Structures and Heats of Formation of Simple Alkaline Earth Metal Compounds II: Fluorides, Chlorides, Oxides, and Hydroxides for Ba, Sr, and Ra

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Table S1. Energy Contribution to the Total Atomization Energies in kcal/mol for the Ground States of the Alkaline Earth Compounds Calculated at the CCSD(T)/awCV*n*Z Level

Compound	$\Delta E_{n=D}$[a]	$\Delta E_{n=T}$[a]	$\Delta E_{n=Q}$[a]	$\Delta E_{n=5}$[a]	$\Delta E_{CBS\text{-}DTQ}$[b]	$\Delta E_{awCVTZ\text{-}DK}$[a,c]
SrO ($^1\Sigma^+$)	78.63	90.80	95.36	97.16	98.02	92.10
BaO ($^1\Sigma^+$)	98.44	121.11	129.40	132.05	134.22	119.22
RaO ($^1\Sigma^+$)	77.35	95.20	101.81	104.37	105.66	97.42
SrF ($^2\Sigma^+$)	120.81	124.72	127.08	127.85	128.53	124.74
BaF ($^2\Sigma^+$)	126.61	133.28	136.78	137.90	138.92	133.03
RaF ($^2\Sigma^+$)	117.03	122.94	126.03	127.12	127.92	123.75
SrCl ($^2\Sigma^+$)	90.49	94.84	98.13	99.14	100.21	94.74
BaCl ($^2\Sigma^+$)	97.41	102.98	106.95	108.21	109.44	103.14
RaCl ($^2\Sigma^+$)	89.89	94.22	97.95	99.07	100.32	94.44
SrF_2 ($^1A_1$)	252.87	259.64	263.99	265.36	266.70	259.39
BaF_2 ($^1A_1$)	258.43	270.07	276.17	278.06	279.89	270.04
RaF_2 ($^1A_1$)	241.92	252.80	258.48	260.33	261.94	253.89
$SrCl_2$ ($^1\Sigma_g$)	197.94	205.14	211.33	213.21	215.28	204.93
$BaCl_2$ ($^1A_1$)	205.58	215.13	222.46	224.64	227.09	215.26
$RaCl_2$ ($^1A_1$)	191.75	199.92	206.99	209.02	211.48	200.07
SrOH ($^2\Sigma^+$)	189.75	198.25	201.85	202.90	203.99	198.08
BaOH ($^2\Sigma^+$)	195.50	206.57	211.29	212.60	214.10	206.47
RaOH ($^2\Sigma^+$)	185.55	195.72	200.06	201.29	202.64	196.35
$Sr(OH)_2$ ($^1A_1$)	391.32	407.44	414.27	416.17	418.33	406.76
$Ba(OH)_2$ ($^1A_1$)	395.33	415.58	424.09	426.41	429.14	415.55
$Ra(OH)_2$ ($^1A_1$)	378.74	398.10	406.26	408.46	411.11	398.71

[a] Calculated as the energy difference between the ground states of the atoms ($^1S_0$ for Sr, Ba , Ra, $^3P_2$ for O, $^2P_{3/2}$ for Cl, and $^2P_{3/2}$ for F) and the metal compound (MO, MX, MOH, $M(OH)_2$ where X = Cl and F) at the CCSD(T) level with the appropriate basis set.

[b] Extrapolated CCSD(T) energies with n = D, T, and Q using Eq. 2.

[c] Valence electronic energies at CCSD(T)-DK/awCVTZ-DK level.

Table S2. T1 diagnostic values at CCSD(T)/awCVQZ Level.

Molecule	T1
SrO ($^1\Sigma^+$)	0.033
BaO ($^1\Sigma^+$)	0.030
RaO ($^1\Sigma^+$)	0.024
SrF ($^2\Sigma^+$)	0.020
BaF ($^2\Sigma^+$)	0.024
RaF ($^2\Sigma^+$)	0.022
SrCl ($^2\Sigma^+$)	0.010
BaCl ($^2\Sigma^+$)	0.021
RaCl ($^2\Sigma^+$)	0.018
SrF_2 ($^1A_1$, C_{2v})	0.012
BaF_2 ($^1A_1$, C_{2v})	0.013
RaF_2 ($^1A_1$, C_{2v})	0.013
$SrCl_2$ ($^1\Sigma_g$, $D_{\infty h}$)	0.006
$BaCl_2$ ($^1A_1$, C_{2v})	0.006
$RaCl_2$ ($^1A_1$, C_{2v})	0.006
SrOH ($^2\Sigma^+$, $C_{\infty v}$)	0.021
BaOH ($^2\Sigma^+$, $C_{\infty v}$)	0.025
RaOH ($^2\Sigma^+$, $C_{\infty v}$)	0.023
$Sr(OH)_2$ ($^1A_1$, C_{2v})	0.012
$Ba(OH)_2$ ($^1A_1$, C_{2v})	0.013
$Ra(OH)_2$ ($^1A_1$, C_{2v})	0.013

Table S3. Calculated ZPE in kcal/mol for molecules other except diatomics.

Molecule	ΔE_{ZPE} Harmonic[a]	Anharmonic correction to the ΔE_{ZPE}[b]
SrF_2	-1.46	0.006
BaF_2	-1.35	0.004
RaF_2	-1.28	0.004
$SrCl_2$	-0.82	0.016
$BaCl_2$	-0.76	0.004
$RaCl_2$	-0.71	0.001
SrOH	-7.53	0.109
BaOH	-7.37	0.097
RaOH	-7.32	0.093
$Sr(OH)_2$	-15.29	0.270
$Ba(OH)_2$	-14.88	0.401
$Ra(OH)_2$	-14.78	0.229

[a] CCSD(T)/awCVTZ.

[b] MP2/awCVTZ/wCVTZ-PP(Sr, Ba, Ra).

Table S4. Calculated and Experimental Vibrational Frequencies in cm^{-1} for the Alkaline Earth Alkaline Earth Dihalides.

Molecule	MP2/awCVTZ/wCVTZ-PP			Calculated CCSD(T)/ awCVTZ	Anharm corrected
	E(harm)	E(anhar)	Δ(Harmonic – anharmonic)		
SrF_2	475.5	471.0	4.6	478.3	473.7
	468.8	464.1	4.7	469.9	465.2
	75.6	72.4	3.2	75.9	72.7
BaF_2	441.9	438.3	3.7	437.4	433.7
	421.1	417.5	3.7	418.5	414.8
	92.3	90.6	1.7	88.0	86.3
RaF_2	417.0	413.7	3.2	418.4	415.2
	395.9	392.7	3.1	397.4	394.3
	79.2	77.4	1.8	79.8	78.0
$SrCl_2$[a]	319.7	317.7	2.1	313.0	310.9
	269.2	266.5	2.6	262.7	260.1
	20.0	1.6	18.4	26.1	7.7
$BaCl_2$	279.9	279.0	0.9	259.7	258.8
	275.4	272.6	2.8	270.0	267.2
	43.3	41.9	1.4	41.1	39.7
$RaCl_2$	252.5	251.7	0.8	248.0	247.2
	252.0	251.3	0.7	247.6	246.9
	38.2	38.3	-0.1	37.7	37.8

[a] The frequencies for $SrCl_2$ were evaluated at 160°.

Table S5. Calculated and Experimental Vibrational Frequencies in cm^{-1} for the Alkaline Earth Hydroxides.

Molecule	MP2/awCVTZ/wCVTZ-PP			Calculated CCSD(T)/ awCVTZ	CCSD(T) with anhar from MP2
	E(harm)	E(anhar)	Δ(Harmonic – anharmonic)		
SrOH	3930.5	3761.7	168.8	3935.7	3766.9
	534.6	521.6	13.0	536.6	523.6
	403.2 π	377.9 π	25.3	400.6 π	375.3 π
BaOH	3897.4	3728.3	169.1	3904.0	3734.9
	493.7	483.2	10.5	493.6	483.1
	383.6 π	367.4 π	16.2	379.9 π	363.7 π
RaOH	3900.0	3730.0	170.0	3903.7	3733.7
	460.8	450.9	9.9	461.5	451.6
	380.6 π	368.4 π	12.2	378.7 π	366.5 π
$Sr(OH)_2$	3925.3	3757.2	168.1	3931.8	3763.7
	3926.0	3758.0	168.0	3930.7	3762.7
	506.5	494.2	12.3	508.7	496.4
	500.3	489.0	11.3	500.3	489.0
	470.4	435.0	35.4	454.6	419.2
	462.4	431.3	31.1	449.7	418.6
	455.0	425.5	29.5	444.8	415.3
	454.8	419.8	35.0	440.2	405.2
	49.0	47.2	1.8	44.8	43.0
$Ba(OH)_2$	3900.1	3728.5	171.6	3897.4	3725.8
	3900.0	3728.3	171.7	3897.0	3725.3
	499.6	417.3	82.3	469.7	387.4
	485.2	417.7	67.5	442.2	374.7
	477.9	442.7	35.2	425.0	389.8
	473.1	410.2	62.9	422.1	359.2
	456.9	369.5	87.4	405.3	317.9
	445.2	430.6	14.6	384.9	370.3
	66.2	70.4	-4.2	72.2	76.4
$Ra(OH)_2$	3895.3	3728.0	167.3	3898.0	3730.7
	3895.5	3728.4	167.1	3897.8	3730.7
	452.0	442.4	9.6	451.6	442.0
	422.6	402.6	20.0	422.4	402.4
	422.6	404.4	18.2	416.0	397.8
	422.3	411.3	10.9	415.6	404.7
	406.6	382.4	24.2	399.5	375.3
	385.3	364.5	20.7	378.6	357.9
	70.4	70.6	-0.2	67.1	67.3

Table S6. Calculated Heats of Formation at 0K and 298K from the Total Atomization Energies in kcal/mol at CCSD(T)/CBS-DTQ Level

Molecule	$\Sigma D_{0,0K}$	$\Delta H_{f,0K}$	$\Delta H_{f,298K}$
SrO	98.02	0.1	-0.4
BaO	134.22	-29.2	-29.7
RaO	105.66	-11.5	-12.0
SrF	128.44	-69.7	-70.1
BaF	138.92	-76.1	-76.6
RaF	127.92	-72.9	-73.3
SrCl	100.21	-30.9	-31.3
BaCl	109.44	-36.8	-37.2
RaCl	100.32	-34.4	-34.8
SrF_2	266.70	-188.0	-188.5
BaF_2	279.89	-197.8	-198.4
RaF_2	261.94	-187.7	-188.2
$SrCl_2$	215.28	-116.1	-117.2
$BaCl_2$	227.09	-124.6	-125.0
$RaCl_2$	211.48	-115.7	-116.1
SrOH	203.99	-46.3	-47.2
BaOH	214.10	-52.9	-53.9
RaOH	202.64	-48.9	-49.8
$Sr(OH)_2$	418.33	-141.7	-144.3
$Ba(OH)_2$	424.14	-150.0	-152.6
$Ra(OH)_2$	411.11	-139.2	-140.8

Table S7. Calculated Heats of Formation at 0K and 298K from the Total Atomization Energies in kcal/mol at CCSD(T)/CBS-TQ5 Level

Molecule	$\Sigma D_{0,0K}$	$\Delta H_{f,0K}$	$\Delta H_{f,298K}$
SrO	98.37	-0.1	-0.6
BaO	130.53	-28.6	-29.1
RaO	107.00	-11.7	-12.2
SrF	127.22	-69.4	-69.9
BaF	137.24	-75.8	-76.2
RaF	127.56	-72.7	-73.2
SrCl	98.36	-30.5	-30.8
BaCl	107.87	-36.3	-36.7
RaCl	98.73	-33.8	-34.2
SrF_2	263.67	-187.4	-188.0
BaF_2	276.99	-197.1	-197.6
RaF_2	260.43	-187.1	-187.7
$SrCl_2$	211.61	-115.1	-116.3
$BaCl_2$	223.60	-123.4	-123.8
$RaCl_2$	207.96	-114.4	-114.8
SrOH	195.70	-45.8	-46.7
BaOH	205.76	-52.2	-53.1
RaOH	195.18	-48.2	-49.2
$Sr(OH)_2$	401.12	-140.6	-143.2
$Ba(OH)_2$	412.80	-148.6	-151.2
$Ra(OH)_2$	395.35	-137.8	-139.5

Table S8. Total CCSD(T) and CBS Energies in Hartrees

compound	aug-cc-pwCVDZ	aug-cc-pwCVTZ	aug-cc-pwCVQZ	aug-cc-pwCV5Z	CBS-DTQ[a]	CBS-TQ5[b]	CBS-Q5[c]	aug-cc-pwCVTZ-DK
SrO	-105.601563	-105.771518	-105.842450	-105.869206	-105.884528	-105.884785	-105.890932	-3252.866793
BaO	-100.372207	-100.586028	-100.649492	-100.668788	-100.684986	-100.679974	-100.684456	-8207.568549
RaO	-98.904663	-99.112636	-99.163574	-99.190717	-99.190795	-99.206606	-99.212758	-25062.871106
SrF	-130.296148	-130.479207	-130.554799	-130.582792	-130.599574	-130.59908	-130.605521	-3277.607260
BaF	-125.044463	-125.259046	-125.323056	-125.342779	-125.358894	-125.35422	-125.358794	-8232.279002
RaF	-123.595259	-123.810464	-123.863975	-123.891653	-123.892685	-123.90785	-123.914128	-25087.601527
SrCl	-490.425058	-490.696469	-490.812541	-490.856703	-490.881629	-490.88242	-490.892563	-3639.150898
BaCl	-485.175160	-485.475650	-485.579387	-485.615134	-485.639115	-485.63591	-485.644160	-8593.822819
RaCl	-483.729242	-484.029587	-484.123094	-484.166602	-484.175904	-484.19202	-484.201931	-25449.146267
SrF_2	-230.095874	-230.383892	-230.490666	-230.528629	-230.552884	-230.55071	-230.559454	-3377.598793
BaF_2	-224.843799	-225.166712	-225.262863	-225.292846	-225.316674	-225.31024	-225.317193	-8332.274296
RaF_2	-223.383563	-223.707097	-223.792725	-223.830648	-223.839392	-223.85279	-223.861442	-25187.585862
$SrCl_2$	-950.362779	-950.826796	-951.014488	-951.084859	-951.125330	-951.12583	-951.142000	-4100.694895
$BaCl_2$	-945.114028	-945.608932	-945.785013	-945.847054	-945.886922	-945.88313	-945.897431	-9055.369910
$RaCl_2$	-943.658062	-944.152585	-944.318401	-944.388205	-944.413376	-944.42892	-944.444885	-25910.682992
SrOH	-106.278647	-106.442743	-106.512154	-106.537710	-106.553406	-106.552583	-106.558461	-3253.535680
BaOH	-101.026880	-101.222224	-101.279999	-101.297154	-101.312287	-101.307093	-101.311084	-8208.207588
RaOH	-99.577090	-99.772827	-99.820142	-99.845171	-99.845339	-99.85982	-99.865494	-25063.528769

$Sr(OH)_2$	-182.061780	-182.312166	-182.406550	-182.439622	-182.461694	-182.458852	-182.466477	-3329.456734
$Ba(OH)_2$	-176.807242	-177.091344	-177.174983	-177.199918	-177.221680	-177.214366	-177.220166	-8284.129289
$Ra(OH)_2$	-175.346878	-175.631389	-175.704632	-175.737370	-175.744279	-175.75649	-175.763954	-25139.439751

[a] Extrapolated CCSD(T)/awCV*n*Z energies with *n* = D, T, and Q using Eq. 2.

[b] Extrapolated CCSD(T)/awCV*n*Z energies with *n* = T, Q, and 5 using Eq. 2.

[c] Extrapolated CCSD(T)/awCV*n*Z energies with *n* = Q and 5 using Eq. 1.

Table S9. NPAs form NBOs at B3LYP/awCVTZ/wCVTZ(Be,Mg)/wCVTZ-PP(Ca,Sr,Ba,Ra) Level.

Molecules	M charge	M valence d (α/β)	M valence s (α/β)	M valence p (α/β)
SrO ($^1\Sigma$, $C_{\infty v}$)	1.54	0.38	0.04	0.07
BaO ($^1\Sigma$, $C_{\infty v}$)	1.55	0.39	0.02	0.08
RaO ($^1\Sigma$, $C_{\infty v}$)	1.63	0.28	0.02	0.10
SrF ($^2\Sigma$, $C_{\infty v}$)	0.95	0.09 (0.05/0.04)	0.92 (0.91/0.01)	0.04 (0.04/0.00)
BaF ($^2\Sigma$, $C_{\infty v}$)	0.94	0.12 (0.07/0.05)	0.92 (0.91/0.01)	0.02 (0.01/0.01)
RaF ($^2\Sigma$, $C_{\infty v}$)	0.96	0.08 (0.05/0.03)	0.93 (0.93/0.01)	0.02 (0.02/0.00)
SrCl ($^2\Sigma$, $C_{\infty v}$)	0.90	0.10 (0.06/0.04)	0.96 (0.93/0.03)	0.04 (0.04/0.00)
BaCl ($^2\Sigma$, $C_{\infty v}$)	0.89	0.15 (0.10/0.05)	0.94 (0.92/0.02)	0.02 (0.02/0.00)
RaCl ($^2\Sigma$, $C_{\infty v}$)	0.92	0.09 (0.06/0.03)	0.96 (0.94/0.03)	0.02 (0.02/0.00)
SrOH ($^2\Sigma$, $C_{\infty v}$)	0.97	0.08 (0.04/0.04)	0.93 (0.92/0.01)	0.03 (0.03/0.00)
BaOH ($^2\Sigma$, $C_{\infty v}$)	0.96	0.10 (0.06/0.04)	0.93 (0.92/0.01)	0.02 (0.02/0.00)
RaOH ($^2\Sigma$, $C_{\infty v}$)	0.98	0.07 (0.04/0.03)	0.94 (0.93/0.01)	0.02 (0.02/0.00)
BeF_2 ($^1\Sigma_g^+$, $D_{\infty h}$)	1.74	-	0.14	0.11
MgF_2 ($^1\Sigma_g^+$, $D_{\infty h}$)	1.88	0.01	0.09	0.02
CaF_2 ($^1A_1$, C_{2v})	1.85	0.13	0.01	-
SrF_2 ($^1A_1$, C_{2v})	1.87	0.13	0.01	-
BaF_2 ($^1A_1$, C_{2v})	1.84	0.15	0.01	0.01
RaF_2 ($^1A_1$, C_{2v})	1.88	0.11	0.01	0.01
$BeCl_2$ ($^1\Sigma_g^+$, $D_{\infty h}$)	1.45	-	0.36	0.18
$MgCl_2$ ($^1\Sigma_g^+$, $D_{\infty h}$)	1.68	0.01	0.26	0.05
$CaCl_2$ ($^1\Sigma_g^+$, $D_{\infty h}$)	1.78	0.15	0.06	0.01
$SrCl_2$ ($^1\Sigma_g$, $D_{\infty h}$)	1.83	0.13	0.04	-
$BaCl_2$ ($^1A_1$, C_{2v})	1.79	0.17	0.03	-
$RaCl_2$ ($^1A_1$, C_{2v})	1.83	0.12	0.04	-
$Sr(OH)_2$ ($^1A_1$, C_{2v})	1.91	0.09	0.01	-
$Ba(OH)_2$ ($^1A_1$, C_{2v})	1.89	0.12	0.01	0.01
$Ra(OH)_2$ ($^1A_1$, C_{2v})	1.92	0.08	0.01	0.01

Table S10. Calculated DFT Geometry Parameters for all the Alkaline Earth Halides (Fluorides and Chlorides)

compound	Method (DFT functional/basis sets)	M–X (Å)	∠XMX(°)
BeF_2 ($^1\Sigma_g^+$, $D_{\infty h}$)	B3LYP/DZVP	1.444	180.0
MgF_2 ($^1\Sigma_g^+$, $D_{\infty h}$)	B3LYP/DZVP	1.762	180.0
CaF_2 ($^1A_1$, C_{2v})	B3LYP/DZVP	2.010	146.0
SrF_2 ($^1A_1$, C_{2v})	B3LYP/aug-cc-pVDZ/Stuttgart	2.132	129.7
BaF_2 ($^1A_1$, C_{2v})	B3LYP/aug-cc-pVDZ/Stuttgart	2.248	121.0
RaF_2 ($^1A_1$, C_{2v})	B3LYP/aug-cc-pVDZ/Stuttgart	2.370	117.2
$BeCl_2$ ($^1\Sigma_g^+$, $D_{\infty h}$)	B3LYP/DZVP	1.890	180.0
$MgCl_2$ ($^1\Sigma_g^+$, $D_{\infty h}$)	B3LYP/DZVP	2.198	180.0
$CaCl_2$ ($^1\Sigma_g^+$, $D_{\infty h}$)	B3LYP/DZVP	2.480	180.0
$SrCl_2$ ($^1A_1$, C_{2v})	B3LYP/aug-cc-pVDZ/Stuttgart	2.643	161.1
$BaCl_2$ ($^1A_1$, C_{2v})	B3LYP/aug-cc-pVDZ/Stuttgart	2.768	129.0
$RaCl_2$ ($^1A_1$, C_{2v})	B3LYP/aug-cc-pVDZ/Stuttgart	2.898	128.1

Table S11. Calculated $SrCl_2$ CCSD(T)/awCVTZ Frequencies at Different Angles.

Angle	Energy in Hartees	Energy difference	ν_1(asym stretch - b_2)	ν_2(sym stretch - a_1)	ν_3(bending - a_1)
130	-950.825108	1.10	298.8	270.7	60.1
140	-950.826234	0.39	304.7	267.7	51.6
150	-950.826733	0.08	309.5	264.9	40.4
155	-950.826826	0.02	311.4	263.7	33.7
160	-950.826855	0.00	313.0	262.7	26.1
165	-950.826848	0.00	314.2	261.9	17.2
170	-950.826825	0.02	315.1	261.3	2.4(i)
176	-950.826802	0.03	315.7	260.9	14.8(i)
179.8	-950.826796	0.04	315.8	260.8	16.0(i)
180	-950.826796	0.04	315.6	260.7	15.4(x2)(i)