4$ (α)[†]	11,929	20.522	3.27	600-679	[6]
$ThCl_4$ (β)[†]	11,859	22.146	3.88	679-1042	[6]
UCl_4[‡]	7223±15	6.77 ±0.02			[38]
UCl_4	10,427	13.2995			[18]
UCl_4[†]	11,571	23.637	4.01	600-863	[6]
UCl_4	11,350	23.21	3.02	298-863	[39]
$NpCl_4$	8920	12.17			[31]

Table S12d. Experimental Tetravalent Actinide (An^{IV}) Liquid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	T range (K)	Ref
$ThCl_4$	7987	9.57			[18]
$ThCl_4$[†]	10,137	30.514	7.20	1042-1224	[6]
$ThCl_4$	7980	9.57		1043-1186	[5]
UCl_4	7205	9.65			[18]
UCl_4[†]	9720	29.332	6.68	863-1068	[6]
UCl_4	9950	28.96	5.53	863-1062	[39]
$NpCl_4$	6220	8.64			[31]

Table S12e. Experimental Pentavalent Actinide (An^{V}) Solid (s) or Liquid (l) Phase Vapor Pressure Coefficients.[§, ‖]

Compound	A	B	C	T range (K)	Ref
$PaCl_5$ (s)	11,162	23.87			[40]
$PaCl_5$ (l)	7377	17.27			[40]
UCl_5 (s)	3307	3.361			[39]
UCl_5 (s)[†]	6957	23.014	4.04		[6]
UCl_5 (s - α)[†]	2586	11.356	1.68	298-367	[6]
UCl_5 (s - β)[†]	2591	11.446	1.71	367-600	[6]

Table S12f. Experimental Hexavalent Uranium (U^{VI}) Solid Phase Vapor Pressure Coefficients.[§, %, &, ‖]

Compound	A	B	C	T range (K)	Ref
UCl_6 (s)	4000	10.20		298-450	[39]
UCl_6 (s)	3788	9.52			[36]
UCl_6 (s)	2422	6.634			[36]
UCl_6 (s)[†]	4710	19.197	3.96		[6]
UCl_6 (s - S_1)[†]	2907	14.417	2.54	298-368	[6]
UCl_6 (s - S_2)[†]	2907	14.417	2.54	368-451	[6]

Table S13a. Computed Tetravalent Actinide (An^{IV}) Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
$(UCl_4)_2$ (G_1)	12,410	31.646	7.50	700-863	[6]
$(UCl_4)_2$ (G_2)	8940	41.426	12.20	863-1154	[6]
$PuCl_4$ (G_1)	9351	17.819	3.47	600-1033	[6]
$PuCl_4$ (G_2)	6948	21.762	5.55	1033-2000	[6]

Table S13b. Computed Pentavalent Uranium (U^V) Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
$(UCl_5)_2$ (G_1)	4587	15.116	3.48	298-600	[6]
$(UCl_5)_2$ (G_2)	4587	15.116	3.48	600-863	[6]
$(UCl_5)_2$ (G_3)	1696	30.352	9.81	863-1154	[6]
$(UCl_5)_2$ (G_4)	5237	8.421	1.14	1154-1700	[6]

Table S13c. Computed Hexavalent Uranium (U^{VI}) Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
UCl_6 (G_1)	1958	7.356	2.25	298-863	[6]
UCl_6 (G_2)	463	14.344	5.22	863-1154	[6]
UCl_6 (G_3)	4118	6.703	0.69	1154-2000	[6]

Table S14a. Thermodynamic Crystalline Phase Trivalent Actinide (An^{III}) Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$AcCl_3$¶	–1053	148.7±6.0	–980.7[Δ, *]		[27]
UCl_3	–863.700±2.000	163.900±2.000	–797.832±2.088	102.520±0.500	[41]
UCl_3	–861.9	159.0	–794.6[Δ, *]	102.5	[6]
$NpCl_3$	–896.800±3.000	160.400±4.000	–829.811±3.237	101.850±4.000	[41]
$PuCl_3$	–959.600±1.800	161.700±3.000	–891.806±2.024	101.200±4.000	[41]
$PuCl_3$	–961.5	159.0	–1008.9	102.9	[6]
$AmCl_3$	–977.800±1.300	146.200±6.000	–905.105±2.290	103.000±10.000	[41]
$CmCl_3$	–974±4	163±6	–901.7[Δ, *]		[42]
$CmCl_3$¶	–969.6±6.7	163.1±6.0	–897.3[Δ, *]		[27]
$BkCl_3$¶	–952±15	164.6±6.0	–878.0[Δ, *]		[27]
$CfCl_3$¶	–965±20	167.2±6.0	–890.9[Δ, *]		[43]
$EsCl_3$¶	–950±24				[27]
$FmCl_3$¶	–963±44				[27]
$MdCl_3$¶	–864±50				[27]
$NoCl_3$¶	–716±50				[27]

Table S14b. Thermodynamic Gas Phase Trivalent Actinide (An^{III}) Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
UCl_3	–523.000±20.000	380.300±10.000	–521.652±20.221	82.400±5.000	[41]
UCl_3	–580.7	357.0	–572.4[Δ, *]	76.1[¶]	[6]
$NpCl_3$	–589.000±10.400	362.800±10.000	–582.357±10.822	78.500±5.000	[41]
$PuCl_3$	–647.400±1.868	368.620±10.000	–641.299±3.598	78.470±5.000	[41]

Table S14c. Thermodynamic Crystalline Phase Tetravalent Actinide (An^{IV}) Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).[‖]

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ThCl_4$ (β)	–1186.300±1.300	183.500±5.000	–1092.293±1.984	120.3±6.0	[44]
$ThCl_4$	–1186.8	190.4	–1095.1[Δ, *]	120.3	[6]
$PaCl_4$	–1044.3				[45]
$PaCl_4$	–1044±13	193.7±4.2	–954±13		[46]
UCl_4	–1018.800±2.500	197.200±0.800	–929.605±2.512	121.800±0.400	[41]
UCl_4	–1018.8	197.2	–929.6[Δ, *]	120.8	[6]
$NpCl_4$	–984.000±1.800	200.000±8.000	–895.562±2.998	122.000±6.000	[41]
$PuCl_4$	–963.6±7.5				[46]
$PuCl_4$	–968.700±5.000	201.000±10.000	–879.368±5.826	121.400±4.000	[41]

Table S14d. Thermodynamic Gas Phase Tetravalent Actinide (An^{IV}) Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ThCl_4$	–951.400±5.166	403.400±4.000	–922.956±5.304	101.4±3.0	[44]
$ThCl_4$	–967.9	397.6	–938.0[Δ, *]	101.6	[6]
UCl_4	–815.400±4.717	409.300±5.000	–789.442±4.947	103.500±3.000	[41]
UCl_4	–1018.8	197.2	–929.6[Δ, *]	120.8	[6]
$(UCl_4)_2$	–1891.6	581.3	–1768.9[Δ, *]	165.0	[6]
$NpCl_4$	–787.000±4.600	423.000±10.000	–765.050±5.487	105.000±5.000	[41]
$PuCl_4$	–792.000±10.000	409.000±10.000	–764.683±10.438	103.400±5.000	[41]
$PuCl_4$	–793.7	412.5	–767.4[Δ, *]	98.0[¶]	[6]

Table S14e. Thermodynamic Crystalline (cr) or Gas (g) Phase Pentavalent Actinide (An^V) Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$PaCl_5$ (cr)	–1147.8±14.4	238.8±8	–1037.2[Δ, *]		[27]
$PaCl_5$ (g)	–1042±15	440.8	–991.7[Δ, *]		[27]
UCl_5 (cr)	–1039.000±3.000	242.700±8.400	–930.115±3.908	150.600±8.400	[41]
UCl_5 (cr)	–1041.5	246.9	–933.9[Δ, *]	114.6	[6]
UCl_5 (g)	–900.000±15.000	438.700±10.000	–849.552±15.074	123.600±5.000	[41]
$(UCl_5)_2$ (g)	–1960.2	707.2	–1808.5[Δ, *]	263.4	[6]

Table S14f. Thermodynamic Crystalline (cr) or Gas (g) Phase Hexavalent Uranium (U^{VI}) Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
UCl_6 (s)	–1066.500±3.000	285.500±1.700	–937.120±3.043	175.700±4.200	[41]
UCl_6 (s)	–1068.2	285.8	–938.9[Δ, *]	175.6	[6]
UCl_6 (g)	–985.500±5.000	438.000±5.000	–901.588±5.218	147.200±3.000	[41]
UCl_6 (g)	–987.8	432.7	–902.3[Δ, *]	142.7	[6]

Table S15a. Di- and Trivalent Actinide (An^{II} and An^{III}) Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap), and Sublimation (sub).[‖]

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
Divalent Actinide							
$AmCl_2$ (α)	17.2						[47]
$AmCl_2$ (β)	15.8						[47]
Trivalent Actinides							
UCl_3	49	43.7	225.9	205.0	263.6	238.5	[18, 47]
UCl_3	48.6	43.7	175.9	95.0	224.5[◊]	138.7[◊]	[6]
$NpCl_3$	50						[47]
$PuCl_3$	63.6	61.5	241.0	241.8	304.6	263.6	[1, 6, 18]
$PuCl_3$	49, 55						[27, 47]
$AmCl_3$	48.1±0.4						[27]
$CmCl_3$	47.9±0.4						[27]

Table S15b. Tetravalent Actinide (An^{IV}) Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap), and Sublimation (sub).[‖]

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
$ThCl_4$	43.9		146.4		190.4[◊]		[1]
$ThCl_4$	94.2[◊]	80.7[◊]	152.7	151.9	246.9	232.6	[18]
$ThCl_4$			146.4	122.6			[18]
$ThCl_4$	61.5	59.0	120.8	98.7	182.3[◊]	157.7[◊]	[6, 27]
$ThCl_4$	94.14	90.8	152.7	127.6	246.9	218.4[◊]	[48]
UCl_4	44.8, 49.8						[1]
UCl_4	49.8	49.8[◊]	150.6	174.5	193.7	224.3	[18, 27]
UCl_4	54.4	63.0	126.8	118.7	181.2[◊]	181.7[◊]	[6]
UCl_4	61.5		138.1		199.6		[48]
$NpCl_4$	59.6	82.1[◊]	123.5±0.8	176.1±7.1	189.5±1.7	258.2±2.1	[27, 49]
$NpCl_4$	55.5[◊]		115.2±3.3		170.7 ±3.4		[31]
$ThCl_{4avg}$[ϕ]	*73.4±25.0*	*76.8±16.2*	*143.8±13.2*	*125.2±21.8*	*216.6±35.1*	*202.9±39.8*	
UCl_{4avg}[ϕ]	*52.1±6.3*		*138.5±11.9*		*191.5±9.4*		

Table S15c. Penta- and Hexavalent Actinide (An^{V} and An^{VI}) Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap), and Sublimation (sub).[‖]

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
Pentavalent Actinides							
$PaCl_5$	31.5	54.7[◊]	61.29	88.3	92.76	143	[27, 40]
UCl_5	35.6	59.3		192.9		252.2[◊]	[6, 27]
Hexavalent Actinide							
UCl_6	20.9	46.4					[6, 27]

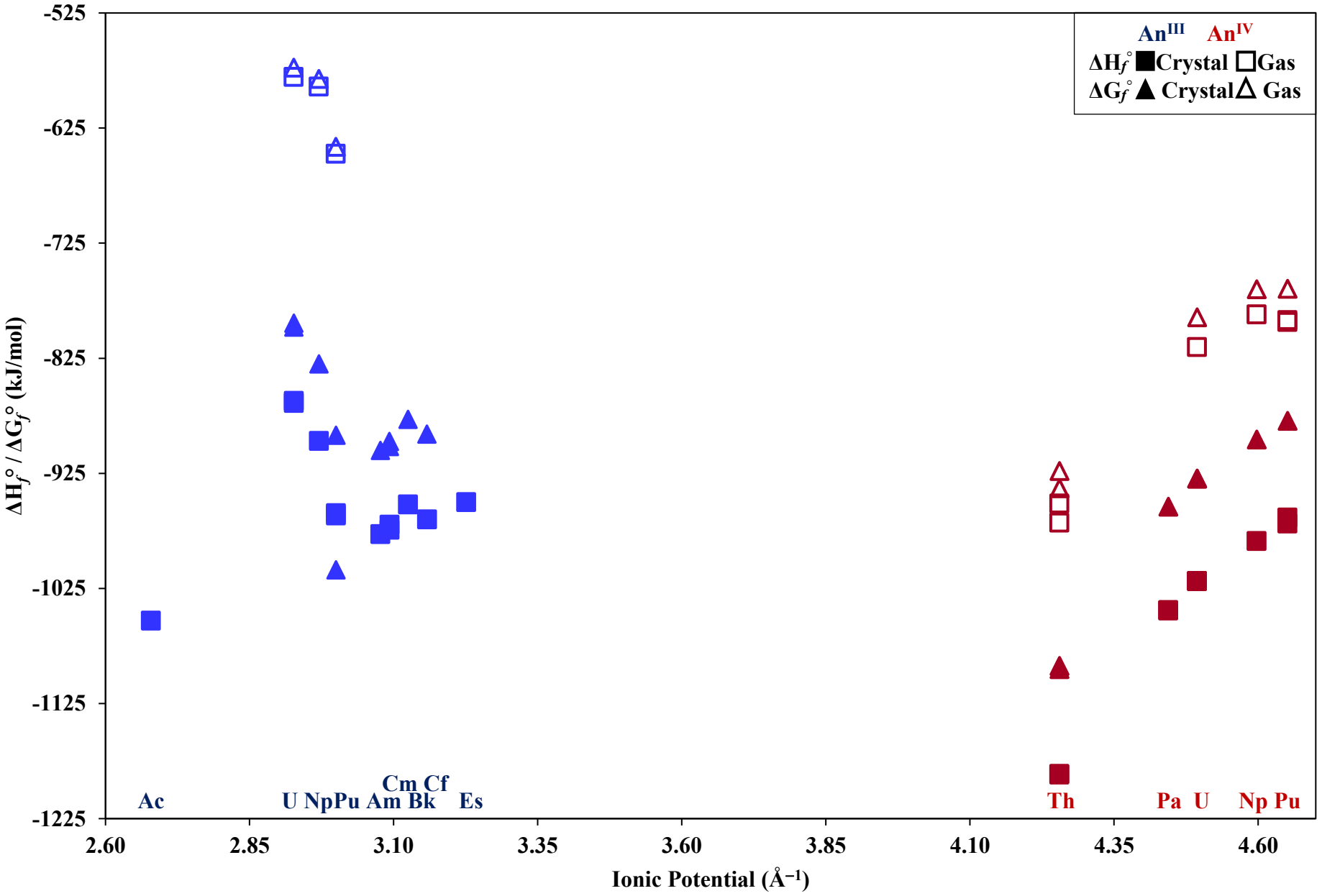

Figure S2. Graphical depiction of enthalpies and Gibbs free energies of formation ($\Delta H_f°$, squares, $\Delta G_f°$, triangles) for the crystalline (solid shapes) and gas phases (empty shapes) in kJ/mol for **An**Cl_x (x = 3, 4) by ionic potential (IP, $Å^{-1}$) using 6-coordinate Shannon ionic radii (CN_6).

CONTAMINANT PRODUCT (CONP) ELEMENT DATA

RARE EARTH (RE) ELEMENTS

FISSION PRODUCTS (FPS)

Table S16. Melting (T_M) and Boiling (T_B) Phase Change Temperatures of Di- and Trivalent Rare Earths.

Compound	T_M (K)	T_B (K)	Ref
Divalent Rare Earths			
$SmCl_2$	1131	2233	[6]
$EuCl_2$	1004		[1]
$YbCl_2$	994	~2200	[1, 6]
Trivalent Rare Earths			
$ScCl_3$	1240	1359	[1, 6]
YCl_3	994	1755	[1]
$LaCl_3$	1131	2023	[1, 48]
$CeCl_3$	1080	2003	[1, 19]
$PrCl_3$	1059	1973	[1, 3]
$NdCl_3$	1032	1873	[1]
$PmCl_3$	928	1943	[1, 48]
$SmCl_3$	955		[1]
$EuCl_3$	896	(dec)	[1, 3]
$GdCl_3$	875	1853	[1, 3]
$TbCl_3$	855	1869	[1, 6]
$DyCl_3$	991	1803	[1]
$HoCl_3$	993	1773	[1]
$ErCl_3$	1049	1750	[1, 6]
$TmCl_3$	1118	1800	[1, 6]
$YbCl_3$	1127	>1573 (dec)	[1, 6]
$LuCl_3$	1198	~1750	[1, 6]

Table S17a. Experimental Solid Phase Vapor Pressure Coefficients of Di- and Trivalent Rare Earths.[§]

Compound	A	B	C	T range (K)	Ref
		Divalent Rare Earths			
$SmCl_2$[†]	17,205	22.728	4.34	1000-1013	[6]
		Trivalent Rare Earths			
$ScCl_3$[†]	13,490	20.350	3.24	700-1240	[6]
$ScCl_3$	14,200	14.37		1065-1233	[5]
YCl_3[†]	16,208	19.289	2.77	900-994	[6]
$LaCl_3$[†]	18,843	27.350	5.04	900-1131	[6]
$LaCl_3$	19,040	36.20	7.05	298-1131	[5]
$CeCl_3$[†]	18,142	25.358	4.54	900-1080	[6]
$CeCl_3$	18,750	36.38	7.05	298-1080	[5]
$PrCl_3$[†]	18,151	28.097	5.39	900-1059	[6]
$PrCl_3$	18,490	36.31	7.05	298-1059	[5]
$NdCl_3$[†]	17,856	26.563	4.90	900-1032	[6]
$NdCl_3$	18,220	36.27	7.05	298-1032	[5]
$SmCl_3$[†]	5362	13.153	2.98	400-950	[6]
$EuCl_3$[†]	15,213	23.117	3.85	800-897	[6]
$GdCl_3$[†]	16,949	22.850	3.77	875	[6]
$TbCl_3$[†,a]	16,247	25.385	4.78	800-855	[6]
$DyCl_3$[†]	17,297	21.583	3.22	900-924	[6]
$HoCl_3$[†]	15,695	19.188	2.79	800-993	[6]
$ErCl_3$[†]	15,816	21.658	3.57	800-1049	[6]
$TmCl_3$[†]	15,992	19.386	2.90	900-1101	[6]
$YbCl_3$[†]	17,268	19.980	2.58	900-1148	[6]

[a]Designated as "B" in the primary literature.

Table S17b. Experimental Liquid Phase Vapor Pressure Coefficients for Di- and Trivalent Rare Earths.[§]

Compound	A	B	C	T range (K)	Ref
		Divalent Rare Earths			
$SmCl_2$	16,807	24.709	5.13	1013-2000	[6]
		Trivalent Rare Earths			
$ScCl_3$	12,104	31.467	7.20	1240-1359	[6]
YCl_3	17,157	38.319	8.80	994-1757	[6]
$LaCl_3$	17,750	38.476	9.00	1131-2045	[6]
$CeCl_3$	17,705	37.481	8.67	1080-1997	[6]
$PrCl_3$	15,442	25.266	5.30	1059-1982	[6]
$NdCl_3$	16,105	30.893	6.90	1032-1976	[6]
$EuCl_3$	13,395	27.498	6.02	897-1300	[6]
$GdCl_3$	15,971	30.648	6.80	875-1919	[6]
$TbCl_3$	15,664	30.596	6.79	855-1869	[6]
$DyCl_3$	16,585	32.586	7.19	924-1810	[6]
$HoCl_3$	15,270	31.917	7.18	993-1780	[6]
$ErCl_3$	15,605	34.537	7.90	1049-1750	[6]
$TmCl_3$	16,009	34.611	7.90	1101-1800	[6]
$YbCl_3$	14,971	24.283	4.64	1148-1300	[6]

Table S18a. Divalent Rare Earth (RE^{II}) Thermodynamic Crystalline Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$LaCl_2$	–501.732	125.94	–455.82[Δ, *]	75.82	[52]
$CeCl_2$	–554.807	131.80	–506.14[Δ, *]	76.26	[52]
$PrCl_2$	–669.969	131.78	–620.94[Δ, *]	77.03	[52]
$NdCl_2$	–693.128	130.82	–644.32[Δ, *]	77.20	[52]
$NdCl_2$		140.1±0.5		77.77±0.30	[54]
$PmCl_2$	–754.793	127.69	–705.05[Δ, *]	78.64	[52]
$SmCl_2$	–802.961	122.59	–752.27[Δ, *]	84.64	[52]
$SmCl_2$		132.2±0.4		84.41±0.3	[54]
$EuCl_2$	–822.635	127.85	–771.07[Δ, *]	75.00	[52]
$EuCl_2$		138.3±0.8		75.23±0.4	[54]
$GdCl_2$	–488.280	134.58	–441.61[Δ, *]	82.10	[52]
$TbCl_2$	–596.497	140.28	–550.00[Δ, *]	75.92	[52]
$DyCl_2$	–687.686	145.21	–641.95[Δ, *]	76.60	[52]
$DyCl_2$		144.2±0.6		77.30±0.3	[54]
$HoCl_2$	–664.380	144.20	–618.43[Δ, *]	76.51	[52]
$TmCl_2$	–712.281	137.07	–664.59[Δ, *]	76.77	[52]
$TmCl_2$		135.1±0.3		76.68±0.2	[54]
$YbCl_2$	–782.489	119.98	–733.90[Δ, *]	75.76	[52, 62]
$YbCl_2$	–799.6	130.5	–754.1[Δ, *]	82.9	[62]
$YbCl_2$	–799.1	122.6	–751.3[Δ, *]	74.2	[6]
$YbCl_2$		120.0±0.6		75.73±0.4	[54]
$LuCl_2$	–431.872	125.17	–387.49[Δ, *]	75.70	[52]
$YbCl_{2avg}$[ϕ]	*–791.0±9.7*	*123.5±5.0*	*–744.0±10.9*	*78.1±3.9*	

Table S18b. Trivalent Rare Earth (RE^{III}) Thermodynamic Crystalline Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ScCl_3$	–925.1	127.2	–852.9	91.6	[1, 50]
$ScCl_3$	–918.8	121.3	–844.8$^{\Delta, *}$	92.1	[6]
YCl_3	–1000.0	140.2	–928.8$^{\Delta, *}$	92.0	[1][6]
YCl_3	–973.6	137.7	–901.6$^{\Delta, *}$	92.0	[51]
$LaCl_3$	–1071.6±1.5	137.90	–996.0$^{\Delta, *}$	97.81	[52]
$LaCl_3$	–1070.7	137.7	–995.0$^{\Delta, *}$	98.1	[6]
$LaCl_3$	–1072.2			108.8	[1]
$CeCl_3$	–1060.1±1.5	151.83	–984.2$^{\Delta, *}$	98.11	[52]
$CeCl_3$	–1053.5	150.6	–977.2$^{\Delta, *}$	87.8	[6]
$CeCl_3$	–1060.5	151.0	–984.8	87.4	[1]
$PrCl_3$	–1057.5±1.5	154.34	–982.0$^{\Delta, *}$	98.46	[52]
$PrCl_3$	–1056.9	153.3	–981.0$^{\Delta, *}$	98.9	[6]
$PrCl_3$	–1056.9	153.3	–980.8	98.97	[1, 53]
$NdCl_3$	–1041.1±1.0	154.25	–966.0$^{\Delta, *}$	99.40	[52]
$NdCl_3$	–1041.8	153.5	–966.5$^{\Delta, *}$	99.2	[6]
$NdCl_3$	–1041.0	143.9	–962.8$^{\Delta, *}$	96.2	[51]
$NdCl_3$	–1041.8	153.4	–966.6	99.1	[55]
$NdCl_3$	–1041.0			113.0	[1]
$PmCl_3$	–1033.7±10	153.57	–958.4$^{\Delta, *}$	98.74	[52]
$SmCl_3$	–1025.3±2.0	150.47	–949.7$^{\Delta, *}$	99.45	[52]
$SmCl_3$	–1025.9	147.7	–949.4$^{\Delta, *}$	99.5	[6]
$SmCl_3$	–1025.9	150.1	–950.2	99.5	[1, 56]
$EuCl_3$	–935.4±3.0	144.18	–855.5$^{\Delta, *}$	106.93	[52]
$EuCl_3$	–936.0	144.1	–856.0$^{\Delta, *}$	107.0	[1][6]
$EuCl_3$	–922.2	125.5	–836.6$^{\Delta, *}$	98.3	[51]

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$GdCl_3$	–1023.3±1.5	151.95	–948.6[Δ, *]	97.42	[52]
$GdCl_3$	–1008.0	151.5	–933.1[Δ, *]	97.8	[6]
$GdCl_3$	–1008.0	151.4	–993.1	88.0	[1][57]
$TbCl_3$	–1010.6±3.0	155.38	–935.4[Δ, *]	97.76	[52]
$TbCl_3$	–997.0	153.1	–921.0[Δ, *]	97.5	[6]
$TbCl_3$	–997.0	153.1	–921.1	97.5	[1, 58]
$DyCl_3$	–992.4±3.0	168.80	–920.4[Δ, *]	98.90	[52]
$DyCl_3$	–998.3	150.8	–920.9[Δ, *]	97.1	[6]
$DyCl_3$	–989.9	154.0	–913.7	97.1	[59]
$DyCl_3$	–1000.0				[1]
$HoCl_3$	–997.5±2.5	167.86	–925.4[Δ, *]	99.28	[52]
$HoCl_3$	–1005.4	154.0	–929.1[Δ, *]	96.2	[6]
$HoCl_3$	–1005.4	154.0	–929.2	96.2	[60]
$HoCl_3$	–1105.4			88.0	[1]
$ErCl_3$	–995.5±2.0	166.71	–923.6[Δ, *]	99.15	[52]
$ErCl_3$	–994.5	154.8	–919.1[Δ, *]	98.1	[6]
$ErCl_3$	–994.5	152.7	–918.5	98.1	[59]
$ErCl_3$	–998.7			100.0	[1]
$TmCl_3$	–996.2±2.5	164.47	–923.4[Δ, *]	99.23	[52]
$TmCl_3$	–988.1	159.0	–913.7[Δ, *]	97.7[¶]	[6]
$TmCl_3$	–986.6	146.9	–908.5	97.7	[1, 61]
$YbCl_3$	–959.2±3.0	159.48	–889.1[Δ, *]	99.49	[52]
$YbCl_3$	–961.1	135.1	–883.7[Δ, *]	95.4	[6]
$YbCl_3$	–959.8	147.7	–886.2	95.3	[1, 62]
$LuCl_3$	–984.2±2.5	142.75	–911.8[Δ, *]	98.23	[52]
$LuCl_3$	–987.1 ±2.5	84.22	–897.3[Δ, *]		[63, 64]
$LuCl_3$	–945.6				[1]

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ScCl_{3avg}^{\phi}$	–923.0±3.6				
YCl_{3avg}^{ϕ}	–991.2±15.2				
$LaCl_{3avg}^{\phi}$	–1071.5±0.8			101.6±6.3	
$CeCl_{3avg}^{\phi}$	–1058.0±3.9	151.1±0.6	–982.1±4.2	91.1±6.1	
$PrCl_{3avg}^{\phi}$	–1056.9±0.0			99.3±0.6	
$NdCl_{3avg}^{\phi}$	–1041.3±0.4	151.3±4.9	–965.5±1.8	101.4±6.6	
$SmCl_{3avg}^{\phi}$	–1025.8±0.3	149.4±1.5	–949.8±0.4	99.5±0.0	
$EuCl_{3avg}^{\phi}$	–932.4±6.8	137.9±10.8	–849.4±11.0	104.1±5.0	
$GdCl_{3avg}^{\phi}$	–1011.8±7.6	151.6±0.3	–958.3±31.2	92.8±5.6	
$TbCl_{3avg}^{\phi}$	–1000.4±6.8	153.9±1.3	–925.8±8.3	97.6±0.2	
$DyCl_{3avg}^{\phi}$	–995.2±4.8	157.9±9.6	–918.3±4.0	97.7±1.0	
$HoCl_{3avg}^{\phi}$	–1028.4±51.5	158.6±8.0	–927.9±2.2	94.9±4.8	
$ErCl_{3avg}^{\phi}$	–995.8±2.0	158.1±7.6	–920.4±2.8	98.8±0.9	
$TmCl_{3avg}^{\phi}$	–989.4±4.6	156.8±9.0	–915.2±7.6	98.2±0.9	
$YbCl_{3avg}^{\phi}$	–960.0±1.0	147.4±12.2	–886.3±2.7	96.7±2.4	
$LuCl_{3avg}^{\phi}$	–972.3±23.2				

Table S18c. Divalent Rare Earth (RE^{II}) Gas Phase Enthalpy of Formation (ΔH_f^o, kJ/mol).

Compound	ΔH_f^o	Ref
$LaCl_2$	–326.632	[52]
$CeCl_2$	–320.473	[52]
$PrCl_2$	–353.737	[52]
$NdCl_2$	–355.198	[52]
$PmCl_2$	–417.371	[52]
$SmCl_2$	–463.376	[52]
$EuCl_2$	–480.500	[52]
$GdCl_2$	–315.709	[52]
$TbCl_2$	–310.258	[52]
$DyCl_2$	–361.738	[52]
$HoCl_2$	–360.580	[52]
$ErCl_2$	–362.122	[52]
$TmCl_2$	–386.234	[52]
$YbCl_2$	–453.600	[52]
$LuCl_2$	–281.362	[52]

Table S18d. Trivalent Rare Earth (RE^{III}) Thermodynamic Gas Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
YCl_3	–698.2	351.5	–690.0[Δ, *]	77.8	[6]
$LaCl_3$	–730.3	364.5	–722.2[Δ, *]	78.4	[6]
$LaCl_3$	–731.3				[52]
$CeCl_3$	–723.0	370.7	–712.3[Δ, *]	78.4	[6]
$CeCl_3$	–729.0				[52]
$PrCl_3$	–731.0	374.0	–720.9[Δ, *]	78.4	[6]
$PrCl_3$	–727.9				[52]
$NdCl_3$	–719.1	374.4	–709.6[Δ, *]	78.3	[6]
$NdCl_3$	–718.8	374.4	–709.5	78.3	[55]
$NdCl_3$	–709.3				[52]
$PmCl_3$	–701.7				[52]
$SmCl_3$	–710.3				[52]
$EuCl_3$	–658.1	363.7	–643.6[Δ, *]	88.0	[6]
$EuCl_3$	–660.4				[52]
$GdCl_3$	–696.6	371.5	–687.3[Δ, *]	78.2	[6]
$GdCl_3$	–709.8				[52]
$TbCl_3$	–691.2	375.3	–803.1	78.2	[6, 58]
$TbCl_3$	–702.3				[52]
$DyCl_3$	–677.4	379.9	–668.4[Δ, *]	78.2	[6]
$DyCl_3$	–677.4	376.5	–667.5	78.1	[59]
$DyCl_3$	–691.5				[52]
$HoCl_3$	–712.9	363.6	–699.1[Δ, *]	78.2	[6]
$HoCl_3$	–682.4	377.4	–672.8	78.2	[60]
$HoCl_3$	–694.2				[52]

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ErCl_3$	–703.9	363.6	–690.7[Δ, *]	78.1	[6]
$ErCl_3$	–674.0	376.2	–664.6	78.1	[59]
$ErCl_3$	–693.1				[52]
$TmCl_3$	–691.1	364.6	–678.0[Δ, *]	78.1	[6]
$TmCl_3$	–665.7	374.1	–655.4	78.1	[61]
$TmCl_3$	–694.7				[52]
$YbCl_3$	–638.9	370.0	–749.2	78.1	[6, 62]
$YbCl_3$	–652.3				[52]
$LuCl_3$	–626.3	352.5	–616.4[Δ, *]	78.1	[6]
$LuCl_3$	–678.4				[52]
$NdCl_{3avg}$[ϕ]	*–715.7±5.6*				
$TbCl_{3avg}$[ϕ]	*–694.9±6.4*				
$DyCl_{3avg}$[ϕ]	*–682.1±8.1*				
$HoCl_{3avg}$[ϕ]	*–696.5±15.4*				
$ErCl_{3avg}$[ϕ]	*–690.3±15.1*				
$TmCl_{3avg}$[ϕ]	*–683.8±15.8*				
$YbCl_{3avg}$[ϕ]	*–643.4±7.7*				

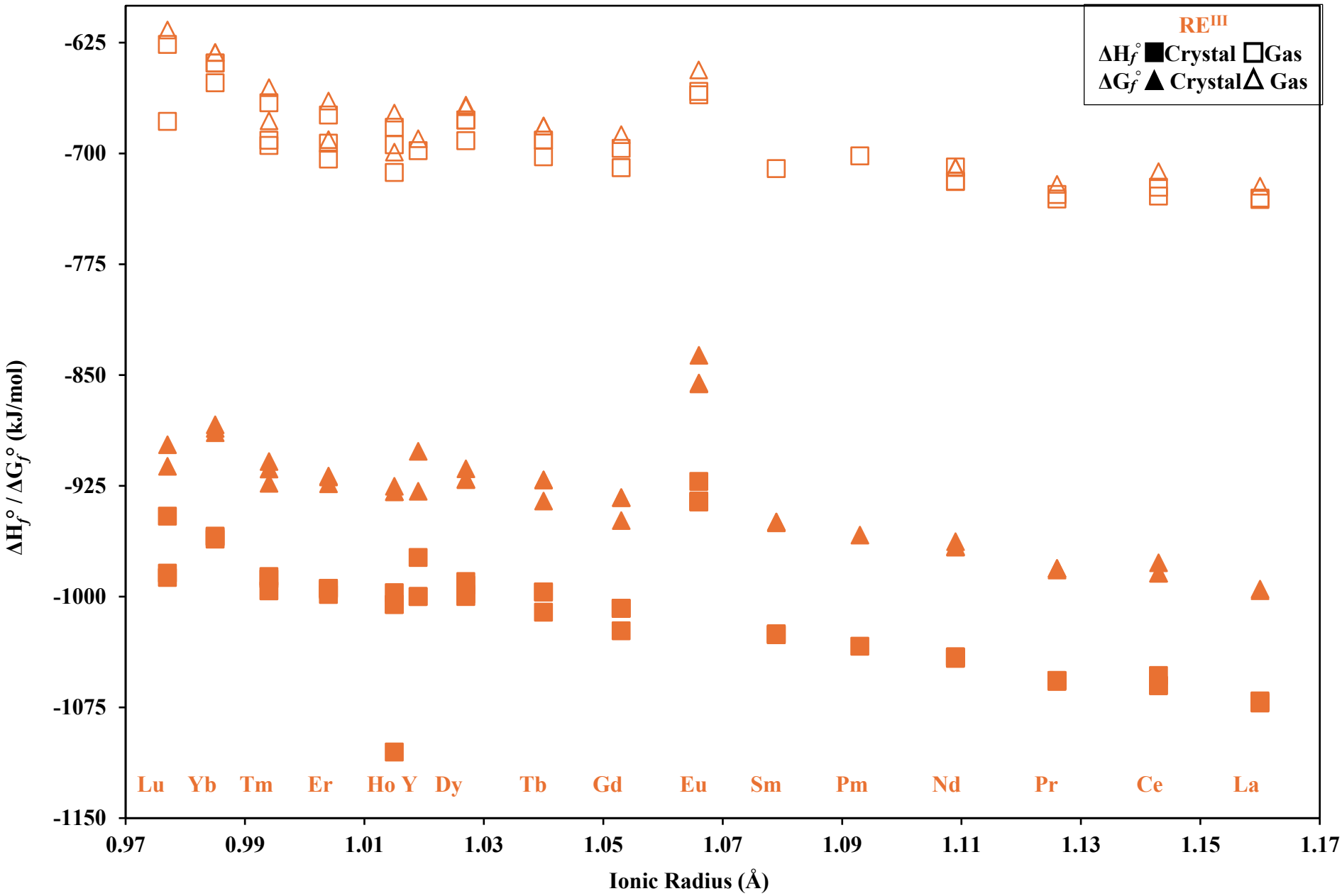

Figure S3. Graphical depiction of enthalpies and Gibbs free energies of formation ($\Delta H_f°$, squares, $\Delta G_f°$, triangles) for the crystalline (solid shapes) and gas phases (empty shapes) in kJ/mol of rare earth chlorides, $\mathbf{RE^{III}}Cl_3$, by 8-coordinate Shannon ionic radii (CN_8).

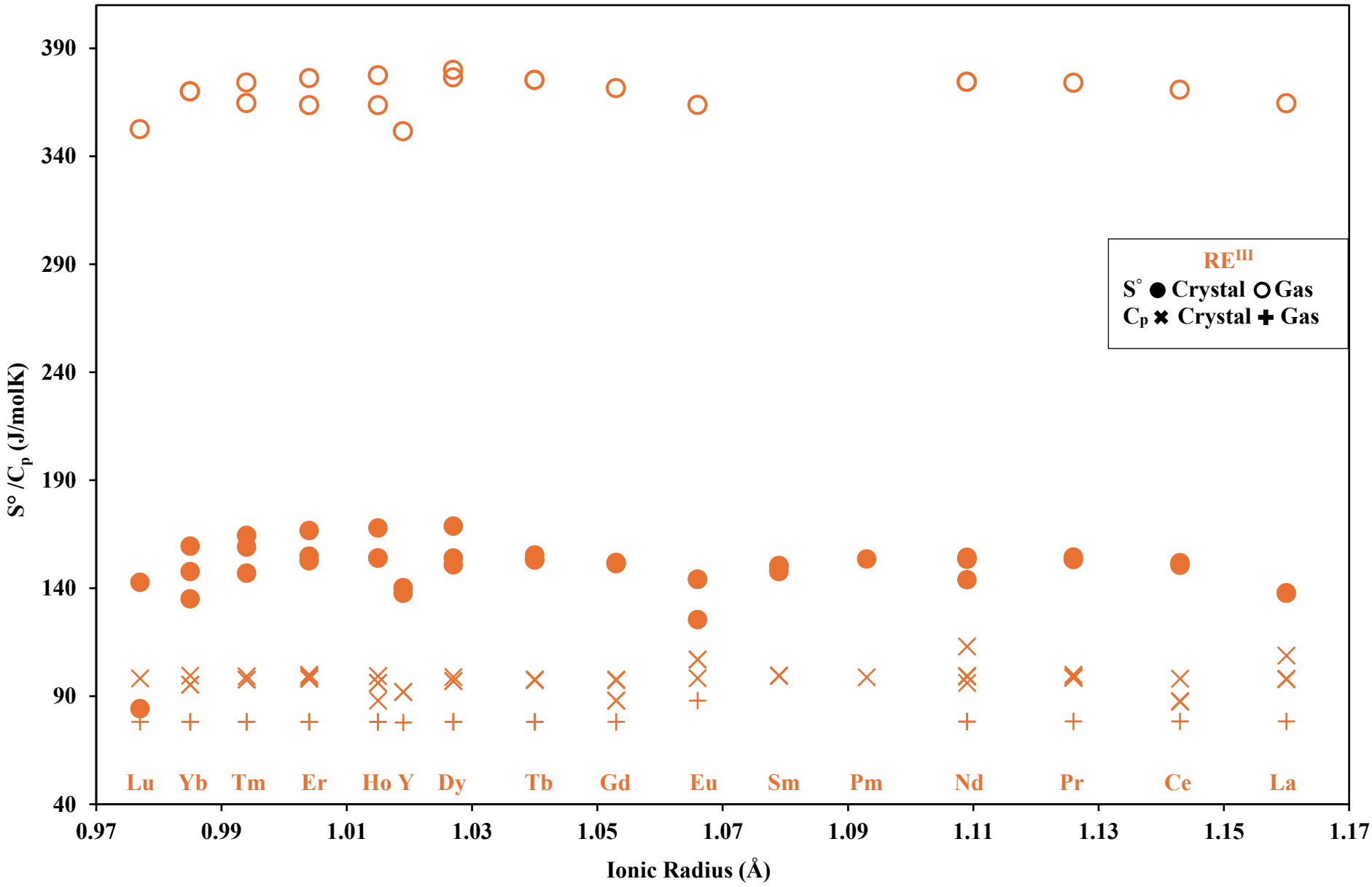

Figure S4. Graphical depiction absolute entropies (S°, circles) and molar heat capacities (C_p, ×, +) for crystalline (solid shapes) and gas phases (empty shapes) in J/molK of rare earth chlorides, $\mathbf{RE^{III}Cl_3}$, by 8-coordinate Shannon ionic radii (CN_8).

Table S19a. Divalent Rare Earth (RE^{II}) Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap) and Sublimation (sub).

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
$LaCl_2$	38.0		137.1◊		175.1		[52]
$CeCl_2$	38.3		197.2◊		235.5		[52]
$PrCl_2$	38.7		277.2◊		315.9		[52]
$NdCl_2$	39.0		298.7◊		337.7		[52]
$PmCl_2$	39.4		298.2◊		337.6		[52]
$SmCl_2$	14.2	14.0	324.5◊	101.3	338.7	115.3◊	[6, 52]
$EuCl_2$	23.0		320.7◊		343.7		[52]
$GdCl_2$	40.6		133.1◊		173.7		[52]
$TbCl_2$	35.0		253.2◊		288.2		[52]
$DyCl_2$	34.1		292.6◊		326.7		[52]
$HoCl_2$	33.3		270.3◊		303.6		[52]
$ErCl_2$	32.4		246.1◊		278.5		[52]
$TmCl_2$	31.1		294.4◊		325.5		[52]
$YbCl_2$	31.1		297.3◊		328.4		[52]
$LuCl_2$	29.8		119.9◊		149.7		[52]

Table S19a. Trivalent Rare Earth (RE^{III}) Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap) and Sublimation (sub).

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
$ScCl_3$	67.4	54.3	150.4	110.6	217.8◊	164.9◊	[6]
YCl_3	31.5	31.7	200.1	113.7	231.6◊	231.8◊	[6]
$LaCl_3$	58.0	51.3		91.2		142.5◊	[6]
$LaCl_3$	55.7		284.6◊		340.3		[52]
$CeCl_3$	45.2	41.8		97.8		139.6◊	[6]
$CeCl_3$	55.5		275.6◊		331.1		[52]
$PrCl_3$	50.6	47.8		105.1		152.9◊	[6]
$PrCl_3$	52.1		277.5◊		329.6		[52]
$NdCl_3$	50.2	48.7		98.7		147.4◊	[6]
$NdCl_3$	48.1		283.7◊		331.8		[52]
$PmCl_3$	47.8		284.2◊		332.0		[52]
$SmCl_3$	46.0	48.4					[6]
$SmCl_3$	47.6		267.4◊		315.0		[52]
$EuCl_3$	51.0	56.9					[6]
$EuCl_3$	45.0		230.0◊		275.0		[52]
$GdCl_3$	40.7	46.5		102.9		149.4◊	[6]
$GdCl_3$	40.6		272.9◊		313.5		[52]
$TbCl_3$	25.0	29.3	194.9	104.3	219.9◊	133.6◊	[6]
$TbCl_3$	33.4		274.9◊		308.3		[52]
$DyCl_3$	24.2		276.9◊		300.9		[52]
$DyCl_3$	43.9	47.5	209.5	115.7	253.4◊	163.2◊	[6]
$HoCl_3$	30.543		272.8◊		303.3		[52]
$HoCl_3$	44.3	44.6	186.2	104.6	230.5◊	149.2◊	[6]
$ErCl_3$	36.4		266.0◊		302.4		[52]
$ErCl_3$	41.7	39.8	183.8	105.0	225.5◊	144.8◊	[6]
$TmCl_3$	35.6		265.9◊		301.5		[52]
$TmCl_3$	45.3	41.2	188.3	104.6	233.6◊	145.8◊	[6]
$YbCl_3$	35.982		270.9◊		306.9		[52]
$YbCl_3$	63.6	55.4	243.3		306.9◊		[6, 52]
$LuCl_3$	39.33		266.47◊		305.8		[52]

TRANSITION METAL (TM) ELEMENTS

FISSION PRODUCTS (FPS)

Table S20. Melting (T_M), Boiling (T_B), Sublimation (T_{sub}), and Triple Point (T_{TP}) Phase Change Temperatures.

Compound	T_M (K)	T_B (K)	T_{sub} (K)	T_{TP} (K)	Ref
$ZrCl_2$	995	1564			[1, 6]
$ZrCl_3$	900				[1]
$ZrCl_4$	700[a]		604	710	[1, 6]
$MoCl_2$	773 (dec)				[1]
$MoCl_3$	673 (dec)				[1, 48]
$MoCl_4$	590	595	554		[1, 6, 48]
$MoCl_5$	467	541			[1]
$TcCl_4$		573			[3]
$TcCl_5$		505			[19]
$RuCl_3$	~773 (dec)				[1, 19]
$RhCl_3$	~723	990			[1]
$PdCl_2$	952				[1]
AgCl	728	1820			[1]
$CdCl_2$	841	1237			[1]

[a]Under increased pressure, 17.9 bar.

Table S21a. Experimental Solid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	D	T range (K)	Ref
$ZrCl_2$[†]	12,761	17.490	2.66		700-1000	[6]
$ZrCl_2$	8500	16.61	1.50		298-995	[5]
$ZrCl_3$[†]	6979	23.644	4.86		400-714	[6]
$ZrCl_4$[†]	6134	17.869	2.80		400-609	[6]
$MoCl_2$[†]	10,792	31.381	7.30		600-1219	[6]
$MoCl_3$[†]	12,630	55.648	14.16		500-926	[6]
$MoCl_4$[†]	6279	20.785	3.73		400-603	[6]
$MoCl_5$[†]	4978	22.315	4.79		298-470	[6]
$MoCl_5$	5210	13.1			298-467	[5]
$RuCl_3$[†]	8870	15.800	2.59		500-1123	[6]
$RuCl_3$	16,750	30.53	4.63		298-1000	[5]
$RhCl_3$[†]	10,151	18.377	3.26		500-1221	[6]
$PdCl_2$[†]	9418	15.215	2.37		600-952	[6]
AgCl	11,830	12.39	0.30	–1.02	298-455	[5]
$CdCl_2$[†]	10,179	17.689	2.79		600-842	[6]
$CdCl_2$	9270	17.46	2.11		298-842	[5]

Table S21b. Experimental Liquid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	T range (K)	Ref
$ZrCl_2$[†]	10,851	17.831	3.41	1000-1564	[6]
$ZrCl_2$	8440	26.37	5.03	995-1564	[5]
$PdCl_2$[†]	8765	16.819	3.14	952-1232	[6]
AgCl[†]	10,750	13.332	2.29	730-1835	[6]
AgCl	11,320	17.34	2.55	455-1547	[5]
$CdCl_2$[†]	9335	25.579	5.83	842-1236	[6]
$CdCl_2$	9183	25.907	5.04	842-1236	[5]

Table S22. Computed Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
$ZrCl_2$	12,637	7.429	0.93	1564-2000	[6]
$ZrCl_3$ (G_1)	10,369	18.859	2.96	600-714	[6]
$ZrCl_3$ (G_3)	6681	2.898	0.10	1564-2000	[6]
$ZrCl_4$	17,718	3.328	–0.37	1400-2000	[6]
$MoCl_2$ (G_1)	20,008	21.784	3.93	1100-1219	[6]
$MoCl_2$ (G_2)	16,089	14.465	2.60	1219-2000	[6]
$MoCl_3$ (G_1)	16,243	38.973	9.23	800-926	[6]
$MoCl_3$ (G_3)	7357	3.979	0.51	1219-2000	[6]
$MoCl_4$ (G_1)	4237	30.870	8.20	603-926	[6]
$MoCl_4$ (G_2)	11,183	2.538	–0.51	1219-2000	[6]
$MoCl_4$ (G_3)	7280	3.636	0.42	1219-2000	[6]
$RuCl_3$ (G_1)	16,502	32.048	6.15	800-1123	[6]
$PdCl_2$ (G_1)	15,653	18.146	2.50	800-952	[6]
$PdCl_2$ (G_2)	15,024	19.898	3.31	952-1232	[6]
$PdCl_2$ (G_3)	6303	3.579	0.32	1232-1825	[6]

Table S23a. Thermodynamic Crystalline Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ZrCl_2$	–502.0				[1]
$ZrCl_2$	–431.0	110.0	–385.7[Δ, *]	72.6	[6, 65]
$ZrCl_3$	–711.9	145.9	–644.0[Δ, *]	96.2	[6]
$ZrCl_3$	–714.2	145.8	–646.3	96.2	[65]
$ZrCl_4$	–980.5	181.6	–889.9	119.8	[1]
$ZrCl_4$	–980.5	181.6	–890.0[Δ, *]	119.9	[6]
$MoCl_2$	–279.7	116.3	–239.3[Δ, *]	74.6	[6]
$MoCl_3$	–428.1	124.7	–356.9[Δ, *]	94.8	[6]
$MoCl_4$	–494.7	182.9	–407.6[Δ, *]	124.4	[6]
$MoCl_4$	–477.0	223.8	–402.2	129.7	[65]
$MoCl_5$	–527.1	238.5	–423.4[Δ, *]	155.5	[6]
$MoCl_5$	–527.2	238.5	–423.5	155.6	[65]
$MoCl_6$	–523.0	255.2	–391.0	175.3	[65]
$RuCl_3$	–205.0				[1]
$RuCl_3$	–246.7	121.9	–174.8[Δ, *]	115.1[¶]	[6]
$RuCl_3$	–230.1	127.1	–159.7	92.2	[66]
$RhCl_3$	–299.2	126.8	–227.8	92.2	[1, 66]
$RhCl_3$	–274.6	122.1	–201.8[Δ, *]	92.2[¶]	[6]
$PdCl_2$	–173.2	104.5	–126.6[Δ, *]	75.3[¶]	[6]
$PdCl_2$	–198.7	104.2	–152.0	75.3	[53]
AgCl	–127.0	96.3	–109.8	50.8	[1]
AgCl	–127.1	96.2	–109.8[Δ, *]	53.0	[6]
$CdCl_2$	–391.5	115.3	–343.9	74.7	[1]
$CdCl_2$	–391.5	115.3	–343.9[Δ, *]	74.6	[6]
$RuCl_{3avg}$[ϕ]	*–227±21*				

Table S23b. Thermodynamic Liquid Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ZrCl_2$	–411.6	122.5	–370.0	91.0	[65]
$MoCl_4$	–462.8	245.5	–394.5	146.4	[65]
$MoCl_5$	–510.1	273.8	–416.9	175.7	[65]

Table S23c. Thermodynamic Gas Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$ZrCl_2$	–195.1	292.6	–204.2[Δ, *]	57.7	[6]
$ZrCl_2$	–186.2	292.6	–195.3	57.7	[65]
$ZrCl_3$	–522.0	339.3	–511.8[Δ, *]	76.0	[6]
$ZrCl_3$	–524.3	339.3	–514.1	76.0	[65]
$ZrCl_4$	–870.0	367.7	–835.0[Δ, *]	98.2	[6, 65]
$MoCl_2$	+83.1	294.0	+70.5[Δ, *]	67.4	[6]
$MoCl_3$	–149.6	332.5	–140.4[Δ, *]	76.1	[6]
$MoCl_4$	–384.1	371.8	–353.4[Δ, *]	98.1	[6]
$MoCl_4$	–384.9	371.9	–354.3	98.1	[65]
$MoCl_5$	–447.3	398.2	–391.2[Δ, *]	121.2	[6]
$MoCl_5$	–447.7	397.8	–391.5	119.5	[65]
$MoCl_6$	–461.4	419.8	–378.5[Δ, *]	142.7	[6]
$MoCl_6$	–439.3	419.7	–356.4	144.1	[65]
$RuCl_3$	+56.1	397.6	+45.8[Δ, *]	55.8[¶]	[6]
$RuCl_3$	+79.1	328.4	+89.4	55.2	[66]
$RuCl_4$	–79.9	374.2	–49.9	63.4	[66]
$PdCl_2$	+117.6	307.0	+103.8[Δ, *]	60.6[¶]	[6]
AgCl	+89.0	246.1	+61.6[Δ, *]	35.8[b]	[6]
$CdCl_2$	–205.2	294.7	–211.1[Δ, *]	58.1	[6]

Table S24. Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap) and Sublimation (sub).

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
$ZrCl_2$	42.7	42.7	163.6	104.6	206.3◊	147.3◊	[6]
$ZrCl_4$					103.1	169.2	[6]
$MoCl_4$					101.5	168.4	[6]
$MoCl_5$		40.2					[6]
$PdCl_2$	18.4	19.3					[6]
AgCl	13.2	18.1	171.7	93.6	184.9◊	111.7◊	[6]
$CdCl_2$	37.3	44.3	118.9	96.2	156.2◊	140.5◊	[6]

CORROSION PRODUCTS (CORPS)

Table S25. Melting (T_M), Boiling (T_B), and Sublimation (T_{sub}) Phase Change Temperatures.

Compound	T_M (K)	T_B (K)	T_{sub} (K)	Ref
$TiCl_2$	1308	1773		[1]
$TiCl_3$	698 (dec)	1233		[1]
$TiCl_4$	249.03	409.60		[1]
VCl_2	1623		1183	[1]
VCl_3	773 (dec)			[1]
VCl_4	245	424		[1]
$CrCl_2$	1097	1393		[1]
$CrCl_3$	1100	1573 (dec)		[1]
$MnCl_2$	923	1463		[1]
$FeCl_2$	950	1296		[1]
$FeCl_3$	580.75	~589		[1]
$CoCl_2$	1010	1322		[1]
$NiCl_2$	1304		1258	[1]
CuCl	696	1763		[1]
$CuCl_2$	871	1266		[1]
$NbCl_3$			763	[67]
$NbCl_4$	1073 (dec)		548[a]	[1]
$NbCl_5$	478.95	520.56		[1]
$TaCl_3$	713 (dec)			[1]
$TaCl_4$	573 (dec)			[1]
$TaCl_5$	489	512		[1]
WCl_2	773 (dec)			[1]
WCl_3	823 (dec)			[1]
WCl_4	723 (dec)			[1]
WCl_5	526	559		[1]
WCl_6	555	610		[1]

[a]Under reduced pressure, ca. 10^{-4} mmHg.

Table S26a. Experimental Solid Phase Vapor Pressure Coefficients.[§, %, &]

Compound	A	B	C	D	T range (K)	Ref
$TiCl_2$ (S_1)[†]	12,980	21.437	3.56		700-1166	[6]
$TiCl_2$ (S_2)[†]	13,299	23.489	4.14		1166-1246	[6]
$TiCl_2$	15,230	19.36	2.51		298-1308	[5]
$TiCl_3$	9620	21.47	3.27		298-698	[5]
VCl_2[†]	9720	5.735			800-1620	[6]
VCl_3[†]	9659	20.260	3.28		500-916	[6]
$CrCl_2$[†]	14,005	17.727	2.53		800-1088	[6]
$CrCl_2$	14,000	15.14	0.62	–0.58	298-1097	[5]
$CrCl_3$[†]	15,876	23.851	3.83		800-1088	[6]
$CrCl_3$	13,950	17.49	0.73	–0.77	298-1218	[5]
$MnCl_2$[†]	11,792	17.628	2.81		700-923	[6]
$FeCl_2$	9890	11.10			670-740	[5]
Fe_2Cl_6	9540	45.53	9.5		298-580	[5]
$CoCl_2$	14,150	30.10	5.03		298-1010	[5]
$NiCl_2$[†]	12,715	17.305	2.25		700-1228	[6]
$NiCl_2$	13,300	21.88	2.68		298-1258	[5]
$CuCl_2$ (S_1)[†]	8419	9.044	–0.12		500-683	[6]
$CuCl_2$ (S_2)[†]	8940	8.984	–0.41		683-709	[6]
$CuCl_2$ (S_3)[†]	9569	9.017	–0.71		709-862	[6]
$NbCl_4$[†]	6870	9.425			400-602	[6]
$NbCl_4$[†]	6800	17.845	2.91		400-602	[6]
$NbCl_4$	6870	12.30			577-631	[5]
$NbCl_5$	5296	18.617	2.99		298-479	[6]
$NbCl_5$	4370	11.51			403-479	[5]
$TaCl_3$[†]	8877	19.414	3.27		500-912	[6]
$TaCl_4$[†]	5622	18.905	3.22		298-559	[6]
$TaCl_5$[†]	5288	18.359	2.88		298-490	[6]
$TaCl_5$	6275	34.305	7.04		298-490	[5]

Compound	A	B	C	D	T range (K)	Ref
WCl_2†	13,493	18.300	3.33		800-862	[6]
WCl_4†	7287	25.764	5.65		400-771	[6]
WCl_4	3253	8.195			555-598	[5]
WCl_4 (S_1)	3996	9.615			458-503	[5]
WCl_4 (S_2)	3588	8.795			503-554	[5]
WCl_5	3670	9.50			413-526	[5]
WCl_6 (S_1)†	5867	23.653	4.87		298-450	[6]
WCl_6 (S_2)†	6029	29.293	6.86		450-503	[6]
WCl_6 (S_3)†	4629	19.377	4.22		503-555	[6]
WCl_6 (S_1)	4580	10.73			425-503	[5]
WCl_6 (S_2)	4080	9.73			503-555	[5]

Table S26b. Experimental Liquid Phase Vapor Pressure Coefficients.§

Compound	A	B	C	T range (K)	Ref
$TiCl_2$	13,110	17.93	2.51	1308-1773	[5]
$TiCl_4$†	2915	22.641	5.94	298-409	[6]
$TiCl_4$	2919	25.129	5.788	298-410	[5]
VCl_4†	3255	26.458	7.16	298-427	[6]
$CrCl_2$†	12,501	22.449	4.54	1088-1576	[6]
$CrCl_2$	13,800	27.70	5.03	1097-1575	[5]
$MnCl_2$†	10,257	19.226	3.91	923-1509	[6]
$MnCl_2$	10,606	23.68	4.33	923-1463	[5]
$CoCl_2$	11,050	27.06	5.03	1010-1322	[5]
CuCl	10,170	8.04		1000-1922	[5]
Cu_3Cl_3	3750	4.90		900-1800	[5]
$NbCl_5$†	5147	39.053	10.73	479-519	[6]
$NbCl_5$	2870	8.37		479-520	[5]
$TaCl_5$†	5124	39.007	10.68	490-506	[6]
$TaCl_5$	2975	8.68		490-512	[5]
WCl_5	2760	7.72		526-559	[5]
WCl_6†	4619	23.229	5.63	555-613	[6]
WCl_6	3050	7.87		555-610	[5]

Table S27. Computed Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
$TiCl_2$ (G_1)	15,633	22.129	3.82	800-1246	[6]
$TiCl_2$ (G_2)	6471	4.694	0.57	1246-1939	[6]
$TiCl_3$ (G_1)	9851	16.393	2.42	600-1017	[6]
$(TiCl_3)_2$ (G_1)	10,772	20.681	3.40	600-1017	[6]
$(TiCl_3)_2$ (G_2)	4458	5.855	0.69	1017-2000	[6]
$TiCl_4$	9043	3.389		800-2000	[6]
$CrCl_3$ (G_1)	12,631	19.538	3.11	700-1279	[6]
$FeCl_2$ (G_1)	10,901	17.819	2.83	600-950	[6]
$FeCl_2$ (G_2)	9422	21.831	4.70	950-1293	[6]
$(FeCl_2)_2$ (G_1)	13,914	26.033	4.73	700-950	[6]
$(FeCl_2)_2$ (G_2)	10,978	34.198	8.51	950-1293	[6]
$(FeCl_2)_2$ (G_3)	3876	4.393	0.35	1293-2000	[6]
$FeCl_3$ (G_1)	8141	21.485	3.80	400-577	[6]
$FeCl_3$ (G_2)	6502	25.492	6.28	577-604	[6]
$(FeCl_3)_2$ (G_1)	8047	29.026	5.52	400-577	[6]
$(FeCl_3)_2$ (G_2)	4776	37.136	10.51	577-604	[6]
$(FeCl_3)_2$ (G_3)	4109	6.874	1.01	604-2000	[6]
$CoCl_2$ (G_1)	11,865	18.509	2.92	700-994	[6]
$CoCl_2$ (G_2)	9985	19.525	3.89	994-1354	[6]
$(CoCl_2)_2$ (G_1)	15,153	26.775	4.94	700-994	[6]
$(CoCl_2)_2$ (G_2)	11,436	29.150	6.98	994-1354	[6]
$(CoCl_2)_2$ (G_3)	4212	4.628	0.31	1354-2000	[6]
CuCl (G_1)	11,765	16.471	3.22	800-1482	[6]
$(CuCl)_3$ (G_1)	8584	27.024	6.20	500-683	[6]
$(CuCl)_3$ (G_2)	7864	27.862	6.85	683-709	[6]
$(CuCl)_3$ (G_3)	6942	28.044	7.37	709-1482	[6]
$(CuCl)_3$ (G_4)	9429	7.003	0.73	1482-2000	[6]

Compound	A	B	C	T range (K)	Ref
$TaCl_3$ (G_1)	12,581	20.733	3.55	700-912	[6]
$TaCl_4$ (G_1)	7568	18.463	2.92	400-559	[6]
$TaCl_5$ (G_1)	4889	4.561		506-2000	[6]
WCl_5 (G_1)	5963	25.427	5.34	298-526	[6]
WCl_5 (G_2)	5124	26.771	6.42	526-558	[6]
$(WCl_5)_2$ (G_1)	9304	38.321	8.16	400-526	[6]
$(WCl_5)_2$ (G_2)	7670	41.691	10.54	526-558	[6]
$(WCl_5)_2$ (G_3)	1248	5.467	1.01	558-2000	[6]
WCl_6	2862	4.644	0.44	613-2000	[6]

Table S28a. Thermodynamic Crystalline Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and molar heat capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$TiCl_2$	–515.5	87.4	–465.9[Δ, *]	69.8	[6]
$TiCl_2$	–513.8	87.4	–464.4	87.4	[1]
$TiCl_3$	–721.7	139.7	–654.4[Δ, *]	97.1	[6]
$TiCl_3$	–720.9	139.7	–653.5	97.2	[1]
VCl_3	–581.2	131.0	–511.9[Δ, *]	93.2	[6]
VCl_3	–580.7	131.0	–511.2	93.2	[1]
$CrCl_2$	–395.4	115.3	–356.2[Δ, *]	69.3	[6]
$CrCl_3$	–556.5	123.0	–486.1	91.8	[1]
$MnCl_2$	–481.3	118.2	–440.5[Δ, *]	73.0	[6]
$MnCl_2$	–481.3	118.2	–440.5	72.9	[1]
$FeCl_2$	–341.6	117.9	–302.1[Δ, *]	76.5	[6]
$FeCl_2$	–341.8	118.0	–302.3	76.7	[1]
$FeCl_3$	–399.3	147.8	–335.5[Δ, *]	96.9	[6]
$FeCl_3$	–399.5	142.3	–334.0	96.7	[1]

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$CoCl_2$	–312.5	109.2	–269.8	78.5	[1, 6]
$NiCl_2$	–305.3	98.0	–259.1[Δ, *]	71.7	[6]
$NiCl_2$	–305.3	97.7	–259.0	71.7	[1]
CuCl	–136.8	87.4	–119.7[Δ, *]	53.3	[6]
CuCl	–137.2	86.2	–119.9	48.5	[1]
$CuCl_2$	–218.0	108.0	–173.7[Δ, *]	71.7	[6]
$CuCl_2$	–220.1	108.1	–175.7	71.9	[1]
$TaCl_5$	–859.0	221.7	–746.4[Δ, *]	147.9	[1, 6]
WCl_2	–260.3	130.5	–223.0[Δ, *]	77.8	[6]
WCl_4	–443.1	198.3	–359.5[Δ, *]	129.7	[6]
WCl_5	–513.0	217.6	–401.9[Δ, *]	155.6	[6]
WCl_6	–593.7	238.5	–455.5[Δ, *]	175.4	[6]
WCl_6	–602.5				[1]

Table S28b. Thermodynamic Liquid Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and molar heat capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$TiCl_4$	–804.2	252.3	–737.2	145.2	[1]
VCl_4	–570.1	258.6	–505.6[Δ, *]	156.9	[6]
VCl_4	–569.4	255.0	–503.7		[1]

Table S28c. Thermodynamic Gas Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and molar heat capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$TiCl_2$	–237.2	278.3	–244.5[Δ, *]	57.7	[6]
$TiCl_3$	–539.3	316.8	–524.8[Δ, *]	72.5	[6]
$(TiCl_3)_2$	–1247.5	482.1	–1173.4[Δ, *]	169.7	[6]
$TiCl_4$	–763.2	354.8	–726.8[Δ, *]	95.5	[6]
$TiCl_4$	–763.2	353.2	–726.3	95.4	[1]
VCl_4	–525.5	366.5	–493.1[Δ, *]	93.2	[6]
VCl_4	–525.5	362.4	–492.0	96.2	[1]
$CrCl_2$	–136.2	307.9	–154.4[Δ, *]	57.7	[6]
$CrCl_3$	–325.2	317.6	–313.0[Δ, *]	76.0	[6]
$MnCl_2$	–264.1	295.4	–276.1[Δ, *]	57.1	[6]
$FeCl_2$	–140.9	299.3	–155.5[Δ, *]	57.6	[6]
$(FeCl_2)_2$	–431.4	464.5	–420.6[Δ, *]	125.9	[6]
$FeCl_3$	–254.0	344.2	–248.7[Δ, *]	77.70	[6]
$(FeCl_3)_2$	–660.5	537.1	–604.8[Δ, *]	173.7	[6]
$CoCl_2$	–93.7	298.5	–107.2[Δ, *]	59.6	[6]
$(CoCl_2)_2$	–349.7	450.4	–333.1[Δ, *]	127.5	[6]
$NiCl_2$	–70.2	298.2	–83.7[Δ, *]	60.6	[6]
CuCl	+91.2	237.2	+63.6[Δ, *]	35.1	[6]
$(CuCl)_3$	–263.7	429.5	–262.3[Δ, *]	124.3	[6]
$NbCl_5$	–703.3	404.1	–646.6[Δ, *]	119.0	[6]
$NbCl_5$	–703.7	400.6	–646.0	120.8	[1]
$TaCl_3$	–322.2	346.0	–313.2[a]	75.5	[6]
$TaCl_4$	–574.1	377.3	–541.2[Δ, *]	99.0	[6]
$TaCl_5$	–764.8	413.0	–709.3[Δ, *]	120.1	[6]
WCl_2	–12.6	309.4	–28.6[Δ, *]	58.4	[6]
WCl_4	–335.8	379.3	–306.1[Δ, *]	98.8	[6]
WCl_5	–412.5	405.5	–357.4[Δ, *]	120.2	[6]
$(WCl_5)_2$	–869.1	711.4	–729.2[Δ, *]	263.3	[6]
WCl_6	–493.6	419.3	–409.3[Δ, *]	143.8	[6]
WCl_6	–513.8				[1]

Table S29. Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap) and Sublimation (sub).

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
$TiCl_4$			35.8	87.5			[6]
VCl_4			37.1	86.8			[6]
$CrCl_2$	46.9	43.1	179.9	114.1	226.8◊	157.2◊	[6]
$MnCl_2$	37.7	40.8	147.4	97.7	185.1◊	138.5◊	[6]
$FeCl_2$	43.0	45.2					[6]
$FeCl_3$	43.1	74.7					[6]
$CoCl_2$	43.9	44.2					[6]
$NiCl_2$		59.4		119.9◊	220.1	179.3	[6]
CuCl	6.9	9.7					[6]
$NbCl_5$	33.9	70.7	52.3	100.7	86.2◊	171.4◊	[6]
$TaCl_5$	35.1	71.7	53.2	105.1	88.3◊	176.8◊	[6]
WCl_5					20.6	39.1	[6]
WCl_6	6.7	12.1	59.8	97.6	66.5◊	109.7◊	[6]

MAIN GROUP (MG) ELEMENT DATA

FISSION PRODUCTS (FPS)

Table S30. Melting (T_M), Boiling (T_B), and Triple Point (T_{TP}) Phase Change Temperatures.

Compound	T_M (K)	T_B (K)	T_{TP} (K)	Ref
SCl_2	151	332.75		[1]
S_2Cl_2	196	410		[1]
$SnCl_2$	520	896		[1]
$SnCl_4$	307.22	387.30		[1]
$SbCl_3$	346.55	493.45		[1]
$SbCl_5$	277	413 (dec)		[1]
$TeCl_2$	481	601		[1]
$TeCl_4$	497	660		[1]
ICl	300.53	370 (dec)		[1]
ICl_3	336	370 (dec)	374[a]	[1]

[a]Under increased pressure, 16 atmospheres.

Table S31a. Experimental Crystalline Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	D	T range (K)	Ref
$SnCl_2$[†]	7335	19.781	3.67		400-520	[6]
$SbCl_3$[†]	4161	20.495	4.26		298-346	[6]
$SbCl_3$	3460	2.81	–1.02	–5.6		[5]
$TeCl_2$[†]	4539	17.421	3.40		298-448	[6]
$TeCl_4$[†]	6846	25.915	5.35		400-497	[6]

Table S31b. Experimental Liquid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	D	T range (K)	Ref
SCl_2[†]	2306	18.846	4.72		298-332	[6]
S_2Cl_2[†]	2917	22.530	5.90		298-410	[6]
$SnCl_2$[†]	6925	23.120	5.19		520-885	[6]
$SnCl_4$[†]	3262	32.036	9.10		298-382	[6]
$SnCl_4$	1925	7.865			298-387	[5]
$SbCl_3$[†]	3644	21.741	5.34		346-496	[6]
$SbCl_3$	3770	29.48	7.04		346-493	[5]
$SbCl_5$[†]	2779	19.861	5.02		298-413	[6]
$SbCl_5$	2530	8.56			277-350	[5]
$TeCl_2$[†]	4163	19.472	4.49		448-593	[6]
$TeCl_2$	3350	8.51			481-601	[5]
$TeCl_4$[†]	8211	58.025	16.24		497-687	[6]

Table S32. Computed Gas Phase Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
SCl_2 (G_1)	783	–5.841	–1.61	332-717	[6]
SCl_2 (G_2)	2831	2.003	0.04	717-2000	[6]
S_2Cl_2 (G_1)	587	–11.537	–3.37	410-717	[6]
S_2Cl_2 (G_2)	3868	4.714	0.50	717-2000	[6]
$SnCl_2$	1967	8.386	1.24	885-2000	[6]
$SnCl_4$	7251	6.435	0.73	600-2000	[6]
$SbCl_5$ (G_1)	1017	–10.387	–4.34	413-496	[6]
$SbCl_5$ (G_2)	2349	5.929	0.58	496-1000	[6]
$TeCl_2$	6562	0.899	–0.21	700-2000	[6]
$TeCl_4$	2452	3.434	0.05	687-2000	[6]

Table S33a. Thermodynamic Crystalline Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
$SnCl_2$	–325.1	134.1	–283.3[Δ, *]		[1]
$SnCl_2$	–328.0	134.1	–286.2[Δ, *]	78.0	[6]
$SnCl_2$	–328.026	78.047	–286.222	78.047	[56]
$SbCl_3$	–382.2	184.1	–323.7	107.9	[1]
$SbCl_3$	–382.2	184.1	–323.7[Δ, *]	107.5	[6]
$TeCl_2$	–190.2	161.4	–157.0[Δ, *]	83.7[¶]	[6]
$TeCl_4$	–326.4			138.5	[1]
$TeCl_4$	–323.8	203.0	–236.5[Δ, *]	138.5	[6]
$TeCl_4$	–323.8	200.8	–235.9	138.5	[58]
ICl	–35.4	97.9	–14.049	55.229	[65]
ICl_3	–89.5	167.4	–22.3	100.8	[68, 69]
$SnCl_{2avg}$[ϕ]	*–327.0±1.7*	*115.4±32.4*	*–285.2±1.7*		
$TeCl_{4avg}$[ϕ]	*–324.7±1.5*			*138.5±0.0*	

Table S33b. Thermodynamic Liquid Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
SCl_2	–50.0	183.7	–28.7[Δ, *]	91.0	[1, 6]
S_2Cl_2	–57.9	224.4	–39.1[Δ, *]	124.3	[6]
S_2Cl_2	–58.2	223.8	–39.26	124.29	[50, 70]
$SnCl_4$	–511.3	258.7	–440.1[Δ, *]	165.3	[6]
$SnCl_4$	–511.29	258.74	–440.12	165.27	[56]
$SbCl_5$	–440.2	301.2	–350.2	159.0[¶]	[6, 71]
ICl	–23.9	135.2	–14.0	102.8	[65]

Table S33c. Thermodynamic Gas Phase Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and Molar Heat Capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
Gas Phase					
SCl_2	–17.6	281.3	–25.4[Δ, *]	50.9	[6]
S_2Cl_2	–16.7	327.2	–28.6[Δ, *]	73.0	[6]
$SeCl_2$	–33.5	295.7	–42.5[Δ, *]	53.7	[6]
$SeCl_2$	–33.5	295.7	–42.5	53.5	[50]
$SnCl_2$	–197.9	305.9	–207.3[Δ, *]	54.6	[6]
$SnCl_2$	–197.945	305.855	–207.350	54.632	[56]
$SnCl_4$	–471.5	365.0	–432.0[Δ, *]	98.4	[6]
$SnCl_4$	–471.54	364.95	–432.04	98.45	[56]
$SbCl_3$	–313.1	339.1	–300.8[Δ, *]	76.8[¶]	[6]
$SbCl_3$	–313.8	337.7	–301.2	76.7	[71]
$SbCl_5$	–399.4	401.8	–339.3[Δ, *]	112.6[¶]	[6]
$SbCl_5$	–388.82	401.77	–328.73	120.92	[50]
$TeCl_2$	–113.0	305.7	–122.822	54.346	[58]
ICl	+17.1	247.6	–5.7	35.5	[65]

Table S34. Enthalpic (ΔH, kJ/mol) and Entropic (ΔS, J/molK) Heats of Fusion (fus), Vaporization (vap) and Sublimation (sub).

Compound	ΔH_{fus}	ΔS_{fus}	ΔH_{vap}	ΔS_{vap}	ΔH_{sub}	ΔS_{sub}	Ref
SCl_2			31.0	93.4			[6]
S_2Cl_2			35.8	87.3			[6]
$SnCl_2$	14.6	28.2	93.7	105.9	108.3[◊]	134.1[◊]	[6]
$SnCl_4$		38.2	33.5	87.7		125.9[◊]	[6]
$SbCl_3$	13.0	37.5	47.8	96.3	60.8[◊]	133.8[◊]	[6]
$SbCl_5$			36.1	87.3			[6]
$TeCl_2$	11.3	25.2	57.6	97.1	68.9[◊]	122.3[◊]	[6]
$TeCl_4$	18.9	38.0	64.4	93.8	83.3[◊]	131.8[◊]	[6]
ICl_3	11.4		41.3		52.8		[69]

CORROSION PRODUCTS (CORPS)

Table S35. Melting (T_M), Boiling (T_B), and Sublimation (T_{sub}) Phase Change Temperatures.

Compound	T_M (K)	T_B (K)	T_{sub} (K)	Ref
$AlCl_3$	465	454	453	[1, 6]

Table S36. Experimental Solid Phase Vapor Pressure Coefficients.[§]

Compound	A	B	C	D	T range (K)	Ref
Al_2Cl_6	6360	9.66	–3.77	–6.12	298-453	[5]

Table S37. Computed Vapor Pressure Coefficients.[§, %, &, †]

Compound	A	B	C	T range (K)	Ref
$AlCl_3$ (G_1)	6720	19.415	2.97	400-454	[6]
$AlCl_3$ (G_2)	11,177	4.206	0.16	900-2000	[6]
$(AlCl_3)_2$ (G_1)	6642	25.842	4.22	298-454	[6]
$(AlCl_3)_2$ (G_2)	3433	6.927	1.00	454-2000	[6]

Table S38. Thermodynamic Data for Enthalpy of Formation (ΔH_f^o, kJ/mol), Standard Entropy (S^o, J/molK), Gibbs Free Energy of Formation (ΔG_f^o, kJ/mol), and molar heat capacity (C_p, J/molK).

Compound	ΔH_f^o	S^o	ΔG_f^o	C_p	Ref
Crystalline Phase					
$AlCl_3$	–705.4	109.3	–629.8[Δ, *]	91.1	[6]
$AlCl_3$	–704.2	109.3	–628.8	91.1	[1]
Gas Phase					
$AlCl_3$	–584.6	314.5	–570.2[Δ, *]	71.0	[6]
$(AlCl_3)_2$	–1295.7	475.0	–1220.9[Δ, *]	158.3	[6]

Table S39. Entropic (ΔS, J/molK) Heat of Fusion (fus).

Compound	ΔS_{fus}	Ref
$AlCl_3$	75.9	[6]

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