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Exploring the Properties of New Super-chalcogens Based on Multiple Electron Counting Rules: A Combined DFT and *Ab Initio* Study on $[M(B_2C_4X_6)_2]^{2-}$ Dianion Clusters

Supporting Information

Part I

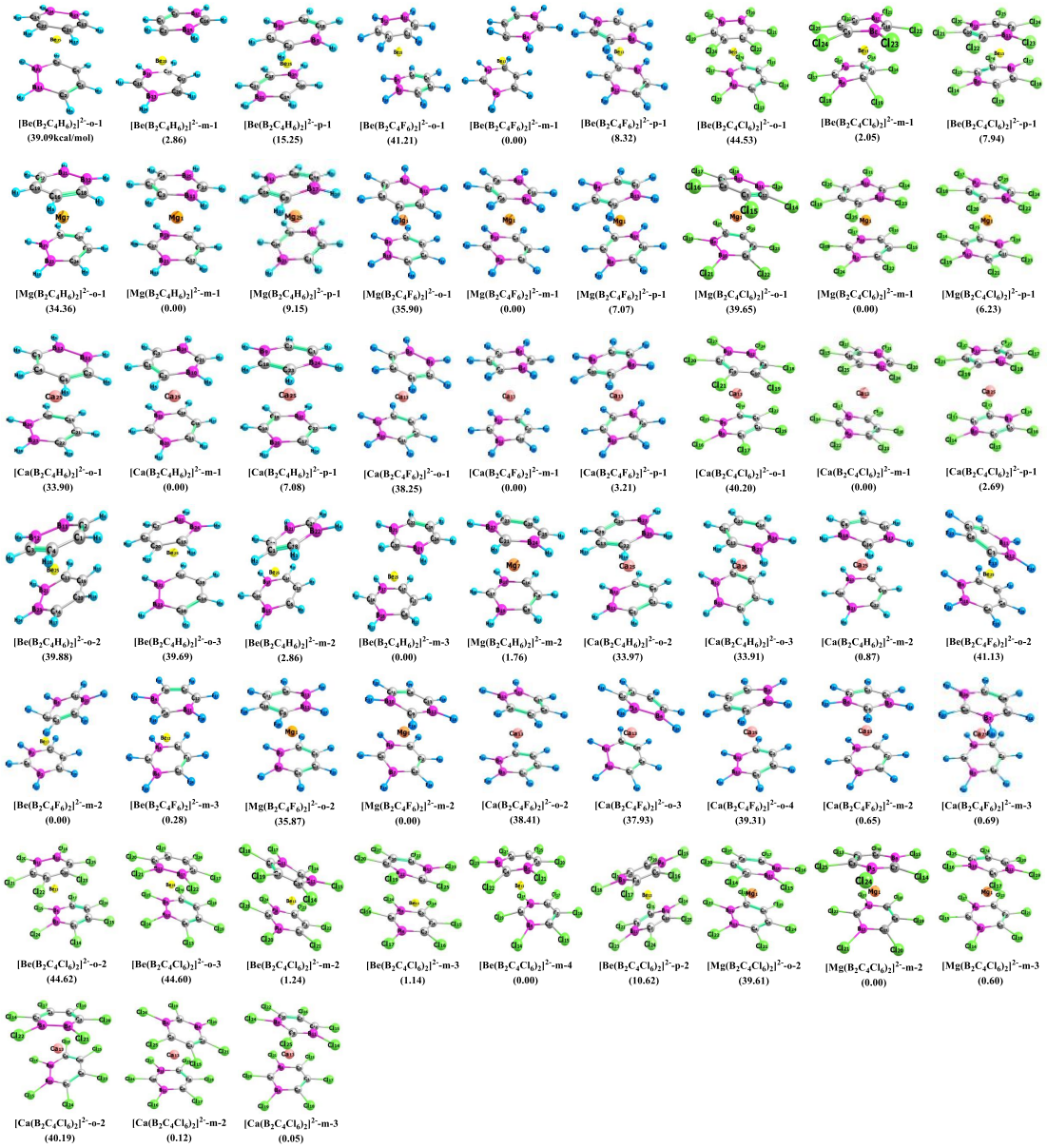


Figure S1. All 3D geometries and relative energies of dianion clusters $[M(B_2C_4X_6)_2]^{2-}$ (M = Be, Mg, Ca; X = H, F, Cl) at B3LYP-D3(BJ)/ 6-311++G(d,p) level.

Table S1. FVDE values (eV) for all $[M(B_2C_4X_6)_2]^{2-}$ clusters as well as $[B_2C_4X_6]^{2-}$, $[MX_4]^{2-}$ clusters (M = Be, Mg and Ca; X = H, F and Cl) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

Clusters	FVDE	Clusters	FVDE	Clusters	FVDE
$[Be(B_2C_4H_6)_2]^{2-}$-m-1	-0.72	$[Mg(B_2C_4H_6)_2]^{2-}$-m-1	-0.57	$[Ca(B_2C_4H_6)_2]^{2-}$-m-1	-0.04
$[Be(B_2C_4H_6)_2]^{2-}$-m-2	-0.71	$[Mg(B_2C_4H_6)_2]^{2-}$-m-2	-0.57	$[Ca(B_2C_4H_6)_2]^{2-}$-m-2	-0.03
$[Be(B_2C_4H_6)_2]^{2-}$-m-3	-1.23	$[Mg(B_2C_4H_6)_2]^{2-}$-o-1	-0.67	$[Ca(B_2C_4H_6)_2]^{2-}$-o-1	-0.53
$[Be(B_2C_4H_6)_2]^{2-}$-o-1	-1.32	$[Mg(B_2C_4H_6)_2]^{2-}$-p-1	-0.63	$[Ca(B_2C_4H_6)_2]^{2-}$-o-2	-0.59
$[Be(B_2C_4H_6)_2]^{2-}$-o-2	-1.00			$[Ca(B_2C_4H_6)_2]^{2-}$-o-3	-0.53
$[Be(B_2C_4H_6)_2]^{2-}$-o-3	-1.40			$[Ca(B_2C_4H_6)_2]^{2-}$-p-1	-0.63
$[Be(B_2C_4H_6)_2]^{2-}$-p-1	-1.03				
$[Be(B_2C_4F_6)_2]^{2-}$-m-1	0.71	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	0.76	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	1.04
$[Be(B_2C_4F_6)_2]^{2-}$-m-2	0.71	$[Mg(B_2C_4F_6)_2]^{2-}$-m-2	0.92	$[Ca(B_2C_4F_6)_2]^{2-}$-m-2	1.10
$[Be(B_2C_4F_6)_2]^{2-}$-m-3	0.09	$[Mg(B_2C_4F_6)_2]^{2-}$-o-1	0.58	$[Ca(B_2C_4F_6)_2]^{2-}$-m-3	1.06
$[Be(B_2C_4F_6)_2]^{2-}$-o-1	0.37	$[Mg(B_2C_4F_6)_2]^{2-}$-o-2	0.60	$[Ca(B_2C_4F_6)_2]^{2-}$-o-1	0.62
$[Be(B_2C_4F_6)_2]^{2-}$-o-2	0.34	$[Mg(B_2C_4F_6)_2]^{2-}$-p-1	0.42	$[Ca(B_2C_4F_6)_2]^{2-}$-o-2	0.65
$[Be(B_2C_4F_6)_2]^{2-}$-p-1	0.32			$[Ca(B_2C_4F_6)_2]^{2-}$-o-3	0.48
				$[Ca(B_2C_4F_6)_2]^{2-}$-o-4	0.63
				$[Ca(B_2C_4F_6)_2]^{2-}$-p-1	0.50
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1	1.25	$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1	1.27	$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-1	1.35
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-2	1.02	$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-2	1.34	$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-2	1.64
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-3	1.02	$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-3	1.47	$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-3	1.64
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-4	0.74	$[Mg(B_2C_4Cl_6)_2]^{2-}$-o-1	1.19	$[Ca(B_2C_4Cl_6)_2]^{2-}$-o-1	1.28
$[Be(B_2C_4Cl_6)_2]^{2-}$-o-1	0.98	$[Mg(B_2C_4Cl_6)_2]^{2-}$-o-2	1.25	$[Ca(B_2C_4Cl_6)_2]^{2-}$-o-2	1.28
$[Be(B_2C_4Cl_6)_2]^{2-}$-o-2	1.02	$[Mg(B_2C_4Cl_6)_2]^{2-}$-p-1	0.76	$[Ca(B_2C_4Cl_6)_2]^{2-}$-p-1	1.14
$[Be(B_2C_4Cl_6)_2]^{2-}$-o-3	1.02				
$[Be(B_2C_4Cl_6)_2]^{2-}$-p-1	0.90				
$[Be(B_2C_4Cl_6)_2]^{2-}$-p-2	0.47				
$[BeCl_4]^{2-}$	0.86	$[MgCl_4]^{2-}$	1.53	$[CaCl_4]^{2-}$	1.89
$[BeF_4]^{2-}$	0.50	$[MgF_4]^{2-}$	1.28	$[CaF_4]^{2-}$	1.56
$[BeH_4]^{2-}$	-2.00	$[MgH_4]^{2-}$	-1.08	$[CaH_4]^{2-}$	-0.89
$[B_2C_4H_6]^{2-}$-m	-3.15	$[B_2C_4F_6]^{2-}$-m	-2.07	$[B_2C_4Cl_6]^{2-}$-m	-1.24
$[B_2C_4H_6]^{2-}$-o	-3.28	$[B_2C_4F_6]^{2-}$-o	-1.71	$[B_2C_4Cl_6]^{2-}$-o	-1.04
$[B_2C_4H_6]^{2-}$-p	-2.68	$[B_2C_4F_6]^{2-}$-p	-2.36	$[B_2C_4Cl_6]^{2-}$-p	-0.62

Table S2. FVDE values (eV) calculated from different methods for selected structures.

Clusters	OVGF(PS)	B3LYP-D3(BJ)	ωB97XD	MP2	(HF+MP2)/2	Δ^1	Δ^2	Δ^3
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1	1.12(0.89)	1.25	1.36	1.69	0.92	0.13	0.24	-0.20
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-2	1.12(0.89)	1.02	1.36	1.69	0.92	-0.10	0.24	-0.20
$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1	1.22(0.89)	1.27	1.71	2.10	1.50	0.05	0.49	0.28
$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-2	1.22(0.89)	1.34	1.71	2.12	1.51	0.12	0.49	0.29
$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-1	1.65(0.89)	1.35	2.53	2.27	1.85	-0.30	0.88	0.20
$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-2	1.65(0.89)	1.64	2.53	2.27	1.85	-0.01	0.88	0.20

Δ^1 refers to the difference between B3LYP-D3(BJ) and OVGF results.

Δ^2 refers to the difference between ωB97XD and OVGF results.

Δ^3 refers to the difference between (HF+MP2)/2 and OVGF results.

Table S3. FVDE value of partial clusters $[M(B_2C_4X_6)_2]^{2-}$ (M = Be, Mg and Ca; X = H, F and Cl) and the corresponding maximum difference among H, F and Cl substituents.

Clusters	H	F	Cl	Maximum ΔFVDE
$[Be(B_2C_4X_6)_2]^{2-}$-m-1	-0.72	0.71	1.25	1.97
$[Be(B_2C_4X_6)_2]^{2-}$-o-1	-1.32	0.04	0.67	1.99
$[Be(B_2C_4X_6)_2]^{2-}$-p-1	-1.03	0.32	0.90	1.93
$[Mg(B_2C_4X_6)_2]^{2-}$-m-1	-0.57	0.76	1.27	1.84
$[Mg(B_2C_4X_6)_2]^{2-}$-o-1	-0.67	0.58	1.19	1.86
$[Mg(B_2C_4X_6)_2]^{2-}$-p-1	-0.83	0.42	0.76	1.59
$[Ca(B_2C_4X_6)_2]^{2-}$-m-1	-0.04	1.04	1.35	1.39
$[Ca(B_2C_4X_6)_2]^{2-}$-o-1	-0.53	0.62	1.28	1.81
$[Ca(B_2C_4X_6)_2]^{2-}$-p-1	-0.63	0.50	1.14	1.77

Table S4. FVDE value of partial clusters $[M(B_2C_4X_6)_2]^{2-}$ (M = Be, Mg and Ca; X = H, F and Cl) and the corresponding maximum difference among Be, Mg and Ca central atoms.

Clusters	Be	Mg	Ca	Maximum ΔFVDE
$[M(B_2C_4H_6)_2]^{2-}$-m-1	-0.72	-0.57	-0.04	0.68
$[M(B_2C_4F_6)_2]^{2-}$-m-1	0.71	0.76	1.04	0.33
$[M(B_2C_4Cl_6)_2]^{2-}$-m-1	1.25	1.27	1.35	0.10
$[M(B_2C_4H_6)_2]^{2-}$-o-1	-1.32	-0.67	-0.53	0.79
$[M(B_2C_4F_6)_2]^{2-}$-o-1	0.04	0.58	0.62	0.58
$[M(B_2C_4Cl_6)_2]^{2-}$-o-1	0.67	1.19	1.28	0.61
$[M(B_2C_4H_6)_2]^{2-}$-p-1	-1.03	-0.83	-0.63	0.40
$[M(B_2C_4F_6)_2]^{2-}$-p-1	0.32	0.42	0.50	0.18
$[M(B_2C_4Cl_6)_2]^{2-}$-p-1	0.90	0.76	1.14	0.38

Table S5. FVDE value of partial clusters $[M(B_2C_4X_6)_2]^{2-}$ (M = Be, Mg and Ca; X = H, F and Cl) and the corresponding maximum difference among m, o and p positions.

Clusters	m	o	p	Maximum ΔFVDE
$[Be(B_2C_4H_6)_2]^{2-}$	-0.72	-1.32	-1.03	0.60
$[Be(B_2C_4F_6)_2]^{2-}$	0.71	0.04	0.32	0.67
$[Be(B_2C_4Cl_6)_2]^{2-}$	1.25	0.67	0.90	0.58
$[Mg(B_2C_4H_6)_2]^{2-}$	-0.57	-0.67	-0.83	0.26
$[Mg(B_2C_4F_6)_2]^{2-}$	0.76	0.58	0.42	0.34
$[Mg(B_2C_4Cl_6)_2]^{2-}$	1.27	1.19	0.76	0.51
$[Ca(B_2C_4H_6)_2]^{2-}$	-0.04	-0.53	-0.63	0.59
$[Ca(B_2C_4F_6)_2]^{2-}$-	1.04	0.62	0.50	0.54
$[Ca(B_2C_4Cl_6)_2]^{2-}$	1.35	1.28	1.14	0.21

Table S6. The electron affinity(eV) of substitute H, F, Cl and the ionization energy(eV) of Be, Mg, Ca

	H	F	Cl	IE	Be	Mg	Ca
EA	-0.35	1.25	2.48	FIE	8.04	6.60	5.12
				SIE	18.12	14.72	11.31

FIE=First Ionization Energy, $\Delta E_1=E(X^+)-E(X0)$

SIE=Second Ionization Energy, $\Delta E_2= E(X^{2+})-E(X^+)$

Table S7. The kinetic energies of molecular orbitals for partial mono-anion and dianion structures.

		anion (a.u.)		dianion (a.u.)	$LUMO_{anin,Beta}$-$HOMO_{dianion}$	
		Alpha	Beta		a.u.	eV
$[Be(B_2C_4H_6)_2]^{2-}$-m-1	LUMO+1	0.853068	0.112257	0.066969	0.031562	0.86
	LUMO	0.118825	0.916096	0.060279		
	HOMO	1.041259	0.981102	0.884534		
	HOMO-1	0.98573		1.015431		
$[Be(B_2C_4F_6)_2]^{2-}$-m-1	LUMO+1	1.10255	1.646936	0.357791	0.034726	0.94
	LUMO	1.659678	1.625729	0.410067		
	HOMO	1.705064	1.690984	1.591003		
	HOMO-1	1.703791		1.78118		
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1	LUMO+1	1.991046	1.720635	1.494181	0.030101	0.82
	LUMO	1.661447	1.563239	1.436874		
	HOMO	1.716185	1.678025	1.533138		
	HOMO-1	1.770209		1.730486		
$[Mg(B_2C_4H_6)_2]^{2-}$-m-1	LUMO+1	0.07578	0.103992	0.047765	0.004076	0.11
	LUMO	0.106806	0.993017	0.04318		
	HOMO	1.057945	0.897329	0.988941		
	HOMO-1	1.018425		0.90006		
$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	LUMO+1	1.374667	1.115211	0.124725	0.008507	0.23
	LUMO	1.130422	1.685461	0.431154		
	HOMO	1.795147	1.648497	1.676954		
	HOMO-1	1.795823		1.64076		
$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1	LUMO+1	1.548158	1.787017	0.738806	0.001703	0.05
	LUMO	1.810217	1.628693	0.931814		
	HOMO	1.762346	1.635621	1.626990		
	HOMO-1	1.803826		1.632241		

$[Ca(B_2C_4H_6)_2]^{2-}$-m-1	LUMO+1	0.056605	0.030274	0.021253	0.00747	0.20
	LUMO	0.030219	0.976600	0.020505		
	HOMO	0.942232	1.007931	0.969130		
	HOMO-1	0.949805		0.989624		
$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	LUMO+1	1.638326	1.225157	0.023316	0.011988	0.37
	LUMO	1.237057	1.729191	0.026279		
	HOMO	1.739507	1.688072	1.717203		
	HOMO-1	1.702604		1.667075		
$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-1	LUMO+1	1.629114	1.57743	0.050573	0.006934	0.19
	LUMO	1.55513	1.625812	0.048509		
	HOMO	1.686884	1.647126	1.618878		
	HOMO-1	1.721739		1.62481		

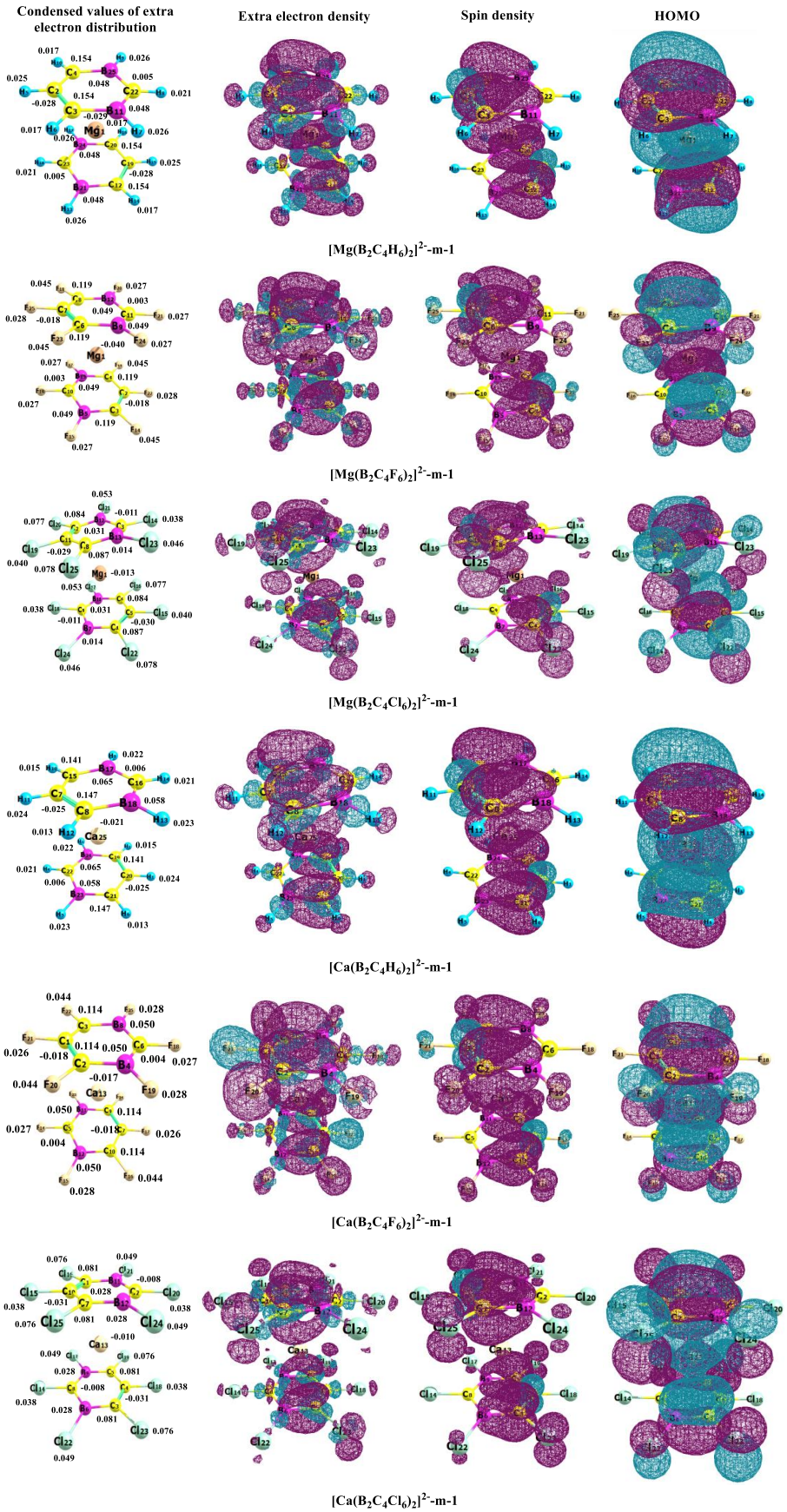


Figure S2. The distribution of extra electron, spin density and contribution of HOMO orbitals of $[Mg(B_2C_4X_6)_2]^{2-}$-m-1 (X = H, F, Cl) and $[Ca(B_2C_4X_6)_2]^{2-}$-m-1 (X = H, F, Cl) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

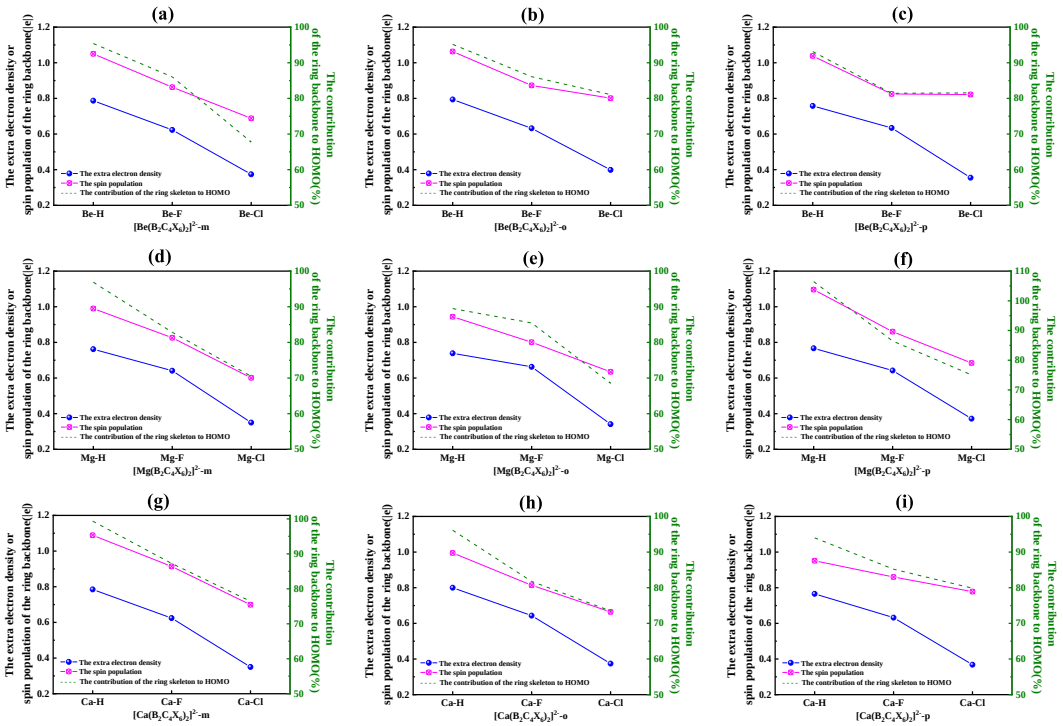


Figure S3. Comparison of extra electron density, spin density and contribution to HOMO for the ring backbone atoms of $[M(B_2C_4X_6)_2]^{2-}$ (M = Be, Mg and Ca; X = H, F and Cl) clusters: (a) $[Be(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-m-1, (b) $[Be(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-o-1, (c) $[Be(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-p-1, (d) $[Mg(B_2C_4X_6)_2]^{2-}$(X= H, F and Cl)-m-1, (e) $[Mg(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-o-1, (f) $Mg(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-p-1, (g) $[Ca(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-m-1, (h) $[Ca(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-o-1, (i) $[Ca(B_2C_4X_6)_2]^{2-}$(X = H, F and Cl)-p-1.

Table S8. First extra electron (FEE) of all C and B atoms on the aromatic ring backbone in $[M(B_2C_4X_6)_2]^{2-}$-m-1 (M=Be, Mg and Ca; X=H, F and Cl) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

First extra electron (FEE)					
Clusters	FEE	Clusters	FEE	Clusters	FEE
$[Be(B_2C_4H_6)_2]^{2-}$-o-1	0.794	$[Mg(B_2C_4H_6)_2]^{2-}$-o-1	0.739	$[Ca(B_2C_4H_6)_2]^{2-}$-o-1	0.800
$[Be(B_2C_4F_6)_2]^{2-}$-o-1	0.632	$[Mg(B_2C_4F_6)_2]^{2-}$-o-1	0.663	$[Ca(B_2C_4F_6)_2]^{2-}$-o-1	0.643
$[Be(B_2C_4Cl_6)_2]^{2-}$-o-1	0.399	$[Mg(B_2C_4Cl_6)_2]^{2-}$-o-1	0.341	$[Ca(B_2C_4Cl_6)_2]^{2-}$-o-1	0.374
$[Be(B_2C_4H_6)_2]^{2-}$-m-1	0.787	$[Mg(B_2C_4H_6)_2]^{2-}$-m-1	0.762	$[Ca(B_2C_4H_6)_2]^{2-}$-m-1	0.785
$[Be(B_2C_4F_6)_2]^{2-}$-m-1	0.623	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	0.641	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	0.624
$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1	0.374	$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1	0.350	$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-1	0.350
$[Be(B_2C_4H_6)_2]^{2-}$-p-1	0.758	$[Mg(B_2C_4H_6)_2]^{2-}$-p-1	0.767	$[Ca(B_2C_4H_6)_2]^{2-}$-p-1	0.766
$[Be(B_2C_4F_6)_2]^{2-}$-p-1	0.634	$[Mg(B_2C_4F_6)_2]^{2-}$-p-1	0.642	$[Ca(B_2C_4F_6)_2]^{2-}$-p-1	0.632
$[Be(B_2C_4Cl_6)_2]^{2-}$-p-1	0.355	$[Mg(B_2C_4Cl_6)_2]^{2-}$-p-1	0.372	$[Ca(B_2C_4Cl_6)_2]^{2-}$-p-1	0.368

Table S9. First extra electron (FEE) of all C and B atoms on the aromatic ring backbone and contribution of the aromatic ring backbone to the HOMO orbital and spin population of aromatic ring backbone in $[M(B_2C_4X_6)_2]^{2-}$-m-1 (M=Be, Mg and Ca; X=H, F and Cl) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

First extra electron (FEE)					
Clusters	FEE	Clusters	FEE	Clusters	FEE
$[Be(B_2C_4H_6)_2]^{2-}$-m-1	0.787	$[Be(B_2C_4F_6)_2]^{2-}$-m-1	0.623	$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1	0.374
$[Mg(B_2C_4H_6)_2]^{2-}$-m-1	0.762	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	0.641	$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1	0.350
$[Ca(B_2C_4H_6)_2]^{2-}$-m-1	0.785	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	0.624	$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-1	0.350
Spin population number					
Clusters	Spin population	Clusters	Spin population	Clusters	Spin population
$[Be(B_2C_4H_6)_2]^{2-}$-m-1	1.050	$[Be(B_2C_4F_6)_2]^{2-}$-m-1	0.863	$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1	0.688
$[Mg(B_2C_4H_6)_2]^{2-}$-m-1	0.990	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	0.826	$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1	0.601
$[Ca(B_2C_4H_6)_2]^{2-}$-m-1	1.089	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	0.914	$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-1	0.699
Contribution of the aromatic ring backbone to the HOMO orbitals					
Clusters	Contribution	Clusters	Contribution	Clusters	Contribution
$[Be(B_2C_4H_6)_2]^{2-}$-m-1	95.39	$[Be(B_2C_4F_6)_2]^{2-}$-m-1	86.04	$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1	67.74
$[Mg(B_2C_4H_6)_2]^{2-}$-m-1	96.88	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	82.84	$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1	70.47
$[Ca(B_2C_4H_6)_2]^{2-}$-m-1	99.38	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	87.28	$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-1	76.44

Table S10. First extra electron (FEE) of all C and B atoms on the aromatic ring backbone and contribution of the aromatic ring backbone to the HOMO orbital and spin population of aromatic ring backbone in $[M(B_2C_4F_6)_2]^{2-}$ (M=Be, Mg and Ca) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

First extra electron (FEE)					
Clusters	FEE	Clusters	FEE	Clusters	FEE
$[Be(B_2C_4F_6)_2]^{2-}$-m-1	0.623	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	0.641	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	0.624
$[Be(B_2C_4F_6)_2]^{2-}$-o-1	0.632	$[Mg(B_2C_4F_6)_2]^{2-}$-o-1	0.663	$[Ca(B_2C_4F_6)_2]^{2-}$-o-1	0.643
$[Be(B_2C_4F_6)_2]^{2-}$-p-1	0.634	$[Mg(B_2C_4F_6)_2]^{2-}$-p-1	0.642	$[Ca(B_2C_4F_6)_2]^{2-}$-p-1	0.632
Spin population number					
Clusters	Spin population	Clusters	Spin population	Clusters	Spin population
$[Be(B_2C_4F_6)_2]^{2-}$-m-1	0.863	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	0.826	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	0.914
$[Be(B_2C_4F_6)_2]^{2-}$-o-1	0.873	$[Mg(B_2C_4F_6)_2]^{2-}$-o-1	0.801	$[Ca(B_2C_4F_6)_2]^{2-}$-o-1	0.814
$[Be(B_2C_4F_6)_2]^{2-}$-p-1	0.825	$[Mg(B_2C_4F_6)_2]^{2-}$-p-1	0.860	$[Ca(B_2C_4F_6)_2]^{2-}$-p-1	0.860
Contribution of the aromatic ring backbone to the HOMO orbitals					
Clusters	Contribution	Clusters	Contribution	Clusters	Contribution
$[Be(B_2C_4F_6)_2]^{2-}$-m-1	86.04	$[Mg(B_2C_4F_6)_2]^{2-}$-m-1	82.84	$[Ca(B_2C_4F_6)_2]^{2-}$-m-1	87.28
$[Be(B_2C_4F_6)_2]^{2-}$-o-1	86.09	$[Mg(B_2C_4F_6)_2]^{2-}$-o-1	85.44	$[Ca(B_2C_4F_6)_2]^{2-}$-o-1	81.77
$[Be(B_2C_4F_6)_2]^{2-}$-p-1	81.43	$[Mg(B_2C_4F_6)_2]^{2-}$-p-1	86.46	$[Ca(B_2C_4F_6)_2]^{2-}$-p-1	85.20

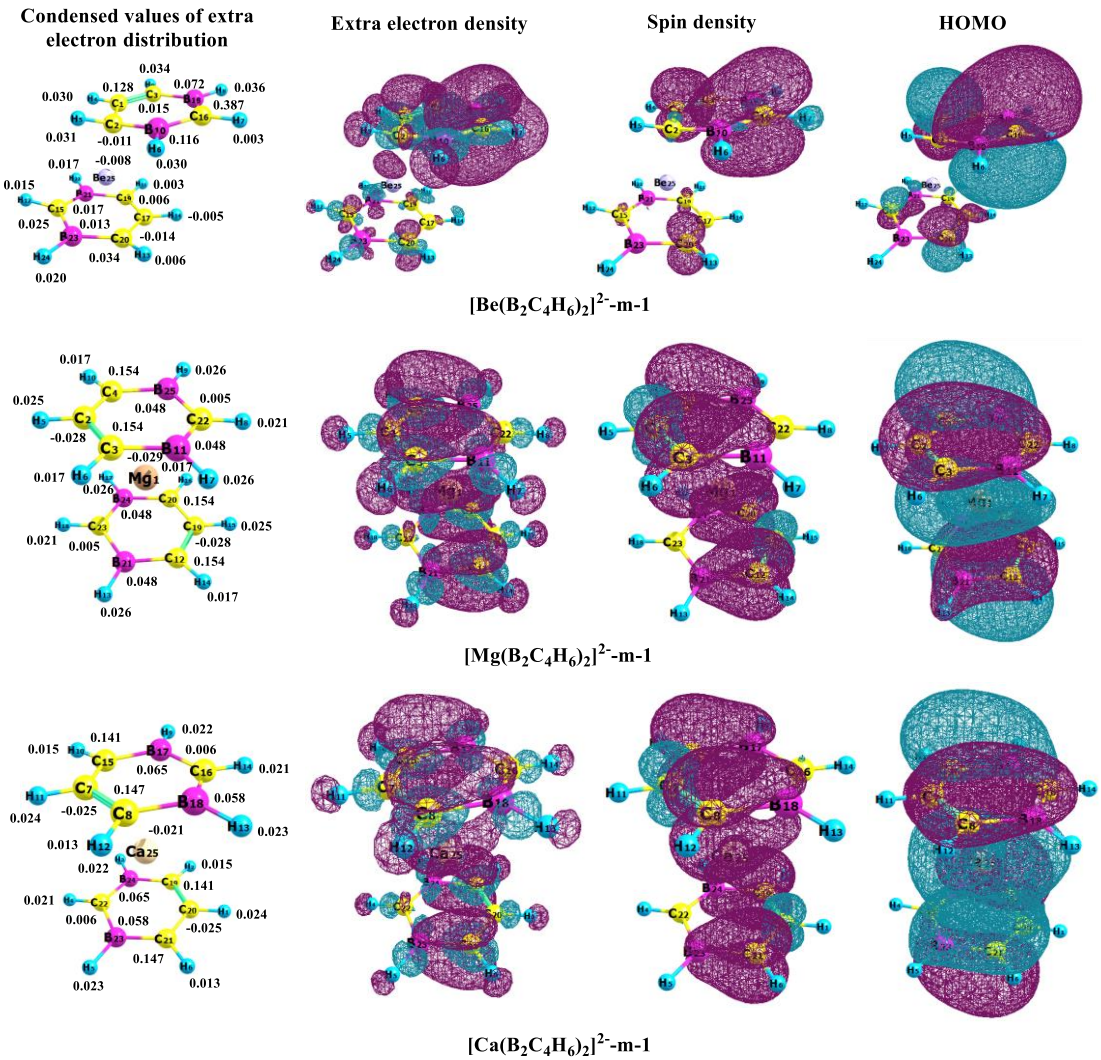


Figure S4. The distribution of the extra electron, the spin density and the contribution of HOMO orbitals of $[M(B_2C_4H_6)_2]^{2-}$-m-1 (M = Be, Mg, Ca) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

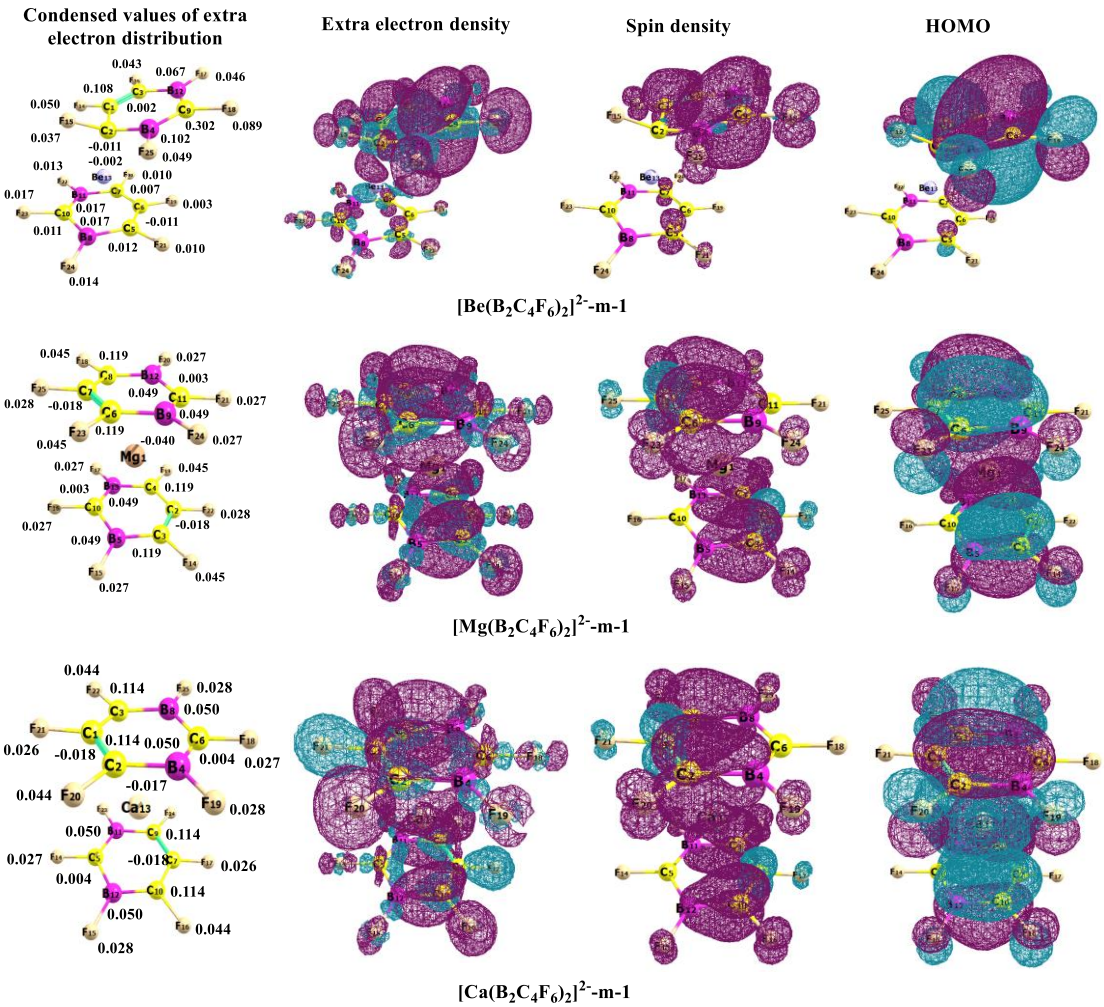


Figure S5. The distribution of the extra electron, the spin density and the contribution of HOMO orbitals of $[M(B_2C_4F_6)_2]^{2-}$-m-1 (M = Be, Mg, Ca) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

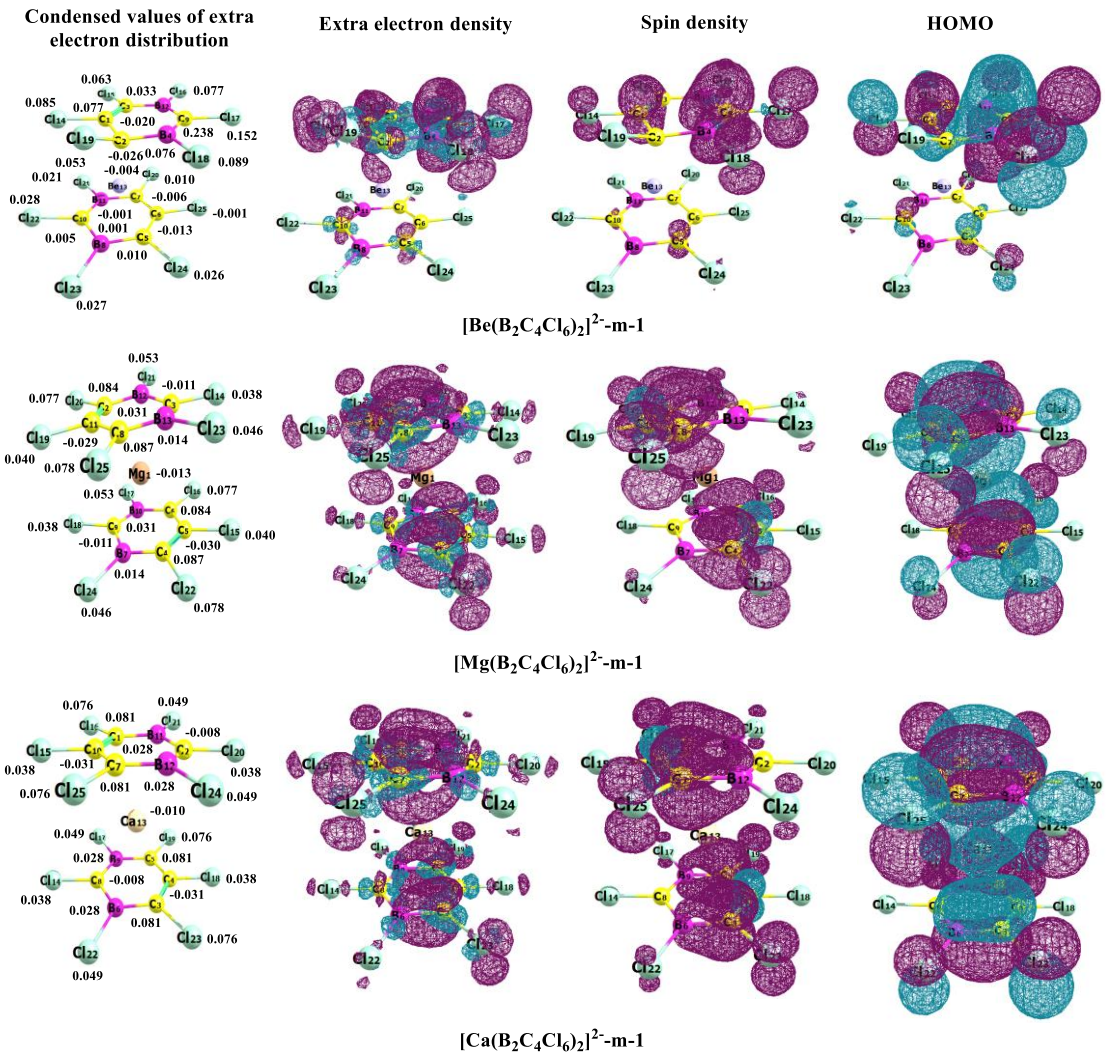


Figure S6. The distribution of the extra electron, the spin density and the contribution of HOMO orbitals of $[M(B_2C_4Cl_6)_2]^{2-}$-m-1 (M = Be, Mg, Ca) at the B3LYP-D3(BJ)/6-311++G(d,p) level.

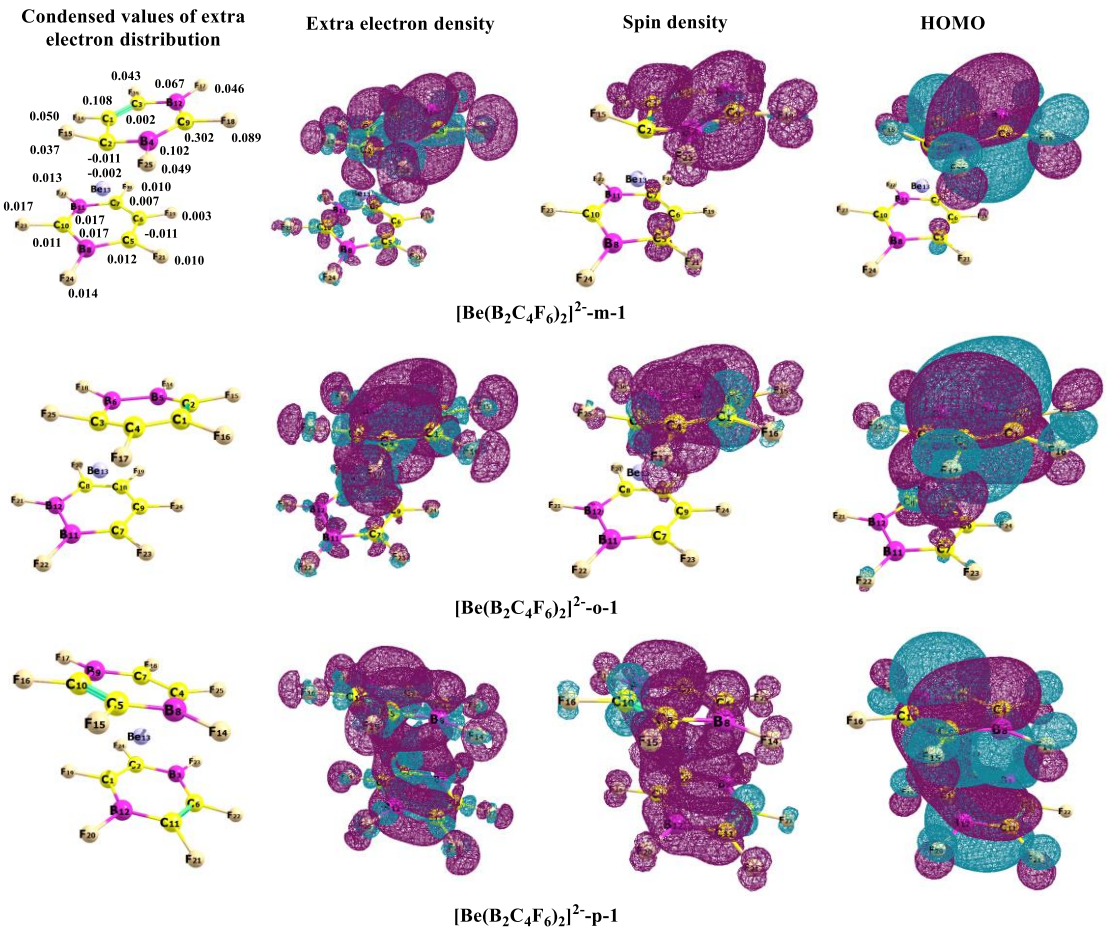


Figure S7. The distribution of the extra electron, the spin density and the contribution of HOMO orbitals of $Be(B_2C_4F_6)_2]^{2-}$ at the B3LYP-D3(BJ)/6-311++G(d,p) level.

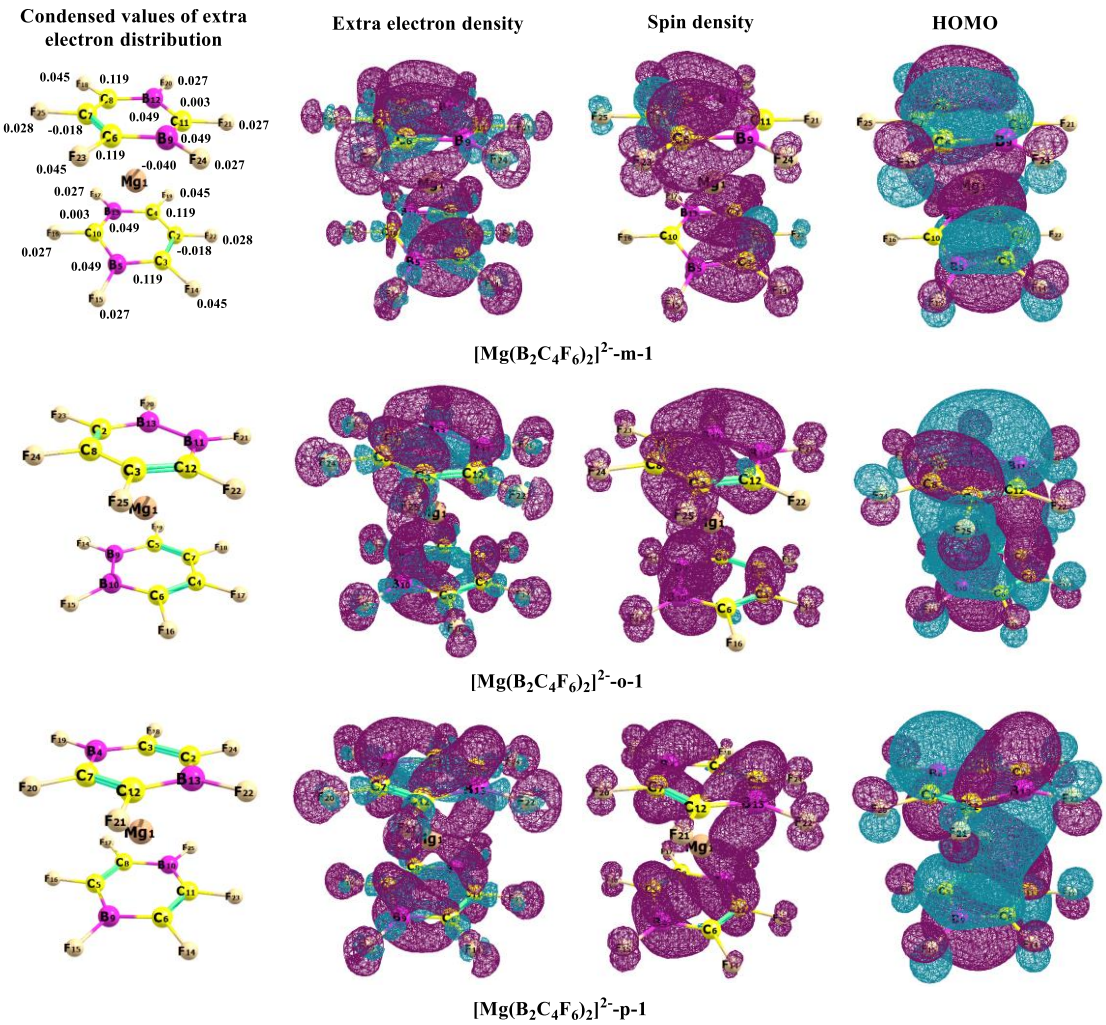


Figure S8. The distribution of the extra electron, the spin density and the contribution of HOMO orbitals of $Mg(B_2C_4F_6)_2]^{2-}$ at the B3LYP-D3(BJ)/6-311++G(d,p) level.

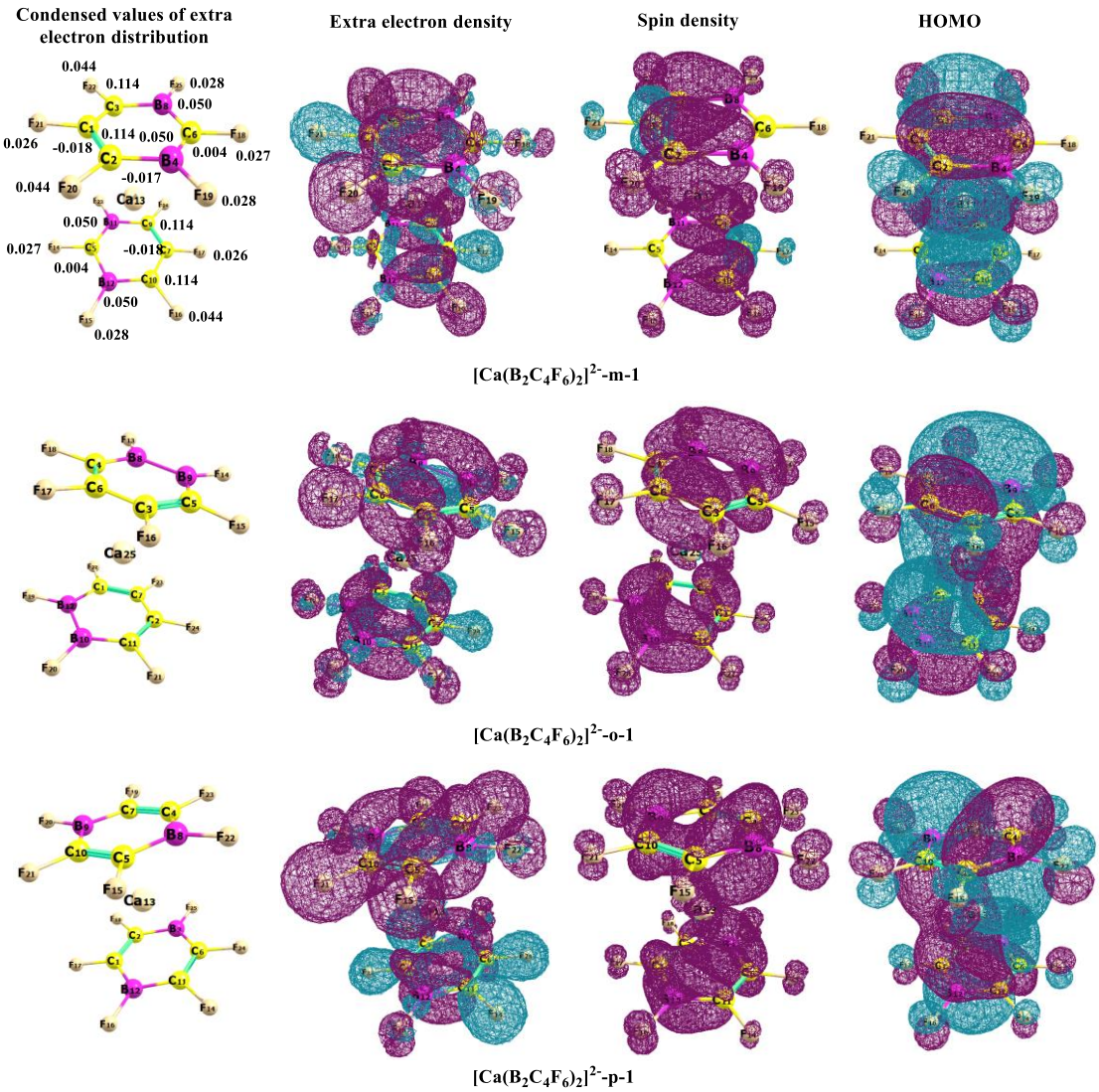


Figure S9. The distribution of the extra electron, the spin density and the contribution of HOMO orbitals of $Ca(B_2C_4F_6)_2]^{2-}$ at the B3LYP-D3(BJ)/6-311++G(d,p) level.

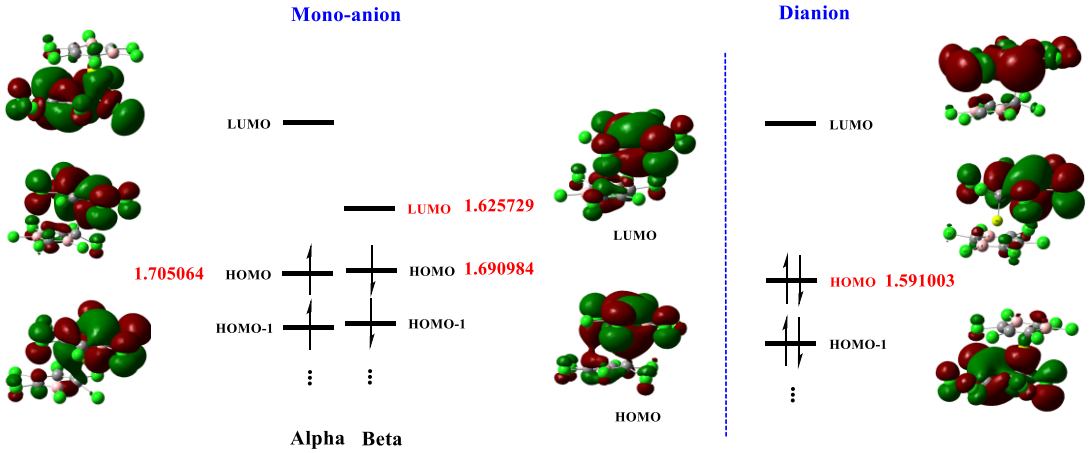


Figure S10. The kinetic energies (a.u.) of partial molecular orbitals for mono-anion $[Be(B_2C_4F_6)_2]^-$-m-1 and dianion $[Be(B_2C_4F_6)_2]^{2-}$-m-1.

In addition, in order to estimate electronic kinetic energy of the extra electron, we have also analyzed kinetic energies of molecular orbitals for partial mono-anion and dianion structures as shown in Figure S9 and Table S5. Taking $[Be(B_2C_4Cl_6)_2]^{2-}$-m-1 as an example (in Table S5), the kinetic energy of HOMO orbital on dianion is 1.533138 a.u., and that of HOMO alpha/beta orbital, LUMO beta orbital on mono-anion form is 1.716185/1.678025, 1.563239 a.u. Taking $[Be(B_2C_4F_6)_2]^{2-}$-m-1 as an example, the kinetic energies of HOMO orbital on dianion and HOMO alpha/beta orbital, LUMO beta orbital on mono-anion are 1.591003 and 1.705064/1.690984, 1.625729 a.u. respectively. Taking $[Be(B_2C_4H_6)_2]^{2-}$-m-1 as an example, the kinetic energies of HOMO orbital on dianion and HOMO alpha/beta orbital, LUMO beta orbital on mono-anion are 0.884534 and 1.041259/0.981102, 0.916096 a.u. respectively. Significantly, the kinetic energies of HOMO orbital on dianion indeed have been decreased in the process of getting extra electron from the mono-anion to the dianion as shown in Figure S9.

Here, the approximated approach was also employed to estimate the kinetic energies of extra electron, i.e., the decreased value of kinetic energies from LUMO beta orbital of mono-anion to HOMO orbital of dianion. For example, in $[Be(B_2C_4F_6)_2]^{2-}$-m-1 and $[Be(B_2C_4Cl_6)_2]^{2-}$-m-1, the decreased values are 0.034726 a.u. (0.95 eV) and 0.030101 a.u. (0.82 eV) respectively. Significantly, the kinetic energies of extra electron have been also decreased. Moreover, from H to halogens, these values gradually increase overall, consistent with FVDE and FEE values. For example, In $[Be(B_2C_4H_6)_2]^{2-}$-m-1 and $[Be(B_2C_4F_6)_2]^{2-}$-m-1, the decreased values are 0.031562 a.u.(0.86 eV) and 0.034726 a.u. (0.95 eV) respectively (in Table S5). Similar situations exist in $[Mg(B_2C_4X_6)_2]^{2-}$-m-1 and $[Ca(B_2C_4X_6)_2]^{2-}$-m-1 as shown in Table S5. It is noted that the clusters concluding Cl-substituent have close value of decreased kinetic energies with $[M(B_2C_4H_6)_2]^{2-}$-m-1. For example, the decreased value of kinetic energies in $[Be(B_2C_4Cl_6)_2]^{2-}$-m-1 (0.030101 a.u. (0.82 eV)) is close to that of $[Be(B_2C_4H_6)_2]^{2-}$-m-1 (0.031562 a.u.(0.86 eV)). This poor performance may be induced by other more complexed factor. Thus, in the future similar work, the comprehensive analysis methods will be employed to provide more reasonable explanation. In this revised manuscript, this idea of the approximated approach, i.e., the decreased value of kinetic energies from LUMO beta orbital on mono-anion form to HOMO orbital on dianion, to estimate the kinetic energies of extra electron.

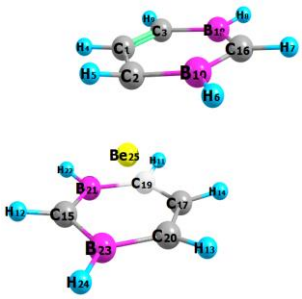
Table S11. NICS(0) values (ppm) for $[M(B_2C_4X_6)_2]^{2-}$ (M = Be, Mg, Ca; X = H, F, Cl) clusters at B3LYP-D3(BJ)/6-311++G (d,p) level.

Be-H	ring 1	ring 2	Be-F	ring 1	ring 2	Be-Cl	ring 1	ring 2
o-1	-2.84	-9.00	o-1	-12.75	-20.70	o-1	-7.51	-12.79
o-2	-2.84	-9.00	o-2	--	--	o-2	-7.51	-12.79
m-1	-1.58	-8.25	m-1	-9.04	-20.25	m-1	-4.99	-12.29
m-2	-1.58	-8.25	m-2	-9.04	-20.25	m-2	-4.99	-12.29
p-1	-4.68	-4.68	p-1	-16.17	-16.17	p-1	-9.09	-9.09
Mg-H	ring 1	ring 2	Mg-F	ring 1	ring 2	Mg-Cl	ring 1	ring 2
o-1	-4.90	-4.90	o-1	--	--	o-1	-9.99	-9.99
o-2	--	--	o-2	-17.32	-17.32	o-2	--	--
m-1	-3.66	-3.66	m-1	-16.00	-16.00	m-1	-8.87	-8.87
p-1	-3.43	-3.43	p-1	-15.99	-15.99	p-1	-8.89	-8.89
Ca-H	ring 1	ring 2	Ca-F	ring 1	ring 2	Ca-Cl	ring 1	ring 2
o-1	-5.80	-5.80	o-1	-19.17	-19.17	o-1	-11.52	-11.52
o-2	-5.90	-5.90	o-2	-19.12	-19.12	o-2	-11.52	-11.52
m-1	-5.35	-5.35	m-1	-18.59	-18.59	m-1	-11.04	-11.06
p-1	-6.25	-6.25	p-1	-19.71	-19.71	p-1	-11.92	-11.92

Part II

Optimized coordinates and corresponding energies at B3LYP/6-311++G(d,p) level.

$[Be(B_2C_4H_6)_2]^{2-}$-m-1



E (B3LYP/6-311++G(d,p)) = -426.44400127

Zero-point correction=	0.182897 (Hartree/Particle)
Thermal correction to Energy=	0.194958
Thermal correction to Enthalpy=	0.195902
Thermal correction to Gibbs Free Energy=	0.144470
Sum of electronic and zero-point Energies=	-426.261104
Sum of electronic and thermal Energies=	-426.249043
Sum of electronic and thermal Enthalpies=	-426.248099
Sum of electronic and thermal Free Energies=	-426.299532

Charge = -2 Multiplicity = 1

C	-1.45612700	-1.30773700	0.75273100
C	-0.79498700	-0.11363400	1.27494500
C	-2.46253100	-1.26883400	-0.17926300
H	-1.08444200	-2.27974900	1.09999700
H	-0.33325900	-0.26364600	2.26185700
H	-0.93205300	2.26040200	1.47956400
H	-2.91451000	2.32675900	-0.40566400
H	-3.94228500	0.04566000	-1.52222900
H	-2.82827900	-2.23787100	-0.53948200
B	-1.40410600	1.27624200	0.92466200
H	0.48479100	-1.04853100	-2.18167800
H	2.96733600	-1.34348500	1.52540900
H	1.62352700	2.53563100	-0.25638900
H	0.46612800	1.33469500	-1.97821100
C	2.59458100	-0.76548000	0.67421900
C	-2.49915600	1.35408000	-0.10725200
C	1.16828300	0.78060900	-1.35835800
B	-3.04076000	0.07889900	-0.68188900
C	1.18745500	-0.62784900	-1.46643400
C	1.85203000	1.47476000	-0.33146600

B	1.96690800	-1.50347700	-0.48849200
H	1.90002000	-2.71074600	-0.56271700
B	2.66383200	0.74623600	0.73233400
H	3.15922500	1.36286300	1.65224900
Be	0.74178800	-0.03174200	0.35987100

$[Be(B_2C_4H_6)_2]^{2-}$-m-2

E (B3LYP/6-311++G(d,p)) = -426.44400128

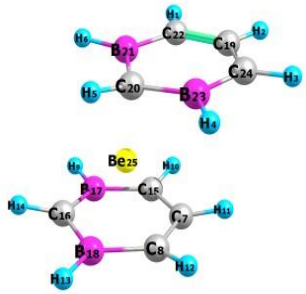
Zero-point correction=	0.182897 (Hartree/Particle)
Thermal correction to Energy=	0.194958
Thermal correction to Enthalpy=	0.195902
Thermal correction to Gibbs Free Energy=	0.144470
Sum of electronic and zero-point Energies=	-426.261104
Sum of electronic and thermal Energies=	-426.249043
Sum of electronic and thermal Enthalpies=	-426.248099
Sum of electronic and thermal Free Energies=	-426.299531

Charge = -2 Multiplicity = 1

C	1.45598900	-1.30778300	0.75252400
H	1.08420100	-2.27981700	1.09960200
H	2.82824800	-2.23778400	-0.53966300
H	3.94271600	0.04567000	-1.52170800
H	0.93203100	2.26026300	1.47976500
C	-1.18780100	-0.62832900	-1.46632800
H	-1.90034300	-2.71087900	-0.56168300
H	-0.48532900	-1.04934400	-2.18157100
H	-0.46618100	1.33393600	-1.97883100
H	-1.62318500	2.53567100	-0.25726800
H	-3.15868300	1.36368700	1.65203100
H	-2.96694300	-1.34268100	1.52625700
C	-1.16833900	0.78017200	-1.35869100
C	-1.85183900	1.47480600	-0.33194300
B	-1.96709000	-1.50357500	-0.48790300

C	-2.59437400	-0.76504600	0.67473100
B	-2.66352300	0.74670900	0.73222900
C	2.46247500	-1.26877900	-0.17937800
H	0.33300800	-0.26380300	2.26166300
H	2.91438400	2.32688700	-0.40556500
B	1.40406500	1.27619100	0.92469800
B	3.04089600	0.07898700	-0.68169100
C	0.79494900	-0.11369300	1.27487800
C	2.49910700	1.35415100	-0.10721600
Be	-0.74166600	-0.03158900	0.35971200

$[Be(B_2C_4H_6)_2]^{2-}$-m-3



E (B3LYP/6-311++G(d,p)) = -426.44948309

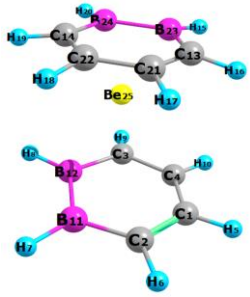
Zero-point correction=	0.183065 (Hartree/Particle)
Thermal correction to Energy=	0.195059
Thermal correction to Enthalpy=	0.196003
Thermal correction to Gibbs Free Energy=	0.145399
Sum of electronic and zero-point Energies=	-426.266418
Sum of electronic and thermal Energies=	-426.254424
Sum of electronic and thermal Enthalpies=	-426.253480
Sum of electronic and thermal Free Energies=	-426.304084

Charge = -2 Multiplicity = 1

H	-2.87064600	2.13443300	0.61891700
H	-3.58210100	-0.00728300	1.44348800
H	-2.81574200	-2.13057300	0.61569200
H	-0.98542400	-2.37709100	-1.40226300
H	-0.16885400	0.03927700	-2.38718800
H	-1.04245100	2.43053900	-1.39438900
C	1.09991700	-0.83127800	1.31591600
C	1.85115700	-1.45615100	0.29301800
H	1.77351500	2.71381900	0.73383300
H	0.32449700	0.93582600	2.19605200
H	0.39567600	-1.43643000	1.88405500
H	1.66388400	-2.52048600	0.16311700

H	3.22412800	-1.20929800	-1.63288000
H	2.94199400	1.48241800	-1.38417600
C	1.06703700	0.57063100	1.49132100
C	2.55528600	0.85216100	-0.57771700
B	1.86511700	1.51548500	0.59489600
B	2.67309200	-0.65170800	-0.70480800
C	-2.83200500	0.00361900	0.63682500
C	-0.74687800	0.03067000	-1.45145200
B	-1.37343800	1.34415100	-0.94601400
C	-2.41171700	1.25456800	0.15653300
B	-1.34390800	-1.29873800	-0.95101300
C	-2.37513400	-1.23903900	0.15678000
Be	0.69780700	0.07195400	-0.38672700

$[Be(B_2C_4H_6)_2]^{2-}$-o-1



E (B3LYP/6-311++G(d,p)) = -426.38683558

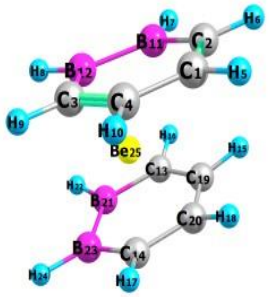
Zero-point correction=	0.183174 (Hartree/Particle)
Thermal correction to Energy=	0.195213
Thermal correction to Enthalpy=	0.196157
Thermal correction to Gibbs Free Energy=	0.145051
Sum of electronic and zero-point Energies=	-426.203662
Sum of electronic and thermal Energies=	-426.191623
Sum of electronic and thermal Enthalpies=	-426.190678
Sum of electronic and thermal Free Energies=	-426.241785

Charge = -2 Multiplicity = 1

C	-2.43486800	-1.08581400	0.20308200
C	-2.84924800	0.19762200	0.67987900
C	-0.80597000	-0.16323900	-1.43206200
C	-1.49874300	-1.27367300	-0.79395500
H	-2.86793900	-1.98658200	0.65271100
H	-3.60129900	0.16170000	1.48170900
H	-2.72175800	2.54284300	0.57309000
H	-0.60169400	2.15925200	-1.73325400

H	-0.26791200	-0.43969900	-2.34952400
H	-1.23268300	-2.29459000	-1.07253600
B	-2.29999400	1.47801200	0.12226200
B	-1.17741000	1.28459400	-1.10218900
C	1.41800700	-1.32368400	0.90571400
C	2.19026200	1.30917000	-0.06521700
H	2.65559900	-2.41862800	-0.75115200
H	0.89848100	-2.22249700	1.24161200
H	0.10228400	-0.17470600	2.20905200
H	0.75964200	1.99630200	1.42824900
H	2.24296500	2.33593600	-0.43219100
H	3.47730500	0.41223100	-1.80092100
C	0.92883700	-0.12930400	1.50727000
C	1.30720000	1.14441800	1.04068700
B	2.40508400	-1.34089100	-0.24461900
B	2.83771300	0.15245200	-0.79874100
Be	0.69929600	0.00115600	-0.40069800

$[Be(B_2C_4H_6)_2]^{2-}$-o-2



E (B3LYP/6-311++G(d,p)) = -426.38552848

Zero-point correction=	0.183164 (Hartree/Particle)
Thermal correction to Energy=	0.195250
Thermal correction to Enthalpy=	0.196194
Thermal correction to Gibbs Free Energy=	0.144998
Sum of electronic and zero-point Energies=	-426.202365
Sum of electronic and thermal Energies=	-426.190278
Sum of electronic and thermal Enthalpies=	-426.189334
Sum of electronic and thermal Free Energies=	-426.240531

Charge = -2 Multiplicity = 1

C	-2.61589200	-0.50878600	-0.64851200
C	-1.95326800	-1.44594100	0.14432800
C	-1.76679700	1.43025300	0.61541400
C	-2.51885700	0.88691300	-0.42766700

H	-3.25495000	-0.84251000	-1.47363200
H	-2.16347800	-2.49672500	-0.10202000
H	-0.44916000	-1.94734000	1.89066300
H	-0.31974200	1.15933900	2.45835600
H	-1.82354600	2.52307600	0.70809900
H	-3.07899800	1.54358700	-1.10147300
B	-1.01587000	-1.05021900	1.28508100
B	-0.92764500	0.58311500	1.57158400
C	2.24193100	-1.22734200	0.21431300
C	1.34569000	1.24706200	-1.02389800
H	0.84095200	-2.13451300	-1.18743000
H	2.33847600	-2.20507000	0.69153600
H	0.78148400	2.08105800	-1.44410000
H	0.08808500	-0.08806100	-2.19573900
C	1.34767600	-1.22059700	-0.89530600
C	0.91589000	-0.02415800	-1.49542600
B	2.85154200	0.02563600	0.80429900
H	3.51870100	-0.09807600	1.81450100
B	2.34555900	1.43060600	0.10102800
H	2.56206300	2.56565300	0.47865100
Be	0.67848600	0.04237000	0.43828900

$[Be(B_2C_4H_6)_2]^{2-}$-o-3

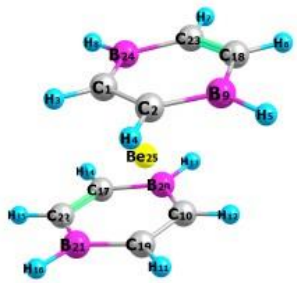
E (B3LYP/6-311++G(d,p)) = -426.38576463

Zero-point correction=	0.183098 (Hartree/Particle)
Thermal correction to Energy=	0.195184
Thermal correction to Enthalpy=	0.196128
Thermal correction to Gibbs Free Energy=	0.144936
Sum of electronic and zero-point Energies=	-426.202667
Sum of electronic and thermal Energies=	-426.190581
Sum of electronic and thermal Enthalpies=	-426.189636
Sum of electronic and thermal Free Energies=	-426.240829

Charge = -2 Multiplicity = 1

H	1.27561600	-2.30180600	1.08905800
H	0.26106500	-0.45968100	2.33616900
H	0.55689700	2.14301000	1.71628000
H	2.65627700	2.54739400	-0.61213400
H	3.58357000	0.17731000	-1.49659300
H	2.90106800	-1.97883100	-0.64618400
C	-2.53154300	0.63306700	0.66583300
C	-1.84229200	1.38585900	-0.32818900
H	-1.61393700	-2.79773100	-0.72309100
H	-3.15949900	-1.40912000	1.61561000
H	-2.88035200	1.23761800	1.50766900
H	-1.70042500	2.45411700	-0.19627100
H	-0.45619600	1.38183700	-1.95660000
H	-0.30674000	-1.00085100	-2.19549300
C	-1.05774700	-0.65668600	-1.48417800
C	2.45690500	-1.08350500	-0.19799100
C	0.82061800	-0.17589700	1.43498900
C	2.83841400	0.20339400	-0.68813100
C	1.52939500	-1.27982500	0.80578400
C	-1.11632600	0.76157400	-1.36048800
B	1.15309000	1.27626100	1.08969400
B	2.26374500	1.47952500	-0.14190300
B	-2.63322400	-0.87695000	0.65539200
B	-1.81339800	-1.60863000	-0.57711300
Be	-0.63823900	-0.01804700	0.33636500

$[Be(B_2C_4H_6)_2]^{2-}$-p-1



E (B3LYP/6-311++G(d,p)) = -426.42419437

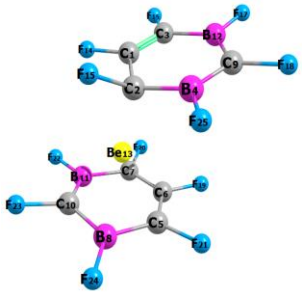
Zero-point correction=	0.182496 (Hartree/Particle)
Thermal correction to Energy=	0.194802
Thermal correction to Enthalpy=	0.195746
Thermal correction to Gibbs Free Energy=	0.144408
Sum of electronic and zero-point Energies=	-426.241698
Sum of electronic and thermal Energies=	-426.229393

Sum of electronic and thermal Enthalpies=	-426.228449
Sum of electronic and thermal Free Energies=	-426.279786

Charge = -2 Multiplicity = 1

C	0.96932300	-0.28360200	1.54383700
C	1.49314700	-1.37473000	0.72900400
H	0.33875800	-0.55104500	2.39320900
H	1.18415600	-2.38619900	1.00511300
H	2.73695200	-2.01361400	-1.19226500
H	3.38634500	0.61273600	-1.59426500
H	2.52277300	2.41304000	-0.26693600
H	0.81628200	2.07184400	1.83189300
B	2.36235300	-1.11097700	-0.46595500
C	-0.96942400	-0.28281300	-1.54403500
H	-1.18316700	-2.38552200	-1.00659400
H	-0.33844200	-0.54983900	-2.39321400
H	-0.81742400	2.07317300	-1.83099500
H	-2.52372900	2.41230700	0.26820700
H	-3.38586700	0.61117100	1.59494300
H	-2.73544400	-2.01483500	1.19142200
C	-2.24698300	1.39106500	-0.02371700
C	2.74237000	0.35060200	-0.74321200
C	-1.49267500	-1.37438300	-0.72991400
B	-1.28752100	1.15282500	-1.20119200
B	-2.36152700	-1.11163100	0.46547000
C	-2.74215000	0.34968300	0.74355500
C	2.24641300	1.39150000	0.02435500
B	1.28692500	1.15215900	1.20151000
Be	-0.00061700	-0.42725700	0.00026900

$[Be(B_2C_4F_6)_2]^{2-}$-m-1



E (B3LYP/6-311++G(d,p)) = -1617.97818967

Zero-point correction=	0.096406 (Hartree/Particle)
Thermal correction to Energy=	0.119939

Thermal correction to Enthalpy=	0.120883
Thermal correction to Gibbs Free Energy=	0.041432
Sum of electronic and zero-point Energies=	-1617.881784
Sum of electronic and thermal Energies=	-1617.858250
Sum of electronic and thermal Enthalpies=	-1617.857306
Sum of electronic and thermal Free Energies=	-1617.936757

Charge = -2 Multiplicity = 1

C	-1.28714200	1.26424600	-0.98161000
C	-0.54091600	0.03168800	-1.24437400
C	-2.45273900	1.29271700	-0.31598000
B	-1.32729000	-1.32450100	-0.97383000
C	1.73068700	-1.42558500	0.95288900
C	1.09484900	-0.45526400	1.74328000
C	1.28629400	0.92129700	1.53730500
B	2.73875100	-1.07139100	-0.12526400
C	-2.59150300	-1.29879200	-0.20536400
C	2.84982600	0.40895600	-0.37469500
B	2.26784500	1.47162400	0.51853100
B	-3.21566700	-0.00039300	0.12087400
Be	0.89323200	0.01099000	-0.22601900
F	-0.67344600	2.44175500	-1.33990000
F	-0.04747500	0.06238800	-2.62350900
F	-2.95398000	2.52934700	0.06401600
F	-4.42402600	0.17891700	0.77568000
F	-3.27085100	-2.51058800	0.10917800
F	0.18449000	-0.85333900	2.65454900
F	0.49679000	1.74823100	2.30079400
F	1.35909400	-2.72427400	1.19719400
F	2.44652400	2.82061200	0.35469400
F	3.56939700	0.82706100	-1.50132500
F	3.34556700	-2.04141800	-0.88156600
F	-0.74622400	-2.46271800	-1.49493700

$[Be(B_2C_4F_6)_2]^{2-}$-m-2

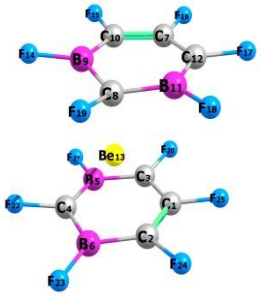
E (B3LYP/6-311++G(d,p)) = -1617.97818967

Zero-point correction=	0.096406 (Hartree/Particle)
Thermal correction to Energy=	0.119939
Thermal correction to Enthalpy=	0.120883
Thermal correction to Gibbs Free Energy=	0.041433
Sum of electronic and zero-point Energies=	-1617.881784
Sum of electronic and thermal Energies=	-1617.858250
Sum of electronic and thermal Enthalpies=	-1617.857306
Sum of electronic and thermal Free Energies=	-1617.936757

Charge = -2 Multiplicity = 1

C	1.28712500	1.26423500	-0.98161900
C	-1.28640300	0.92156000	1.53712500
C	-1.09475800	-0.45493500	1.74335900
C	-1.73047300	-1.42549800	0.95316500
B	-2.26804200	1.47155200	0.51825500
C	-2.84988900	0.40862900	-0.37475500
B	-2.73860700	-1.07165500	-0.12503700
C	2.45272000	1.29270600	-0.31598300
B	1.32728000	-1.32451300	-0.97385000
B	3.21564900	-0.00040400	0.12086700
C	0.54090500	0.03167600	-1.24439300
C	2.59149000	-1.29880300	-0.20538100
Be	-0.89324100	0.01095900	-0.22603300
F	-1.35869000	-2.72408700	1.19771200
F	-3.34530600	-2.04191100	-0.88113800
F	-3.56953600	0.82641700	-1.50145400
F	-2.44690900	2.82048300	0.35415500
F	-0.49700100	1.74875100	2.30044000
F	-0.18432400	-0.85270600	2.65468600
F	0.74621300	-2.46273000	-1.49495800
F	3.27084000	-2.51060000	0.10915900
F	0.04746500	0.06238300	-2.62352600
F	0.67342900	2.44174400	-1.33990700
F	2.95395600	2.52933500	0.06402000
F	4.42400300	0.17890600	0.77568200

$[Be(B_2C_4F_6)_2]^{2-}$-m-3



E (B3LYP/6-311++G(d,p)) = -1617.97874704

Zero-point correction=	0.096145 (Hartree/Particle)
Thermal correction to Energy=	0.119741
Thermal correction to Enthalpy=	0.120685
Thermal correction to Gibbs Free Energy=	0.042438
Sum of electronic and zero-point Energies=	-1617.882602
Sum of electronic and thermal Energies=	-1617.859006
Sum of electronic and thermal Enthalpies=	-1617.858062
Sum of electronic and thermal Free Energies=	-1617.936309

Charge = -2 Multiplicity = 1

C	1.12629700	-1.25408000	1.28870500
C	2.18975600	-1.23627700	0.37883700
C	0.56121000	-0.07310600	1.80670700
C	2.20442200	1.29036600	0.46432800
B	1.13808000	1.30432300	1.52752500
B	2.86979700	0.04796200	-0.05952200
C	-2.70253400	0.00720400	0.01555300
C	-0.33269900	0.04237900	-1.64569200
B	-1.06344500	1.36262100	-1.33976700
C	-2.22257000	1.24966500	-0.39672100
B	-0.99980100	-1.30114900	-1.30441200
C	-2.16522200	-1.22117100	-0.36787800
Be	0.68998800	0.12267900	-0.17712500
F	-0.67274100	2.56616100	-1.89327300
F	-2.93764800	2.36239400	0.06019800
F	-3.78343300	-0.00828100	0.85933300
F	-2.81730000	-2.35527500	0.13025900
F	-0.53930200	-2.50068400	-1.81332100
F	0.56947200	0.04884800	-2.76790300
F	-0.53836300	-0.24743700	2.60895300
F	0.60466300	2.43153900	2.09239800
F	2.62635100	2.52182900	-0.05357600
F	3.90227100	0.03028600	-0.96533000
F	2.54304900	-2.45764900	-0.14849500

F	0.55019700	-2.43499400	1.59368200

$[Be(B_2C_4F_6)_2]^{2-}$-o-1

E (B3LYP/6-311++G(d,p)) = -1617.91306536

Zero-point correction=	0.095828 (Hartree/Particle)
Thermal correction to Energy=	0.119411
Thermal correction to Enthalpy=	0.120355
Thermal correction to Gibbs Free Energy=	0.041982
Sum of electronic and zero-point Energies=	-1617.817237
Sum of electronic and thermal Energies=	-1617.793654
Sum of electronic and thermal Enthalpies=	-1617.792710
Sum of electronic and thermal Free Energies=	-1617.871083

Charge = -2 Multiplicity = 1

C	-2.67942500	-0.06955300	-0.05854800
C	-1.01781000	-1.14248500	1.39211100
C	2.52515200	-0.60223600	-0.08563700
C	1.56006500	1.44846300	-0.99528800
C	1.61673000	-1.42843200	-0.72468400
C	2.49782600	0.79234200	-0.21618100
C	-2.04234700	-1.22753400	0.45160000
B	0.48493700	0.72821800	-1.79709000
B	0.51831000	-0.91195500	-1.64055800
B	-1.19052600	1.43171900	1.53270500
C	-0.55989300	0.10722700	1.88059600
B	-2.39864700	1.32968500	0.42142200
F	-0.30150600	1.47665100	-2.69309600
F	-0.25151700	-1.84684500	-2.35915900
F	1.84734000	-2.78927600	-0.55397100
F	3.46367900	-1.13546300	0.76469300
F	3.40920600	1.50940300	0.52113100
F	1.72972200	2.82366300	-1.07459900
F	-3.06098600	2.38852900	-0.18459100
F	-0.62845700	2.59075500	2.04388700

F	0.57230100	0.00440300	2.66209400
F	-3.54043800	-0.33928900	-1.10451500
F	-2.38005800	-2.45158300	-0.01876200
F	-0.41237100	-2.28610900	1.78559600
Be	-0.62359900	0.08534000	-0.13614400

$[Be(B_2C_4F_6)_2]^{2-}$-o-2

E (B3LYP/6-311++G(d,p)) = -1617.91186248

Zero-point correction=	0.095606 (Hartree/Particle)
Thermal correction to Energy=	0.119331
Thermal correction to Enthalpy=	0.120275
Thermal correction to Gibbs Free Energy=	0.040649
Sum of electronic and zero-point Energies=	-1617.816257
Sum of electronic and thermal Energies=	-1617.792531
Sum of electronic and thermal Enthalpies=	-1617.791587
Sum of electronic and thermal Free Energies=	-1617.871213

Charge = -2 Multiplicity = 1

C	1.60997300	1.43705800	-0.83301200
C	2.54432600	0.69238200	-0.12699100
C	1.60830400	-1.45035000	-0.83115500
C	-2.45586000	-0.61192400	-0.03224800
C	-1.56203100	1.44085100	0.96854600
C	-1.69862300	-1.43154500	0.83718900
C	-2.39011400	0.77880600	0.03116500
C	2.54353800	-0.70584400	-0.12625900
B	-0.74881500	0.73472500	2.02392000
B	-0.82685000	-0.90366700	1.94913400
B	0.52928700	0.81559500	-1.70316900
B	0.52863400	-0.82845800	-1.70208700
F	1.79695000	-2.82396100	-0.76944000
F	-0.27447200	-1.67640500	-2.48818100
F	-1.77654700	-2.77229100	0.53065800
F	-3.22118800	-1.17207200	-1.00089200

F	-3.09901100	1.49494300	-0.87512900
F	-1.51237800	2.80524300	0.78453700
F	1.80180100	2.81051700	-0.77460300
F	-0.27034800	1.66419600	-2.49315600
F	-0.09161100	-1.80866600	2.70173100
F	0.06718300	1.49424700	2.85107500
F	3.47783200	-1.33685300	0.65771500
F	3.48030000	1.32332900	0.65497100
Be	-0.50373700	-0.00190300	-0.04399400

$[Be(B_2C_4F_6)_2]^{2-}$-p-1

E (B3LYP/6-311++G(d,p)) = -1617.96630816

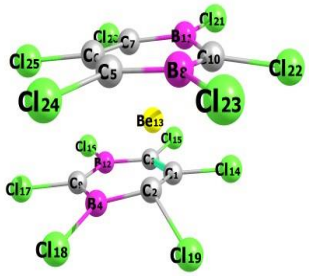
Zero-point correction=	0.095939 (Hartree/Particle)
Thermal correction to Energy=	0.119540
Thermal correction to Enthalpy=	0.120484
Thermal correction to Gibbs Free Energy=	0.042815
Sum of electronic and zero-point Energies=	-1617.870369
Sum of electronic and thermal Energies=	-1617.846768
Sum of electronic and thermal Enthalpies=	-1617.845824
Sum of electronic and thermal Free Energies=	-1617.923493

Charge = -2 Multiplicity = 1

C	-0.48411100	-0.33662000	-1.77468700
C	-1.23356600	-1.38877300	-1.11886900
B	-2.35684000	-1.09789400	-0.18041500
C	0.48412300	-0.33661900	1.77470700
C	1.99399300	1.38449400	0.62577600
C	-2.69662400	0.38392300	-0.00827200
C	1.23357400	-1.38878300	1.11889400
B	0.80825500	1.11079700	1.55245000
B	2.35682300	-1.09790400	0.18040400
C	2.69661200	0.38391400	0.00825900
C	-1.99398200	1.38450000	-0.62576500
B	-0.80823500	1.11079800	-1.55242700

Be	0.00007000	-0.46301300	-0.00001600
F	0.13752100	2.13521700	2.18537500
F	2.38370300	2.68701300	0.39090700
F	3.73631600	0.74777700	-0.82596700
F	3.07393700	-2.07894100	-0.48040800
F	0.86689000	-2.68739500	1.44793300
F	0.43844400	-0.73664700	-2.73153200
F	-0.13750000	2.13521900	-2.18537100
F	-2.38368700	2.68702100	-0.39089700
F	-3.73634100	0.74779100	0.82593800
F	-3.07397100	-2.07893200	0.48039300
F	-0.86688300	-2.68738800	-1.44790600
F	-0.43847500	-0.73664000	2.73150800

$[Be(B_2C_4Cl_6)_2]^{2-}$-m-1



E (B3LYP/6-311++G(d,p)) = -5942.29478853

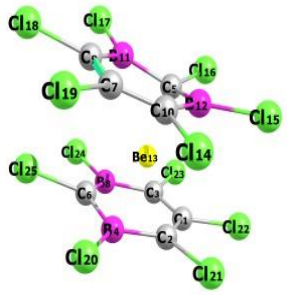
Zero-point correction=	0.080993 (Hartree/Particle)
Thermal correction to Energy=	0.108501
Thermal correction to Enthalpy=	0.109445
Thermal correction to Gibbs Free Energy=	0.019993
Sum of electronic and zero-point Energies=	-5942.213795
Sum of electronic and thermal Energies=	-5942.186287
Sum of electronic and thermal Enthalpies=	-5942.185343
Sum of electronic and thermal Free Energies=	-5942.274796

Charge = -2 Multiplicity = 1

C	-0.93163400	1.27197700	-1.32435300
C	-0.15026600	0.02634200	-1.47017900
C	-2.16955500	1.28575800	-0.76900600
B	-0.93392000	-1.32541100	-1.32060700
C	2.04729800	-1.35773200	0.90062700
C	0.84601200	-1.12670700	1.61135000
C	0.39041400	0.18891700	1.86343900
B	2.94833300	-0.22980000	0.42950500

C	-2.26568800	-1.31256600	-0.68497900
C	2.39281700	1.14789200	0.62728000
B	1.20627100	1.42169200	1.50275000
B	-2.92120400	-0.02276700	-0.40069100
Be	0.90414400	0.02389600	-0.06180900
Cl	-0.11008500	2.78571100	-1.73522900
Cl	-2.93446900	2.84367100	-0.38624900
Cl	-4.58102200	0.10427400	0.35150100
Cl	-3.11447800	-2.85610400	-0.32182000
Cl	-0.11111500	-2.86049500	-1.84922900
Cl	0.96829200	0.05754500	-2.94290200
Cl	-1.19769400	0.40313200	2.59167500
Cl	0.63333600	3.07249200	1.93048100
Cl	3.24246500	2.52299200	-0.12482700
Cl	4.48121300	-0.57117800	-0.46269800
Cl	2.52624300	-3.02339000	0.57346400
Cl	-0.15976600	-2.48202900	2.06215000

$[Be(B_2C_4Cl_6)_2]^{2-}$-m-2



E (B3LYP/6-311++G(d,p)) = -5942.28654985

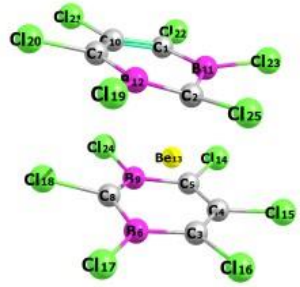
Zero-point correction=	0.081956 (Hartree/Particle)
Thermal correction to Energy=	0.109007
Thermal correction to Enthalpy=	0.109951
Thermal correction to Gibbs Free Energy=	0.021078
Sum of electronic and zero-point Energies=	-5942.198195
Sum of electronic and thermal Energies=	-5942.171144
Sum of electronic and thermal Enthalpies=	-5942.170200
Sum of electronic and thermal Free Energies=	-5942.259073

Charge = -2 Multiplicity = 1

C	-2.26619000	-1.05030800	0.80857800
C	-1.02877200	-1.39533400	1.40999400
C	-2.66127600	0.30057700	0.67461200
B	-0.09251400	-0.35814100	2.01505500

C	-0.15217000	0.05972500	-1.60178100
C	-0.47631600	1.06491700	1.72967000
C	2.66216200	-0.02465400	-0.51911900
B	-1.83724100	1.45839800	1.22807100
C	2.10022600	1.21077900	-0.86593500
C	1.98653900	-1.22287900	-0.78360600
B	0.68315900	1.32521800	-1.49355900
B	0.60389500	-1.24844600	-1.49272800
Be	-0.77414000	0.06909600	0.08601700
Cl	2.72551200	-2.72791100	-0.34914000
Cl	-0.01396100	-2.77564000	-2.15286800
Cl	-1.60403500	0.10417800	-2.67266900
Cl	0.10108200	2.90017900	-2.06002500
Cl	3.02688600	2.65670800	-0.62927300
Cl	4.24014500	-0.07411400	0.23426100
Cl	1.46700300	-0.83745500	2.75627700
Cl	-0.55900300	-3.09012200	1.45095400
Cl	-3.24305200	-2.30592700	0.08591500
Cl	-4.14958900	0.65843300	-0.18775100
Cl	-2.37479700	3.15447900	1.03629800
Cl	0.69703400	2.34787000	2.09138900

$[Be(B_2C_4Cl_6)_2]^{2-}$-m-3



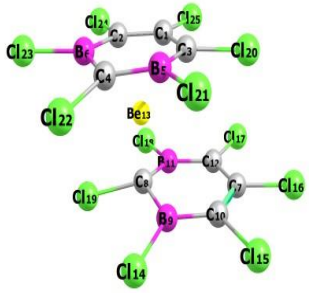
E (B3LYP/6-311++G(d,p)) = -5942.28654831

Zero-point correction=	0.081957 (Hartree/Particle)
Thermal correction to Energy=	0.109007
Thermal correction to Enthalpy=	0.109951
Thermal correction to Gibbs Free Energy=	0.021078
Sum of electronic and zero-point Energies=	-5942.198195
Sum of electronic and thermal Energies=	-5942.171144
Sum of electronic and thermal Enthalpies=	-5942.170200
Sum of electronic and thermal Free Energies=	-5942.259073

Charge = -2 Multiplicity = 1

C	-1.98653200	-1.22287900	-0.78358400
C	0.15216600	0.05972800	-1.60177000
C	2.66127200	0.30068000	0.67464000
C	2.26627400	-1.05023700	0.80856300
C	1.02887600	-1.39536300	1.40996300
B	1.83715100	1.45842900	1.22811800
C	-2.10023700	1.21077600	-0.86592200
C	0.47625300	1.06484000	1.72970200
B	0.09253700	-0.35825200	2.01503300
C	-2.66216600	-0.02465800	-0.51910400
B	-0.60391000	-1.24843800	-1.49274800
B	-0.68316700	1.32522000	-1.49353200
Be	0.77417500	0.06907000	0.08601000
Cl	0.55921600	-3.09018200	1.45085300
Cl	3.24322400	-2.30576800	0.08586700
Cl	4.14956700	0.65865700	-0.18770300
Cl	2.37458000	3.15454700	1.03637200
Cl	-0.69718700	2.34770400	2.09144600
Cl	-0.10107900	2.90017800	-2.05996700
Cl	-3.02690000	2.65670100	-0.62926500
Cl	-4.24014700	-0.07412800	0.23427700
Cl	-2.72546100	-2.72791200	-0.34905700
Cl	0.01389800	-2.77561600	-2.15298000
Cl	-1.46696700	-0.83769700	2.75618000
Cl	1.60401100	0.10419900	-2.67268700

$[Be(B_2C_4Cl_6)_2]^{2-}$-m-4



E (B3LYP/6-311++G(d,p)) = -5942.29829286

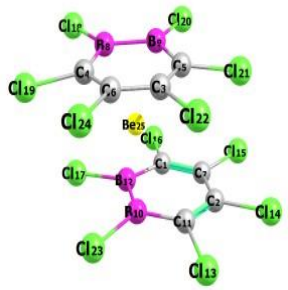
Zero-point correction=	0.080773 (Hartree/Particle)
Thermal correction to Energy=	0.108318
Thermal correction to Enthalpy=	0.109262
Thermal correction to Gibbs Free Energy=	0.020231
Sum of electronic and zero-point Energies=	-5942.217520
Sum of electronic and thermal Energies=	-5942.189975

Sum of electronic and thermal Enthalpies=	-5942.189031
Sum of electronic and thermal Free Energies=	-5942.278062

Charge = -2 Multiplicity = 1

C	0.77545100	-1.19376000	1.58494400
C	2.02222200	-1.28010200	0.92925400
C	0.18561600	0.06076300	1.87469600
C	2.15776000	1.25730700	0.80937500
B	0.89731100	1.38034400	1.61301500
B	2.84651200	-0.05266900	0.58105200
C	-2.67970700	0.04026500	-0.49956800
C	0.02228800	-0.04462500	-1.63684900
B	-0.72127200	1.28746400	-1.50017300
C	-2.05804400	1.25459100	-0.81696200
B	-0.77345500	-1.33464500	-1.42694300
C	-2.11043400	-1.21504900	-0.76116600
Be	0.77819800	0.06626800	-0.02719800
Cl	-0.01482900	2.84202900	-2.10994500
Cl	-2.90338500	2.78214100	-0.47148900
Cl	-4.28592600	0.09158800	0.26344300
Cl	-3.03369900	-2.68794300	-0.36587300
Cl	-0.12162400	-2.95064600	-1.94128400
Cl	1.46065600	-0.10677700	-2.76177900
Cl	-1.42470400	0.08751600	2.58412700
Cl	0.14916300	2.94924500	2.07222200
Cl	2.93065300	2.74073600	0.19558200
Cl	4.46826200	-0.21144200	-0.19781800
Cl	2.64282200	-2.87524600	0.49965400
Cl	-0.11734200	-2.65790000	1.93149500

$[Be(B_2C_4Cl_6)_2]^{2-}$-o-1



E (B3LYP/6-311++G(d,p)) = -5942.22557038

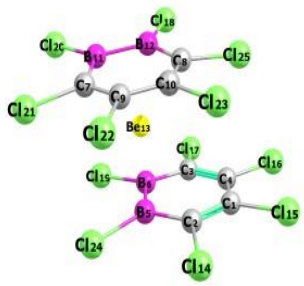
Zero-point correction=	0.080274 (Hartree/Particle)
Thermal correction to Energy=	0.107902

Thermal correction to Enthalpy=	0.108846
Thermal correction to Gibbs Free Energy=	0.018474
Sum of electronic and zero-point Energies=	-5942.145296
Sum of electronic and thermal Energies=	-5942.117668
Sum of electronic and thermal Enthalpies=	-5942.116724
Sum of electronic and thermal Free Energies=	-5942.207096

Charge = -2 Multiplicity = 1

C	-1.16075900	1.45228800	1.30056700
C	-2.43882600	-0.56873500	0.70790900
C	0.74617800	-1.23103200	-1.62792300
C	2.59678700	0.07192400	-0.62779900
C	0.02487800	-0.03914000	-1.95185900
C	2.00439400	-1.17478200	-0.99494500
C	-2.29883400	0.84000600	0.77137200
B	2.03838100	1.40085200	-1.03976900
B	0.59395500	1.33862200	-1.78548500
B	-0.11960800	-0.94884100	1.70068000
C	-1.43638900	-1.43650900	1.14478500
B	0.02294500	0.66279700	1.81461800
Cl	-1.80293500	-3.18391400	1.17272900
Cl	-3.93233000	-1.23008500	0.02197000
Cl	-3.60945400	1.83727800	0.12414100
Cl	-1.16533900	3.22113300	1.46885500
Cl	1.41119900	1.50073300	2.67786200
Cl	2.87284000	2.94550200	-0.58619900
Cl	4.05608300	-0.00884300	0.37823500
Cl	-0.37924900	2.79904400	-2.23375900
Cl	-1.62133800	-0.24952000	-2.57982000
Cl	0.04430400	-2.79654900	-1.97664800
Cl	1.09488100	-2.13003800	2.42669000
Cl	2.82930500	-2.67877200	-0.63861000
Be	0.63290600	-0.04818100	-0.03135600

$[Be(B_2C_4Cl_6)_2]^{2-}$-o-2



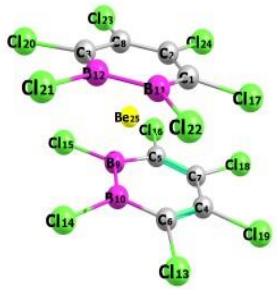
E (B3LYP/6-311++G(d,p)) = -5942.22640934

Zero-point correction=	0.080286 (Hartree/Particle)
Thermal correction to Energy=	0.107889
Thermal correction to Enthalpy=	0.108833
Thermal correction to Gibbs Free Energy=	0.019453
Sum of electronic and zero-point Energies=	-5942.146123
Sum of electronic and thermal Energies=	-5942.118520
Sum of electronic and thermal Enthalpies=	-5942.117576
Sum of electronic and thermal Free Energies=	-5942.206956

Charge = -2 Multiplicity = 1

C	2.45282900	-0.61958200	-0.60337300
C	1.43323600	-1.45073100	-1.06635100
C	1.29470800	1.44244200	-1.28875900
C	2.39199100	0.79193100	-0.72656600
B	0.16290500	-0.91506400	-1.68431600
B	0.07745200	0.70101100	-1.79806200
C	-2.58671700	-0.48185800	0.61862400
C	-0.18726600	0.52857800	1.88738700
C	-1.58917600	-1.36645400	1.13390700
C	-0.42423400	-0.87337700	1.76009500
B	-2.54532100	1.00496000	0.80443800
B	-1.19520600	1.57377400	1.50664500
Be	-0.69129200	0.01750300	-0.00292900
Cl	1.71251200	-3.21322400	-1.02810900
Cl	3.86700300	-1.32607100	0.19742200
Cl	3.76445100	1.73986300	-0.12791800
Cl	1.39729300	3.20317600	-1.51610200
Cl	-0.82213100	3.33673600	1.70347800
Cl	-1.26437300	1.59083200	-2.68839200
Cl	-3.87187700	2.06308100	0.15848600
Cl	-3.92254200	-1.22376100	-0.28325600
Cl	-1.77677100	-3.09815000	0.96205100
Cl	0.78127000	-2.01381700	2.31423700
Cl	-1.05601900	-2.05682600	-2.45957300
Cl	1.40023100	1.01468400	2.50758100

$[Be(B_2C_4Cl_6)_2]^{2-}$-o-3



E (B3LYP/6-311++G(d,p)) = -5942.22640067

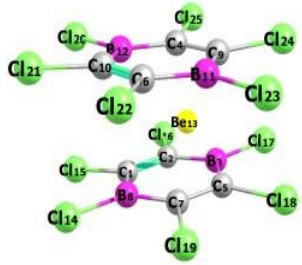
Zero-point correction=	0.080268 (Hartree/Particle)
Thermal correction to Energy=	0.107879
Thermal correction to Enthalpy=	0.108823
Thermal correction to Gibbs Free Energy=	0.019421
Sum of electronic and zero-point Energies=	-5942.146133
Sum of electronic and thermal Energies=	-5942.118522
Sum of electronic and thermal Enthalpies=	-5942.117578
Sum of electronic and thermal Free Energies=	-5942.206980

Charge = -2 Multiplicity = 1

C	-0.18340000	0.52017700	-1.88922900
C	-0.42830900	-0.88008200	-1.75881500
C	-2.58845700	-0.47398300	-0.61826900
C	2.39176800	0.79101900	0.72678500
C	1.43129300	-1.45055600	1.06863500
C	1.29490900	1.44277700	1.28846600
C	2.45158200	-0.62058800	0.60484400
C	-1.59562200	-1.36525100	-1.13101600
B	0.16134000	-0.91347200	1.68604800
B	0.07695200	0.70282200	1.79807300
B	-1.18552900	1.57188500	-1.51124400
B	-2.53879400	1.01212600	-0.80780200
Cl	1.39920900	3.20355100	1.51551100
Cl	-1.26460700	1.59410400	2.68747500
Cl	-1.05803900	-2.05318400	2.46374000
Cl	1.70989000	-3.21340400	1.03304500
Cl	1.40703600	0.99559400	-2.51063600
Cl	3.86487800	-1.32895200	-0.19586200
Cl	3.76458400	1.73772400	0.12700100
Cl	-3.92890600	-1.20623400	0.28488700
Cl	-3.85972800	2.07919400	-0.16504900
Cl	-0.80309000	3.33232700	-1.71308900
Cl	-1.79229700	-3.09544300	-0.95434800
Cl	0.76959700	-2.02854500	-2.31295500

Be	-0.68935100	0.01691600	0.00274700

$[Be(B_2C_4Cl_6)_2]^{2-}$-p-1



E (B3LYP/6-311++G(d,p)) = -5942.28580343

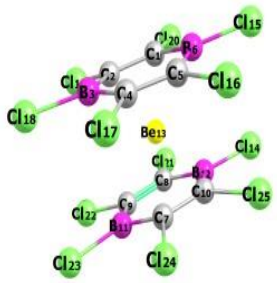
Zero-point correction=	0.080710 (Hartree/Particle)
Thermal correction to Energy=	0.108258
Thermal correction to Enthalpy=	0.109202
Thermal correction to Gibbs Free Energy=	0.020389
Sum of electronic and zero-point Energies=	-5942.205093
Sum of electronic and thermal Energies=	-5942.177546
Sum of electronic and thermal Enthalpies=	-5942.176602
Sum of electronic and thermal Free Energies=	-5942.265414

Charge = -2 Multiplicity = 1

C	1.92414400	-1.35949900	0.99730000
C	2.67513200	-0.29364000	0.56633500
B	2.19389600	1.15308500	0.72081200
C	-0.06010700	0.24673100	-1.81862900
C	0.89075000	1.37023200	1.41137400
C	-2.67510400	-0.29402200	-0.56648000
C	0.06009700	0.24640200	1.81874100
B	0.53758300	-1.16234000	1.61677000
C	-0.89108000	1.37037800	-1.41123000
C	-1.92385700	-1.35967400	-0.99755600
B	-2.19423700	1.15284500	-0.72080100
B	-0.53729800	-1.16214300	-1.61691400
Be	-0.00032300	0.50940900	0.00008900
Cl	-0.45655100	-2.57221600	2.15292400
Cl	2.55775700	-3.00815300	0.86720400
Cl	4.25894400	-0.57151900	-0.18012200
Cl	3.20299600	2.54397600	0.13415500
Cl	0.33551700	3.01639800	1.78385500
Cl	-1.41692500	0.54728700	2.76096800
Cl	0.45719500	-2.57173400	-2.15313700

Cl	-2.55710100	-3.00848100	-0.86763700
Cl	-4.25884700	-0.57237400	0.17994200
Cl	-3.20377600	2.54342600	-0.13416700
Cl	-0.33614300	3.01669500	-1.78342400
Cl	1.41703400	0.54808900	-2.76049200

$[Be(B_2C_4Cl_6)_2]^{2-}$-p-2



E (B3LYP/6-311++G(d,p)) = -5942.27160630

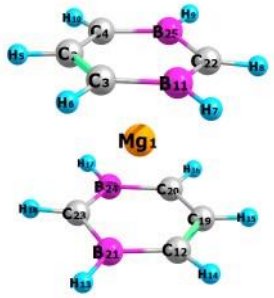
Zero-point correction=	0.081389 (Hartree/Particle)
Thermal correction to Energy=	0.108608
Thermal correction to Enthalpy=	0.109552
Thermal correction to Gibbs Free Energy=	0.020466
Sum of electronic and zero-point Energies=	-5942.190217
Sum of electronic and thermal Energies=	-5942.162999
Sum of electronic and thermal Enthalpies=	-5942.162054
Sum of electronic and thermal Free Energies=	-5942.251140

Charge = -2 Multiplicity = 1

C	0.12923900	0.78041800	1.84899000
C	0.03770200	-0.62728100	1.88227900
B	1.18680600	-1.52359200	1.45940700
C	2.35985900	-0.80637300	0.81797800
C	2.42923200	0.59862300	0.73796800
B	1.36440200	1.50015100	1.33575500
C	0.13380200	-0.44714100	-1.69335400
C	-2.51638900	0.44364600	-0.67230300
C	-2.30493500	-0.90092200	-0.81880100
C	-0.10363100	0.95238300	-1.57825700
B	-0.97193500	-1.44871900	-1.34923300
B	-1.44571000	1.47194200	-1.05934700
Be	0.62879700	-0.00614700	0.07994000
Cl	-1.75880200	3.21920600	-0.96777900
Cl	1.47121700	3.27962300	1.27118900
Cl	3.77658700	1.34669600	-0.10462000

Cl	3.63522800	-1.77853700	0.10960000
Cl	1.10098100	-3.30161400	1.57698700
Cl	-1.45377800	-1.38182500	2.41306100
Cl	-1.24657800	1.74179600	2.35475500
Cl	-4.05108000	1.03784700	-0.06093800
Cl	-3.57413400	-2.05086800	-0.43232800
Cl	-0.71757700	-3.18865000	-1.59458300
Cl	1.54384500	-1.01021600	-2.60017900
Cl	1.02866300	2.09039900	-2.28279300

$[Mg(B_2C_4H_6)_2]^{2-}$-m-1



E (B3LYP/6-311++G(d,p)) = -611.821244398

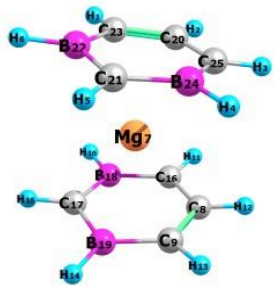
Zero-point correction=	0.180048 (Hartree/Particle)
Thermal correction to Energy=	0.193231
Thermal correction to Enthalpy=	0.194175
Thermal correction to Gibbs Free Energy=	0.138165
Sum of electronic and zero-point Energies=	-611.641196
Sum of electronic and thermal Energies=	-611.628014
Sum of electronic and thermal Enthalpies=	-611.627070
Sum of electronic and thermal Free Energies=	-611.683080

Charge = -2 Multiplicity = 1

Mg	-0.00000700	-0.00001500	0.00069800
C	-2.22817200	1.27734100	-0.00298200
C	-2.13395100	0.61328200	-1.24603600
C	-2.13546000	0.61821800	1.24281500
H	-2.32209000	2.36872700	-0.00521000
H	-2.17267900	1.24889200	-2.13291400
H	-1.86391200	-1.45528300	-2.40407700
H	-1.49945300	-2.69278100	0.00534500
H	-1.86679500	-1.44572800	2.40936000
H	-2.17529000	1.25735000	2.12711300
B	-1.94120300	-0.90109400	-1.32135800
C	2.13396800	-0.61327300	-1.24603700

H	1.86388700	1.45528900	-2.40407300
H	2.17271400	-1.24888000	-2.13291600
H	2.32214900	-2.36871500	-0.00521500
H	2.17532300	-1.25734700	2.12711100
H	1.86676900	1.44572500	2.40936300
H	1.49940100	2.69277500	0.00535000
C	2.22820400	-1.27733100	-0.00298500
C	2.13547600	-0.61821400	1.24281400
B	1.94118900	0.90109900	-1.32135500
C	-1.73600000	-1.62273600	0.00306200
C	1.73597000	1.62273400	0.00306500
B	1.94276500	0.89583000	1.32436700
B	-1.94277900	-0.89583000	1.32436600

$[Mg(B_2C_4H_6)_2]^{2-}$-m-2



E (B3LYP/6-311++G(d,p)) = -611.82043871

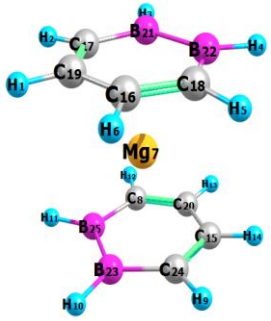
Zero-point correction=	0.180290 (Hartree/Particle)
Thermal correction to Energy=	0.193378
Thermal correction to Enthalpy=	0.194322
Thermal correction to Gibbs Free Energy=	0.140157
Sum of electronic and zero-point Energies=	-611.640149
Sum of electronic and thermal Energies=	-611.627061
Sum of electronic and thermal Enthalpies=	-611.626117
Sum of electronic and thermal Free Energies=	-611.680282

Charge = -2 Multiplicity = 1

H	2.28011700	0.44948600	-2.39122100
H	1.99959400	-1.82508500	-1.65338500
H	1.70470700	-2.48050000	0.64532000
H	1.69965500	-0.71879100	2.73673500
H	1.80549000	1.87822000	1.88619300
H	2.32656100	2.59670300	-0.69810400
Mg	-0.00000300	0.19771400	0.00000000
C	-2.04335000	-1.04141700	0.88999700

C	-2.20056300	0.29582300	1.31295600
H	-1.69966000	-0.71887300	-2.73671500
H	-1.70470200	-2.48051700	-0.64525400
H	-1.99958800	-1.82503900	1.65343800
H	-2.28011200	0.44955300	2.39120900
H	-2.32656900	2.59672100	0.69802800
H	-1.80549600	1.87816200	-1.88625000
C	-1.86359100	-1.41591400	-0.46182900
C	-1.91335800	1.08379000	-1.13954700
B	-1.85355300	-0.37220300	-1.57796700
B	-2.19782900	1.44819100	0.30921400
C	2.04335300	-1.04144100	-0.88996600
C	1.91335600	1.08382600	1.13951300
B	2.19782700	1.44818400	-0.30925700
C	2.20056600	0.29578700	-1.31296300
B	1.85355300	-0.37215700	1.57797700
C	1.86359400	-1.41590200	0.46186800

$[Mg(B_2C_4H_6)_2]^{2-}$-o-1



E (B3LYP/6-311++G(d,p)) = -611.76826237

Zero-point correction=	0.180107 (Hartree/Particle)
Thermal correction to Energy=	0.193320
Thermal correction to Enthalpy=	0.194265
Thermal correction to Gibbs Free Energy=	0.139943
Sum of electronic and zero-point Energies=	-611.588155
Sum of electronic and thermal Energies=	-611.574942
Sum of electronic and thermal Enthalpies=	-611.573998
Sum of electronic and thermal Free Energies=	-611.628319

Charge = -2 Multiplicity = 1

H	-2.37634300	0.53277500	-2.27961100
H	-2.19303200	2.38533900	-0.73689800
H	-1.84814700	2.16146100	1.91487900

H	-1.57004400	-0.86970800	2.77513000
H	-1.73250300	-2.49469400	0.64704300
H	-2.15243500	-1.77992000	-1.62422500
Mg	0.00003700	0.12655300	0.00002700
C	2.13733800	1.38806500	0.28728600
H	1.73220400	-2.49462400	-0.64751900
H	1.57005600	-0.86922800	-2.77531500
H	1.84848400	2.16174100	-1.91449400
H	2.19328600	2.38509000	0.73733800
H	2.37628400	0.53222000	2.27972100
H	2.15210800	-1.78032100	1.62390200
C	2.12790100	-1.02652700	0.83647200
C	-2.12808200	-1.02627100	-0.83665900
C	-2.13718500	1.38822300	-0.28703200
C	-1.87227400	-1.41678200	0.50896800
C	-2.25747500	0.31738900	-1.21721600
C	2.25744700	0.31704500	1.21728000
B	-1.94344200	1.17111400	1.20697700
B	-1.79644800	-0.42481400	1.66054500
B	1.79645900	-0.42456900	-1.66063900
C	1.87210900	-1.41675800	-0.50924100
B	1.94362500	1.17125400	-1.20676800

$[Mg(B_2C_4F_6)_2]^{2-}$-m-1

E (B3LYP/6-311++G(d,p)) = -1803.34836827

Zero-point correction=	0.093234 (Hartree/Particle)
Thermal correction to Energy=	0.117996
Thermal correction to Enthalpy=	0.118940
Thermal correction to Gibbs Free Energy=	0.036986
Sum of electronic and zero-point Energies=	-1803.255135
Sum of electronic and thermal Energies=	-1803.230372
Sum of electronic and thermal Enthalpies=	-1803.229428
Sum of electronic and thermal Free Energies=	-1803.311383

Charge = -2 Multiplicity = 1

Mg	0.00000000	0.00002300	0.00000000
C	-2.47426400	0.00024300	0.89920100
C	-2.24354800	1.23246600	0.27156500
C	-2.24375000	-1.23220900	0.27196000
B	-1.82504900	1.32867500	-1.18567800
C	2.24354800	1.23247100	-0.27154400
C	2.47426400	0.00025900	-0.89920100
C	2.24375100	-1.23220400	-0.27198100
B	1.82504900	1.32865400	1.18570100
C	-1.48976300	-0.00026500	-1.83039900
C	1.48976300	-0.00029700	1.83039900
B	1.82521300	-1.32897000	1.18521200
B	-1.82521300	-1.32894900	-1.18523600
F	-2.52665100	2.35948900	1.03340400
F	-1.72442300	2.54966100	-1.82403500
F	-1.06690000	-0.00051400	-3.17609800
F	-1.72469300	-2.55016300	-1.82317600
F	2.52695100	-2.35892600	-1.03422200
F	-2.52695000	-2.35894500	1.03418100
F	1.72469300	-2.55019500	1.82313100
F	1.06689900	-0.00057000	3.17609700
F	-2.91247700	0.00048800	2.19048000
F	2.52665100	2.35950700	-1.03336300
F	1.72442300	2.54962900	1.82407900
F	2.91247800	0.00052700	-2.19048000

$[Mg(B_2C_4F_6)_2]^{2-}$-m-2

E (B3LYP/6-311++G(d,p)) = -1803.34743795

Zero-point correction=	0.093336 (Hartree/Particle)
Thermal correction to Energy=	0.118025
Thermal correction to Enthalpy=	0.118969
Thermal correction to Gibbs Free Energy=	0.037577
Sum of electronic and zero-point Energies=	-1803.254102

Sum of electronic and thermal Energies=	-1803.229413
Sum of electronic and thermal Enthalpies=	-1803.228469
Sum of electronic and thermal Free Energies=	-1803.309861

Charge = -2 Multiplicity = 1

Mg	-0.00000100	0.24501900	-0.00000400
C	2.16896000	-1.05018200	-0.61014800
C	2.35655800	0.26382200	-1.05739100
C	1.80367000	-1.36412900	0.70908300
C	1.81033000	1.12028800	1.28135600
B	1.70156600	-0.30105800	1.79061100
B	2.27531400	1.45507100	-0.11799700
C	-2.16896000	-1.05016400	0.61017300
C	-1.81033100	1.12026200	-1.28138400
B	-2.27530800	1.45508100	0.11796400
C	-2.35654800	0.26385300	1.05738600
B	-1.70157500	-0.30109700	-1.79060500
C	-1.80367900	-1.36414600	-0.70905200
F	2.55915400	2.73455500	-0.55904800
F	1.68043900	2.17282900	2.21185800
F	-1.68044100	2.17277900	-2.21191300
F	-2.55914200	2.73457600	0.55898600
F	-1.47497000	-0.64077100	-3.11036700
F	-1.68018100	-2.71762800	-0.99318700
F	-2.31427300	-2.06958300	1.50323000
F	2.31427400	-2.06962400	-1.50317900
F	1.68016900	-2.71760500	0.99325200
F	1.47495800	-0.64070000	3.11038000
F	2.69622100	0.40289800	-2.39712500
F	-2.69620600	0.40296100	2.39711900

$[Mg(B_2C_4F_6)_2]^{2-}$-o-1

E (B3LYP/6-311++G(d,p)) = -1803.29016542

Zero-point correction=	0.092868 (Hartree/Particle)
Thermal correction to Energy=	0.117706
Thermal correction to Enthalpy=	0.118651
Thermal correction to Gibbs Free Energy=	0.035996
Sum of electronic and zero-point Energies=	-1803.197297
Sum of electronic and thermal Energies=	-1803.172459
Sum of electronic and thermal Enthalpies=	-1803.171515
Sum of electronic and thermal Free Energies=	-1803.254170

Charge = -2 Multiplicity = 1

Mg	0.00004700	0.30835200	0.00024100
C	-2.42336400	1.29178100	-0.06327000
C	-2.33831300	-1.15295600	-0.24949000
C	2.33871500	-1.15231100	0.25001400
C	2.42288000	1.29221900	0.06256500
C	1.72494800	-1.30284000	-1.01349900
C	2.67612600	0.09466800	0.76477700
C	-2.67614700	0.09371300	-0.76483300
B	1.86509400	1.33550700	-1.34532000
B	1.47083600	-0.14929100	-1.96387700
B	-1.47083000	-0.14858900	1.96400900
C	-1.72451800	-1.30268800	1.01409100
B	-1.86553200	1.33591600	1.34463300
F	1.78303500	2.56901500	-2.00028200
F	0.99743100	-0.42674300	-3.25040800
F	1.51084500	-2.62422100	-1.37879200
F	2.56604500	-2.25318600	1.02723500
F	3.20944000	0.14888100	2.02339400
F	2.85801900	2.43468000	0.72432900
F	-1.78391200	2.56982100	1.99889300
F	-0.99744100	-0.42515300	3.25073000
F	-1.50998600	-2.62380600	1.38006800
F	-2.85887300	2.43371400	-0.72567900
F	-3.20942200	0.14708900	-2.02350200
F	-2.56522100	-2.25425300	-1.02623600

$[Mg(B_2C_4F_6)_2]^{2-}$-o-2

E (B3LYP/6-311++G(d,p)) = -1803.29001814

Zero-point correction=	0.092856 (Hartree/Particle)
Thermal correction to Energy=	0.117704
Thermal correction to Enthalpy=	0.118649
Thermal correction to Gibbs Free Energy=	0.035796
Sum of electronic and zero-point Energies=	-1803.197162
Sum of electronic and thermal Energies=	-1803.172314
Sum of electronic and thermal Enthalpies=	-1803.171370
Sum of electronic and thermal Free Energies=	-1803.254222

Charge = -2 Multiplicity = 1

Mg	-0.00001000	0.00008700	0.00000500
C	2.62255400	0.69506100	-0.59881900
C	2.09754000	1.44715200	0.47407000
C	2.09692600	-1.44712500	0.47494800
C	2.62225300	-0.69592400	-0.59840800
B	1.58415800	0.82819200	1.75945200
B	1.58384500	-0.82716500	1.75996900
C	-2.09753800	1.44715600	-0.47407200
C	-2.09692600	-1.44712800	-0.47495000
C	-2.62254600	0.69506300	0.59882100
C	-2.62224700	-0.69592500	0.59841000
B	-1.58416700	0.82819300	-1.75945800
B	-1.58385500	-0.82716300	-1.75997500
F	2.22249700	2.82028200	0.31057300
F	1.21998000	1.67152400	2.81407900
F	-2.22248500	2.82028600	-0.31056900
F	-1.21999100	1.67152500	-2.81408500
F	-3.09574800	1.33822400	1.70948200
F	-1.21939900	-1.66973500	-2.81513800
F	3.09518900	-1.33996100	-1.70867400
F	-2.22134000	-2.82041000	-0.31231000
F	2.22134800	-2.82040700	0.31231100
F	-3.09518000	-1.33996100	1.70867700
F	1.21938500	-1.66973700	2.81513100

F	3.09575900	1.33822300	-1.70947700

$[Mg(B_2C_4F_6)_2]^{2-}$-p-1

E (B3LYP/6-311++G(d,p)) = -1803.33858226

Zero-point correction=	0.093490 (Hartree/Particle)
Thermal correction to Energy=	0.117888
Thermal correction to Enthalpy=	0.118832
Thermal correction to Gibbs Free Energy=	0.038461
Sum of electronic and zero-point Energies=	-1803.245093
Sum of electronic and thermal Energies=	-1803.220695
Sum of electronic and thermal Enthalpies=	-1803.219750
Sum of electronic and thermal Free Energies=	-1803.300122

Charge = -2 Multiplicity = 1

Mg	0.00000000	0.00001500	0.00000100
C	2.01229200	-0.32395700	1.41053600
C	2.01225600	-1.37139300	0.46237000
B	2.06130400	-1.13596400	-1.02824000
C	-2.01226200	-0.46241100	-1.37137900
C	-2.01232600	1.41054000	0.32383400
C	2.01235800	0.32392800	-1.41048100
C	-2.01232100	-1.41051500	-0.32388800
B	-2.06127800	1.02821400	-1.13603700
B	-2.06132700	-1.02818900	1.13598100
C	-2.01231400	0.46243500	1.37132300
C	2.01231900	1.37136500	-0.46231700
B	2.06130100	1.13593300	1.02829500
F	-2.01024100	2.74177300	0.70307800
F	-2.12355600	1.95843600	-2.16375100
F	-2.01009100	-0.97202100	-2.65835800
F	-2.01022600	-2.74174700	-0.70313300
F	2.01007800	-2.65840100	0.97190600
F	2.12360100	-2.16362400	-1.95851800

F	2.01029900	0.70325100	-2.74169200
F	2.01020300	2.65837400	-0.97185100
F	2.12359900	2.16359400	1.95858000
F	-2.01019100	0.97204600	2.65830200
F	2.01017100	-0.70328000	2.74174600
F	-2.12364900	-1.95841100	2.16369100

$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-1

E (B3LYP/6-311++G(d,p)) = -6127.66966802

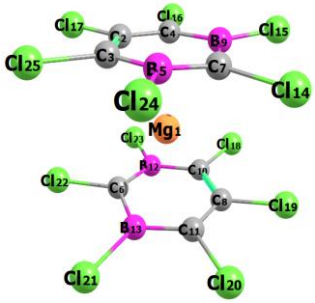
Zero-point correction=	0.078517 (Hartree/Particle)
Thermal correction to Energy=	0.107125
Thermal correction to Enthalpy=	0.108069
Thermal correction to Gibbs Free Energy=	0.014357
Sum of electronic and zero-point Energies=	-6127.591151
Sum of electronic and thermal Energies=	-6127.562543
Sum of electronic and thermal Enthalpies=	-6127.561599
Sum of electronic and thermal Free Energies=	-6127.655311

Charge = -2 Multiplicity = 1

Mg	-0.00032200	0.09668500	-0.00025000
C	-1.93584300	1.01426500	1.25882000
C	0.30643600	0.36917500	2.32327700
C	1.36523600	-1.37817900	-1.45553400
C	2.24233900	-0.34583800	-1.05721900
C	1.93185500	1.01703800	-1.26163700
B	0.07184900	-1.09016100	-2.20221000
C	-1.36006100	-1.37820300	1.45979000
C	-0.30763400	0.36023900	-2.32476100
B	0.67420000	1.45218100	-1.99592900
C	-2.24119000	-0.35038900	1.05859200
B	-0.67958500	1.45637700	1.99134000
B	-0.06763400	-1.08302300	2.20534200
Cl	1.86945100	0.80914000	3.07791100
Cl	3.74094500	-0.76856600	-0.22871300

Cl	3.08345800	2.24586800	-0.70509400
Cl	0.35464400	3.20626600	-2.33698700
Cl	-1.87207800	0.79199800	-3.08118100
Cl	-3.73839800	-0.78132200	0.23177400
Cl	-3.09226700	2.23703400	0.69893400
Cl	-0.36651600	3.21267900	2.32699900
Cl	1.82379900	-3.05961400	-1.13131900
Cl	0.99142500	-2.42924800	2.80309600
Cl	-0.98195700	-2.44223800	-2.79605500
Cl	-1.81233600	-3.06233500	1.14077100

$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-2



E (B3LYP/6-311++G(d,p)) = -6127.66966802

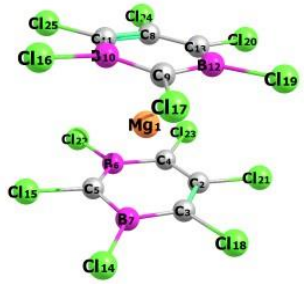
Zero-point correction=	0.078517 (Hartree/Particle)
Thermal correction to Energy=	0.107125
Thermal correction to Enthalpy=	0.108069
Thermal correction to Gibbs Free Energy=	0.014357
Sum of electronic and zero-point Energies=	-6127.591151
Sum of electronic and thermal Energies=	-6127.562543
Sum of electronic and thermal Enthalpies=	-6127.561599
Sum of electronic and thermal Free Energies=	-6127.655311

Charge = -2 Multiplicity = 1

Mg	0.00031600	0.09669800	-0.00024600
C	-2.24232400	-0.34590100	-1.05722600
C	-1.93190500	1.01699500	-1.26160400
C	-1.36517000	-1.37818800	-1.45556800
B	-0.67427300	1.45221900	-1.99588700
C	-0.30643400	0.36913300	2.32329300
C	0.30761200	0.36033500	-2.32475500
C	2.24119400	-0.35037900	1.05857900
B	-0.07179800	-1.09008700	-2.20224000
C	1.36007700	-1.37821000	1.45975900
C	1.93583100	1.01426800	1.25883100

B	0.06765000	-1.08305900	2.20532300
B	0.67957200	1.45635200	1.99136800
Cl	1.87202800	0.79219100	-3.08117900
Cl	0.98207200	-2.44209500	-2.79612200
Cl	-1.82365100	-3.05965400	-1.13140000
Cl	-3.74091600	-0.76872600	-0.22874200
Cl	1.81237000	-3.06233000	1.14070700
Cl	3.73840900	-0.78127900	0.23175800
Cl	3.09223600	2.23706200	0.69896100
Cl	0.36648500	3.21264500	2.32706000
Cl	-1.86944300	0.80906700	3.07795700
Cl	-0.99139100	-2.42930700	2.80305400
Cl	-0.35480000	3.20632900	-2.33689500
Cl	-3.08356600	2.24575500	-0.70502400

$[Mg(B_2C_4Cl_6)_2]^{2-}$-m-3



E (B3LYP/6-311++G(d,p)) = -6127.66937251

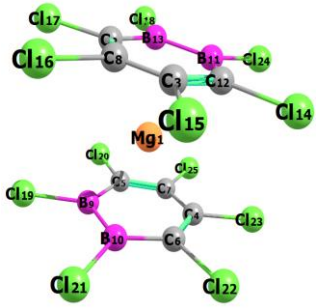
Zero-point correction=	0.078489 (Hartree/Particle)
Thermal correction to Energy=	0.107087
Thermal correction to Enthalpy=	0.108031
Thermal correction to Gibbs Free Energy=	0.015024
Sum of electronic and zero-point Energies=	-6127.590884
Sum of electronic and thermal Energies=	-6127.562286
Sum of electronic and thermal Enthalpies=	-6127.561342
Sum of electronic and thermal Free Energies=	-6127.654349

Charge = -2 Multiplicity = 1

Mg	-0.00007600	0.23105200	0.00000100
C	1.76565700	-1.04847000	1.27271300
C	2.20021300	0.29038100	1.16220000
C	0.50747900	-1.38108300	1.82256600
C	0.00319100	1.10434700	2.20308200
B	-0.41815200	-0.32565300	2.40564300
B	1.38324100	1.44777000	1.71436400

C	-1.76801300	-1.04620000	-1.27164000
C	-0.00063000	1.10160700	-2.20417800
B	-1.38000100	1.44865700	-1.71614000
C	-2.19960300	0.29374600	-1.16270100
B	0.41758500	-0.32953600	-2.40501000
C	-0.51051300	-1.38222200	-1.82093700
Cl	2.02440000	3.14564900	1.66622500
Cl	-1.07840600	2.41836400	2.76050900
Cl	-2.01742300	3.14800100	-1.67013200
Cl	1.08399000	2.41258100	-2.76286600
Cl	3.77837100	0.61438000	0.42014200
Cl	1.98108300	-0.80401200	-3.19484000
Cl	-0.05340200	-3.09272300	-1.91712300
Cl	2.79877700	-2.33793400	0.65675400
Cl	-1.98259800	-0.79574300	3.19625000
Cl	0.04652800	-3.09044800	1.92067300
Cl	-2.80409800	-2.33265400	-0.65435600
Cl	-3.77717200	0.62210200	-0.42129000

$[Mg(B_2C_4Cl_6)_2]^{2-}$-o-1



E (B3LYP/6-311++G(d,p)) = -6127.60526467

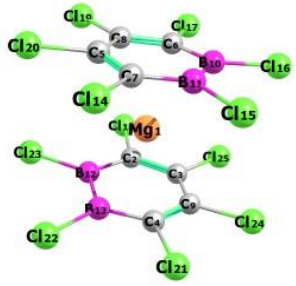
Zero-point correction=	0.077957 (Hartree/Particle)
Thermal correction to Energy=	0.106713
Thermal correction to Enthalpy=	0.107658
Thermal correction to Gibbs Free Energy=	0.013137
Sum of electronic and zero-point Energies=	-6127.527308
Sum of electronic and thermal Energies=	-6127.498551
Sum of electronic and thermal Enthalpies=	-6127.497607
Sum of electronic and thermal Free Energies=	-6127.592128

Charge = -2 Multiplicity = 1

Mg	0.00004800	0.15355000	0.00003400
C	-1.62122300	1.38689200	1.37916200
C	-1.99756700	-1.03618700	1.02530600

C	1.99749600	-1.03628300	-1.02536100
C	1.62132300	1.38683300	-1.37911700
C	0.81173700	-1.38817400	-1.73962000
C	2.38896000	0.30375000	-0.85281600
C	-2.38892700	0.30388400	0.85280400
B	0.39715700	1.18084600	-2.22744300
B	-0.05747200	-0.37278100	-2.42684800
B	0.05740600	-0.37288500	2.42687100
C	-0.81185000	-1.38819900	1.73957500
B	-0.39709700	1.18078100	2.22751500
Cl	-0.43646800	-3.12338400	1.88273700
Cl	-2.97479200	-2.30130200	0.28752400
Cl	-3.83544900	0.64334100	-0.09327000
Cl	-2.22263400	3.03502500	1.06846400
Cl	0.50295600	2.60491700	2.93626300
Cl	-0.50279100	2.60508400	-2.93611700
Cl	2.22287500	3.03490900	-1.06838400
Cl	-1.52785800	-0.89115400	-3.38157400
Cl	0.43623600	-3.12332600	-1.88286200
Cl	2.97464100	-2.30150100	-0.28764800
Cl	1.52773600	-0.89140900	3.38160500
Cl	3.83553200	0.64306500	0.09323400

$[Mg(B_2C_4Cl_6)_2]^{2-}$-o-2



E (B3LYP/6-311++G(d,p)) = -6127.60526482

Zero-point correction=	0.077952 (Hartree/Particle)
Thermal correction to Energy=	0.106711
Thermal correction to Enthalpy=	0.107655
Thermal correction to Gibbs Free Energy=	0.013080
Sum of electronic and zero-point Energies=	-6127.527313
Sum of electronic and thermal Energies=	-6127.498554
Sum of electronic and thermal Enthalpies=	-6127.497609
Sum of electronic and thermal Free Energies=	-6127.592185

Charge = -2 Multiplicity = 1

Mg	0.00007000	0.15437400	-0.00004900
C	0.81099100	-1.38755800	1.73961000
C	1.99682800	-1.03738800	1.02464100
C	1.62384700	1.38629900	1.37777600
C	-2.38984000	0.30203800	-0.85140000
C	-0.81100200	-1.38764000	-1.73957300
C	-1.62384800	1.38622600	-1.37779900
C	-1.99679600	-1.03744900	-1.02454300
C	2.38987800	0.30209300	0.85147100
B	0.05656000	-0.37098400	-2.42702000
B	-0.39989600	1.18203900	-2.22687800
B	-0.05662500	-0.37087900	2.42695200
B	0.39983900	1.18213600	2.22677100
Cl	-2.22737300	3.03347700	-1.06641700
Cl	0.49779800	2.60758400	-2.93579900
Cl	1.52702400	-0.88723000	-3.38278100
Cl	-0.43334700	-3.12227800	-1.88346400
Cl	0.43334100	-3.12219400	1.88353900
Cl	-2.97197800	-2.30410700	-0.28671300
Cl	-3.83635900	0.63927000	0.09547900
Cl	2.22739400	3.03354000	1.06638100
Cl	-0.49791800	2.60770600	2.93555600
Cl	-1.52713900	-0.88709300	3.38264600
Cl	3.83646300	0.63929100	-0.09532300
Cl	2.97206100	-2.30407000	0.28691700

$[Mg(B_2C_4Cl_6)_2]^{2-}$-p-1

E (B3LYP/6-311++G(d,p)) = -6127.66016417

Zero-point correction=	0.078354 (Hartree/Particle)
Thermal correction to Energy=	0.106896
Thermal correction to Enthalpy=	0.107840
Thermal correction to Gibbs Free Energy=	0.014789

Sum of electronic and zero-point Energies=	-6127.581810
Sum of electronic and thermal Energies=	-6127.553268
Sum of electronic and thermal Enthalpies=	-6127.552324
Sum of electronic and thermal Free Energies=	-6127.645375

Charge = -2 Multiplicity = 1

Mg	0.00000000	0.00000300	0.00002700
C	-1.95346800	1.40449100	-0.40504100
C	-1.95346400	0.40195900	-1.40560100
B	-2.01199200	-1.06793700	-1.06565800
C	-1.95318200	-1.40497700	0.40489700
C	-1.95347900	-0.40244400	1.40545800
B	-2.01231300	1.06743900	1.06551100
C	1.95341400	-0.40473500	-1.40466300
C	1.95323600	0.40522000	1.40480100
C	1.95330200	1.40577400	0.40226200
C	1.95364200	-1.40528900	-0.40212400
B	2.01206600	1.06582700	-1.06762300
B	2.01224000	-1.06533000	1.06776500
Cl	1.89679300	3.11285600	0.88301300
Cl	1.89651300	0.88930600	3.11093500
Cl	2.06471200	-2.34873900	2.35370200
Cl	-2.06487300	2.35336100	2.34893200
Cl	-1.89702300	3.11063600	-0.88912100
Cl	2.06433400	2.34924900	-2.35355700
Cl	-1.89715400	0.88272700	-3.11268400
Cl	1.89691700	-0.88883500	-3.11080000
Cl	-2.06417300	-2.35387100	-2.34908300
Cl	1.89753400	-3.11238400	-0.88287700
Cl	-1.89640800	-3.11110900	0.88898300
Cl	-1.89717200	-0.88319900	3.11254600

$[Ca(B_2C_4H_6)_2]^{2-}$-m-1

E (B3LYP/6-311++G(d,p)) = -1089.36618591

Zero-point correction=	0.179690 (Hartree/Particle)
Thermal correction to Energy=	0.192722
Thermal correction to Enthalpy=	0.193666
Thermal correction to Gibbs Free Energy=	0.138306
Sum of electronic and zero-point Energies=	-1089.186496
Sum of electronic and thermal Energies=	-1089.173464
Sum of electronic and thermal Enthalpies=	-1089.172520
Sum of electronic and thermal Free Energies=	-1089.227880

Charge = -2 Multiplicity = 1

C	2.32028200	1.41624900	-0.00016400
C	2.31721800	0.74565300	1.24333800
C	2.31718100	0.74537100	-1.24351900
H	2.28638600	2.51216300	-0.00029000
H	2.29593400	1.38280500	2.13113000
H	2.39888400	-1.33379200	2.40610200
H	2.31478700	-2.63257200	0.00029100
H	2.39881200	-1.33433600	-2.40581800
H	2.29587300	1.38232800	-2.13145100
B	2.38068000	-0.78250500	1.31595200
C	-2.31721800	-0.74565000	1.24333900
H	-2.39888500	1.33379700	2.40609900
H	-2.29593400	-1.38280200	2.13113100
H	-2.28638600	-2.51216300	-0.00028600
H	-2.29587200	-1.38233200	-2.13144900
H	-2.39881100	1.33433100	-2.40582100
H	-2.31478700	2.63257200	0.00028600
C	-2.32028200	-1.41624900	-0.00016200
C	-2.31718000	-0.74537400	-1.24351900
B	-2.38068000	0.78250700	1.31595000
C	2.32441400	-1.53531400	0.00016700
C	-2.32441400	1.53531400	0.00016300
B	-2.38064000	0.78280000	-1.31579200
B	2.38064000	-0.78280200	-1.31579000
Ca	0.00000000	0.00000000	0.00003100

$[Ca(B_2C_4H_6)_2]^{2-}$-m-2

E (B3LYP/6-311++G(d,p)) = -1089.36637831

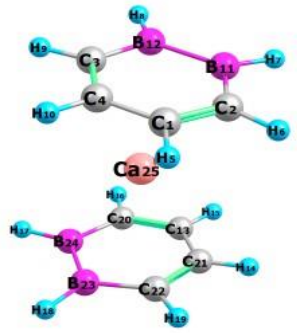
Zero-point correction=	0.179768 (Hartree/Particle)
Thermal correction to Energy=	0.192756
Thermal correction to Enthalpy=	0.193700
Thermal correction to Gibbs Free Energy=	0.139886
Sum of electronic and zero-point Energies=	-1089.186610
Sum of electronic and thermal Energies=	-1089.173623
Sum of electronic and thermal Enthalpies=	-1089.172678
Sum of electronic and thermal Free Energies=	-1089.226492

Charge = -2 Multiplicity = 1

H	2.32436800	-2.48755600	-0.49395800
H	2.11326100	-1.77928900	1.80166600
H	2.06988600	0.52534500	2.50912300
H	2.32604200	2.64126900	0.79986300
H	2.46858400	1.85868900	-1.81813900
H	2.61396900	-0.76079800	-2.59197600
C	-2.21964200	1.00469300	1.03342700
C	-2.33395800	1.40922000	-0.31558500
H	-2.32608400	-2.64121100	0.80004500
H	-2.06993000	-0.52517100	2.50914700
H	-2.11325700	1.77941000	1.80153300
H	-2.32436000	2.48751800	-0.49414100
H	-2.61393700	0.76060700	-2.59203500
H	-2.46856700	-1.85881200	-1.81801800
C	-2.18711200	-0.34852500	1.43684300
C	-2.41156000	-1.08296200	-1.04444000
B	-2.34101800	-1.48029500	0.41782700
B	-2.49862800	0.37974400	-1.43672200
C	2.21963900	-1.00462000	1.03350900
C	2.41156800	1.08288400	-1.04451600
B	2.49864900	-0.37985300	-1.43669200
C	2.33396800	-1.40924600	-0.31547500
B	2.34099600	1.48032700	0.41773000
C	2.18708900	0.34862800	1.43683200

Ca	0.00000400	-0.00000200	-0.17737000

$[Ca(B_2C_4H_6)_2]^{2-}$-o-1



E (B3LYP/6-311++G(d,p)) = -1089.31299000

Zero-point correction=	0.179730 (Hartree/Particle)
Thermal correction to Energy=	0.192766
Thermal correction to Enthalpy=	0.193710
Thermal correction to Gibbs Free Energy=	0.139130
Sum of electronic and zero-point Energies=	-1089.133260
Sum of electronic and thermal Energies=	-1089.120224
Sum of electronic and thermal Enthalpies=	-1089.119280
Sum of electronic and thermal Free Energies=	-1089.173860

Charge = -2 Multiplicity = 1

C	-2.19404600	-1.17261700	-0.79849700
C	-2.21284100	-1.36359600	0.61302500
C	-2.42574400	1.29419000	-0.63199600
C	-2.29607900	0.09691100	-1.39359400
H	-2.07415900	-2.03104400	-1.46226500
H	-2.10271100	-2.40776500	0.92958200
H	-2.38613100	-0.48321100	2.78446100
H	-2.61320300	2.37425300	1.44627700
H	-2.47570300	2.20989800	-1.23315300
H	-2.25094300	0.14689400	-2.48333200
B	-2.38612700	-0.21428000	1.59048200
B	-2.50650700	1.29212300	0.88503900
C	2.29608300	0.09691400	1.39359200
H	2.07416400	-2.03103900	1.46226800
H	2.25095000	0.14690000	2.48333000
H	2.47570600	2.20990100	1.23314600
H	2.61319800	2.37424900	-1.44628400
H	2.38612400	-0.48321700	-2.78446000
H	2.10271000	-2.40776600	-0.92957600

C	2.42574500	1.29419100	0.63199200
C	2.19404900	-1.17261300	0.79849700
C	2.21284000	-1.36359600	-0.61302200
B	2.38612200	-0.21428500	-1.59048100
B	2.50650400	1.29212100	-0.88504400
Ca	-0.00000100	0.16724200	0.00000200

$[Ca(B_2C_4H_6)_2]^{2-}$-o-2

E (B3LYP/6-311++G(d,p)) = -1089.31292597

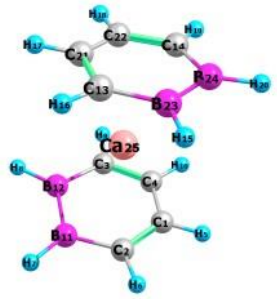
Zero-point correction=	0.179703 (Hartree/Particle)
Thermal correction to Energy=	0.192732
Thermal correction to Enthalpy=	0.193676
Thermal correction to Gibbs Free Energy=	0.139176
Sum of electronic and zero-point Energies=	-1089.133223
Sum of electronic and thermal Energies=	-1089.120194
Sum of electronic and thermal Enthalpies=	-1089.119250
Sum of electronic and thermal Free Energies=	-1089.173750

Charge = -2 Multiplicity = 1

C	2.27871200	-0.82177800	1.13876500
C	2.30175600	-1.47227500	-0.12882600
C	2.35428000	1.45646500	0.15260400
C	2.30386400	0.57766400	1.27335500
H	2.21856800	-1.41469900	2.05368500
H	2.25669700	-2.56684800	-0.07619200
H	2.40942600	-1.36052100	-2.47346100
H	2.46463100	1.78852300	-2.17118500
H	2.34889100	2.52189900	0.41267500
H	2.26266500	0.98719300	2.28480200
B	2.39790300	-0.70792700	-1.43803500
B	2.42757800	0.95191600	-1.27854800
C	-2.27869700	-0.82178200	-1.13876700
H	-2.25669800	-2.56684800	0.07619500
H	-2.21853800	-1.41470500	-2.05368400

H	-2.26263300	0.98718700	-2.28480700
H	-2.34888800	2.52189800	-0.41268600
H	-2.40945800	-1.36051400	2.47345900
C	-2.30384800	0.57766000	-1.27336100
C	-2.35427900	1.45646400	-0.15261300
B	-2.39792200	-0.70792300	1.43803200
C	-2.30175800	-1.47227500	0.12882500
B	-2.42759600	0.95192000	1.27853900
H	-2.46466200	1.78853000	2.17117300
Ca	0.00000000	0.03840600	0.00000900

$[Ca(B_2C_4H_6)_2]^{2-}$-o-3



E (B3LYP/6-311++G(d,p)) = -1089.31299001

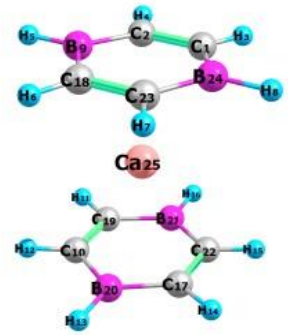
Zero-point correction=	0.179730 (Hartree/Particle)
Thermal correction to Energy=	0.192765
Thermal correction to Enthalpy=	0.193709
Thermal correction to Gibbs Free Energy=	0.139153
Sum of electronic and zero-point Energies=	-1089.133260
Sum of electronic and thermal Energies=	-1089.120225
Sum of electronic and thermal Enthalpies=	-1089.119281
Sum of electronic and thermal Free Energies=	-1089.173837

Charge = -2 Multiplicity = 1

C	-2.29627200	0.09904900	1.39341300
C	-2.42553100	1.29524600	0.63004200
C	-2.21316800	-1.36443100	-0.61105100
C	-2.19449500	-1.17138300	0.80019400
H	-2.25127600	0.15062300	2.48308400
H	-2.47533000	2.21185100	1.22984400
H	-2.61244200	2.37230600	-1.44984900
H	-2.38595700	-0.48718800	-2.78380700
H	-2.10327900	-2.40909400	-0.92606400
H	-2.07493100	-2.02886800	1.46523800
B	-2.50610200	1.29097100	-0.88700500

B	-2.38602800	-0.21650500	-1.59022200
C	2.42553200	1.29524900	-0.63003500
C	2.21316700	-1.36443600	0.61104000
H	2.61245300	2.37229300	1.44986300
H	2.47533100	2.21185900	-1.22983100
H	2.25127000	0.15063900	-2.48308400
H	2.07491900	-2.02885800	-1.46525300
H	2.10327900	-2.40910200	0.92604500
H	2.38596700	-0.48721000	2.78380100
C	2.29626800	0.09905700	-1.39341400
C	2.19449000	-1.17137800	-0.80020400
B	2.50610800	1.29096300	0.88701200
B	2.38603400	-0.21651800	1.59021800
Ca	0.00000000	0.16671800	0.00000500

$[Ca(B_2C_4H_6)_2]^{2-}$-p-1



E (B3LYP/6-311++G(d,p)) = -1089.35603653

Zero-point correction=	0.179677 (Hartree/Particle)
Thermal correction to Energy=	0.192682
Thermal correction to Enthalpy=	0.193626
Thermal correction to Gibbs Free Energy=	0.139433
Sum of electronic and zero-point Energies=	-1089.176360
Sum of electronic and thermal Energies=	-1089.163354
Sum of electronic and thermal Enthalpies=	-1089.162410
Sum of electronic and thermal Free Energies=	-1089.216604

Charge = -2 Multiplicity = 1

C	2.35156600	-0.43803300	1.40479700
C	2.35156200	-1.42109000	0.38187800
H	2.31792800	-0.79998600	2.44011400
H	2.31800400	-2.46998000	0.70237700
H	2.37591800	-1.89204000	-1.96881500
H	2.31794000	0.79998700	-2.44011200

H	2.31804100	2.46997800	-0.70237800
H	2.37591800	1.89204200	1.96881300
B	2.38708300	-1.04937000	-1.09190100
C	-2.35156600	-0.38195400	-1.42106800
H	-2.31793000	-2.44015500	-0.79986000
H	-2.31801800	-0.70250900	-2.46994100
H	-2.37593200	1.96871200	-1.89214700
H	-2.31793800	2.44015600	0.79985400
H	-2.31801600	0.70251000	2.46994100
H	-2.37590100	-1.96871700	1.89214400
C	-2.35157400	1.40482000	0.43795700
C	2.35157100	0.43803200	-1.40479600
C	-2.35156500	-1.40482000	-0.43795800
B	-2.38709000	1.09184500	-1.04942800
B	-2.38708100	-1.09184600	1.04942800
C	-2.35156900	0.38195300	1.42106900
C	2.35157400	1.42108800	-0.38187800
B	2.38708700	1.04936900	1.09190100
Ca	0.00000000	0.00000300	0.00000000

$[Ca(B_2C_4F_6)_2]^{2-}$-m-1

E (B3LYP/6-311++G(d,p)) = -2280.89428093

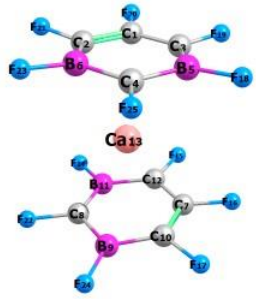
Zero-point correction=	0.092825 (Hartree/Particle)
Thermal correction to Energy=	0.117688
Thermal correction to Enthalpy=	0.118632
Thermal correction to Gibbs Free Energy=	0.035167
Sum of electronic and zero-point Energies=	-2280.801456
Sum of electronic and thermal Energies=	-2280.776593
Sum of electronic and thermal Enthalpies=	-2280.775649
Sum of electronic and thermal Free Energies=	-2280.859114

Charge = -2 Multiplicity = 1

C	-2.38705200	1.38950800	-0.00024900

C	-2.35295300	0.72037800	-1.23115800
C	-2.35299700	0.72081300	1.23089800
B	-2.42527100	-0.79681500	-1.32051800
C	2.34200200	1.51342200	0.00026100
C	-2.34200200	-1.51342200	0.00026500
C	2.38705300	-1.38950800	-0.00024700
B	-2.42531900	-0.79634800	1.32079200
C	2.35299700	-0.72081100	1.23089800
C	2.35295300	-0.72038000	-1.23115700
B	2.42531900	0.79635000	1.32079000
B	2.42527100	0.79681200	-1.32052100
Ca	0.00000000	0.00000000	0.00004200
F	2.37321300	2.92858200	0.00050700
F	2.50891600	1.42694200	-2.55351300
F	2.41549800	-1.53413400	-2.36060500
F	2.44211000	-2.75675800	-0.00048700
F	-2.37321400	-2.92858200	0.00051400
F	-2.50891700	-1.42694700	-2.55351000
F	-2.41549800	1.53412900	-2.36060700
F	-2.44211000	2.75675800	-0.00049200
F	-2.41557700	1.53496300	2.36005700
F	2.50900700	1.42604900	2.55400000
F	2.41557800	-1.53495800	2.36006000
F	-2.50900600	-1.42604300	2.55400400

$[Ca(B_2C_4F_6)_2]^{2-}$-m-2



E (B3LYP/6-311++G(d,p)) = -2280.89452659

Zero-point correction=	0.092862 (Hartree/Particle)
Thermal correction to Energy=	0.117707
Thermal correction to Enthalpy=	0.118651
Thermal correction to Gibbs Free Energy=	0.036449
Sum of electronic and zero-point Energies=	-2280.801664
Sum of electronic and thermal Energies=	-2280.776820
Sum of electronic and thermal Enthalpies=	-2280.775876

Sum of electronic and thermal Free Energies= -2280.858077

Charge = -2 Multiplicity = 1

C	2.29875500	0.94958900	-1.03145500
C	2.36287700	1.39672600	0.29564400
C	2.24247000	-0.40766400	-1.37503300
C	2.41920200	-1.02513800	1.09379300
B	2.39571800	-1.50530900	-0.33236000
B	2.52672400	0.43072900	1.45939200
C	-2.29884200	-0.95067600	-1.03039100
C	-2.41913500	1.02631500	1.09279800
B	-2.52665400	-0.42917200	1.45993300
C	-2.36289000	-1.39641000	0.29719400
B	-2.39571300	1.50496400	-0.33386600
C	-2.24255800	0.40621800	-1.37539600
Ca	-0.00000300	0.00003000	0.17880200
F	-2.45217100	2.83654000	-0.71719600
F	-2.20343600	0.67976800	-2.74043300
F	-2.27790200	-1.88212500	-2.03169300
F	-2.43457900	-2.77786900	0.46570400
F	2.45220800	-2.83729200	-0.71425900
F	2.20329200	-0.68263200	-2.73978400
F	2.27773000	1.87999200	-2.03372600
F	2.43456500	2.77835600	0.46269700
F	-2.52840500	1.99009800	2.12499100
F	2.70243800	0.90614700	2.75090100
F	-2.70226500	-0.90320900	2.75196400
F	2.52857100	-1.98782200	2.12700500

$[Ca(B_2C_4F_6)_2]^{2-}$-o-1

E (B3LYP/6-311++G(d,p)) = -2280.83317162

Zero-point correction= 0.092289 (Hartree/Particle)

Thermal correction to Energy= 0.117263

Thermal correction to Enthalpy=	0.118208
Thermal correction to Gibbs Free Energy=	0.035016
Sum of electronic and zero-point Energies=	-2280.740882
Sum of electronic and thermal Energies=	-2280.715908
Sum of electronic and thermal Enthalpies=	-2280.714964
Sum of electronic and thermal Free Energies=	-2280.798156

Charge = -2 Multiplicity = 1

C	2.18363500	0.24552500	1.35313900
C	2.25091100	-1.10741400	0.93896900
C	2.45346500	1.10136000	-0.93864000
C	2.28039700	1.30443700	0.45302800
B	2.48701800	-1.52066500	-0.49107700
B	2.60294200	-0.26269100	-1.56031700
C	-2.18388900	-0.25152000	1.35192200
C	-2.28176700	-1.30620000	0.44717300
C	-2.45451300	-1.09693600	-0.94340300
B	-2.48549700	1.52322300	-0.48423900
C	-2.24974700	1.10333000	0.94387500
B	-2.60270300	0.27003900	-1.55906900
Ca	0.00016300	-0.00040900	-0.26975500
F	-2.55772000	-2.28134500	-1.67523700
F	-2.81912300	0.36888800	-2.94146900
F	-2.16479600	2.00821300	2.00184800
F	-2.58724700	2.88996400	-0.77982900
F	2.16684800	-2.01710300	1.99290000
F	2.08796200	0.54301200	2.68705900
F	2.27189400	2.57904200	0.95654500
F	2.55556900	2.28907300	-1.66521100
F	2.81943300	-0.35521200	-2.94314300
F	-2.27454500	-2.58310500	0.94495800
F	-2.08865000	-0.55506600	2.68451600
F	2.59004000	-2.88601000	-0.79268800

$[Ca(B_2C_4F_6)_2]^{2-}$-o-2

E (B3LYP/6-311++G(d,p)) = -2280.83325262

Zero-point correction=	0.092328 (Hartree/Particle)
Thermal correction to Energy=	0.117279
Thermal correction to Enthalpy=	0.118223
Thermal correction to Gibbs Free Energy=	0.035350
Sum of electronic and zero-point Energies=	-2280.740924
Sum of electronic and thermal Energies=	-2280.715974
Sum of electronic and thermal Enthalpies=	-2280.715030
Sum of electronic and thermal Free Energies=	-2280.797903

Charge = -2 Multiplicity = 1

C	2.13637100	0.32442700	-1.33167400
C	2.28724200	1.39281000	-0.41405400
C	2.40026200	-1.38920100	0.41423600
C	2.19056800	-1.00972000	-0.93440600
B	2.56971600	1.18750400	1.05201600
B	2.63307800	-0.39710100	1.52401200
C	-2.19062100	1.00949200	-0.93451900
C	-2.40022700	1.38930800	0.41404500
C	-2.13645800	-0.32475500	-1.33146100
C	-2.28727600	-1.39291300	-0.41356800
B	-2.56965600	-1.18724400	1.05247200
B	-2.63298000	0.39748100	1.52408200
Ca	0.00000900	0.00003400	0.33467500
F	-2.44811900	2.77131200	0.60139500
F	2.87228500	-0.87633900	2.82094700
F	2.44817300	-2.77115900	0.60192400
F	2.10887200	-1.97299200	-1.90535500
F	2.00779700	0.59160500	-2.66922800
F	2.23216300	2.65173000	-1.01210700
F	2.74742000	2.31230600	1.87070600
F	-2.23224000	-2.65198100	-1.01131300
F	-2.00797000	-0.59226400	-2.66895700
F	-2.10898200	1.97252400	-1.90571000
F	-2.87210100	0.87704000	2.82091500
F	-2.74731300	-2.31184300	1.87145000

$[Ca(B_2C_4F_6)_2]^{2-}$-o-3

E (B3LYP/6-311++G(d,p)) = -2280.83317590

Zero-point correction=	0.092288 (Hartree/Particle)
Thermal correction to Energy=	0.117263
Thermal correction to Enthalpy=	0.118207
Thermal correction to Gibbs Free Energy=	0.034506
Sum of electronic and zero-point Energies=	-2280.740888
Sum of electronic and thermal Energies=	-2280.715913
Sum of electronic and thermal Enthalpies=	-2280.714969
Sum of electronic and thermal Free Energies=	-2280.798670

Charge = -2 Multiplicity = 1

C	-2.27268500	-1.28892800	-0.49388100
C	-2.45313700	-1.12953900	0.90247500
C	-2.24797400	1.13667900	-0.90405400
C	-2.17464800	-0.20273700	-1.35947500
B	-2.60945500	0.21460100	1.56626500
B	-2.49213000	1.50527900	0.53688400
C	2.45361200	1.12756800	0.90479200
C	2.24747100	-1.13491200	-0.90640300
C	2.27323000	1.28989100	-0.49127500
C	2.17473500	0.20547900	-1.35910200
B	2.60935100	-0.21803200	1.56585900
B	2.49147800	-1.50656100	0.53381100
Ca	0.00001900	0.00024400	0.28190100
F	2.83197300	-0.27030400	2.94994500
F	-2.55504900	-2.33963700	1.59121800
F	-2.83211800	0.26393600	2.95045400
F	2.59901900	-2.86243000	0.87425400
F	-2.07228800	-0.45843000	-2.70147600
F	-2.25868200	-2.54721000	-1.03660400
F	-2.16126700	2.07881100	-1.92883100
F	2.16037000	-2.07491000	-1.93309000
F	2.07249200	0.46396200	-2.70057900
F	2.25974000	2.54929300	-1.03144200
F	2.55600600	2.33623900	1.59599200

F	-2.60022000	2.86042100	0.88009400

$[Ca(B_2C_4F_6)_2]^{2-}$-o-4

E (B3LYP/6-311++G(d,p)) = -2280.83266113

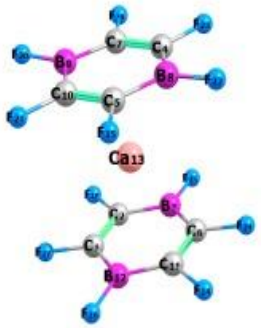
Zero-point correction=	0.092325 (Hartree/Particle)
Thermal correction to Energy=	0.117276
Thermal correction to Enthalpy=	0.118220
Thermal correction to Gibbs Free Energy=	0.036190
Sum of electronic and zero-point Energies=	-2280.740336
Sum of electronic and thermal Energies=	-2280.715385
Sum of electronic and thermal Enthalpies=	-2280.714441
Sum of electronic and thermal Free Energies=	-2280.796471

Charge = -2 Multiplicity = 1

C	2.37166000	1.45283300	0.00316400
C	2.34406900	0.69644300	1.20058900
C	2.37164900	-1.45283600	0.00316300
C	-2.34406700	-0.69644600	-1.20058700
C	-2.37165900	1.45283400	-0.00316400
C	-2.37164800	-1.45283600	-0.00316200
C	-2.34407200	0.69644300	-1.20058800
C	2.34406400	-0.69644600	1.20058800
B	-2.45675800	0.82747000	1.36561200
B	-2.45675200	-0.82747100	1.36561300
B	2.45676300	0.82747000	-1.36561100
B	2.45675700	-0.82747200	-1.36561200
F	2.39814400	-2.83124300	0.21731500
F	2.53128600	-1.66464200	-2.48773500
F	-2.39814700	-2.83124300	-0.21731300
F	-2.38838300	-1.33859700	-2.41113400
F	-2.38839300	1.33859300	-2.41113500
F	-2.39816800	2.83124100	-0.21731700
F	2.39816500	2.83124100	0.21731800
F	2.53129700	1.66464200	-2.48773400

F	-2.53128200	-1.66464100	2.48773600
F	-2.53129300	1.66464100	2.48773400
F	2.38838000	-1.33859800	2.41113400
F	2.38839000	1.33859300	2.41113500
Ca	0.00000100	0.00001000	-0.00000300

$[Ca(B_2C_4F_6)_2]^{2-}$-p-1



E (B3LYP/6-311++G(d,p)) = -2280.89017437

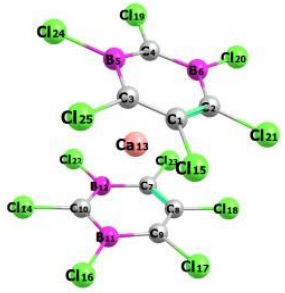
Zero-point correction=	0.092782 (Hartree/Particle)
Thermal correction to Energy=	0.117526
Thermal correction to Enthalpy=	0.118470
Thermal correction to Gibbs Free Energy=	0.036177
Sum of electronic and zero-point Energies=	-2280.797392
Sum of electronic and thermal Energies=	-2280.772648
Sum of electronic and thermal Enthalpies=	-2280.771704
Sum of electronic and thermal Free Energies=	-2280.853998

Charge = -2 Multiplicity = 1

C	-2.37533300	-0.39749000	-1.39136700
C	-2.37535800	-1.39182900	-0.39587500
B	-2.40982700	-1.07770200	1.07896400
C	2.37537200	-0.39593500	1.39180600
C	2.37533500	1.39138600	-0.39743100
C	-2.37535600	0.39749200	1.39136300
C	2.37535400	-1.39138200	0.39742200
B	2.40981900	1.07891900	1.07775000
B	2.40980500	-1.07891600	-1.07775800
C	2.37534100	0.39593800	-1.39181300
C	-2.37535400	1.39182800	0.39586800
B	-2.40979700	1.07770500	-1.07897100
Ca	0.00000000	-0.00001000	0.00002800
F	-2.39916800	2.70889500	0.83886600
F	2.39914600	2.70796600	-0.84188000

F	-2.46723100	2.06057400	-2.06297500
F	-2.39914500	-0.84200200	-2.70792600
F	-2.39917300	-2.70889600	-0.83887200
F	2.39918400	-2.70796200	0.84187300
F	2.46724600	-2.06287400	-2.06067300
F	2.39914300	0.83899600	-2.70886000
F	2.46726500	2.06287900	2.06066600
F	2.39919900	-0.83899400	2.70885200
F	-2.39918500	0.84200400	2.70792200
F	-2.46727900	-2.06057400	2.06297000

$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-2



E (B3LYP/6-311++G(d,p)) = -6605.22192607

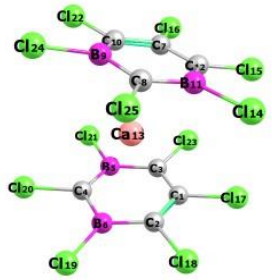
Zero-point correction=	0.077896 (Hartree/Particle)
Thermal correction to Energy=	0.106902
Thermal correction to Enthalpy=	0.107846
Thermal correction to Gibbs Free Energy=	0.012174
Sum of electronic and zero-point Energies=	-6605.144030
Sum of electronic and thermal Energies=	-6605.115024
Sum of electronic and thermal Enthalpies=	-6605.114080
Sum of electronic and thermal Free Energies=	-6605.209752

Charge = -2 Multiplicity = 1

C	-2.12463600	0.97927400	-1.08666400
C	-2.10532200	-0.40259400	-1.36539400
C	-2.28592100	1.47045600	0.22659100
C	-2.47333600	-0.92541600	1.11806000
B	-2.55387400	0.54209800	1.39853800
B	-2.36051700	-1.43918600	-0.28349100
C	2.28332400	-1.47386800	0.20410500
C	2.12176500	-0.96403000	-1.10187700
C	2.10487300	0.42166000	-1.36120100
C	2.47654200	0.90889100	1.12885200
B	2.36331200	1.44249300	-0.26525200

B	2.55435600	-0.56260200	1.38863000
Ca	0.00031000	0.00046200	0.33755800
Cl	2.67775600	2.05623400	2.49749300
Cl	-1.88570500	2.12746400	-2.40957900
Cl	2.39907700	3.22190100	-0.65408900
Cl	1.87248600	0.97113900	-3.03439300
Cl	1.87974300	-2.09295500	-2.44059700
Cl	-2.67111900	-2.09221900	2.47066000
Cl	-2.39401200	-3.21289700	-0.69734800
Cl	-1.87408100	-0.92808600	-3.04637600
Cl	2.81215200	-1.26684600	3.05234800
Cl	2.26742300	-3.23768800	0.43832900
Cl	-2.81114900	1.22245500	3.07224100
Cl	-2.27294200	3.23093900	0.48554000

$[Ca(B_2C_4Cl_6)_2]^{2-}$-m-3



E (B3LYP/6-311++G(d,p)) = -6605.22192586

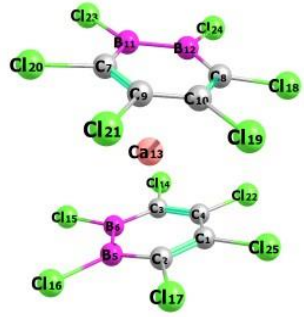
Zero-point correction=	0.077893 (Hartree/Particle)
Thermal correction to Energy=	0.106901
Thermal correction to Enthalpy=	0.107845
Thermal correction to Gibbs Free Energy=	0.012064
Sum of electronic and zero-point Energies=	-6605.144033
Sum of electronic and thermal Energies=	-6605.115025
Sum of electronic and thermal Enthalpies=	-6605.114081
Sum of electronic and thermal Free Energies=	-6605.209862

Charge = -2 Multiplicity = 1

C	2.12395000	0.97244500	-1.09277600
C	2.28539100	1.47119000	0.21755100
C	2.10517900	-0.41101400	-1.36359600
C	2.47428200	-0.91945000	1.12266600
B	2.36124700	-1.44128700	-0.27588700
B	2.55415900	0.54968200	1.39469100
C	-2.12334300	-0.96958600	-1.09583200

C	-2.47498200	0.91635700	1.12433400
B	-2.55452000	-0.55348300	1.39253000
C	-2.28505400	-1.47181100	0.21309200
B	-2.36157700	1.44191200	-0.27279400
C	-2.10481800	0.41455700	-1.36302900
Ca	-0.00007500	0.00002200	0.33750500
Cl	-2.39556600	3.21905800	-0.67178800
Cl	-1.87256200	0.95422800	-3.03941900
Cl	-1.88315100	-2.10642900	-2.42821300
Cl	1.88431800	2.11285700	-2.42223200
Cl	2.27182900	3.23307600	0.46647300
Cl	2.81172100	1.23972800	3.06436800
Cl	2.67298100	-2.07840400	2.48187900
Cl	2.39506000	-3.21737200	-0.67955600
Cl	-2.27112500	-3.23431200	0.45742200
Cl	1.87350900	-0.94623100	-3.04147700
Cl	-2.81252300	-1.24793200	3.06032700
Cl	-2.67441400	2.07169100	2.48649700

$[Ca(B_2C_4Cl_6)_2]^{2-}$-o-1



E (B3LYP/6-311++G(d,p)) = -6605.15722180

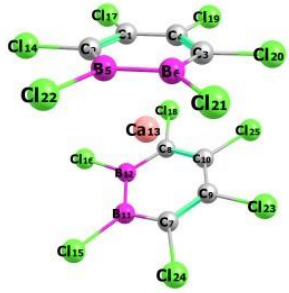
Zero-point correction=	0.077203 (Hartree/Particle)
Thermal correction to Energy=	0.106381
Thermal correction to Enthalpy=	0.107325
Thermal correction to Gibbs Free Energy=	0.011339
Sum of electronic and zero-point Energies=	-6605.080019
Sum of electronic and thermal Energies=	-6605.050841
Sum of electronic and thermal Enthalpies=	-6605.049897
Sum of electronic and thermal Free Energies=	-6605.145883

Charge = -2 Multiplicity = 1

C	2.02627600	-0.39641300	-1.36476400
C	2.19511200	0.96425500	-0.97171700

C	2.37909300	-1.22927800	0.94383900
C	2.10925000	-1.45536500	-0.43935100
B	2.54426300	1.35872700	0.42998100
B	2.64996900	0.13409200	1.49862600
C	-2.38479500	1.20807100	0.96729000
C	-2.18924800	-0.94427600	-0.99341900
C	-2.11474800	1.46402500	-0.41083100
C	-2.02598300	0.42496800	-1.35790700
B	-2.64984400	-0.16768200	1.49337900
B	-2.53782900	-1.36931700	0.39950200
Ca	0.00048400	0.00153000	0.39486000
Cl	2.42426600	-2.66813000	2.00817700
Cl	2.98970900	0.36225100	3.28843900
Cl	2.75964100	3.12462300	0.87642800
Cl	2.02682000	2.20405800	-2.24691100
Cl	-2.01550100	-2.15638000	-2.29407400
Cl	-1.72056100	0.84950500	-3.04298400
Cl	-2.43738900	2.62444900	2.06127100
Cl	-1.88637900	3.12657000	-0.96160500
Cl	1.87439900	-3.10489700	-1.02483800
Cl	-2.99031600	-0.43435600	3.27767800
Cl	-2.74691600	-3.14478800	0.80866500
Cl	1.72150800	-0.78441200	-3.05868500

$[Ca(B_2C_4Cl_6)_2]^{2-}$-o-2



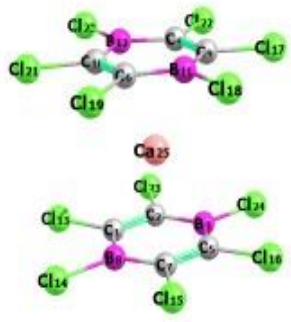
E (B3LYP/6-311++G(d,p)) = -6605.15722236

Zero-point correction=	0.077203 (Hartree/Particle)
Thermal correction to Energy=	0.106381
Thermal correction to Enthalpy=	0.107325
Thermal correction to Gibbs Free Energy=	0.011331
Sum of electronic and zero-point Energies=	-6605.080019
Sum of electronic and thermal Energies=	-6605.050841
Sum of electronic and thermal Enthalpies=	-6605.049897
Sum of electronic and thermal Free Energies=	-6605.145891

Charge = -2 Multiplicity = 1

C	2.11214300	1.45847000	-0.42758100
C	2.38209800	1.21963300	0.95350900
C	2.19216600	-0.95650900	-0.98121900
C	2.02620100	0.40792800	-1.36218300
B	2.65005700	-0.14915500	1.49617800
B	2.54106100	-1.36408200	0.41681800
C	-2.38216900	-1.21791900	0.95614900
C	-2.19210100	0.95484500	-0.98238100
C	-2.11267500	-1.45920700	-0.42459800
C	-2.02667800	-0.41029700	-1.36103400
B	-2.64946000	0.15189300	1.49654900
B	-2.54042400	1.36493200	0.41505800
Ca	0.00008400	0.00001400	0.39473100
Cl	2.43102900	2.64901300	2.03046800
Cl	-2.98901900	0.39967600	3.28375900
Cl	-2.75181400	3.13586500	0.84270100
Cl	1.88060800	3.11370400	-0.99838700
Cl	-2.02090600	2.18061000	-2.27059600
Cl	1.72124300	0.81160700	-3.05243900
Cl	2.02091100	-2.18454000	-2.26726500
Cl	2.75314300	-3.13421000	0.84746800
Cl	2.99030000	-0.39375800	3.28370400
Cl	-1.88193400	-3.11551500	-0.99263200
Cl	-2.43134800	-2.64544800	2.03556500
Cl	-1.72231600	-0.81699500	-3.05067500

$[Ca(B_2C_4Cl_6)_2]^{2-}$-p-1



E (B3LYP/6-311++G(d,p)) = -6605.21583902

Zero-point correction=	0.077612 (Hartree/Particle)
Thermal correction to Energy=	0.106704
Thermal correction to Enthalpy=	0.107648

Thermal correction to Gibbs Free Energy=	0.010188
Sum of electronic and zero-point Energies=	-6605.138227
Sum of electronic and thermal Energies=	-6605.109136
Sum of electronic and thermal Enthalpies=	-6605.108191
Sum of electronic and thermal Free Energies=	-6605.205651

Charge = -2 Multiplicity = 1

C	2.33684500	1.40842000	0.38832400
C	2.33685900	0.42474900	1.39785300
B	2.37679200	-1.04685100	1.07435200
C	-2.33683200	-0.38835600	1.40843400
C	2.33684200	-1.40842000	-0.38836000
C	-2.33685600	0.38835700	-1.40839800
C	2.33683500	-0.42474900	-1.39788900
B	2.37677000	1.04685100	-1.07438800
C	-2.33684600	-1.39787500	0.42475300
C	-2.33684900	1.39787600	-0.42471700
B	-2.37679200	-1.07435900	-1.04684400
B	-2.37677000	1.07436000	1.04688000
Cl	2.29777200	3.12871900	0.84736800
Cl	2.38737500	2.31935900	-2.38034600
Cl	2.29776000	-0.92826600	-3.10570100
Cl	2.29776800	-3.12871900	-0.84740200
Cl	-2.29778400	-3.10569300	0.92825100
Cl	-2.38743200	-2.38030400	-2.31936500
Cl	-2.29779800	0.84741700	-3.12869300
Cl	-2.38737500	2.38030500	2.31940100
Cl	-2.29778900	3.10569300	-0.92821700
Cl	-2.29774200	-0.84741700	3.12872800
Cl	2.29781400	0.92826600	3.10566600
Cl	2.38743100	-2.31935900	2.38031000
Ca	0.00000000	-0.00000200	0.00000000