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Could the increased structural versatility imposed by non-halogen ligands bring something new for polynuclear superhalogens? A case study on binuclear $[Mg_2L_5]^-$ (L=-OH, -OOH and -OF) anions

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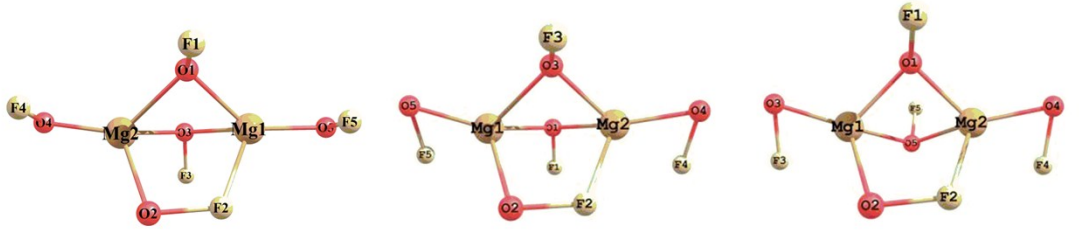
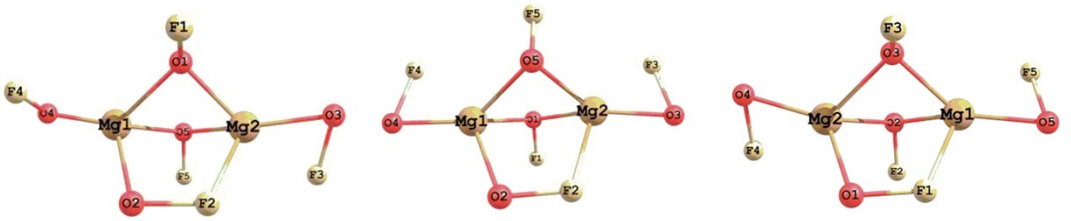
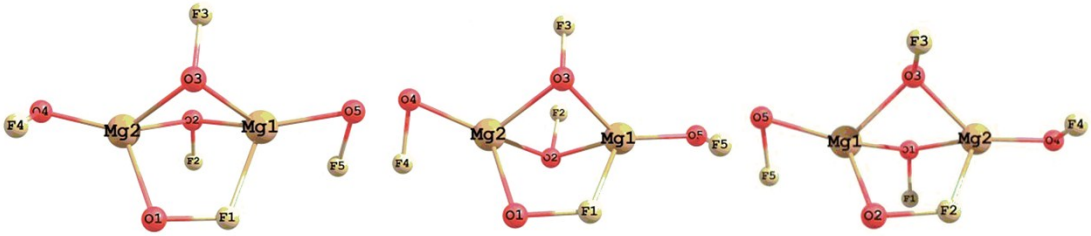


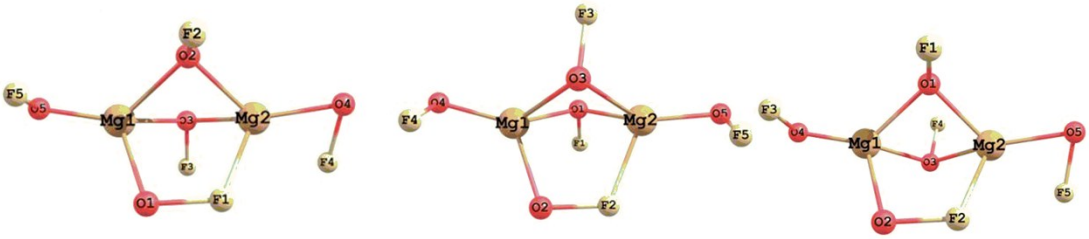
B3_a (C1/ 0 Kcal/mol) B3_b (C1/ 1.88 Kcal/mol) B3_c (C1/ 0.34 Kcal/mol)



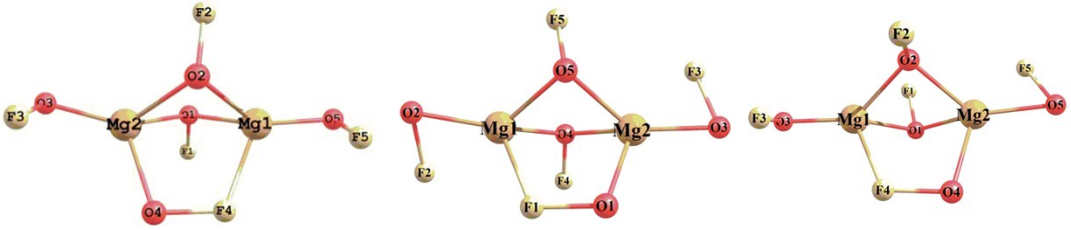
B3_d (C1/ 0.05 K cal/mol) B3_e (C1/ 0.11 Kcal/mol) B3_f (C1/ 0.60 Kcal/mol)



B3_g (C1/ 0.09 Kcal/mol) B3_h (C1/ 1.03 Kal/mol) B3_i (C1/ 0.05 Kcal/mol)



B3_j (C1/ 0.05 Kcal/mol) B3_k (C1/ 0.34 Kcal/mol) B3_l (C1/ 0.13 Kcal/mol)



B3_m (C1/ 0.34 Kcal/mol) B4_a (C1/ 0 Kcal/mol) B4_b (C1/ 0.0001 Kcal/mol)

Fig. S1 The equilibrium structures of isomers of B3_(a-m) and B4_(a-b) at MP2/6-311++G** level, point group and relative energy (Kcal/mol). B3_a and B4_a

represent B3, B4, respectively.

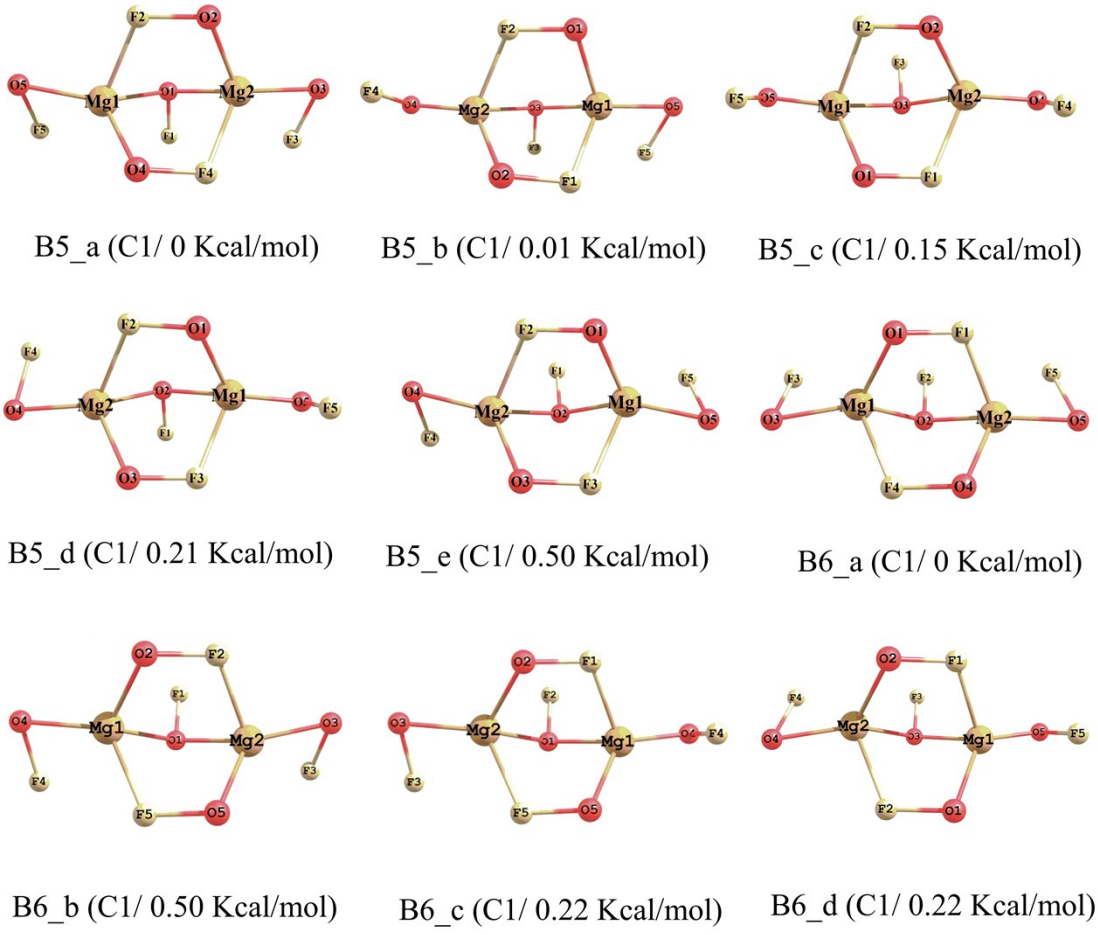


Fig. S2 The equilibrium structures of isomers of B5_(a-e) and B4_(a-d) at MP2/6-311++G** level, point group and relative energy (Kcal/mol). B5_a and B6_a represent B5, B6, respectively.

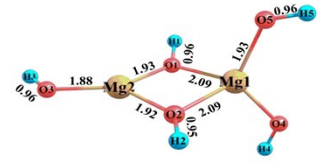
Table. S1 Calculated VDEs of the superhalogen anions of structures similar to **B3**, **B4**, **B5**, **B6** in the manuscript at various theoretical levels (in eV).[a]

	B3LYP	WB97XD	M06-2X	OVGF
B3_a[b]	6.26	6.95	7.38	7.38
B3_b	6.35	7.06	7.47	7.45
B3_c	6.29	7.00	7.41	7.42
B3_d	6.26	6.95	7.38	7.38
B3_e	6.28	6.98	7.39	7.41
B3_f	6.25	6.95	7.37	7.38
B3_g	6.31	7.03	7.44	7.42
B3_h	6.31	7.03	7.44	7.45
B3_i	6.26	6.95	7.38	7.38
B3_j	6.26	6.95	7.38	7.38
B3_k	6.29	7.00	7.41	7.42
B3_l	6.28	6.99	7.42	7.42
B3_m	6.29	7.00	7.41	7.42
B4_a	6.29	7.00	7.40	7.42

B4_b	6.29	7.00	7.40	7.42
B5_a	6.29	7.04	7.46	7.60
B5_c	6.29	7.05	7.46	7.60
B5_d	6.30	7.06	7.47	7.59
B5_e	6.31	7.07	7.48	7.60
B6_a	6.29	7.04	7.46	7.59
B6_b	6.29	7.04	7.45	7.60
B6_c	6.30	7.06	7.47	7.59
B6_d	6.32	7.08	7.47	7.60

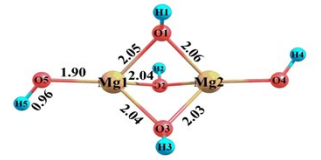
[a] All the calculations are performed on the structures optimized at MP2/6-311++G** level.

[b] B3_a, B4_a, B5_a, B6_a correspond to **B3**, **B4**, **B5**, **B6** respectively.



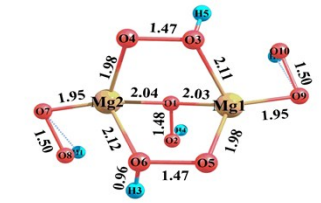
A1 (C1 / 11.94 Kcal/mol)

O1-H2	3.60589	O2-H1	3.52056
O1-H3	3.94081	O3-H1	4.06490
O2-H3	4.35976	O3-H2	3.99682
O5-H4	4.21602	O4-H5	3.49965
O1-H5	3.99502	O5-H1	3.20969
O1-H4	3.75901	O4-H1	4.03299
O2-H5	4.12865	O5-H2	3.94009
O4-H2	3.65509	O2-H4	3.46393



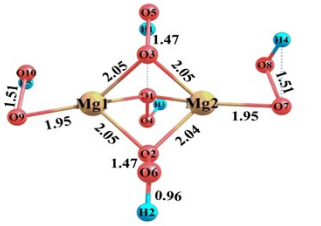
A2 (C1 / 0 Kcal/mol)

O1-H2	3.03875	O1-H3	3.33479
O2-H1	3.65203	O3-H1	3.34037
O2-H3	3.58397	O4-H1	4.11312
O3-H2	3.56555	O1-H4	3.81404
O2-H4	4.21075	O4-H2	4.03742
O3-H4	4.36345	O4-H3	3.93951
O1-H5	4.38335	O5-H1	3.90853
O2-H5	4.10671	O5-H2	4.02107
O3-H5	3.94645	O5-H3	3.99047



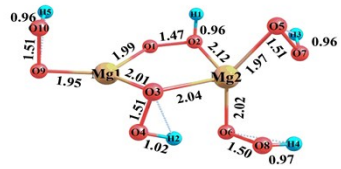
C1 (C1 / 8.38 Kcal/mol)

O7-H1	1.92630	O9-H2	1.90984
O4-H5	1.91302	O1-H4	1.88009
O5-H3	1.90989	O1-H5	3.10861
O5-H4	4.19471	O6-H4	4.13584
O4-H4	4.80773	O3-H4	4.64025
O3-H2	3.64530	O1-H2	3.64530
O5-H2	4.83215	O6-H1	3.53633
O2-H1	2.84214	O1-H1	3.27454



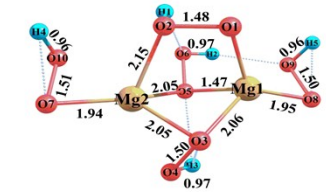
C2 (C1 / 4.43 Kcal/mol)

O9-H5	1.92109	O7-H4	1.92857
O1-H1	2.16079	O6-H4	4.67609
O3-H1	1.90407	O1-H3	1.87560
O3-H3	4.34895	O5-H3	4.32783
O2-H3	4.16747	O3-H2	4.11106
O5-H4	3.40672	O8-H1	3.31305
O7-H1	4.20667	O3-H4	3.48646
O1-H4	4.01179	O2-H4	4.67609



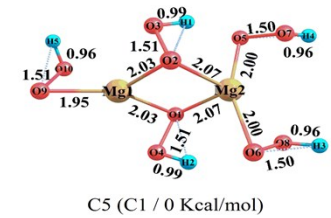
C3 (C1 / 8.06 Kcal/mol)

O9-H5	1.92295	O3-H2	1.95640
O5-H3	1.92611	O6-H4	1.91176
O1-H1	1.91513	O3-H1	3.46323
O4-H1	4.32674	O1-H2	3.51767
O2-H2	3.42986	O6-H2	1.55918
O8-H2	2.38465	O1-H10	3.27937
O3-H10	3.65442	O4-H10	4.05789
O5-H1	2.83061	O7-H1	2.83061
O2-H3	3.02508		



C4 (C1 / 5.28 Kcal/mol)

O4-H7	1.91710	O6-H1	2.35629
O9-H2	2.33132	O5-H3	2.37129
O3-H3	1.95031	O8-H5	1.91644
H1-O1	1.90833	O1-H2	3.51438
H2-O5	1.88099	H2-O2	3.53825
H1-O5	2.69622	H2-O3	4.26883
H3-O6	3.82000	H3-O1	4.37416
H3-O2	4.31204	H1-O10	2.95608
H1-O7	3.74381	H4-O2	2.88862
H4-O6	4.23486	H4-O5	4.18547
O1-H5	3.48414	O6-H5	3.72506



C5 (C1 / 0 Kcal/mol)

O9-H5	1.92264	O2-H1	1.93841
O4-H2	1.99354	O5-H4	1.90563
O6-H3	1.90548	O8-H2	2.64921
O1-H1	3.14363	O4-H1	4.15792
O2-H2	3.11372	O3-H2	4.15808
O5-H1	1.74627	O7-H1	2.64497
O2-H4	4.12137	O3-H4	4.27007
O6-H4	4.05875	O8-H4	3.47482
O5-H3	4.06351	O7-H3	3.47573
O4-H3	4.27038	O1-H3	4.11480
O6-H2	1.74631	O3-H5	3.13802
O2-H5	4.01396	O1-H5	4.26396

Fig. S3 The short contacts between O and H atoms of superhalogen anions of $[Mg_2(OOH)_5]^-$ and $[Mg_2(OH)_5]^-$ at MP2/6-311++G** level. The red mark represents

O H contacts shorter than 3.2 Å.

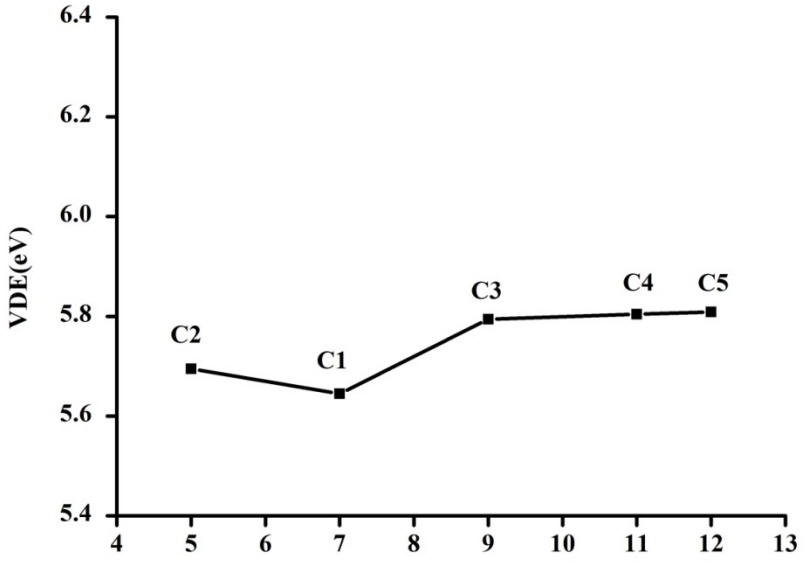
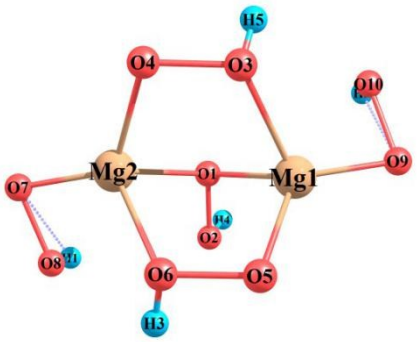


Fig. S4 The correlation between VDE and the number of the intra-molecule hydrogen bonds in $[Mg_2(OOH)_5]^-$

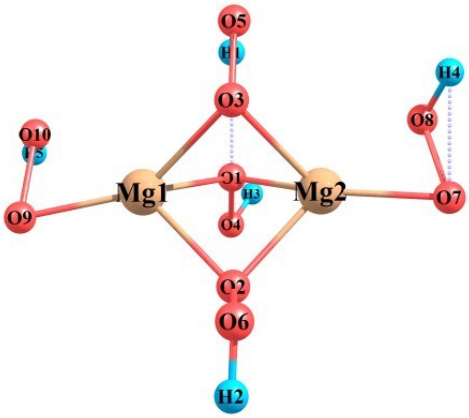
Table. S2 Calculated electronic spatial extent $<R^2>$ of $[Mg_2(OOH)_5]^-$ and $[Mg_2(OH)_5]^-$ at MP2/6-311++G** level.

	R^2		R^2
C1	3120.159	A1	1848.752
C2	3655.900	A2	1566.072
C3	2930.089		
C4	3420.647		
C5	3378.083		



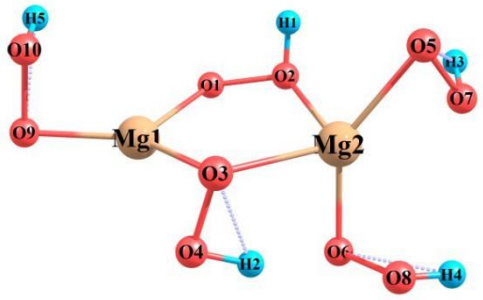
C1 (C1 / 8.38 Kcal/mol)

	Δe（anion-neutral）
O2	0.01
O3	0.05
O4	0.17
O5	0.18
O6	0.06
O7	0.15
O8	0.07
O9	0.14
O10	0.07



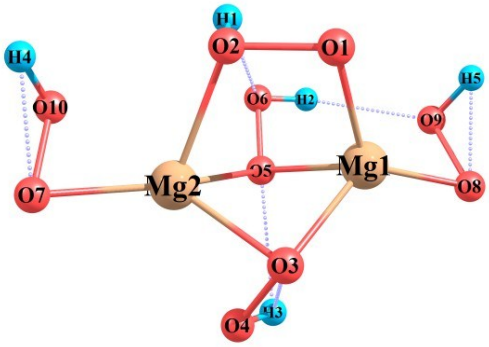
C2 (C1 / 4.43 Kcal/mol)

	Δe（anion-neutral）
O2	0.02
O3	0.08
O4	0.04
O5	0.09
O6	0.03
O7	0.22
O8	0.09
O9	0.23
O10	0.09



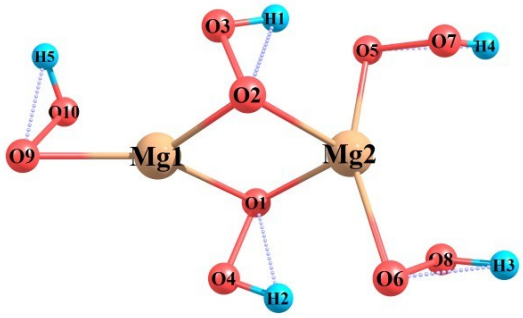
C3 (C1 / 8.06 Kcal/mol)

	Δe（anion-neutral）
O1	0.15
O2	0.05
O4	0.02
O5	0.3
O6	0.01
O7	0.12
O8	0.01
O9	0.17
O10	0.08



C4 (C1 / 5.28 Kcal/mol)

	Δe（anion-neutral）
O1	0.08
O2	0.01
O3	0.03
O4	0.03
O5	0.03
O6	0.04
O7	0.31
O8	0.18
O9	0.08
O10	0.11



C5 (C1 / 0 Kcal/mol)

	Δe（anion-neutral）
O1	0.12
O2	0.17
O3	0.08
O4	0.06
O5	0.01
O7	0.02
O8	0.01
O9	0.29
O10	0.13

Fig. S5 The increase of the negative charge of the O atoms in $[Mg_2(OOH)_5]^-$ at MP2/6-311++G** level.

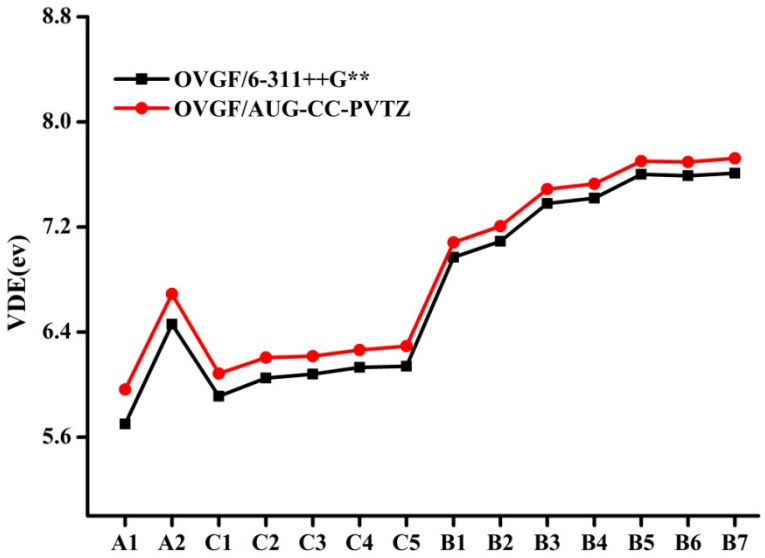


Fig. S6 The comparison between OVGF/6-311++G** and OVGF/aug-cc-pVTZ methods.

Table S3 The Calculated VDE values of the superhalogens under study here at OVGF methods with 6-311++G** and aug-cc-pVTZ basis sets (in eV).

	OVGF		ΔVDE
	6-311++G**	aug-cc-pVTZ	
A1	5.697	5.963	0.266
A2	6.456	6.689	0.233
B1	6.971	7.083	0.112
B2	7.09	7.207	0.117
B3	7.377	7.488	0.111
B4	7.422	7.529	0.107
B5	7.598	7.701	0.103
B6	7.592	7.694	0.102
B7	7.614	7.723	0.109
C1	5.913	6.083	0.170
C2	6.05	6.205	0.155
C3	6.08	6.216	0.136
C4	6.127	6.264	0.137
C5	6.138	6.294	0.156

Table S3

The absolute and relative errors of VDEs at OVGF, (MP2+HF)/2 methods with 6-311++G** basis sets referred to those at CCSD(T)/ 6-311++G** level.

	Absolute error (eV)		Relative error (%)	
	OVGF	(MP2+HF)/2	OVGF	(MP2+HF)/2
A1	0.656	-0.637	13.013	-12.637
A2	0.675	-0.617	11.673	-10.669
B1	0.349	-0.015	5.268	-0.229
B2	0.285	0.533	4.191	7.836
B3	0.345	0.014	4.903	0.196
B4	0.345	0.014	4.869	0.192
B5	0.328	-0.065	4.506	-0.900
B6	0.321	-0.066	4.414	-0.909
B7	0.316	0.538	4.330	7.372
C1	0.268	-0.095	4.751	-1.680
C2	0.355	0.030	6.233	0.526
C3	0.286	0.001	4.940	0.021
C4	0.323	-0.059	5.564	-1.018
C5	0.329	-0.029	5.655	-0.507

Table S4 The absolute and relative errors of VDEs at B3LYP, ωB97XD, M06-2X methods with 6-311+G* basis sets referred to those at CCSD(T)/ 6-311++G** level.

	Absolute error (eV)			Relative error (%)		
	B3LYP	ωB97XD	M06-2X	B3LYP	ωB97XD	M06-2X
A1	-0.549	-0.184	0.037	-10.893	-3.643	0.726
A2	-0.930	-0.213	-0.065	-16.087	-3.682	-1.119
B1	-0.570	0.011	0.410	-8.600	0.170	6.198
B2	-0.683	0.335	0.335	-10.037	4.920	4.920
B3	-0.776	-0.082	0.347	-11.042	-1.171	4.936
B4	-0.786	-0.083	0.322	-11.101	-1.166	4.556
B5	-0.983	-0.232	0.189	-13.527	-3.188	2.604
B6	-0.985	-0.234	0.187	-13.553	-3.221	2.574
B7	-0.815	-0.086	0.194	-11.174	-1.181	2.661

C1	-0.998	-0.313	0.116	-17.680	-5.536	2.052
C2	-0.902	-0.214	0.212	-15.845	-3.764	3.729
C3	-0.859	-0.153	0.213	-14.821	-2.644	3.678
C4	-0.891	-0.072	0.230	-15.353	-1.245	3.957
C5	-1.017	-0.329	0.098	-17.503	-5.659	1.687

Table. S5 The changes of Gibbs free energies of the binuclear superhalogens here along various fragmentation channels at 298 K (in K cal/mol level)

Fragmentation path	△Gr298	Fragmentation path	△Gr298
A1 → $Mg_2(OH)_4 + OH^-$	76.18	B4 → $Mg_2(OF)_4 + OF^-$	97.56
→ $Mg_2(OH)_3O^- + H_2O$	46.18	→ $Mg_2(OF)_3O^- + OF_2$	59.13

	→ $Mg_2(OH)_3^-$ + H_2O_2	841.12		→ $Mg_2F_5^-$ + O_2 + O_3	-240.85
	→ $Mg(OH)_3^-$ + $Mg(OH)_2$	67.35		→ Mg_2F_4 + $2O_2$ + OF^-	-89.08
B1	→ $Mg_2(OF)_4$ + OF^-	87.03		→ $Mg(OF)_3^-$ + $Mg(OF)_2$	72.56
	→ $Mg2(OF)_3O^-$ + OF_2	48.55		→ $Mg_2(OF)_3^-$ + O_2F_2 + Mg	206.81
	→ $Mg_2F_5^-$ + O2 + O3	-251.43	B5	→ $Mg_2(OF)_4$ + OF^-	90.04
	→ Mg_2F_4 + $2O_2$ + OF^-	-99.67		→ $Mg_2(OF)_3O^-$ + OF_2	56.02
	→ $Mg(OF)_3^-$ + $Mg(OF)_2$	61.98		→ $Mg_2F_5^-$ + O_2 + O_3	-248.42
	→ $Mg_2(OF)_3^-$ + O_2F_2 + Mg	196.23		→ Mg_2F_4 + $2O_2$ + OF^-	-96.66
B2	→ $Mg_2(OF)_4$ + OF^-	80.93		→ $Mg(OF)_3^-$ + $Mg(OF)_2$	64.99
	→ $Mg_2(OF)_3O^-$ + OF_2	42.31		→ $Mg_2(OF)_3^-$ + O_2F_2 + Mg	199.24
	→ $Mg_2F_5^-$ + O_2 + O_3	-257.73	B6	→ $Mg_2(OF)_4$ + OF^-	89.98
	→ Mg_2F_4 + $2O_2$ + OF^-	-105.96		→ $Mg_2(OF)_3O^-$ + OF_2	96.53
	→ $Mg(OF)_3^-$ + $Mg(OF)_2$	55.68		→ $Mg_2F_5^-$ + O_2 + O_3	-248.42
	→ $Mg_2(OF)_3^-$ + O_2F_2 + Mg	189.94		→ Mg_2F_4 + $2O_2$ + OF^-	-96.66
B3	→ $Mg_2(OF)_4$ + OF^-	97.34		→ $Mg(OF)_3^-$ + $Mg(OF)_2$	64.99
	→ $Mg_2(OF)_3O^-$ + OF_2	58.92		→ $Mg_2(OF)_3^-$ + O_2F_2 + Mg	199.24
	→ $Mg_2F_5^-$ + O_2 + O_3	-241.06			
	→ Mg_2F_4 + $2O_2$ + OF^-	-89.30			
	→ $Mg(OF)_3^-$ + $Mg(OF)_2$	72.35			
	→ $Mg_2(OF)_3^-$ + O_2F_2 + Mg	206.60			

Lowest normal mode frequencies and optimized coordinates at MP2/6-311++G** level of $Mg_2(OH)_5^-$, $Mg_2(OH)_5^-$, $Mg_2(OH)_5^-$.

A1 / $Mg_2(OH)_5^-$

Lowest normal mode frequency: 31.80cm^{-1}

Mg	-1.32653900	0.00432100	-0.00324700
Mg	1.66619000	-0.03810900	0.00411200
O	0.28180600	0.49227500	1.23865500
O	0.27498700	-0.71827000	-1.12799500
H	0.16766800	1.27926200	1.76901900
H	0.20717400	-1.24418300	-1.92070900
O	3.54164300	-0.03033500	-0.08157100
O	-2.54220600	-1.41594000	0.48160300
H	4.15899100	0.32988200	0.55231300
H	-2.20401900	-2.27939100	0.72030500
O	-1.99075100	1.73083000	-0.56324500
H	-2.92946700	1.85141300	-0.71088000

A2 / $Mg_2(OH)_5^-$

Lowest normal mode frequency: 90.55 cm^{-1}

Mg	-1.30775200	-0.01251800	0.01769000
Mg	1.30884700	0.04538500	0.04282300
O	0.02710100	1.30760300	-0.84077900
O	- 0.01048100	-0.12368500	1.58771100
O	- 0.01865300	1.48953300	-0.49165500
H	0.02910400	-1.60416700	-1.75054500
H	- 0.00315900	-0.88485000	2.16827100
H	- 0.01036900	1.99476600	-1.30313200
O	3.20606400	0.07264200	-0.08668600
O	- 3.20048100	-0.10209600	-0.14115500
H	3.74332100	-0.70553300	-0.22910500
H	- 3.80043300	0.57505200	0.16887000

B1 / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 21.79 cm^{-1}

Mg	1.65043800	-0.14177600	0.14588300
Mg	-1.40709700	0.03796300	-0.01952500
F	0.61411800	-1.96706100	-0.44113700
F	0.80451800	1.77290800	0.63716300
O	0.23071400	-0.72577100	-1.16081100
O	0.17285800	0.60184800	1.30646600
O	-1.92163100	1.42532800	-1.30102000
O	3.53594300	-0.44282200	0.50234700

F	-2.41273800	2.06938900	-0.05193100
F	3.50683700	0.46898700	-0.68666600
O	-2.22718000	-1.26124600	1.19447600
F	-2.65115000	-1.84788400	-0.10720300

B2 / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 19.14 cm^{-1}

Mg	-1.85228500	-0.22959000	-0.06455200
Mg	1.50887200	-0.12233100	0.16665300
F	-0.67328000	1.50288300	-0.79855500
F	0.10425700	-1.20048000	1.45580000
O	-0.14138100	0.14404500	-1.04308000
O	-1.17864400	-0.55452600	1.75424800
F	2.93365000	-0.95531300	-1.35407000
O	2.20079600	-1.85542400	-0.42037100
O	2.05809600	1.35588000	1.31401500
F	2.45677100	1.86340900	-0.03316900
O	-3.58189500	-0.62376200	-0.86930800
F	-3.79193200	0.62209600	-0.05992000

B3 / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 40.17cm^{-1}

Mg	-1.45286100	0.12925100	-0.25548100

Mg	1.47182400	0.15766800	-0.06970900
F	-0.00007600	-2.38479400	-0.41946000
F	-0.72984400	0.08269200	1.67270000
O	0.03766400	-1.04164500	-0.95532500
O	0.74031900	0.10777500	1.81579900
F	-0.08779700	2.66950200	-0.18483200
O	0.00471500	1.39408700	-0.86301800
O	3.35936100	0.45769300	-0.47008100
O	-3.36606000	0.37505900	-0.49882800
F	3.35656100	-0.94258600	0.05180800
F	-3.25390600	-0.95667900	0.17688600

B4 / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 40.63 cm^{-1}

Mg	1.38468100	0.31569500	-0.08013700
Mg	-1.47266600	-0.24977500	-0.21068800
F	0.93492500	-1.27744500	-1.31178500
O	-0.51669600	-1.47575500	-1.51277100
O	3.20773500	0.99092800	-0.07036600
F	3.34658600	-0.42288200	0.40184400
F	-3.24505900	0.73292200	0.58447200
F	0.22234800	-1.51500300	1.87485400
O	-3.39890600	-0.55866600	-0.15468800
O	-0.02605900	-0.23382900	1.25161600

O	-0.22789200	1.27339200	-0.88017200
F	-0.28653700	2.39800800	0.05294200

B5 / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 40.68 cm^{-1}

Mg	-1.53465400	0.13813100	0.08082900
Mg	1.54164100	0.32609000	-0.14404800
O	-0.03183200	-0.51221500	-1.10720200
F	0.03375600	-1.94611200	-0.87097800
F	-0.72516600	1.98088800	-0.49956800
O	0.71332000	2.14383500	-0.24661700
O	3.48555700	0.32146800	-0.30328500
F	3.14830300	-1.11227600	-0.02500100
O	-0.65157800	-0.06648000	1.86416300
F	0.75477300	-0.42744900	1.63067600
F	-3.27408900	-1.11678000	-0.20019600
O	-3.45572200	0.36650700	-0.15153200

B6 / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 40.7cm^{-1}

Mg	1.53435800	0.13884300	0.08305300
Mg	-1.54058500	0.32665000	-0.14642500
O	0.64672300	-0.06083400	1.86447200
O	0.03351500	-0.51393300	-1.10652400
F	-0.75761200	-0.42805300	1.62914900
F	-0.03271900	-1.94750200	-0.86888300
F	3.27252500	-1.11786900	-0.19854400
O	3.45622300	0.36503100	-0.14490600
F	0.72698800	1.98073500	-0.50482500
F	-3.14556100	-1.11514900	-0.03904900
O	-0.71229600	2.14369600	-0.25633100
O	-3.48639600	0.32412000	-0.28173100

B7 / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 40.82 cm^{-1}

Mg	0.15139200	-0.14875900	1.38644000
Mg	0.15139200	-0.14875900	-1.38644000
F	-2.46817500	0.00900600	0.00000000
F	-0.63434300	-2.52006700	0.00000000
O	-1.15509600	0.62538400	0.00000000
O	0.53382800	-1.64823800	0.00000000
F	0.15139200	1.01563700	3.21378300

O	0.07146100	-0.47520500	3.30325600
O	0.07146100	-0.47520500	-3.30325600
O	1.47070100	0.62505900	0.00000000
F	0.15139200	1.01563700	-3.21378300
F	1.51392600	2.07488300	0.00000000

C1 / $Mg_2(OOH)_5^-$

Lowest normal mode frequency: 42.61 cm^{-1}

Mg	1.43945500	-0.26801900	0.39120200
Mg	-1.42249900	0.60702500	-0.16237900
O	0.01653800	-0.54195100	-1.03390700
O	-0.38300200	-1.96024000	-0.94936600
O	1.08755400	1.79975900	0.14220400
O	-0.29871400	2.23310700	-0.10000800
O	0.39897800	-0.62040400	2.03196300
O	-1.00127500	-0.29681000	1.71194100
O	-3.28101800	0.57771700	-0.75979300
O	-3.20043200	-0.77635600	-0.10977300
O	3.28751700	-0.81382000	0.09419700
O	3.30864500	0.25518300	-0.95602500
H	-3.15602900	-1.34005400	-0.89080300
H	3.40109600	-0.29574200	-1.74051500
H	-1.41000800	-1.16839100	1.75817200

H	-0.05124800	-2.25546600	-1.80463600
H	1.53438500	2.14209500	-0.63956200

C2 / $Mg_2(OOH)_5^-$

Lowest normal mode frequency: 49.33 cm^{-1}

Mg	-1.37512100	0.23531300	-0.09412900
Mg	1.36480800	0.26952600	0.08566500
O	-0.04796600	-1.00290100	0.89764700
O	-0.05018200	1.65250700	0.56202100
O	0.09810700	-0.12457300	-1.47970700
O	-0.15708300	-1.21177400	2.34278400
O	0.19164900	-1.53731500	-1.88865800
O	0.00104300	2.85738900	-0.27976600
H	0.09913400	-1.97404500	-1.02700000
H	-0.09985900	3.52003500	0.41196700
H	0.27427600	-2.07103200	2.40534100
O	3.29845300	0.47205200	0.18833700
O	3.13844500	-0.98697900	-0.15260600
O	-3.30201100	0.46044600	0.07057700
O	-3.18425000	-0.96950700	-0.38921200
H	3.45095500	-0.98584700	-1.06492300
H	-3.49039000	-1.42193300	0.40486700

C3 / $Mg_2(OOH)_5^-$

Lowest normal mode frequency: 45.22 cm^{-1}

Mg	-1.90836000	0.20432200	0.07885600
Mg	1.37034800	-0.08765400	-0.24451300
O	-1.15638200	-1.23202400	1.22337100
O	0.24737000	-1.49131500	0.88124800
O	-0.31739100	0.77055100	-1.00280100
O	-0.64992600	1.87892300	-0.02627400
H	0.18882200	-2.34114300	0.43087100
H	0.23013200	1.91565100	0.48597800
O	2.37949400	-1.51321600	-1.15923600
O	1.63269800	1.47841300	1.00816300
O	3.26063300	-1.20423600	0.02052800
O	2.52227600	1.78156300	-0.15795700
O	-3.84838200	0.37982300	0.14551800
O	-3.64579600	-0.73067400	-0.85166200
H	3.19906000	-2.03549800	0.50371900
H	3.38095000	1.60112900	0.24437800
H	-3.93957900	-1.48263000	-0.32424600

C4 / $Mg_2(OOH)_5^-$

Lowest normal mode frequency: 53.31 cm^{-1}

Mg	-1.40079000	0.31141300	0.41334600
Mg	1.41843500	0.34202100	-0.01161400
O	-0.67850200	-0.95790400	1.76042000
O	0.68507700	-1.23242400	1.25600500
O	0.08220000	1.71815700	0.70225800
O	0.59460400	2.39833400	-0.52476600
O	-0.19041700	-0.12514800	-1.19611100
O	-0.36037500	-1.55230500	-1.50398800
H	0.50243100	-1.96444100	0.64957000
H	-1.31795200	-1.56323900	-1.64186900
H	-0.11540500	2.24475200	-1.16518900
O	3.35915400	0.36590900	-0.00213500
O	-3.28977900	0.66451300	0.07548100
O	-3.18874800	-0.69680300	-0.55354600
O	3.11293700	-1.06297900	-0.40447400
H	3.42696000	-1.50937100	0.39028000
H	-3.71697800	-1.20370800	0.07327800

C5 / $Mg_2(OOH)_5^-$

Lowest normal mode frequency: 58.01cm^{-1}

Mg	-1.64288400	-0.23924000	0.13268900
Mg	1.29499100	0.05462900	-0.01041300
O	-0.17930400	-0.90137300	-1.10016400
O	-0.21734100	0.69490900	1.24333700
O	-0.85039200	1.77700800	0.40443100
O	-0.49589400	-2.05563100	-0.18208700
O	1.49638700	1.84351000	-0.87690000
O	1.95011400	-1.64088500	0.81699600
O	2.57032700	1.87347900	0.17026600
O	2.88067700	-1.47162900	-0.34786300
O	-3.54276100	-0.40943800	0.52990800
O	-3.53708900	0.35720600	-0.76754700
H	-0.05234000	2.07783800	-0.10488300
H	0.39683800	-2.18595200	0.23404700
H	3.71341400	-1.40869800	0.13309100
H	3.33789300	1.97252200	-0.40398900
H	-3.81887700	1.22238000	-0.44859300

B6_b / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 37.49 cm^{-1}

Mg	-1.55541400	-0.18022100	-0.11487200
Mg	1.52055100	0.15130700	-0.13034900

F	0.16155200	-1.56795300	1.60362100
O	0.00743600	-0.18924600	1.17159900
O	-0.73200900	-1.24489800	-1.59062900
F	0.71089700	-1.35085200	-1.33847900
O	3.43003300	-0.21879800	-0.19073100
F	3.31726000	0.66797200	1.00441800
F	-3.22779200	0.82837400	0.86515400
O	-3.48544400	-0.39444800	0.04214500
O	0.62175600	1.74754400	-0.93543600
F	-0.77478500	1.72754100	-0.47170600

B6_c / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 39.08 cm^{-1}

Mg	-1.49407800	0.12279700	-0.26604100
Mg	1.54490600	-0.10473800	0.24021100
O	0.17148200	-0.63560500	-1.14482600
F	-0.91012700	-0.79094800	1.50563700
F	0.05621800	-2.08101100	-1.04570500
O	0.49286200	-0.55870100	1.87929500
O	3.46899900	-0.31750800	0.45641000
O	-3.29539200	-0.35405500	-0.83813800
F	3.37356800	0.50180500	-0.79163600
F	-3.53307800	0.51524200	0.35455300

O	-0.65900000	1.92696400	-0.04191000
F	0.78658100	1.77652800	-0.26470400

B6_d / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 42.46 cm^{-1}

Mg	-1.52177700	0.02165400	-0.25763400
Mg	1.54523600	0.20676700	0.09349900
F	-0.73687500	-0.51262700	1.59558100
O	-0.90944100	1.91722600	-0.42217000
O	0.62576900	-0.02570900	1.85311400
F	0.53773800	1.88565500	-0.66751700
F	0.23642000	-2.10041800	-0.77658700
O	0.18363600	-0.68451900	-1.10278600
O	3.43142800	0.66096000	-0.08281100
F	3.43975700	-0.83317400	-0.04532100
F	-3.55913100	0.26514200	0.44135000
O	-3.27422900	-0.75323900	-0.61508800

B5_b / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 40.47cm^{-1}

Mg	1.52012000	0.40527700	-0.12228100
Mg	-1.50623600	-0.19539300	-0.05217500
O	0.44606900	2.08471000	-0.30846400
F	0.76839800	-0.46392900	1.61152500
F	-0.95273500	1.73664100	-0.60225000
O	-0.68167900	-0.28579500	1.76802000
O	0.13558300	-0.64762900	-1.15447000
F	0.36049300	-2.05984000	-0.88809400
F	-3.55600100	0.30112000	0.44074200
O	-3.29611900	-0.73431900	-0.60585000
O	3.44860300	0.69349200	-0.15544700
F	3.31470500	-0.78091200	0.07620600

B5_c / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 43.28 cm^{-1}

Mg	-1.52903600	-0.06995100	-0.24238300
Mg	1.54348500	0.13680000	-0.00980500
O	-0.65421300	-1.82760400	-0.63006300
O	0.66994700	0.08035500	1.78746700
F	0.76638400	-1.57837800	-0.91227500
F	-0.75341800	0.40537600	1.62829300
O	0.01635100	0.95417700	-1.05970200
F	-0.09385600	2.32199900	-0.58002800

F	3.49063800	-0.69636800	0.43961300
F	-3.47242500	-0.70279900	0.47243600
O	3.40870500	0.51481900	-0.43356000
O	-3.39195300	0.45942200	-0.46490500

B5_d / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 38.89 cm^{-1}

Mg	1.49445600	0.12259700	-0.26552100
Mg	-1.54490100	-0.10460800	0.23938100
F	-0.05606500	-2.08045600	-1.04643500
O	0.65919800	1.92661100	-0.04033400
O	-0.17085100	-0.63503200	-1.14546400
F	-0.78647700	1.77700600	-0.26298500
F	0.90943700	-0.79252800	1.50498300
O	-0.49376200	-0.56127100	1.87848400
F	-3.37393100	0.50332800	-0.79117900
O	-3.46894400	-0.31785900	0.45564300
O	3.29591200	-0.35367900	-0.83781000
F	3.53291600	0.51642500	0.35445300

B5_e / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 36.29cm^{-1}

Mg	-1.55173200	0.17371300	0.03497900
Mg	1.54442500	0.14419400	0.06105600
F	-0.01131000	-2.06468800	-0.64706700
O	-0.86395400	-0.01147300	1.89991600
O	-0.00403800	-0.64848700	-0.97486200
F	0.54083900	-0.42833800	1.80945800
F	-0.53212400	1.90246600	-0.59072100
O	0.86766800	2.01243100	-0.15747900
F	3.38957500	-0.24277700	-1.04852600
F	-3.35225900	-0.95865400	-0.36902400
O	3.38858500	-0.34783900	0.44005100
O	-3.41636400	0.53449600	-0.40006300

B4_b / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 40.75 cm^{-1}

Mg	-1.35568400	0.32508000	-0.09559900
Mg	1.46901000	-0.24459300	-0.18340000
F	0.21903100	2.29628200	0.03133200
F	-0.25705300	-1.50573900	1.74943100
O	0.23964200	1.23490800	-1.01182100
O	0.03961100	-0.12816100	1.31937300

F	-3.30579600	-0.37296200	0.42598300
O	-3.18194900	1.02476100	-0.13254200
F	-0.93406400	-1.38189300	-1.17657800
F	3.20296000	0.82034600	0.53927900
O	0.53089800	-1.56364700	-1.41421300
O	3.41109500	-0.52663000	-0.10792700

B3_b / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 39.08 cm^{-1}

Mg	-1.47217500	0.15850200	-0.06857700
Mg	1.45271200	0.12918400	-0.25570900
O	-0.03846700	-1.04162900	-0.95426100
O	-0.73995300	0.11165600	1.81662100
O	-0.00464900	1.39397300	-0.86350800
F	-0.00064000	-2.38442600	-0.41747600
F	0.73004200	0.08267700	1.67279800
F	0.08878200	2.67014600	-0.18688300
O	3.36599200	0.37368500	-0.49930600
F	3.25330300	-0.95804500	0.17624400
F	-3.35458800	-0.94522600	0.04795000
O	-3.36024200	0.45752000	-0.46732900

B3_c / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 36.71 cm^{-1}

Mg	1.47451400	-0.06413200	-0.00138900
Mg	-1.43801200	0.04087000	-0.12486500
O	0.01380300	-0.75570000	-1.27924800
O	0.74176800	-0.88839900	1.69694700
F	-0.06301500	-2.19643500	-1.39021200
F	-0.72332800	-0.96589100	1.52947800
O	3.33733100	-0.03816900	-0.57514600
F	3.41613800	0.66529700	0.73867800
F	-3.28207000	0.64296500	0.83393700
O	-3.34225500	-0.02229700	-0.50412800
O	0.02717200	1.42301400	0.16683400
F	-0.08778900	2.13534800	-1.10377200

B3_d / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 39.53 cm^{-1}

Mg	1.45271400	0.25028800	-0.07891400
Mg	-1.43166600	-0.23927400	-0.26000700
O	0.23213200	-1.19874600	-0.90513700
O	0.73012500	0.14729200	1.80771700
F	0.37984200	-2.49274400	-0.27384200
F	-0.72093700	-0.09124800	1.66768500

F	-3.40587000	0.46537000	0.21230500
F	3.49276200	-0.51770900	0.10430800
O	-3.26392900	-0.83982700	-0.50730400
O	3.26898200	0.83033800	-0.49938400
O	-0.18848300	1.20277500	-0.92829700
F	-0.46615200	2.49557100	-0.34086700

B3_e / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 39.90 cm^{-1}

Mg	1.48765300	-0.18893300	-0.16744200
Mg	-1.42655900	-0.05346800	-0.11518100
O	0.02500700	-0.14033600	1.28090100
O	0.77809800	-1.78179300	-1.19588300
F	-0.04506500	-1.32188700	2.11144400
F	-0.69160600	-1.74729200	-1.05547600
O	-3.35990100	-0.23539000	-0.16906100
O	3.43703100	-0.16020000	-0.06272400
F	-3.14636700	1.12682000	0.40989000
F	3.05346400	1.20630900	0.41204600
O	0.02964800	0.97372100	-1.09689800
F	-0.06066900	2.25391700	-0.39559300

B3_f / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 37.84 cm^{-1}

Mg	1.46514000	-0.05856500	0.01043500
Mg	-1.45198300	0.19994200	-0.12962200
F	0.52122000	0.07042500	1.84747400
F	-0.15092100	-2.45256300	-0.11672400
O	-0.94757500	0.20778500	1.82692900
O	-0.03469900	-1.16643500	-0.76940400
F	0.31473900	2.57842100	-0.19871100
O	0.19265000	1.27412800	-0.81347100
F	-3.42611800	-0.74379800	-0.18124100
O	-3.24777600	0.61588500	-0.77388300
O	3.35625800	-0.22757200	0.40813600
F	3.32899500	-0.26658100	-1.08371000

B3_g / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 37.81 cm^{-1}

Mg	-1.41226700	0.30814300	-0.08162200
Mg	1.47012400	-0.12281800	0.05164200
F	-0.72478500	-1.06388200	-1.46341400
F	-0.38806100	-1.77759600	1.68803600
O	0.74777200	-1.13531400	-1.54756100

O	-0.14150700	-0.40324800	1.30919100
F	0.11568300	2.39848500	0.60945300
O	0.22646000	1.44917800	-0.49616000
O	3.28099100	-0.19574700	0.76892900
F	3.53139300	0.21568400	-0.64332300
F	-3.37198600	-0.57297000	-0.00523200
O	-3.25802500	0.90745800	-0.19814000

B3_h / $Mg_2(OF)_5^-$

Lowest normal mode frequency:33.02 cm^{-1}

Mg	-1.40983800	-0.01131400	-0.17475900
Mg	1.45430400	0.15217900	0.16524200
F	-0.72491400	1.93357100	0.05810400
F	0.02290900	-1.75775800	-1.45960300
O	0.74808100	2.04846700	0.06594500
O	0.18194900	-0.30153700	-1.41429900
F	-0.16914300	-1.82646700	1.51323100
O	-0.15214000	-0.37499800	1.37865400
F	3.50974100	0.45881300	-0.54402900
F	-3.38596900	0.59280600	0.45653300
O	3.24881700	-0.48097100	0.58555900
O	-3.25260700	-0.42834500	-0.62884600

B3_i / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 39.35 cm^{-1}

Mg	1.45242300	-0.25056400	-0.07883000
Mg	-1.43170700	0.24110500	-0.25847000
O	0.23249800	1.20005900	-0.90321800
O	0.73074000	-0.14725700	1.80825100
F	0.38214100	2.49398100	-0.27233700
F	-0.72035400	0.09143400	1.66870800
O	-0.18933900	-1.20144700	-0.92797300
O	-3.26446700	0.83923800	-0.50811200
F	-0.46819100	-2.49352900	-0.33941400
F	-3.40569700	-0.46751100	0.20876700
F	3.49384000	0.51517100	0.10098700
O	3.26753700	-0.83339500	-0.50054800

B3_j / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 39.48 cm^{-1}

Mg	1.45239000	0.25026200	-0.07884200
Mg	-1.43172300	-0.23970900	-0.25959700
O	0.73073500	0.14460900	1.80812300
O	0.23222700	-1.19854000	-0.90563700
F	-0.72016300	-0.09511000	1.66794100

F	0.38055800	-2.49265600	-0.27471500
F	-0.46736600	2.49524400	-0.33828600
O	-0.18898500	1.20311900	-0.92682200
O	-3.26440500	-0.83813500	-0.50880900
F	-3.40562300	0.46651900	0.21187600
F	3.49401300	-0.51571000	0.10252600
O	3.26783100	0.83254500	-0.49970600

B3_k / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 36.94 cm^{-1}

Mg	-1.47507000	-0.06263600	-0.00144300
Mg	1.43708000	0.03917800	-0.12431800
F	0.06013100	-2.19932200	-1.38585200
O	-0.01501900	-0.75831300	-1.27769000
O	-0.74170100	-0.88140100	1.69951700
F	0.72279400	-0.96626000	1.53057800
O	-0.02646500	1.42376200	0.16364900
O	-3.33804400	-0.03826800	-0.57493600
F	0.09383000	2.13194400	-1.10891900
F	-3.41511800	0.66804800	0.73758000
O	3.34167200	-0.02992100	-0.50080000
F	3.28195600	0.64943600	0.83008100

B3_l / $Mg_2(OF)_5^-$

Lowest normal mode frequency: 37.26 cm^{-1}

Mg	1.44992600	0.21681300	0.22243100
Mg	-1.43388500	-0.01464500	-0.16629600
F	0.34161600	-1.83214600	-1.61558900
F	-0.72268900	-1.14294800	1.40950300
O	0.20468300	-0.43390300	-1.27171300
O	0.70426300	-0.92293900	1.72260900
F	3.47162000	-0.51541600	-0.17118700
O	-0.20256600	1.47577400	0.46038300
F	-0.32003400	2.35351100	-0.70286100
O	3.27090800	0.91776400	0.20052700
F	-3.41908400	0.18690700	0.67514900
O	-3.27170900	-0.27109500	-0.74040000

B3_m/$Mg_2(OF)_5^-$

Lowest normal mode frequency: 36.74 cm^{-1}

Mg	1.43713700	0.03857100	-0.12428100
Mg	-1.47517400	-0.06300400	-0.00177400
F	0.06199100	-2.19930500	-1.38604900
F	0.09279300	2.13260200	-1.10713500
O	-0.01474100	-0.75834000	-1.27819700

O	-0.02652900	1.42292700	0.16459500
F	-3.41444900	0.66880200	0.73736000
F	0.72216000	-0.96698500	1.53030500
O	-3.33809900	-0.03734500	-0.57527000
O	-0.74251300	-0.88397000	1.69845300
O	3.34161600	-0.02646000	-0.50168700
F	3.28179000	0.64918600	0.83101900