Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

SI for:

Origins of Observed Specificities in the Addition of B_2Cl_4 and Analogues to Unsaturated Compounds

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Table A SI

B_2	Ethylene	Borane0	Borane90	VdW	TS	g-Product	90 zero diff[a]	TS - Σ R[a]	P - Σ R[a]
B3LYP									
B_2F_4	-78.56317	-449.411255	-449.411072	-527.978638	-527.929016	-528.039368	0.115	28.495	-40.866
B_2Cl_4	-78.56317	-1890.75269	-1890.75659	-1969.31763	-1969.28345	-1969.37500	-2.45	20.337	-34.661
$B_2(OH)_4$	-78.56317	-353.243866	-353.244507		-431.743469	-431.869690	-0.402	39.889	-38.912
$B_2(EG)_2$	-78.56317	-508.000488	-508.000916		-586.494385	-586.619568	-0.268	43.470	-34.814
$B_2(pin)_2$	-78.56317	-822.402710	-822.403320		-900.891479	-901.021606	-0.383	46.687	-34.585
$B_2Cl_4(C_2H_2)$	-77.32771	-1890.75269	-1890.75659	-1968.08252	-1968.05249	-1968.15869	-2.45	17.512	-46.678
ωB97X-D									
B_2F_4	-78.52829	-449.276825	-449.276611	-527.813904	-527.769714	-527.881714	0.134	22.214	-48.200
B_2Cl_4	-78.52829	-1890.66504	-1890.66858	-1969.20300	-1969.17773	-1969.26160	-2.22	12.007	-40.617
$B_2(OH)_4$	-78.52829	-353.122192	-353.122772	-431.656555	-431.597382	-431.726349	-0.364	33.321	-47.243
$B_2(EG)_2$	-78.52829	-507.826752	-507.827087		-586.296509	-586.424377	-0.211	36.940	-43.298
B_2dicat	-78.52829	-812.602539	-812.600891		-891.074768	-891.199158	1.03	34.144	-43.910
B_2diScat	-78.52829	-2104.48413	-2104.48486		-2182.96704	-2183.06665	-0.460	28.935	-33.570
B_2Br_4	-78.52829		-10346.5166		-10425.0264	-10425.1104	----	11.624	-41.070
$B_2Cl_4(C_2H_2)$	-77.29145		-1890.66858	-1967.96558	-1967.94055	-1968.04785		12.222	-55.108

Table A. Energies pertaining to B_2X_4 species and their reaction with ethene or ethyne using the w97Bx-D functional and 6-311G(d,p) basis set. [a]Energies are quoted in a.u.(Hartrees) save for the final three columns where kcal.mol^{-1} is used.

Table B SI

Reactant	Alkene	Reagent	VdW	TS1 - less sub	TS2 - more sub	gP[a]	TS1 - Σ R[b]	TS2 - Σ R[b]	gP - Σ R[b]
B3LYP									
Propene	-117.8647	-1890.75659	-2008.62012	-2008.58618	-2008.58398	-2008.66663	22.06	23.43	-28.42
Z-butene	-157.1636	-1890.75659	-2047.91943	-2047.88123		-2047.95764	24.44		-23.51
E-butene	-157.1657	-1890.75659	-2047.92102	-2047.88354		-2047.95496	24.33		-20.48
2-Mebut-2-ene	-196.4642	-1890.75659	-2087.21973	-2087.17676	-2087.17627	-2087.24634	27.60	27.91	-16.06
WB97xD									
Propene	-117.8168	-1890.66858	-2008.49402	-2008.46875	-2008.46594	-2008.54956	10.41	12.17	-40.30
Z-butene	-157.1030	-1890.66858	-2047.78247	-2047.75391		-2047.83020	11.11		-36.77
E-butene	-157.1047	-1890.66858	-2047.78223	-2047.75623		-2047.82751	10.72		-34.01
2-Mebut-2-ene	-196.3921	-1890.66858	-2087.07300	-2087.03906	-2087.04077	-2087.11060	13.54	12.47	-31.35
Naphthalene	-385.6915	-1890.66858	-2276.37231	-2276.31763		-2276.38330	26.66		-14.55
Benzene	-232.1177	-1890.66858	-2122.79541	-2122.72754		-2122.79004	36.86		-2.36
C60 fullerene	-2285.0725	-1890.54993	-4175.63379	-4175.59814	-4175.57774	-4175.66406	15.24	28.11	-26.12
B3LYP/HBCl2									
Ethylene	-78.56317	-945.968628		-1024.50659		-1024.57739	15.82		-28.61
Propene	-117.8647	-945.968628		-1063.81213	-1063.80469	-1063.87390	13.32	18.00	-25.44
Z-butene	-157.1636	-945.968628	-1103.13306	-1103.10779		-1103.16638	15.33		-21.44
E-butene	-157.1657	-945.968628		-1103.10913		-1103.16736	15.83		-20.71
2-Mebut-2-ene	-196.4642	-945.968628		-1142.41113	-1142.40210	-1142.46216	13.59	19.26	-18.43
WB97xD /HBCl2									
Ethylene	-78.52829	-945.921509	-1024.45410	-1024.43555		-1024.50623	8.943		-35.41
Propene	-117.8168	-945.921509	-1063.74341	-1063.72961	-1063.72278	-1063.79175	5.429	9.719	-33.56
Z-butene	-157.1030	-945.921509	-1103.03210	-1103.01501		-1103.07300	5.975		-30.41
E-butene	-157.1047	-945.921509	-1103.03101	-1103.01611		-1103.07446	6.358		-30.26
2-Mebut-2-ene	-196.3921	-945.921509	-1142.32190	-1142.30884	-1142.30005	-1142.35925	2.968	8.483	-28.67

Table B. Reaction paths for simple alkenes with B_2Cl_4 and $HBCl_2$. [a]For less substituted C-B product. [b]Energies in kcal.mol^{-1}; otherwise in Hartrees.; wB97x- D, 6-311g(d,p) save for C60 where the 6-31g(d,p) basis set was used.

Table C SI

Reactant	Alkene	B_2X_4	VdW	TS	Gauche P	TS - sum R[a]	P -sum R[a]
Dienes B3LYP							
B_2Cl_4							
syn-Butadiene	-155.948227	-1890.75659	-2046.66821	-2046.74866		22.970	-27.509
anti-Butadiene	-155.953705	-1890.75659	-2046.70874	-2046.67090	-2046.74866	24.722	-24.071
1,2 addition-Cpd	-194.061569	-1890.75659	-2084.81787	-2084.78247	-2084.85254	22.396	-21.572
1,4 addition Cpd	-194.061569	-1890.75659	-2084.81787	-2084.76782	-2084.85474	31.588	-22.951
B_2F_4							
1,2-Cpd/ B_2F_4	-194.061569	-449.411255	-643.479309	-643.428467	-643.524597	27.834	-32.488
1,4-Cpd/ B_2F_4	-194.061569	-449.411255	-643.432251	-643.519775		25.460	-29.462
Dienes WB97xD							
B_2Cl_4							
syn-Butadiene	-155.883621	-1890.66858	-2046.56482	-2046.53418	-2046.61438	11.308	-39.018
anti-Butadiene	-155.887970	-1890.66858	-2046.56482	-2046.53687	-2046.61438	12.352	-36.289
1,4-alt BD	-155.887970	-1890.66858		-2046.48572	-2046.61938	44.447	-39.429
1,2-Cpd	-193.988281	-1890.66858	-2084.66797	-2084.64038	-2084.71069	10.341	-33.780
1,4 -Cpd	-193.988281	-1890.66858	-2084.66797	-2084.62109	-2084.70996	22.444	-33.321
B_2F_4							
1,2 addition-BD	-155.887970	-449.276611	-605.175293	-605.128113	-605.230530	22.884	-41.383
1,4 -alt BD	-155.887970	-449.276611	-605.175293	-605.094543	-605.235229	43.949	-44.332
1,2 -Cpd-193.988281	-449.276611	-643.279541		-643.232971	-643.325806	20.031	-38.223
1,4 -Cpd-193.988281	-449.276611	-643.279541		-643.233704	-643.325562	19.571	-38.070

Table C. Reaction paths of butadiene and cyclopentadiene with B_2Cl_4 and B_2F_4. [a]Energies in kcal.mol^{-1}; otherwise in Hartrees.

Table D SI

Entry	Reagent	B–C	B–C'	B'–C'	B–B'	C–C'
1	B_2F_4	1.766	1.830	2.142	1.812	1.397
2	B_2Cl_4	1.718	1.828	2.126	1.846	1.410
3	$B_2(OH)_4$	1.838	1.851	2.170	1.814	1.392
4	B_2EG_2	1.784	1.804	2.224	1.786	1.395
5	B_2Cat_2	1.756	1.807	2.116	1.786	1.402
6	B_2Scat_2	1.640	1.789	1.984	1.843	1.446
7	B_2Br_4	1.700	1.820	2.110	1.850	1.420

Table D. Transition-state interatomic distances in Å observed in B_2X_4 additions to ethene.

Table E SI

Entry	Reactant	B–C	B–C'	B'–C'	B–B'	C–C'
1	C_2H_2	1.689	1.810	2.199	1.810	1.238
2	C_3H_6(prim)	1.652	1.869	2.215	1.850	1.429
3	C_3H_6(sec)	1.719	1.806	2.074	1.853	1.421
4	C_3H_6(prim)	1.718	1.879	2.207	1.817	1.406
5	(E)-C_4H_8	1.654	1.848	2.195	1.849	1.437
6	(Z)-C_4H_8	1.659	1.865	2.140	1.871	1.441
7	C_5H_{10}(sec)	1.615	1.944	2.154	1.949	1.466
8	C_5H_{10}(tert)	1.678	1.852	2.160	1.853	1.444
9	$C_{10}H_8$	1.637	1.899	2.006	1.941	1.474

Table E. Transition state interatomic distances in Å observed for B_2Cl_4 addition to alkenes

Table F SI

Entry	Reactant	B–C	B–C'	C'–H	B–H[a]	C–C'
1	C_2H_4	1.793	1.880	1.798	1.225	1.384
2	C_3H_6(sec)	1.719	1.806	2.074	1.853	1.421
3	C_3H_6(pri)	1.781	1.848	1.717	1.234	1.396
4	E-C_4H_8	1.758	1.890	1.740	1.232	1.403
5	Z-C_4H_8	1.750	1.887	1.729	1.234	1.408
6	C_5H_{10}(sec)	1.779	1.877	1.708	1.236	1.419
7	C_5H_{10}(tert)	1.723	1.934	1.744	1.234	1.412
8	C_2H_4	1.788	1.867	1.682	1.270	1.390

[a] 1.184 Å in $HBCl_2$;

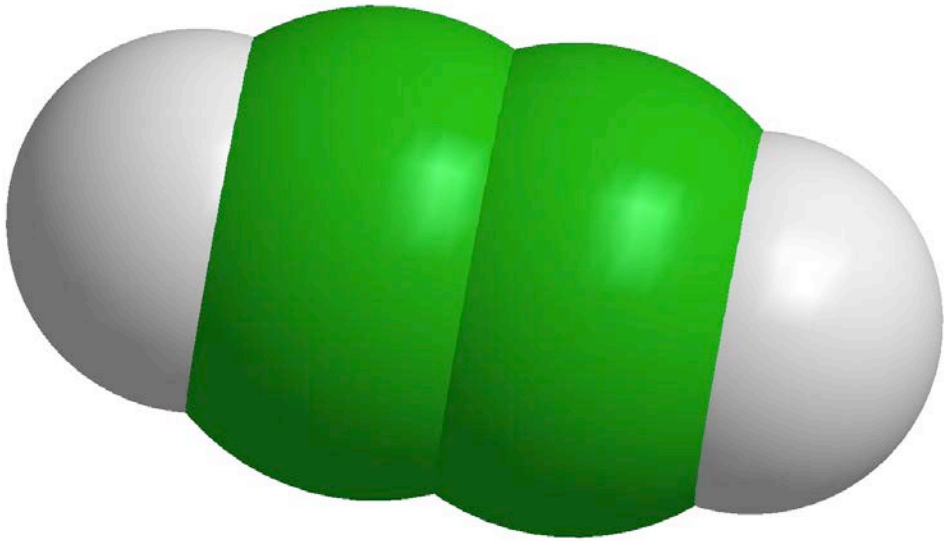
Table F. Transition-state interatomic distances in Å observed for $HBCl_2$ additions to alkenes (ordering as Table E).

Ethyne B3LYP

Zero-point correction= 0.026982 (Hartree/Particle)
Thermal correction to Energy= 0.029792
Thermal correction to Enthalpy= 0.030736
Thermal correction to Gibbs Free Energy= 0.008027
Sum of electronic and zero-point Energies= -77.327716
Sum of electronic and thermal Energies= -77.324906
Sum of electronic and thermal Enthalpies= -77.323962
Sum of electronic and thermal Free Energies= -77.346671

0 1

C	0.00000000	0.00000000	0.59914000
C	0.00000000	0.00000000	-0.59914000
H	0.00000000	0.00000000	1.66209000
H	0.00000000	0.00000000	-1.66209000

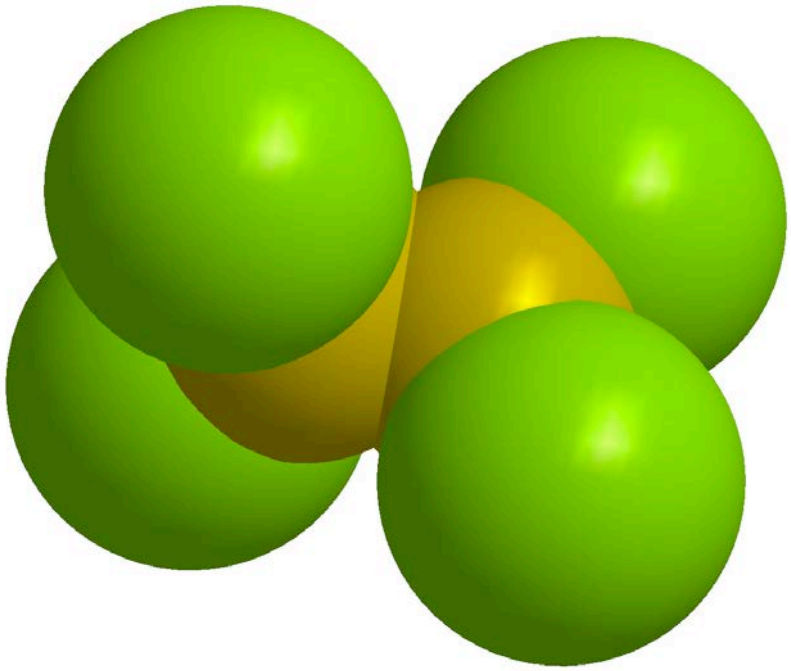


B_2Cl_4 90 B3LYP 6-311G(d,p)

- Zero-point correction= 0.013020 (Hartree/Particle)
- Thermal correction to Energy= 0.020253
- Thermal correction to Enthalpy= 0.021197
- Thermal correction to Gibbs Free Energy= -0.020803
- Sum of electronic and zero-point Energies= -1890.756535
- Sum of electronic and thermal Energies= -1890.749302
- Sum of electronic and thermal Enthalpies= -1890.748358
- Sum of electronic and thermal Free Energies= -1890.790357

- B2Cl490

- 0 1
- B 0.00000000 0.00000000 -0.84229100
- B 0.00000000 0.00000000 0.84229100
- Cl -1.07124100 1.07299800 -1.72923200
- Cl 1.07124100 -1.07299800 -1.72923200
- Cl -1.07124100 -1.07299800 1.72923200
- Cl 1.07124100 1.07299800 1.72923200

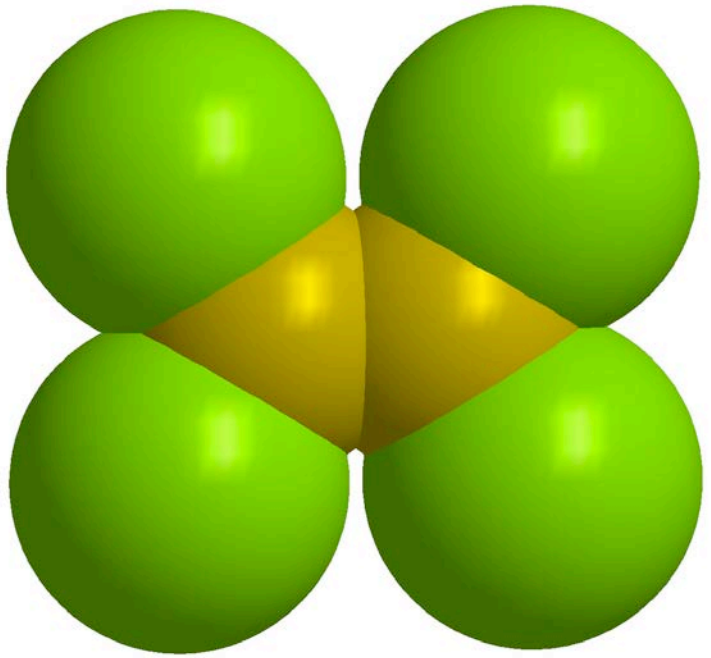


B_2Cl_4 0 B3LYP 6-311g(d,p)

- Zero-point correction= 0.013080 (Hartree/Particle)
- Thermal correction to Energy= 0.019281
- Thermal correction to Enthalpy= 0.020225
- Thermal correction to Gibbs Free Energy= -0.018057
- Sum of electronic and zero-point Energies= -1890.752700
- Sum of electronic and thermal Energies= -1890.746499
- Sum of electronic and thermal Enthalpies= -1890.745555
- Sum of electronic and thermal Free Energies= -1890.783837

- B2Cl400

- 0 1
- B 0.00000000 0.00000000 0.85848000
- B 0.00000000 0.00000000 -0.85848000
- Cl 0.00000000 1.50651600 1.75780700
- Cl 0.00000000 -1.50651600 1.75780700
- Cl 0.00000000 1.50651600 -1.75780700
- Cl 0.00000000 -1.50651600 -1.75780700



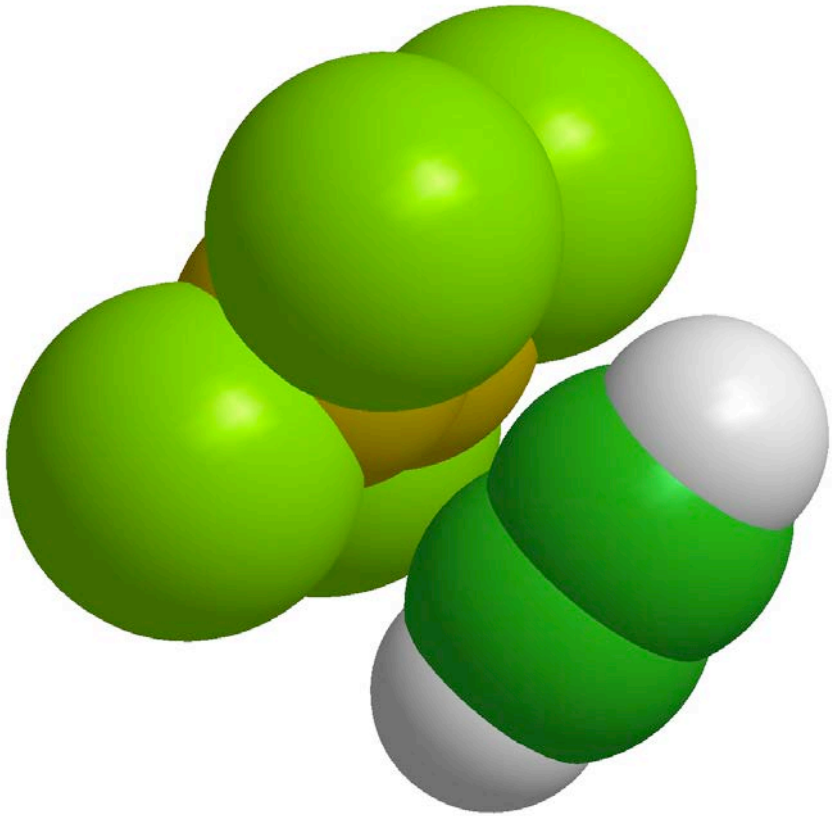
B_2Cl_4 ethyne VdW

Zero-point correction= 0.040855 (Hartree/Particle)
Thermal correction to Energy= 0.052445
Thermal correction to Enthalpy= 0.053389
Thermal correction to Gibbs Free Energy= -0.001221
Sum of electronic and zero-point Energies= -1968.082535
Sum of electronic and thermal Energies= -1968.070945
Sum of electronic and thermal Enthalpies= -1968.070001
Sum of electronic and thermal Free Energies= -1968.124611

B2Cl4AV

0 1

C	0.00265300	-0.58889600	2.77654100
B	0.85677400	-0.00115900	-0.46357700
Cl	1.76320100	-1.50732500	-0.48933900
Cl	1.76025800	1.50600900	-0.51824800
C	0.00166900	0.61080800	2.76929400
B	-0.85754300	-0.00254100	-0.46277200
Cl	-1.76092200	-1.51004400	-0.50802000
Cl	-1.76408400	1.50342000	-0.49637600
H	0.00371400	-1.65237400	2.79038800
H	0.00048500	1.67438200	2.77004600

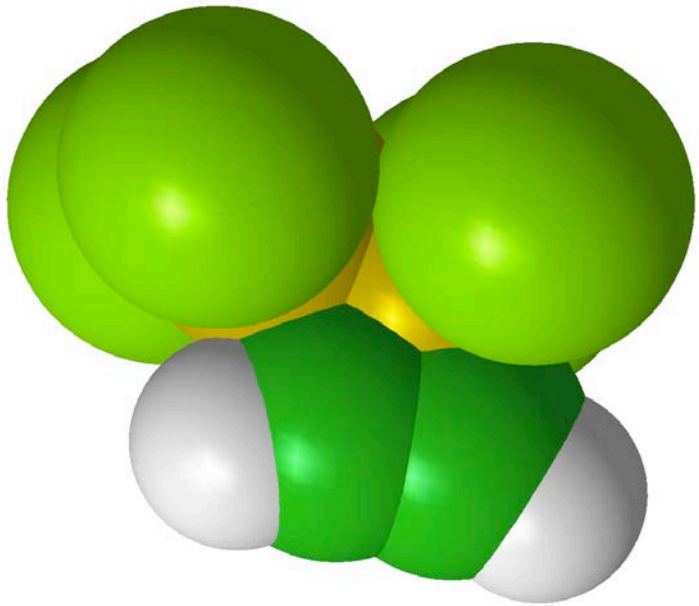


B_2Cl_4 ethyne TS B3LYP

Zero-point correction= 0.041471 (Hartree/Particle)
Thermal correction to Energy= 0.050817
Thermal correction to Enthalpy= 0.051761
Thermal correction to Gibbs Free Energy= 0.004995
Sum of electronic and zero-point Energies= -1968.052505
Sum of electronic and thermal Energies= -1968.043158
Sum of electronic and thermal Enthalpies= -1968.042214
Sum of electronic and thermal Free Energies= -1968.088980

0 1

C	-1.46013000	-0.00142100	1.74142200
C	-0.22462000	-0.00083400	1.87438200
B	0.93634000	0.00044300	0.00996200
B	-0.86502000	-0.00041700	0.17265200
Cl	-1.49051900	1.55493900	-0.63073800
Cl	-1.48842100	-1.55578100	-0.63239800
Cl	1.82658100	1.50187800	-0.16322800
Cl	1.82830800	-1.50008200	-0.16253800
H	-2.48249000	-0.00219600	2.06273200
H	0.74326000	-0.00063800	2.34070200

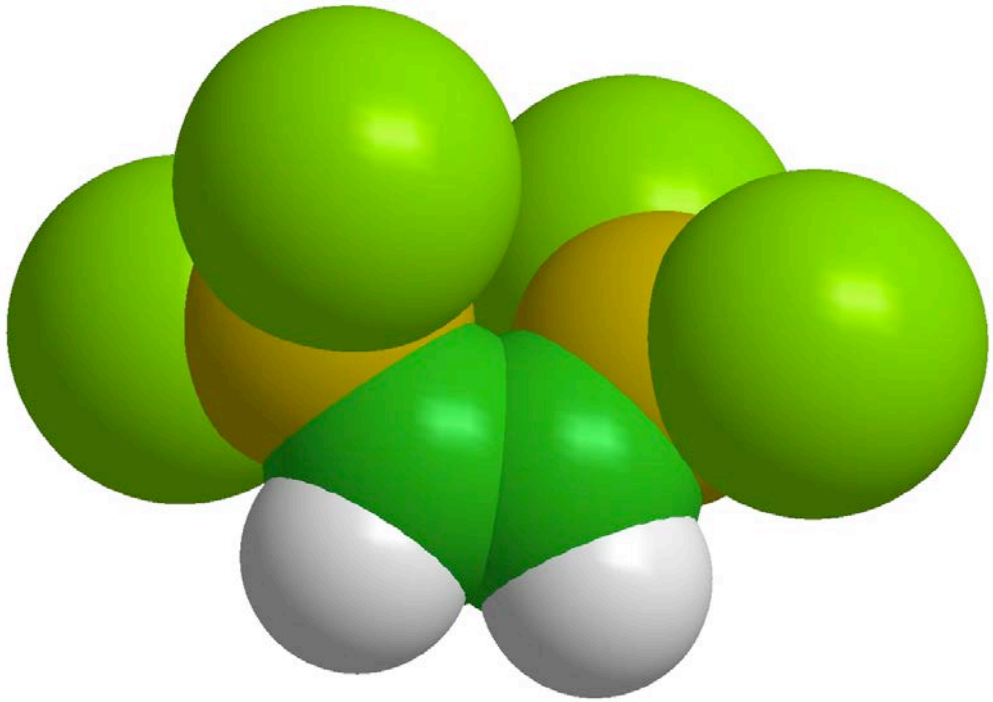


B_2Cl_4 Ethyne Product B3LYP

Zero-point correction=	0.045336 (Hartree/Particle)
Thermal correction to Energy=	0.054604
Thermal correction to Enthalpy=	0.055549
Thermal correction to Gibbs Free Energy=	0.007752
Sum of electronic and zero-point Energies=	-1968.158725
Sum of electronic and thermal Energies=	-1968.149457
Sum of electronic and thermal Enthalpies=	-1968.148513
Sum of electronic and thermal Free Energies=	-1968.196310

0 1

C	-0.61944300	0.16122200	1.52662000
C	0.71887700	-0.08213900	1.52701000
B	1.63443700	-0.27753900	0.27260000
B	-1.59456200	0.27635200	0.28252000
Cl	-1.42757200	1.56998200	-0.92003000
Cl	-3.00953300	-0.79240700	0.22277000
Cl	3.15485800	0.62402000	0.16447000
Cl	1.22825700	-1.44104900	-1.00290000
H	-1.08677200	0.27764200	2.50610000
H	1.20862700	-0.07550900	2.50324000

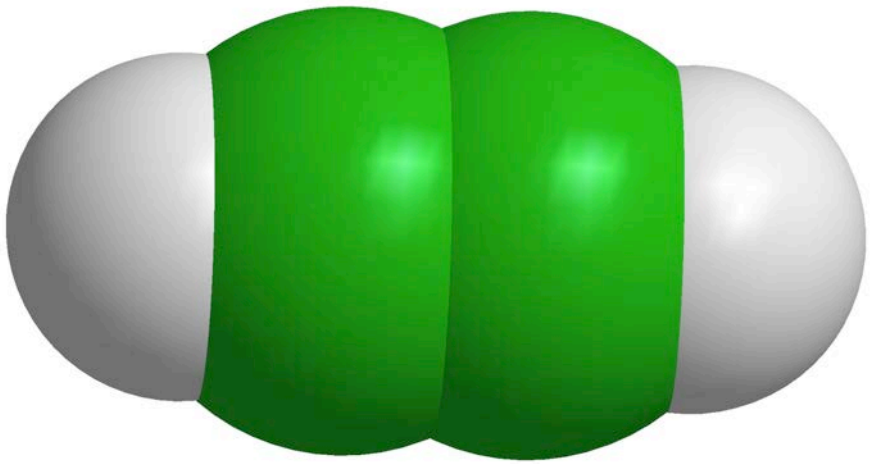


Ethyne ωB97X-D

- Zero-point correction= 0.027184 (Hartree/Particle)
- Thermal correction to Energy= 0.029965
- Thermal correction to Enthalpy= 0.030909
- Thermal correction to Gibbs Free Energy= 0.008243
- Sum of electronic and zero-point Energies= -77.291447
- Sum of electronic and thermal Energies= -77.288665
- Sum of electronic and thermal Enthalpies= -77.287721
- Sum of electronic and thermal Free Energies= -77.310388

- AW

- 0 1
- C 0.00000000 0.00000000 0.59813300
- C 0.00000000 0.00000000 -0.59813300
- H 0.00000000 0.00000000 1.66226300
- H 0.00000000 0.00000000 -1.66226300



B_2Cl_4 90 ωB97x-D

- Zero-point correction= 0.013320 (Hartree/Particle)
- Thermal correction to Energy= 0.020499
- Thermal correction to Enthalpy= 0.021443
- Thermal correction to Gibbs Free Energy= -0.020292
- Sum of electronic and zero-point Energies= -1890.668583
- Sum of electronic and thermal Energies= -1890.661405
- Sum of electronic and thermal Enthalpies= -1890.660460
- Sum of electronic and thermal Free Energies= -1890.702195

- B2Cl49W

- 0 1
- B 0.00000000 0.00000000 -0.84622400
- B 0.00000000 0.00000000 0.84622400
- Cl -1.06876900 -1.06975500 -1.72839000
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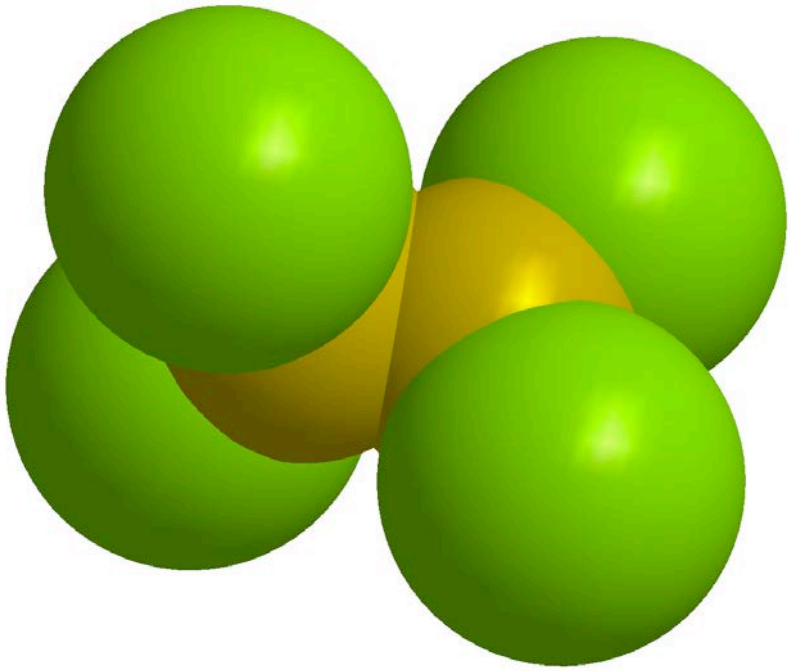
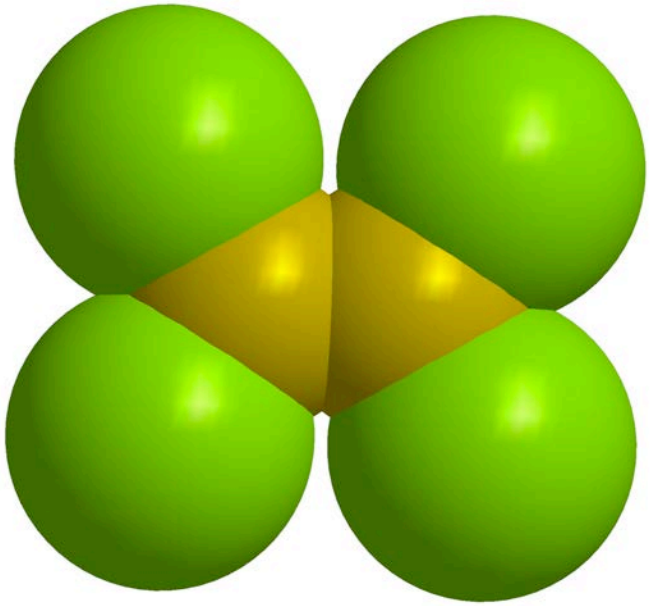


B_2Cl_4 0 ωB97x-D

- Zero-point correction= 0.013347 (Hartree/Particle)
- Thermal correction to Energy= 0.019517
- Thermal correction to Enthalpy= 0.020461
- Thermal correction to Gibbs Free Energy= -0.017768
- Sum of electronic and zero-point Energies= -1890.665098
- Sum of electronic and thermal Energies= -1890.658928
- Sum of electronic and thermal Enthalpies= -1890.657984
- Sum of electronic and thermal Free Energies= -1890.696213

- B2Cl40WB

- 0 1
- B 0.00000000 0.00000000 0.86172100
- B 0.00000000 0.00000000 -0.86172100
- Cl 0.00000000 -1.50209800 1.75747200
- Cl 0.00000000 1.50209800 1.75747200
- Cl 0.00000000 1.50209800 -1.75747200
- Cl 0.00000000 -1.50209800 -1.75747200

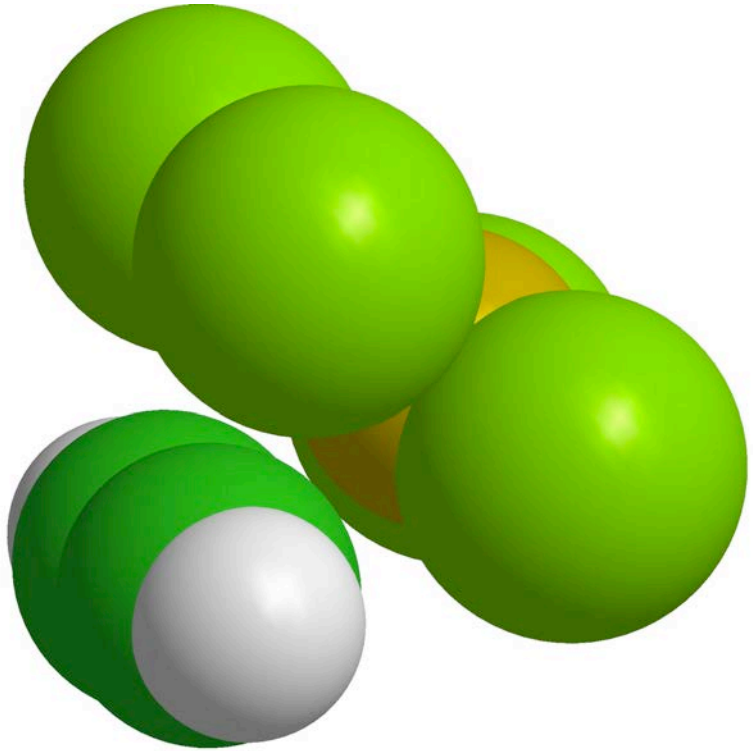


B_2Cl_4 Ethyne VdW ωB97X-D

- Zero-point correction= 0.041233 (Hartree/Particle)
- Thermal correction to Energy= 0.051821
- Thermal correction to Enthalpy= 0.052765
- Thermal correction to Gibbs Free Energy= 0.001688
- Sum of electronic and zero-point Energies= -1967.965541
- Sum of electronic and thermal Energies= -1967.954953
- Sum of electronic and thermal Enthalpies= -1967.954009
- Sum of electronic and thermal Free Energies= -1968.005086

- B2Cl4AVW

- 0 1
- C 0.00037300 0.59628200 2.61309500
- B -0.85994000 0.00035900 -0.43202600
- Cl -1.76262800 1.50344300 -0.46647700
- Cl -1.76170800 -1.50286000 -0.48257600
- C -0.00180600 -0.60207100 2.60979900
- B 0.86022000 0.00068700 -0.43188300
- Cl 1.76201700 1.50390800 -0.48008900
- Cl 1.76293000 -1.50241400 -0.46777100
- H 0.00148500 1.66125000 2.61978100
- H -0.00468900 -1.66705700 2.60991500

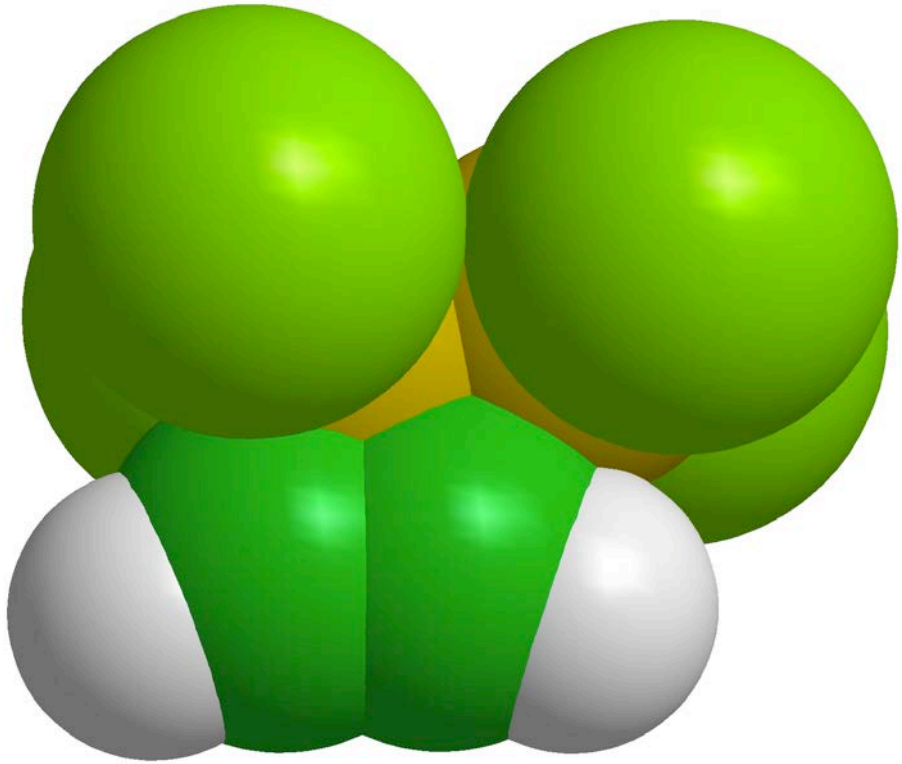


B_2Cl_4 Ethyne TS ωB97X-D

- Zero-point correction= 0.042353 (Hartree/Particle)
- Thermal correction to Energy= 0.051560
- Thermal correction to Enthalpy= 0.052504
- Thermal correction to Gibbs Free Energy= 0.006118
- Sum of electronic and zero-point Energies= -1967.940533
- Sum of electronic and thermal Energies= -1967.931327
- Sum of electronic and thermal Enthalpies= -1967.930382
- Sum of electronic and thermal Free Energies= -1967.976769

- B2Cl4ATSW

- 0 1
- C -1.47242700 0.00001100 1.73546600
- C -0.24114200 -0.00002300 1.86313900
- B 0.93456900 -0.00001500 0.00524500
- B -0.85936300 0.00001000 0.16193700
- Cl -1.48105100 1.54782500 -0.63099600
- Cl -1.48114300 -1.54775500 -0.63101800
- Cl 1.82463700 1.49744700 -0.15647900
- Cl 1.82457800 -1.49751000 -0.15648800
- H -2.50431400 0.00001600 2.02306200
- H 0.73034400 -0.00004700 2.32408900

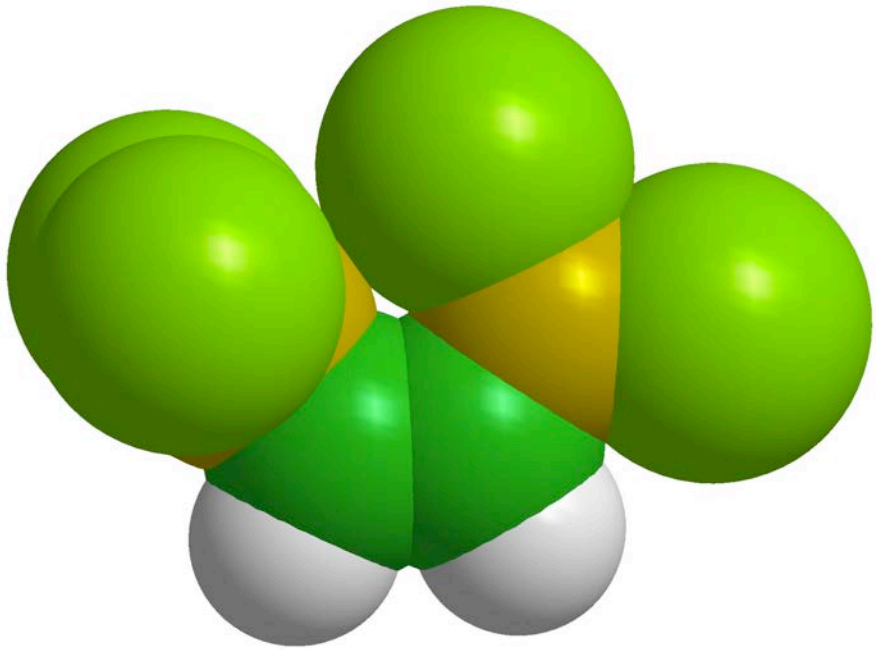


B_2Cl_4 Ethyne product ωB97X-D

- Zero-point correction= 0.046526 (Hartree/Particle)
- Thermal correction to Energy= 0.055780
- Thermal correction to Enthalpy= 0.056724
- Thermal correction to Gibbs Free Energy= 0.008751
- Sum of electronic and zero-point Energies= -1968.047819
- Sum of electronic and thermal Energies= -1968.038566
- Sum of electronic and thermal Enthalpies= -1968.037621
- Sum of electronic and thermal Free Energies= -1968.085594

- B2Cl4APW

- 0 1
- C -0.46670800 -0.01578700 1.54603000
- C 0.87179600 -0.01363900 1.45431500
- B 1.66897400 0.00036700 0.13482500
- B -1.54889300 -0.00553800 0.42210300
- Cl -2.25394900 1.51198600 -0.10383500
- Cl -2.24618600 -1.51412200 -0.13877100
- Cl 3.42453100 -0.00325600 0.16394300
- Cl 0.86534500 0.02024200 -1.43398900
- H -0.90135600 -0.02694900 2.54943500
- H 1.44481600 -0.02307600 2.37894800

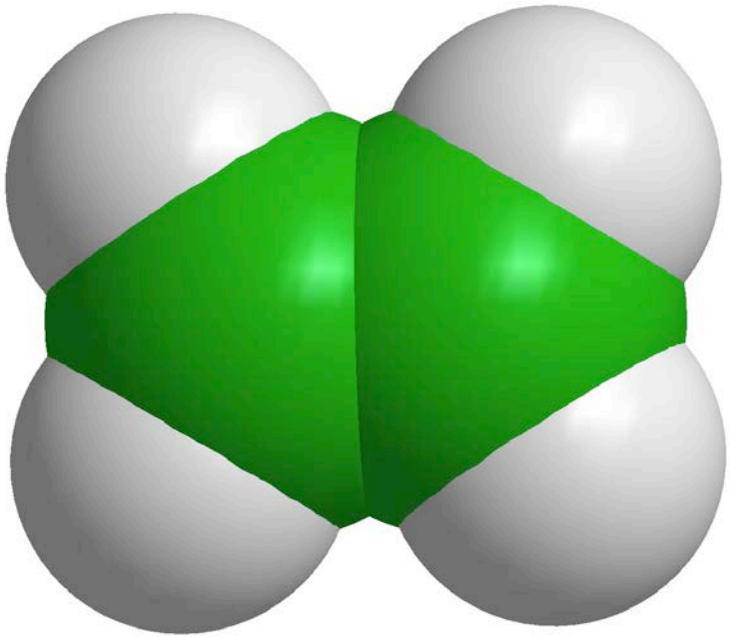


Ethylene B3LYP

Zero-point correction= 0.050809 (Hartree/Particle)
Thermal correction to Energy= 0.053851
Thermal correction to Enthalpy= 0.054795
Thermal correction to Gibbs Free Energy= 0.029941
Sum of electronic and zero-point Energies= -78.563170
Sum of electronic and thermal Energies= -78.560128
Sum of electronic and thermal Enthalpies= -78.559183
Sum of electronic and thermal Free Energies= -78.584038

0 1

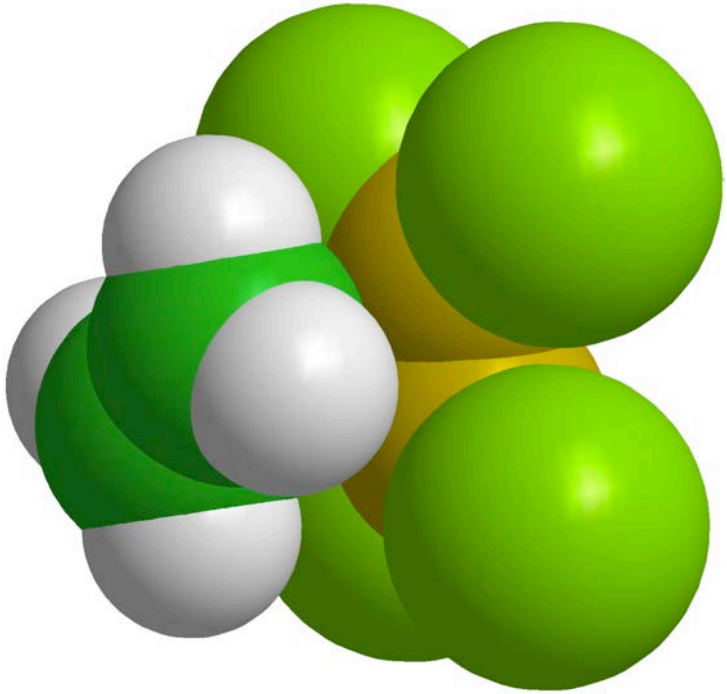
C	0.00000000	0.00000000	0.66347000
C	0.00000000	0.00000000	-0.66347000
H	0.00000000	0.92252000	1.23460000
H	0.00000000	-0.92252000	1.23460000
H	0.00000000	-0.92252000	-1.23460000
H	0.00000000	0.92252000	-1.23460000



B_2Cl_4 Ethene VdW B3LYP

- Zero-point correction= 0.064889 (Hartree/Particle)
- Thermal correction to Energy= 0.076998
- Thermal correction to Enthalpy= 0.077942
- Thermal correction to Gibbs Free Energy= 0.021515
- Sum of electronic and zero-point Energies= -1969.317618
- Sum of electronic and thermal Energies= -1969.305509
- Sum of electronic and thermal Enthalpies= -1969.304565
- Sum of electronic and thermal Free Energies= -1969.360992

- 0 1
- C -0.45281800 0.4744084.64570 2.80701300
- H -1.51406200 0.24908700 2.81834600
- B -0.85575500 -0.03944800 -0.54105700
- Cl -1.82281600 1.40819700 -0.78739000
- Cl -1.69380500 -1.57535500 -0.36873300
- C 0.46573800 -0.48798600 2.80273500
- H 0.19243700 -1.53770200 2.80564600
- B 0.85317500 0.04215700 -0.54344800
- Cl 1.69193800 1.57715200 -0.36655700
- Cl 1.81935800 -1.40439500 -0.79965600
- H 1.52703100 -0.26270300 2.80825000
- H -0.17950700 1.52410900 2.81149600

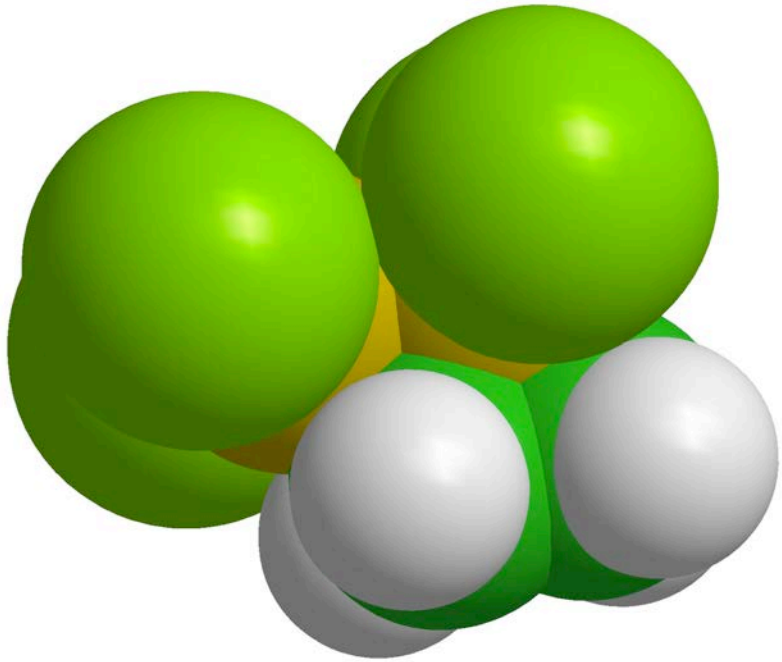


B_2Cl_4 Ethene TS B3LYP

Zero-point correction= 0.067017 (Hartree/Particle)
Thermal correction to Energy= 0.075560
Thermal correction to Enthalpy= 0.076504
Thermal correction to Gibbs Free Energy= 0.032260
Sum of electronic and zero-point Energies= -1969.283452
Sum of electronic and thermal Energies= -1969.274909
Sum of electronic and thermal Enthalpies= -1969.273965
Sum of electronic and thermal Free Energies= -1969.318209

0 1

C	1.58322500	-0.42570000	1.68695100
H	2.29783000	0.30045500	2.01396500
C	0.21396700	-0.01735100	1.79306000
B	-0.92177000	0.11328200	0.08139400
Cl	-2.06098500	-1.23046000	-0.03484900
Cl	-1.56845300	1.71244800	-0.24642600
H	-0.51004900	-0.75297100	2.12880000
H	-0.00274500	1.01826600	2.03262800
B	0.93202300	-0.14723400	0.13484400
Cl	1.69339000	1.38381000	-0.56129900
Cl	1.08974500	-1.64723900	-0.92556800
H	1.76770100	-1.45318900	1.92176200

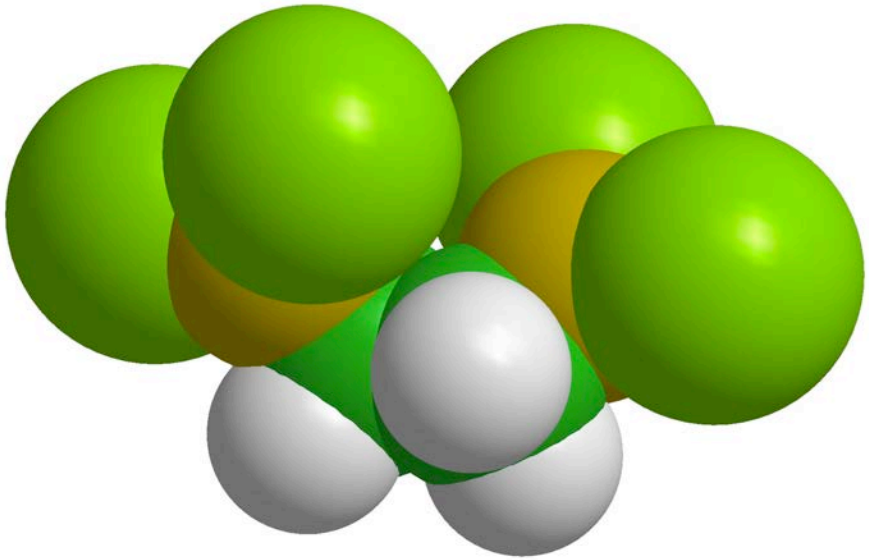


B_2Cl_4 Ethene gauche P B3LYP

- Zero-point correction= 0.068417 (Hartree/Particle)
- Thermal correction to Energy= 0.078205
- Thermal correction to Enthalpy= 0.079149
- Thermal correction to Gibbs Free Energy= 0.028678
- Sum of electronic and zero-point Energies= -1969.374955
- Sum of electronic and thermal Energies= -1969.365167
- Sum of electronic and thermal Enthalpies= -1969.364223
- Sum of electronic and thermal Free Energies= -1969.414693

- B2Cl4EPF

- 0 1
- C 0.71885200 0.27382500 1.38744100
- H 0.72076700 1.36935000 1.41205800
- B 1.68589200 -0.18509900 0.24828200
- Cl 1.29772400 -1.51492400 -0.84686400
- Cl 3.25990000 0.59247500 0.06440900
- C -0.71897300 -0.27471500 1.38716700
- H -1.22149300 0.01325400 2.32348500
- B -1.68585200 0.18506800 0.24822000
- Cl -1.29746600 1.51509000 -0.84646000
- Cl -3.26010800 -0.59217100 0.06419600
- H -0.72087800 -1.37025000 1.41091900
- H 1.22126400 -0.01485400 2.32360100

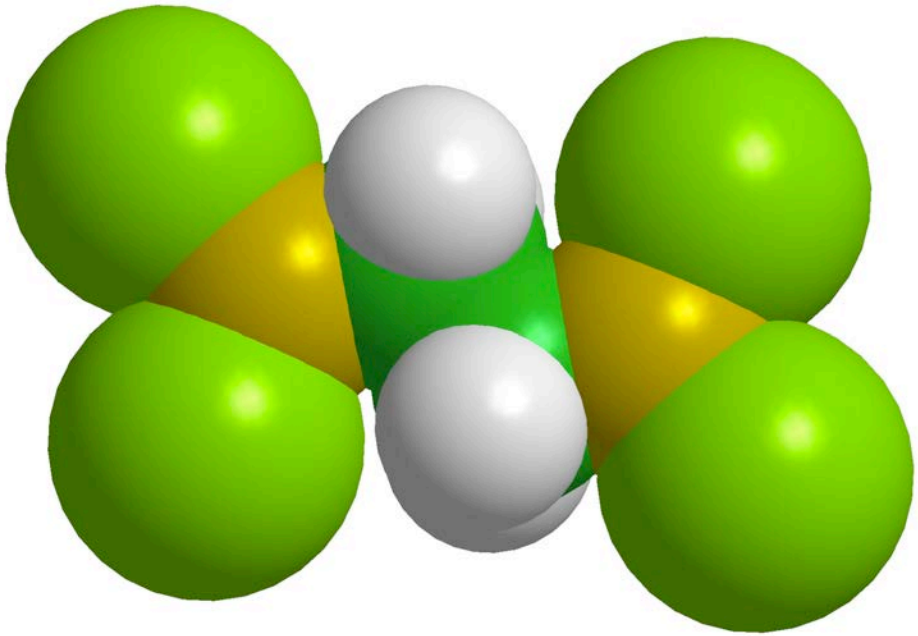


B_2Cl_4 Ethene trans-product B3LYP

- Zero-point correction= 0.068190 (Hartree/Particle)
- Thermal correction to Energy= 0.078187
- Thermal correction to Enthalpy= 0.079131
- Thermal correction to Gibbs Free Energy= 0.027765
- Sum of electronic and zero-point Energies= -1969.375129
- Sum of electronic and thermal Energies= -1969.365132
- Sum of electronic and thermal Enthalpies= -1969.364188
- Sum of electronic and thermal Free Energies= -1969.415554

- B2Cl4EP1F

- 0 1
- C 0.56168000 -0.52498100 0.00005300
- H 0.45850000 -1.19984900 0.86075100
- B 2.03985600 -0.01791300 0.00003500
- Cl 2.46757100 1.69368100 -0.00033900
- Cl 3.36299800 -1.18935200 0.00030200
- C -0.56166800 0.52498800 0.00008600
- H -0.45853100 1.19977400 -0.86069500
- B -2.03982600 0.01788600 0.00002700
- Cl -2.46761000 -1.69368100 -0.00033500
- Cl -3.36297300 1.18935700 0.00029900
- H -0.45846900 1.19981300 0.86080700
- H 0.45851900 -1.19972000 -0.86075900



C_2H_4 M06-2x

- Zero-point correction= 0.051356 (Hartree/Particle)
- Thermal correction to Energy= 0.054386
- Thermal correction to Enthalpy= 0.055330
- Thermal correction to Gibbs Free Energy= 0.029840
- Sum of electronic and zero-point Energies= -78.511071
- Sum of electronic and thermal Energies= -78.508041
- Sum of electronic and thermal Enthalpies= -78.507097
- Sum of electronic and thermal Free Energies= -78.532587

- C2H4M06

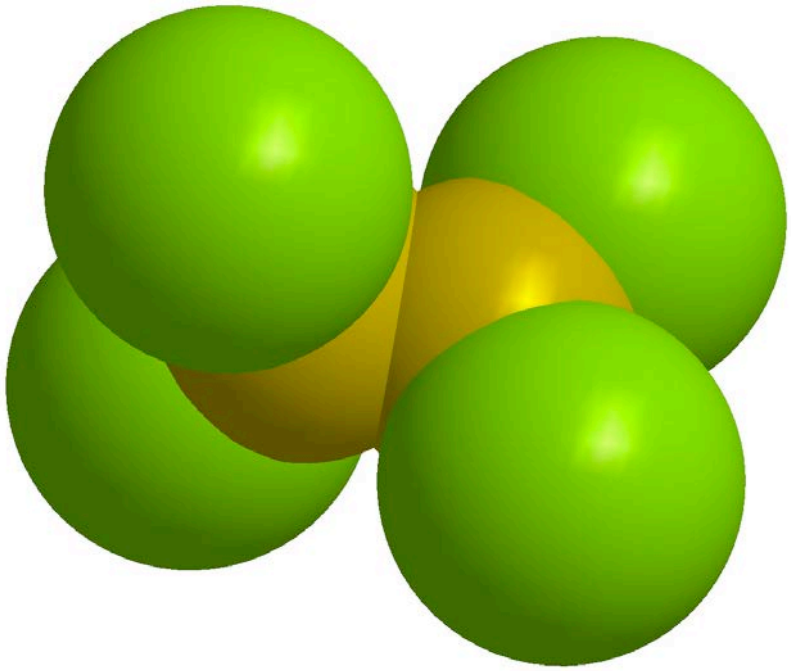
- 0 1
- C 0.00000000 0.66210400 0.00000000
- H 0.92333400 1.23037800 0.00000000
- H -0.92329300 1.23042100 0.00000000
- C 0.00000000 -0.66210400 0.00000000
- H -0.92333400 -1.23037800 0.00000000
- H 0.92329300 -1.23042100 0.00000000

B2Cl4 90 M06-2x

- Zero-point correction= 0.013309 (Hartree/Particle)
- Thermal correction to Energy= 0.020532
- Thermal correction to Enthalpy= 0.021476
- Thermal correction to Gibbs Free Energy= -0.021282
- Sum of electronic and zero-point Energies= -1890.620902
- Sum of electronic and thermal Energies= -1890.613680
- Sum of electronic and thermal Enthalpies= -1890.612735
- Sum of electronic and thermal Free Energies= -1890.655494

- B2Cl490 M06

- 0 1
- B 0.00000000 0.00000000 0.84191600
- B 0.00000000 0.00000000 -0.84191700
- Cl -1.50914500 -0.00005200 1.72099100
- Cl 1.50914500 0.00005200 1.72099100
- Cl 0.00000000 -1.50914500 -1.72099000
- Cl 0.00000000 1.50914500 -1.72099000

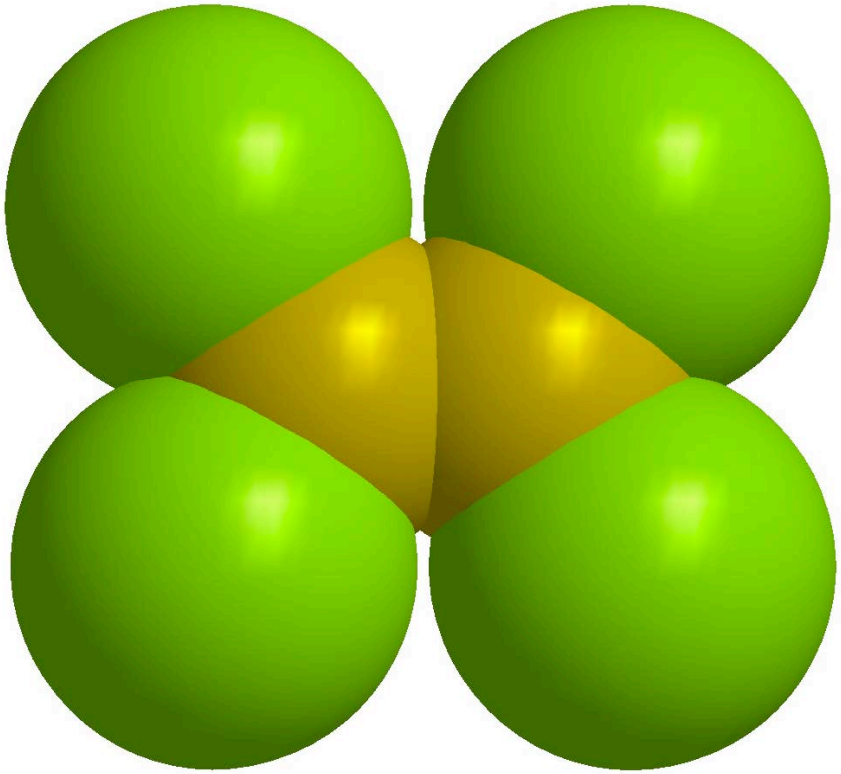


B_2Cl_4 0 M06-2x

- Zero-point correction= 0.013390 (Hartree/Particle)
- Thermal correction to Energy= 0.019552
- Thermal correction to Enthalpy= 0.020496
- Thermal correction to Gibbs Free Energy= -0.017691
- Sum of electronic and zero-point Energies= -1890.618505
- Sum of electronic and thermal Energies= -1890.612344
- Sum of electronic and thermal Enthalpies= -1890.611399
- Sum of electronic and thermal Free Energies= -1890.649586

- B2Cl40 M06

- 0 1
- B 0.00000000 0.00000000 0.85744400
- B 0.00000000 0.00000000 -0.85744400
- Cl 0.00000000 1.50071600 1.74623800
- Cl 0.00000000 -1.50071600 1.74623800
- Cl 0.00000000 1.50071600 -1.74623800
- Cl 0.00000000 -1.50071600 -1.74623800

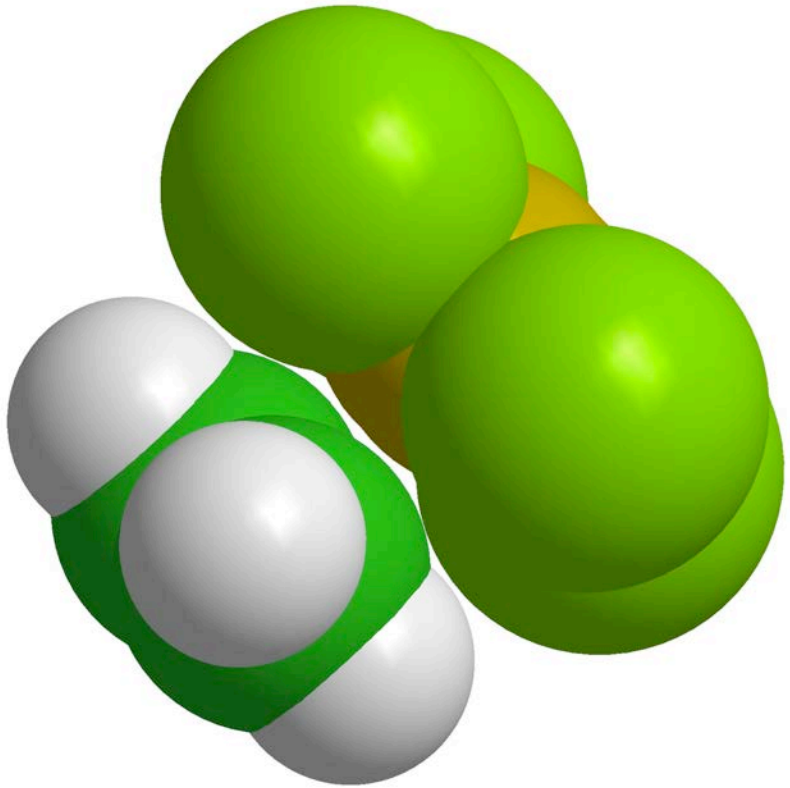


B_2Cl_4 C_2H_4 VdW M06-2x

- Zero-point correction= 0.066065 (Hartree/Particle)
- Thermal correction to Energy= 0.077672
- Thermal correction to Enthalpy= 0.078617
- Thermal correction to Gibbs Free Energy= 0.025299
- Sum of electronic and zero-point Energies= -1969.140420
- Sum of electronic and thermal Energies= -1969.128812
- Sum of electronic and thermal Enthalpies= -1969.127868
- Sum of electronic and thermal Free Energies= -1969.181186

- B2Cl4EtVM

- 0 1
- C 0.48627600 -0.46356400 2.48576800
- H 1.53425100 -0.18060600 2.49364200
- B 0.85115000 0.04882000 -0.47975100
- Cl 1.82755600 -1.39335500 -0.65802000
- Cl 1.66559900 1.59491900 -0.37404700
- C -0.47983600 0.45005500 2.48990000
- B -0.85249000 -0.04609800 -0.47889800
- Cl -1.66673300 -1.59268500 -0.37814300
- Cl -1.82906000 1.39669000 -0.65010100
- H -1.52774300 0.16684500 2.49808400
- H 0.26465900 -1.52552300 2.48087800
- H -0.25826700 1.51203100 2.49191200

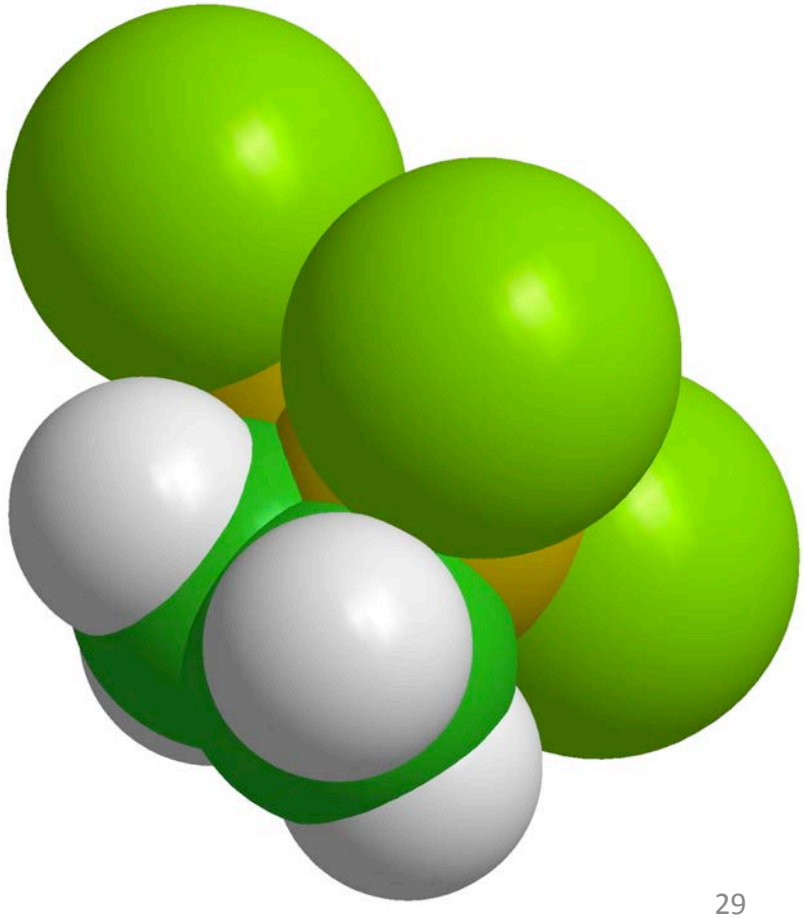


B_2Cl_4 C_2H_4 TS M06-2x

- Zero-point correction= 0.067876 (Hartree/Particle)
- Thermal correction to Energy= 0.077129
- Thermal correction to Enthalpy= 0.078073
- Thermal correction to Gibbs Free Energy= 0.031142
- Sum of electronic and zero-point Energies= -1969.120100
- Sum of electronic and thermal Energies= -1969.110848
- Sum of electronic and thermal Enthalpies= -1969.109904
- Sum of electronic and thermal Free Energies= -1969.156834

- B2Cl4EtTSM

- 0 1
- C 1.67000300 0.00004500 1.65223200
- H 2.21154300 0.92417200 1.79094300
- C 0.26702400 0.00000100 1.79976700
- B -0.92970100 -0.00001100 0.06013200
- Cl -1.82854700 -1.48902000 -0.12507100
- Cl -1.82859600 1.48897200 -0.12505100
- H -0.23304600 -0.92540500 2.06734600
- H -0.23310200 0.92537500 2.06735400
- B 0.90518800 0.00001300 0.11164200
- Cl 1.37393600 1.55558700 -0.73635200
- Cl 1.37399600 -1.55556100 -0.73631800
- H 2.21160000 -0.92404900 1.79094400

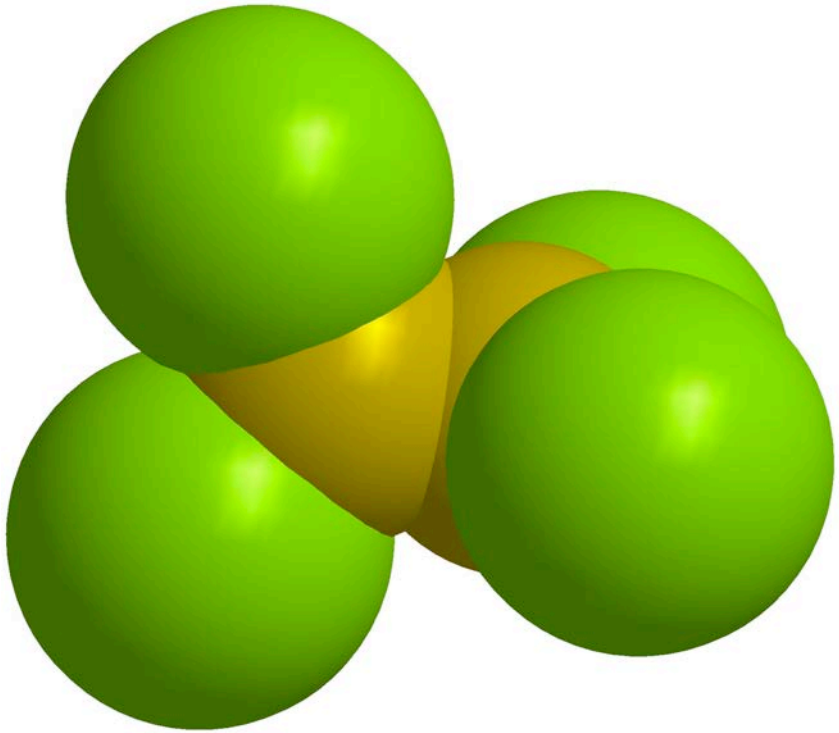


B_2Cl_4 90 B3LYP-D3

- Zero-point correction= 0.012988 (Hartree/Particle)
- Thermal correction to Energy= 0.020233
- Thermal correction to Enthalpy= 0.021177
- Thermal correction to Gibbs Free Energy= -0.021541
- Sum of electronic and zero-point Energies= -1890.762325
- Sum of electronic and thermal Energies= -1890.755080
- Sum of electronic and thermal Enthalpies= -1890.754135
- Sum of electronic and thermal Free Energies= -1890.796854

- B2Cl4B3D

- 0 1
- B 0.00000000 0.00000000 0.84331400
- B 0.00000000 0.00000000 -0.84331400
- Cl 1.51924800 -0.00005200 1.72652900
- Cl -1.51924800 0.00005200 1.72652900
- Cl 0.00000000 -1.51924800 -1.72652900
- Cl 0.00000000 1.51924800 -1.72652900

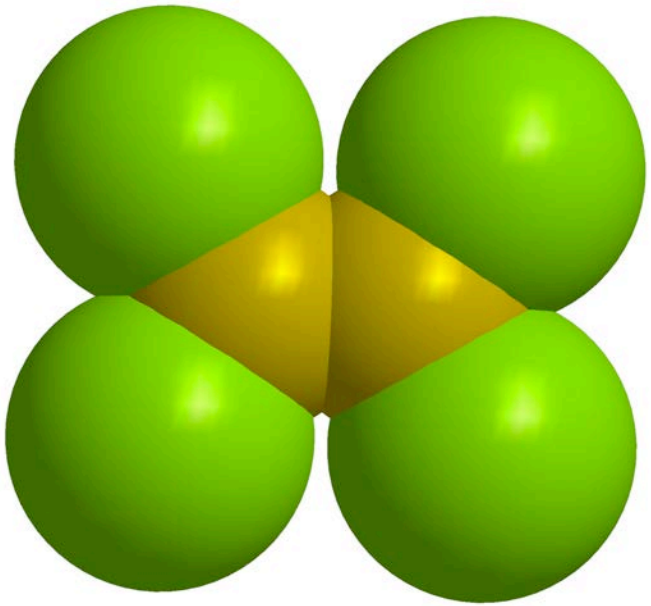


B_2Cl_4 0 B3LYP-D3

- Zero-point correction= 0.013064 (Hartree/Particle)
- Thermal correction to Energy= 0.019250
- Thermal correction to Enthalpy= 0.020194
- Thermal correction to Gibbs Free Energy= -0.018028
- Sum of electronic and zero-point Energies= -1890.758766
- Sum of electronic and thermal Energies= -1890.752580
- Sum of electronic and thermal Enthalpies= -1890.751635
- Sum of electronic and thermal Free Energies= -1890.789857

- B2Cl40D3

- 0 1
- B 0.00000000 0.00000000 0.86014100
- B 0.00000000 0.00000000 -0.86014100
- Cl 0.00000000 -1.50863100 1.75926800
- Cl 0.00000000 1.50863100 1.75926800
- Cl 0.00000000 1.50863100 -1.75926800
- Cl 0.00000000 -1.50863100 -1.75926800

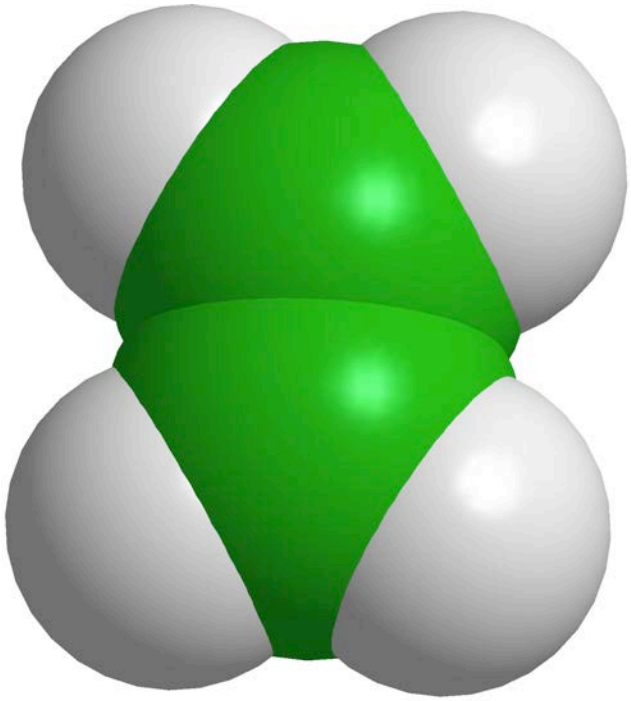


Ethene B3LYP-D3

- Zero-point correction= 0.050802 (Hartree/Particle)
- Thermal correction to Energy= 0.053841
- Thermal correction to Enthalpy= 0.054785
- Thermal correction to Gibbs Free Energy= 0.029279
- Sum of electronic and zero-point Energies= -78.564017
- Sum of electronic and thermal Energies= -78.560978
- Sum of electronic and thermal Enthalpies= -78.560033
- Sum of electronic and thermal Free Energies= -78.585539

- C2H4B3D

- 0 1
- C 0.00000000 0.66360900 0.00000000
- H 0.92282700 1.23482800 0.00000000
- H -0.92278200 1.23488200 0.00000000
- C 0.00000000 -0.66360900 0.00000000
- H -0.92282700 -1.23482800 0.00000000
- H 0.92278200 -1.23488200 0.00000000

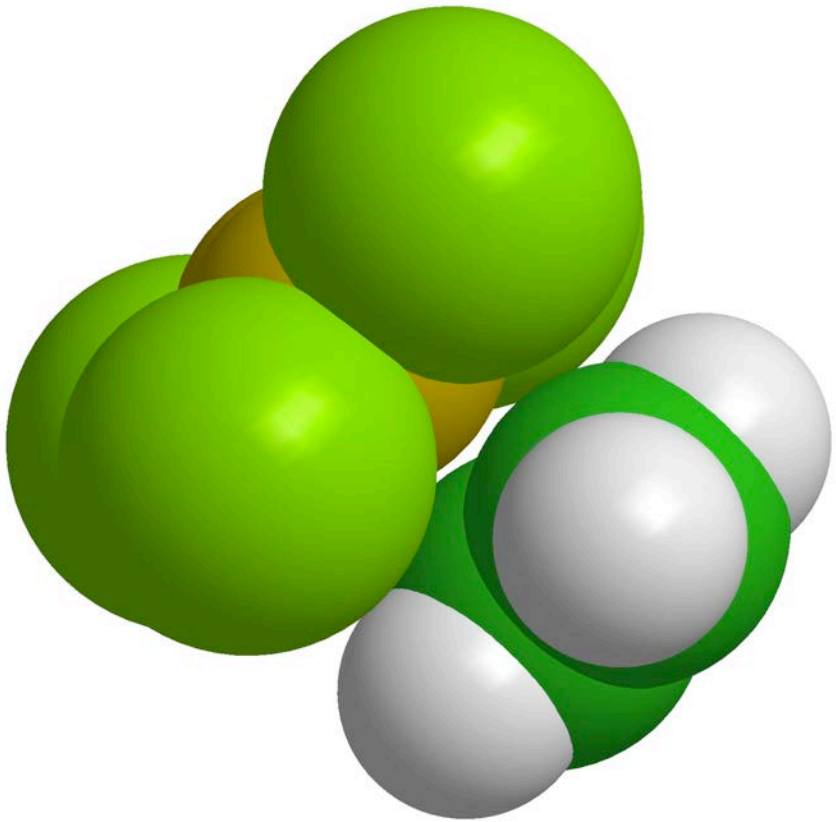


$B_2Cl_4.C_2H_4$ vdW B3LYP-D3

- Zero-point correction= 0.065244 (Hartree/Particle)
- Thermal correction to Energy= 0.077020
- Thermal correction to Enthalpy= 0.077964
- Thermal correction to Gibbs Free Energy= 0.024011
- Sum of electronic and zero-point Energies= -1969.332068
- Sum of electronic and thermal Energies= -1969.320292
- Sum of electronic and thermal Enthalpies= -1969.319348
- Sum of electronic and thermal Free Energies= -1969.373301

- B2Cl4EtVD3

- 0 1
- C -0.46559800 0.47591000 2.51152400
- H -1.52343200 0.23609200 2.51729900
- B -0.85463200 -0.04408300 -0.48105400
- Cl -1.83250200 1.40765500 -0.68444300
- Cl -1.68707000 -1.59231500 -0.35560000
- C 0.46654000 -0.47614200 2.51146800
- H 0.20630300 -1.52883400 2.50634800
- B 0.85442800 0.04410500 -0.48120500
- Cl 1.68688900 1.59235100 -0.35581300
- Cl 1.83230000 -1.40758200 -0.68493700
- H 1.52440000 -0.23642800 2.51695400
- H -0.20540200 1.52860500 2.50620700

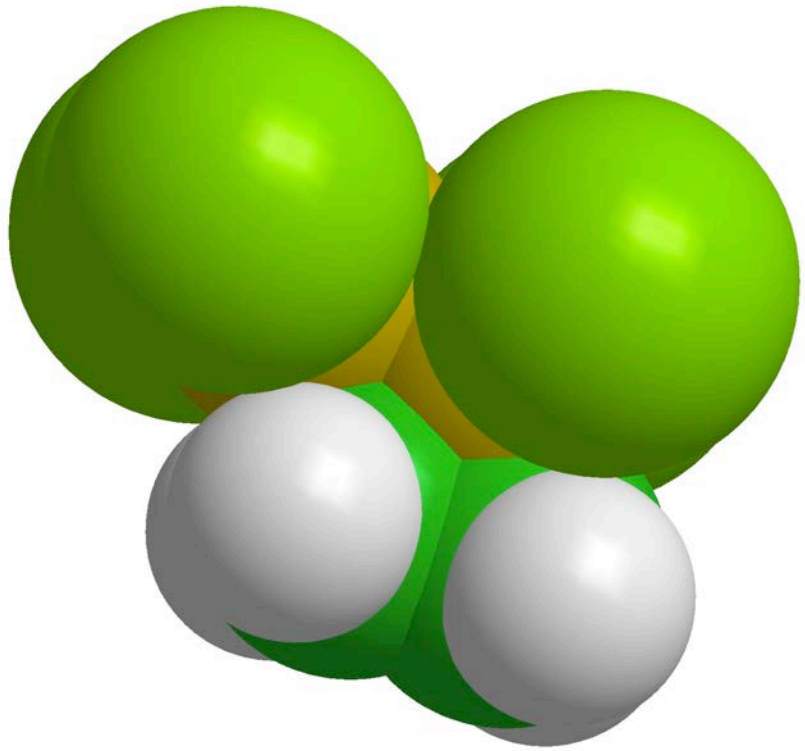


$B_2Cl_4.C_2H_4$ TS B3LYP-D3

- Zero-point correction= 0.067194 (Hartree/Particle)
- Thermal correction to Energy= 0.076517
- Thermal correction to Enthalpy= 0.077461
- Thermal correction to Gibbs Free Energy= 0.030440
- Sum of electronic and zero-point Energies= -1969.301573
- Sum of electronic and thermal Energies= -1969.292250
- Sum of electronic and thermal Enthalpies= -1969.291305
- Sum of electronic and thermal Free Energies= -1969.338326

- B2Cl4ETSD3

- 0 1
- C -1.63277700 0.00015100 1.68105800
- H -2.17172900 -0.91995700 1.85917200
- C -0.21945400 0.00015000 1.82045500
- B 0.94314700 -0.00005100 0.05951200
- Cl 1.84583400 1.49626700 -0.14451000
- Cl 1.84560000 -1.49650200 -0.14452100
- H 0.28118100 0.92324200 2.09219900
- H 0.28117700 -0.92289600 2.09236900
- B -0.92894500 0.00004800 0.12550800
- Cl -1.40985200 -1.56658100 -0.73296700
- Cl -1.40961400 1.56667100 -0.73311700
- H -2.17171400 0.92029400 1.85903900



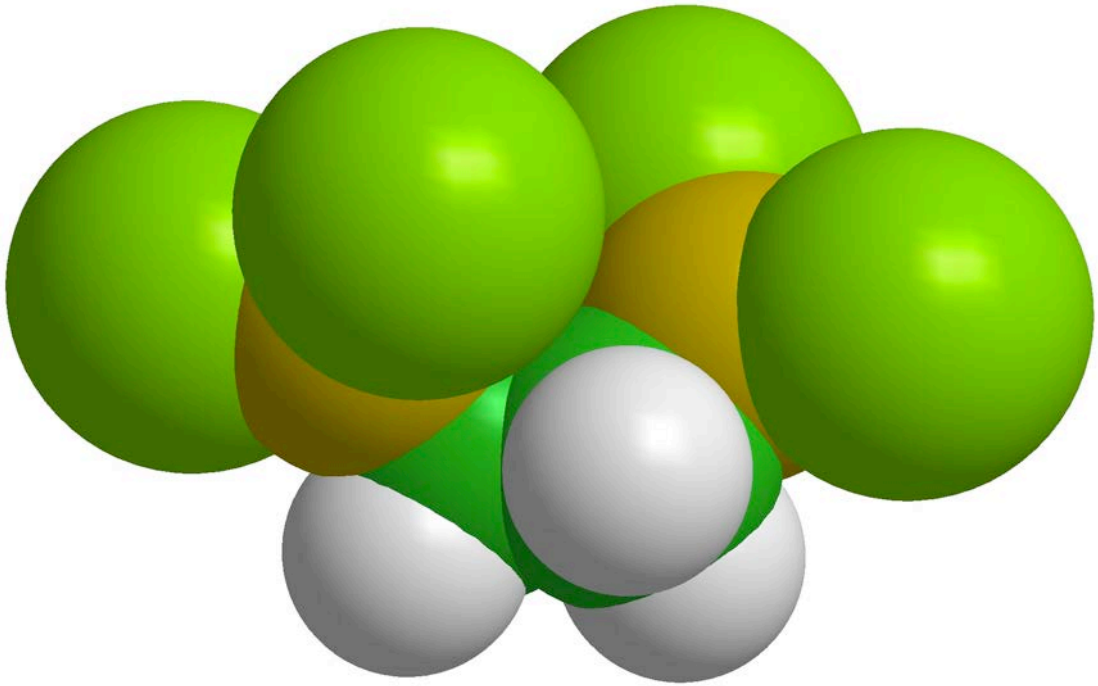
$B_2Cl_4.C_2H_4$ gauche Product B3LYP-D3

Zero-point correction= 0.068583 (Hartree/Particle)
Thermal correction to Energy= 0.078287
Thermal correction to Enthalpy= 0.079232
Thermal correction to Gibbs Free Energy= 0.029247
Sum of electronic and zero-point Energies= -1969.389224
Sum of electronic and thermal Energies= -1969.379519
Sum of electronic and thermal Enthalpies= -1969.378575
Sum of electronic and thermal Free Energies= -1969.428559

B2Cl4EPD3

0 1

C	0.72280400	0.26134400	1.42340300
H	0.74335400	1.35629700	1.45485300
B	1.65407800	-0.20029000	0.25597000
Cl	1.19939000	-1.50477000	-0.84629100
Cl	3.23725200	0.54979800	0.04495700
C	-0.72294800	-0.26224800	1.42317000
H	-1.23425500	0.04628700	2.34724200
B	-1.65411100	0.20013800	0.25595000
Cl	-1.19911500	1.50499500	-0.84573500
Cl	-3.23744500	-0.54951500	0.04457900
H	-0.74349800	-1.35722400	1.45387700
H	1.23403200	-0.04782900	2.34730800

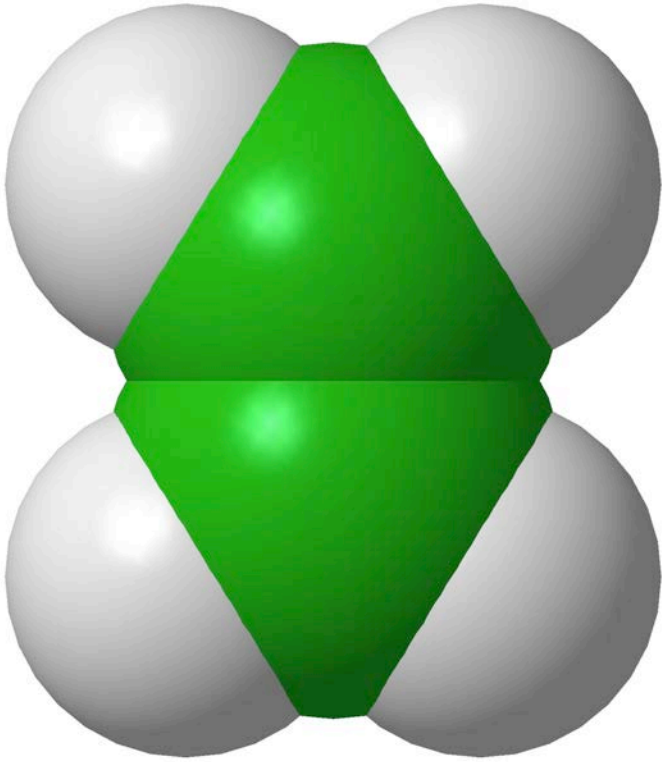


C_2H_4 ωB97X-D

- Zero-point correction= 0.051211 (Hartree/Particle)
- Thermal correction to Energy= 0.054246
- Thermal correction to Enthalpy= 0.055190
- Thermal correction to Gibbs Free Energy= 0.029693
- Sum of electronic and zero-point Energies= -78.528293
- Sum of electronic and thermal Energies= -78.525259
- Sum of electronic and thermal Enthalpies= -78.524315
- Sum of electronic and thermal Free Energies= -78.549812

- C2H4W

- 0 1
- C 0.00000000 0.66217400 0.00000000
- H 0.92415800 1.23108600 0.00000000
- H -0.92411900 1.23112700 0.00000000
- C 0.00000000 -0.66217400 0.00000000
- H -0.92415800 -1.23108600 0.00000000
- H 0.92411900 -1.23112700 0.00000000

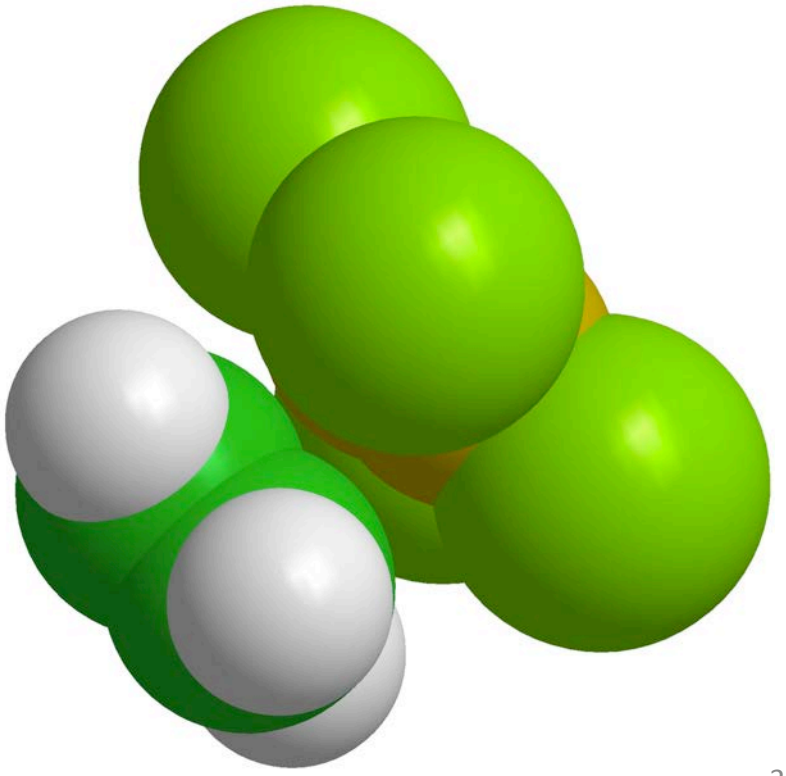


B_2Cl_4 C_2H_4 vdW ωB97X-D

- Zero-point correction= 0.065671 (Hartree/Particle)
- Thermal correction to Energy= 0.077531
- Thermal correction to Enthalpy= 0.078476
- Thermal correction to Gibbs Free Energy= 0.023938
- Sum of electronic and zero-point Energies= -1969.202994
- Sum of electronic and thermal Energies= -1969.191134
- Sum of electronic and thermal Enthalpies= -1969.190190
- Sum of electronic and thermal Free Energies= -1969.244727

- B2Cl4EtVW

- 0 1
- C -0.45829400 0.48025300 2.57291400
- H -1.51960300 0.25254600 2.58144200
- B -0.85738600 -0.04238800 -0.49274800
- Cl -1.82701200 1.40478900 -0.69983600
- Cl -1.68972000 -1.58169700 -0.36593500
- C 0.45911500 -0.48050500 2.57280300
- H 0.18413400 -1.53014100 2.57196800
- B 0.85722500 0.04243700 -0.49297400
- Cl 1.68959500 1.58173600 -0.36625500
- Cl 1.82679800 -1.40472200 -0.70043600
- H 1.52042800 -0.25279900 2.58089500
- H -0.18331500 1.52988900 2.57185400

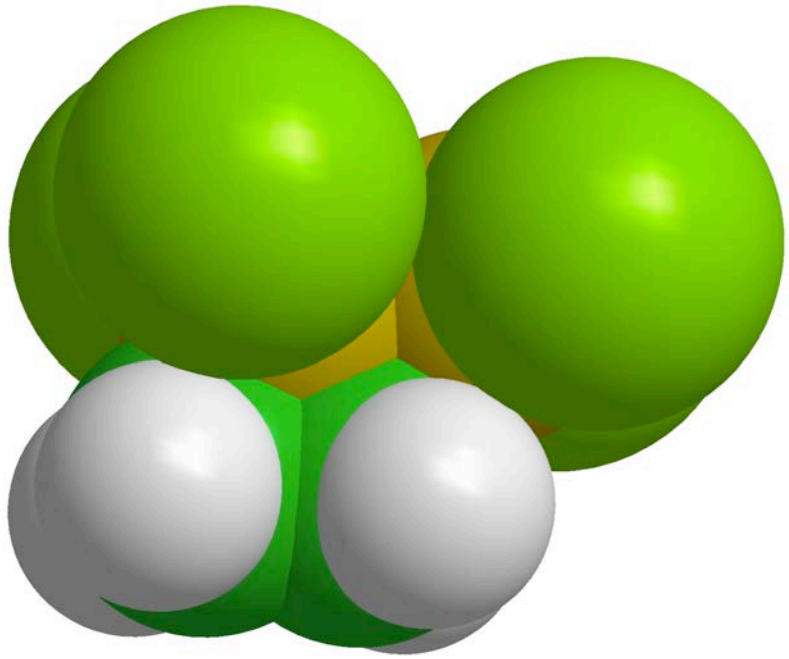


B_2Cl_4 C_2H_4 TS ωB97X-D

- Zero-point correction= 0.068073 (Hartree/Particle)
- Thermal correction to Energy= 0.077316
- Thermal correction to Enthalpy= 0.078260
- Thermal correction to Gibbs Free Energy= 0.031563
- Sum of electronic and zero-point Energies= -1969.177689
- Sum of electronic and thermal Energies= -1969.168446
- Sum of electronic and thermal Enthalpies= -1969.167502
- Sum of electronic and thermal Free Energies= -1969.214200

- B2Cl4ETSW

- 0 1
- C 1.65258100 0.00000900 1.66474000
- H 2.19448200 0.92242000 1.81975600
- C 0.25120000 -0.00000100 1.81993200
- B -0.93387800 -0.00000200 0.05515900
- Cl -1.83889800 -1.49070900 -0.13387500
- Cl -1.83890700 1.49070000 -0.13387100
- H -0.25067200 -0.92465200 2.08666600
- H -0.25068500 0.92464200 2.08666900
- B 0.91117100 0.00000200 0.11525300
- Cl 1.39193300 1.55751000 -0.73592200
- Cl 1.39194500 -1.55750400 -0.73591600
- H 2.19449600 -0.92239400 1.81975500

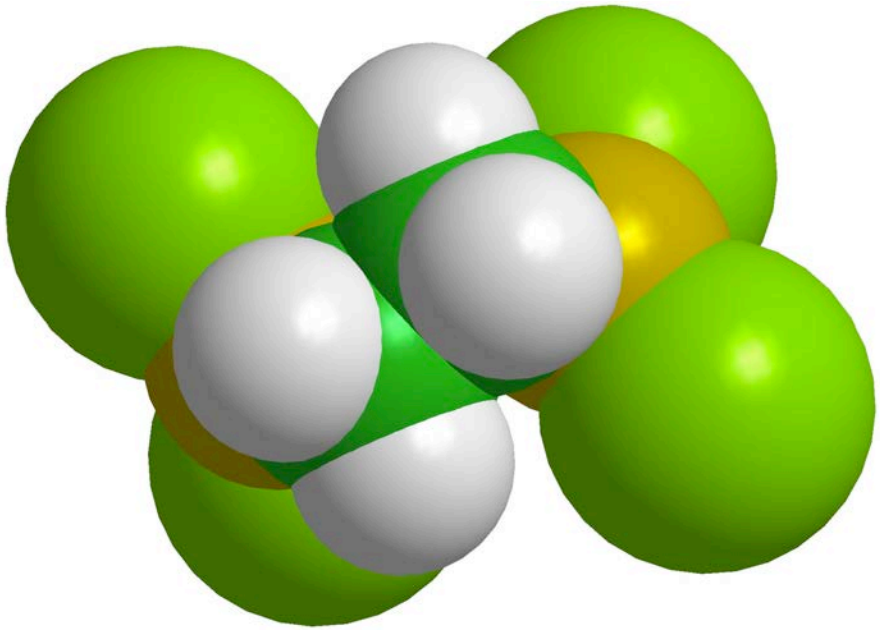


Ethylene B_2Cl_4 gauche product ωB97X-D

- Zero-point correction= 0.069126 (Hartree/Particle)
- Thermal correction to Energy= 0.078859
- Thermal correction to Enthalpy= 0.079803
- Thermal correction to Gibbs Free Energy= 0.029694
- Sum of electronic and zero-point Energies= -1969.266558
- Sum of electronic and thermal Energies= -1969.256825
- Sum of electronic and thermal Enthalpies= -1969.255881
- Sum of electronic and thermal Free Energies= -1969.305989

- B2Cl4EtPW

- 0 1
- C -0.72058400 -0.25813600 1.42749000
- H -1.23187600 0.06453000 2.34636600
- B -1.65083600 0.19790700 0.25640900
- Cl -3.22288400 -0.55835700 0.03278500
- Cl -1.20941800 1.50751400 -0.83661000
- C 0.72111100 0.26110400 1.42668500
- H 1.23270000 -0.05913500 2.34623100
- B 1.65100000 -0.19747200 0.25631400
- Cl 1.20809100 -1.50764600 -0.83541700
- Cl 3.22389900 0.55681500 0.03197900
- H -0.74550400 -1.35248700 1.47289000
- H 0.74597200 1.35558200 1.46932300



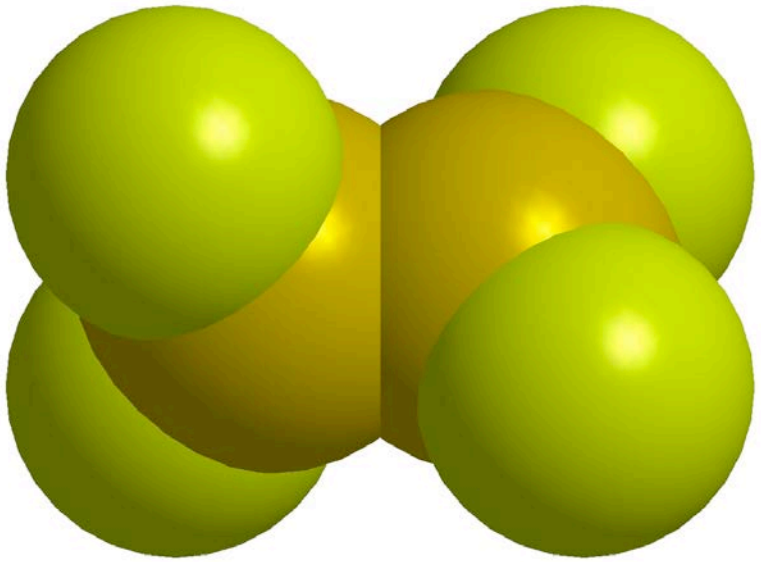
B3LYP B_2F_4, 90˚

Zero-point correction= 0.018962 (Hartree/Particle)
Thermal correction to Energy= 0.024084
Thermal correction to Enthalpy= 0.025029
Thermal correction to Gibbs Free Energy= -0.009231
Sum of electronic and zero-point Energies= -449.411059
Sum of electronic and thermal Energies= -449.405936
Sum of electronic and thermal Enthalpies= -449.404992
Sum of electronic and thermal Free Energies= -449.439251

B2F490

0 1

B	0.00000000	0.00000000	-0.85465400
B	0.00000000	0.00000000	0.85465400
F	-0.78973300	0.80452100	-1.54933400
F	0.78973300	-0.80452100	-1.54933400
F	0.78973300	0.80452100	1.54933400
F	-0.78973300	-0.80452100	1.54933400

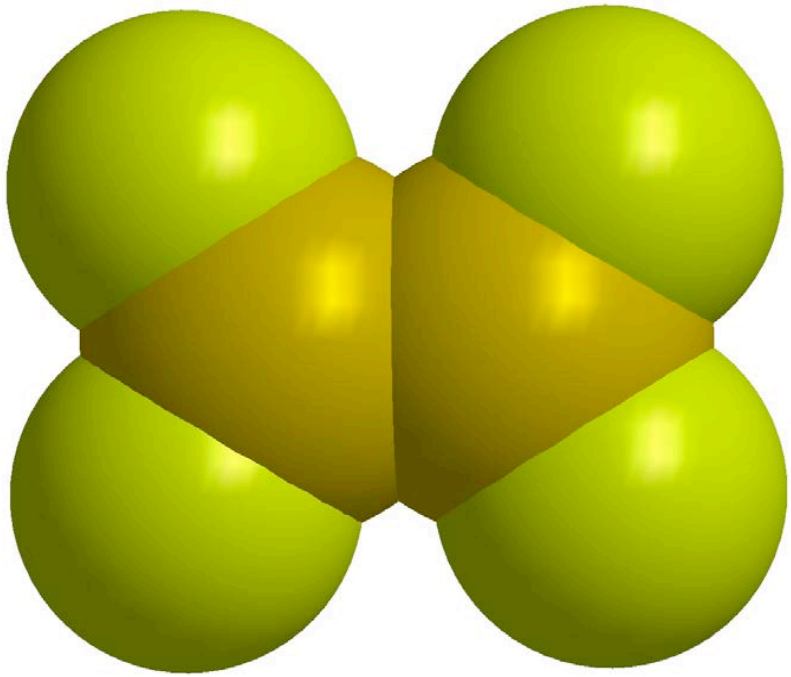


B3LYP B_2F_4 0°

Zero-point correction= 0.019083 (Hartree/Particle)
Thermal correction to Energy= 0.025060
Thermal correction to Enthalpy= 0.026004
Thermal correction to Gibbs Free Energy= -0.011487
Sum of electronic and zero-point Energies= -449.411248
Sum of electronic and thermal Energies= -449.405271
Sum of electronic and thermal Enthalpies= -449.404327
Sum of electronic and thermal Free Energies= -449.441818

0 1

B	0.00000000	0.00000000	0.85725000
B	0.00000000	0.00000000	-0.85725000
F	0.00000000	1.12767000	-1.54725000
F	0.00000000	-1.12767000	-1.54725000
F	0.00000000	-1.12767000	1.54725000
F	0.00000000	1.12767000	1.54725000

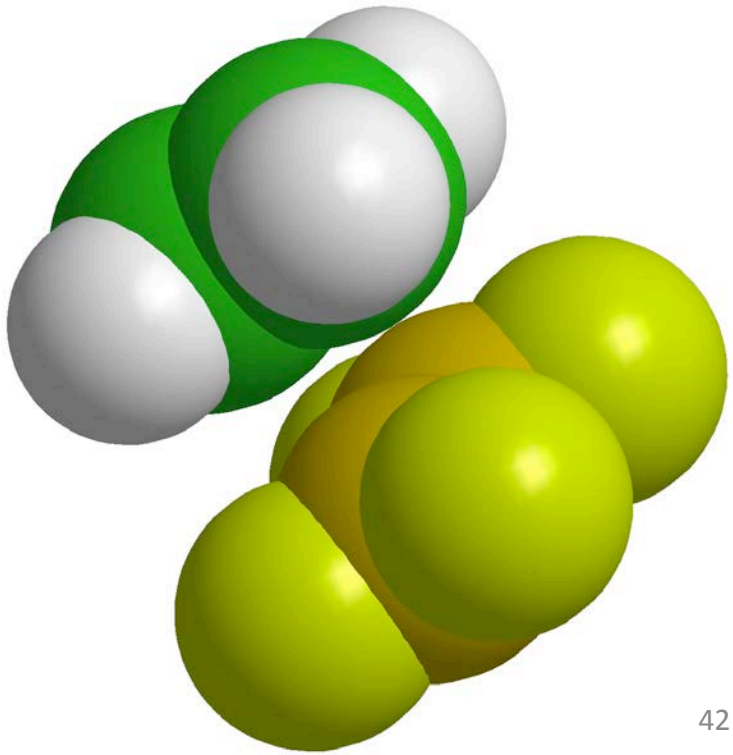


B_2F_4 ethylene VdW B3LYP

- Zero-point correction= 0.071049 (Hartree/Particle)
- Thermal correction to Energy= 0.081849
- Thermal correction to Enthalpy= 0.082793
- Thermal correction to Gibbs Free Energy= 0.031587
- Sum of electronic and zero-point Energies= -527.978610
- Sum of electronic and thermal Energies= -527.967810
- Sum of electronic and thermal Enthalpies= -527.966866
- Sum of electronic and thermal Free Energies= -528.018072

- B2F4EV

- 0 1
- C -2.33414300 -0.04528500 -0.66212500
- H -2.32591600 -0.96926700 -1.23063600
- B 0.82832800 -0.83780600 -0.00078000
- C -2.32957700 -0.04170100 0.66876400
- H -2.31727900 -0.96257000 1.24225700
- B 0.78933700 0.86790400 -0.00156500
- H -2.34846700 0.88206100 1.23738400
- H -2.35688100 0.87545600 -1.23547100
- F 0.77822500 1.56526100 1.12590100
- F 0.77587500 1.56424700 -1.12961000
- F 0.85263700 -1.53378000 1.12728200
- F 0.84243500 -1.53509000 -1.12820000

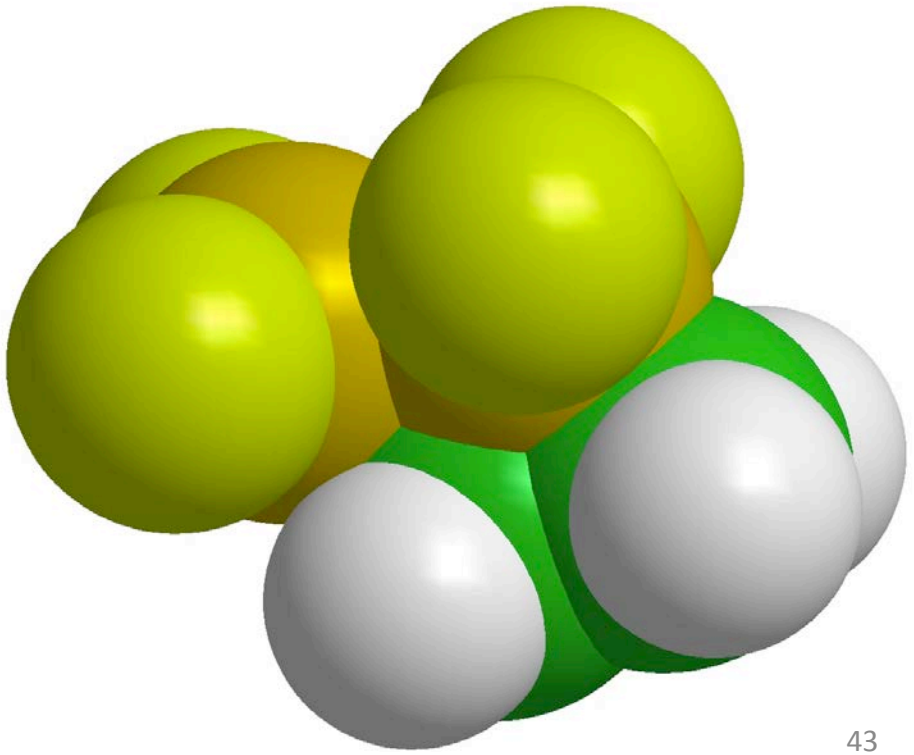


TS ethylene B_2F_4 B3LYP

Zero-point correction= 0.072502 (Hartree/Particle)
Thermal correction to Energy= 0.080675
Thermal correction to Enthalpy= 0.081619
Thermal correction to Gibbs Free Energy= 0.039367
Sum of electronic and zero-point Energies= -527.929042
Sum of electronic and thermal Energies= -527.920870
Sum of electronic and termal Enthalpies= -527.919926
Sum of electronic and thermal Free Energies= -527.962178

0 1

C	1.82027900	-0.00096000	0.97430000
C	0.49788900	-0.00124000	1.44719000
B	-1.09642100	-0.00001800	0.02385000
B	0.68262900	0.00033000	-0.37371000
F	-1.78106000	1.13061200	0.05663000
F	-1.78102200	-1.13072800	0.05501000
F	0.85244800	-1.18631000	-1.07408000
F	0.85254000	1.18827000	-1.07184000
H	2.37560000	0.92593900	0.94209000
H	0.06129800	-0.92191900	1.82241000
H	0.06149000	0.91893100	1.82391000
H	2.37541800	-0.92791100	0.94050000

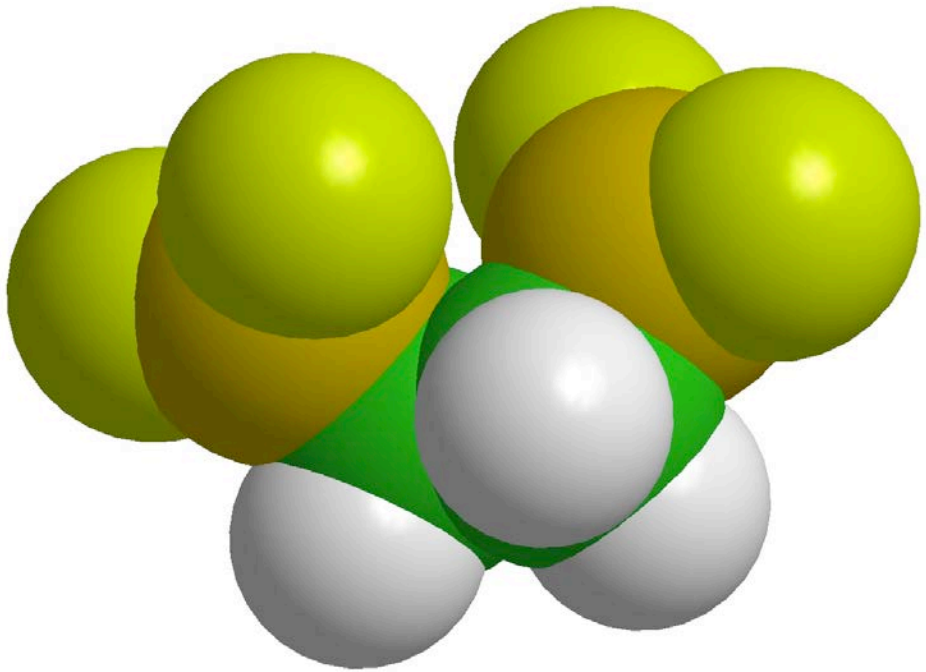


B_2F_4 ethylene product B3LYP

Zero-point correction= 0.074777 (Hartree/Particle)
Thermal correction to Energy= 0.083319
Thermal correction to Enthalpy= 0.084264
Thermal correction to Gibbs Free Energy= 0.039225
Sum of electronic and zero-point Energies= -528.039378
Sum of electronic and thermal Energies= -528.030836
Sum of electronic and thermal Enthalpies= -528.029892
Sum of electronic and thermal Free Energies= -528.074930

0 1

C	0.71393200	1.19308200	-0.28901300
B	1.59195700	-0.02873000	0.12444800
C	-0.71394700	1.19308500	0.28901000
B	-1.59197900	-0.02871000	-0.12448400
F	-2.79953500	-0.23435300	0.38581800
F	-1.18020900	-0.91603400	-1.02769900
F	1.18024700	-0.91599500	1.02774600
F	2.79952000	-0.23434700	-0.38584600
H	0.69285500	1.23582400	-1.38440700
H	-1.25241900	2.10257500	-0.00900500
H	-0.69286500	1.23579300	1.38440500
H	1.25241700	2.10255600	0.00903200

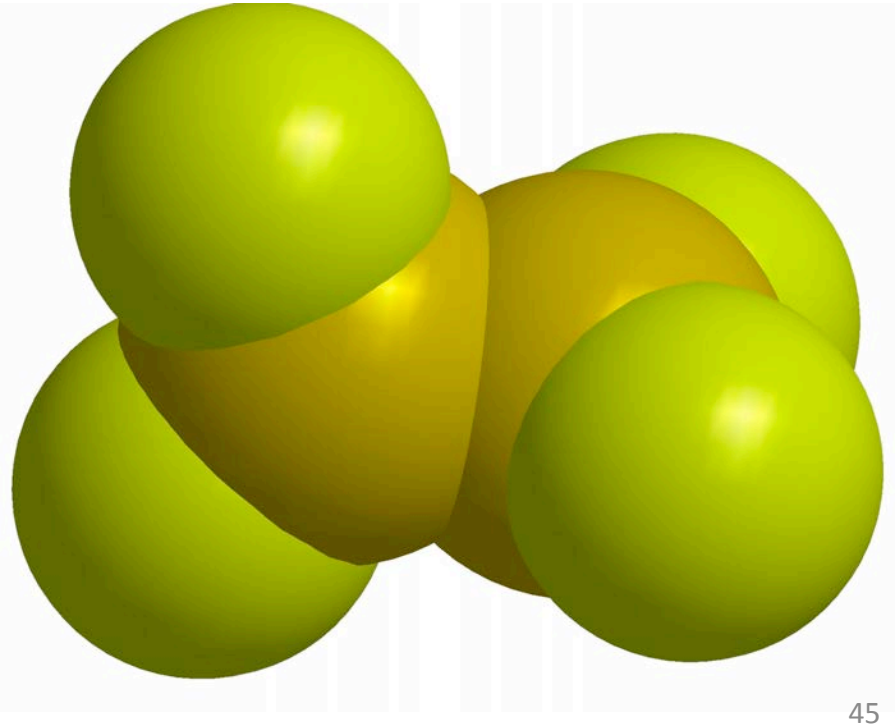


B_2F_4 90 WB97

- Zero-point correction= 0.019048 (Hartree/Particle)
- Thermal correction to Energy= 0.025075
- Thermal correction to Enthalpy= 0.026019
- Thermal correction to Gibbs Free Energy= -0.011817
- Sum of electronic and zero-point Energies= -449.276598
- Sum of electronic and thermal Energies= -449.270572
- Sum of electronic and thermal Enthalpies= -449.269627
- Sum of electronic and thermal Free Energies= -449.307463

- B2F490W

- 0 1
- B 0.00000000 0.00000000 -0.85620000
- B 0.00000000 0.00000000 0.85620000
- F -0.79131100 0.80180100 -1.54932800
- F 0.79131100 -0.80180100 -1.54932800
- F 0.79131100 0.80180100 1.54932800
- F -0.79131100 -0.80180100 1.54932800

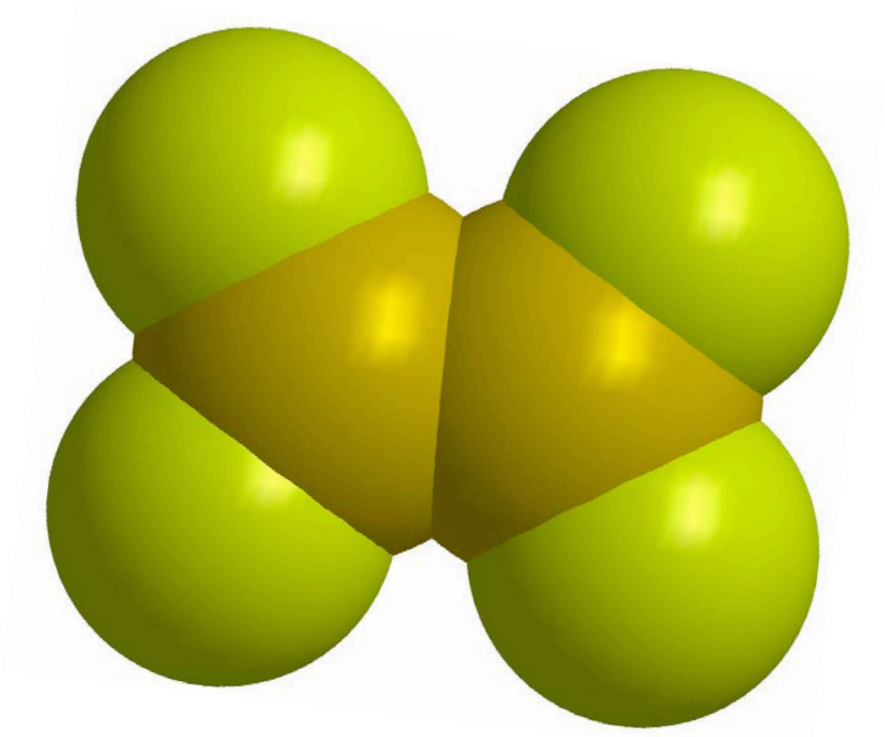


B_2F_4 0 deg WB97-xD

- Zero-point correction= 0.019143 (Hartree/Particle)
- Thermal correction to Energy= 0.025119
- Thermal correction to Enthalpy= 0.026063
- Thermal correction to Gibbs Free Energy= -0.011684
- Sum of electronic and zero-point Energies= -449.276821
- Sum of electronic and thermal Energies= -449.270845
- Sum of electronic and thermal Enthalpies= -449.269901
- Sum of electronic and thermal Free Energies= -449.307648

- B2F40W

- 0 1
- B 0.00000000 0.00000000 -0.85913300
- B 0.00000000 0.00000000 0.85913300
- F -0.00388400 1.12683000 -1.54764100
- F 0.00388400 -1.12683000 -1.54764100
- F 0.00388400 1.12683000 1.54764100
- F -0.00388400 -1.12683000 1.54764100

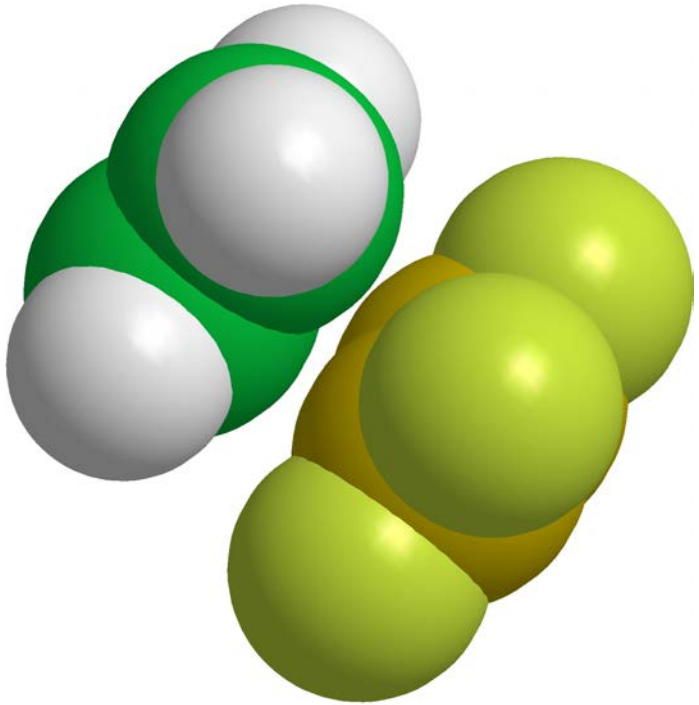


B_2F_4 C_2H_4 VdW WB97xD

- Zero-point correction= 0.071640 (Hartree/Particle)
- Thermal correction to Energy= 0.082325
- Thermal correction to Enthalpy= 0.083269
- Thermal correction to Gibbs Free Energy= 0.032574
- Sum of electronic and zero-point Energies= -527.813882
- Sum of electronic and thermal Energies= -527.803197
- Sum of electronic and thermal Enthalpies= -527.802253
- Sum of electronic and thermal Free Energies= -527.852948

- B2Cl4EVW1

- 0 1
- C -2.23666800 0.16287700 -0.65668900
- H -2.34608400 -0.79921600 -1.14621100
- B 0.68020000 -0.92490000 0.01004100
- C -2.21166800 0.27251300 0.66667800
- H -2.29692500 -0.59602100 1.31141300
- B 0.86605400 0.77357200 -0.01368100
- H -2.10705700 1.23508300 1.15639200
- H -2.15330300 1.03152100 -1.30153600
- F 0.95282200 1.47998700 1.10362600
- F 0.92972800 1.45148900 -1.14982100
- F 0.60458200 -1.60127900 1.14652100
- F 0.60865800 -1.63320400 -1.10719200

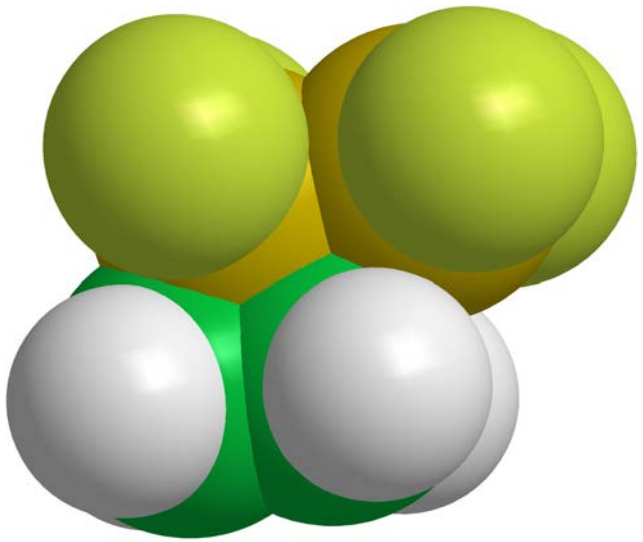


B_2F_4 C_2H_4 TS WB97xD

- Zero-point correction= 0.073200 (Hartree/Particle)
- Thermal correction to Energy= 0.081314
- Thermal correction to Enthalpy= 0.082258
- Thermal correction to Gibbs Free Energy= 0.040081
- Sum of electronic and zero-point Energies= -527.769726
- Sum of electronic and thermal Energies= -527.761612
- Sum of electronic and thermal Enthalpies= -527.760668
- Sum of electronic and thermal Free Energies= -527.802845

- B2F4TSW

- 0 1
- C 1.81044200 -0.00008500 0.97924800
- C 0.49454300 -0.00004500 1.44807100
- B -1.09623100 -0.00000200 0.01378300
- B 0.67438200 0.00001800 -0.37256500
- F -1.78291200 1.12872100 0.05155500
- F -1.78289900 -1.12873500 0.05148800
- F 0.86336800 -1.18627100 -1.06722500
- F 0.86339600 1.18639300 -1.06706900
- H 2.36283700 0.92829900 0.94059400
- H 0.05253700 -0.92195900 1.81504600
- H 0.05261700 0.92190300 1.81506000
- H 2.36276000 -0.92851100 0.94054600

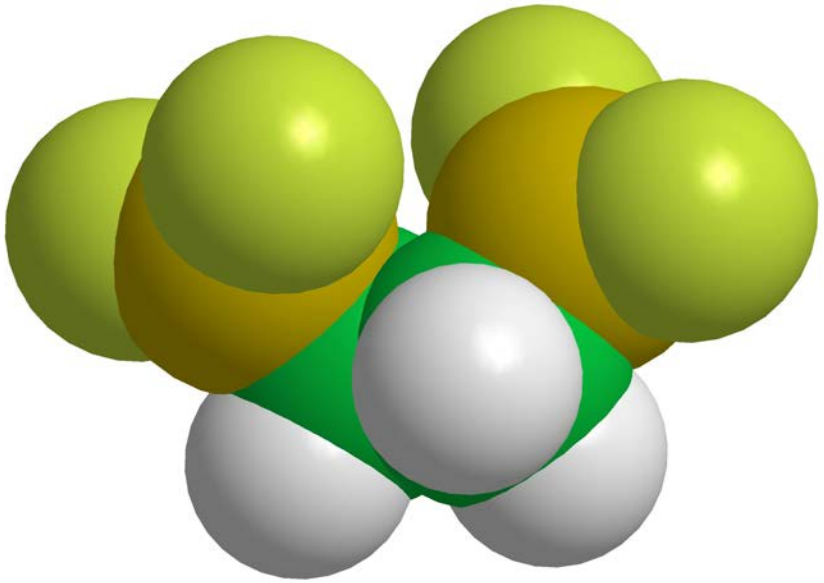


B_2F_4 C_2H_4 gauche-product WB97xD

- Zero-point correction= 0.075285 (Hartree/Particle)
- Thermal correction to Energy= 0.083815
- Thermal correction to Enthalpy= 0.084759
- Thermal correction to Gibbs Free Energy= 0.039805
- Sum of electronic and zero-point Energies= -527.881706
- Sum of electronic and thermal Energies= -527.873176
- Sum of electronic and thermal Enthalpies= -527.872232
- Sum of electronic and thermal Free Energies= -527.917186

- B2F4EtPW

- 0 1
- C 0.70928900 1.19121300 -0.29284400
- C -0.70959600 1.19120400 0.29179600
- B -1.58720700 -0.02985300 -0.12468900
- B 1.58723100 -0.02927100 0.12462100
- H 0.68231100 1.22565200 -1.38773200
- H -0.68250400 1.22604600 1.38668700
- H -1.25017300 2.09998600 -0.00077800
- H 1.24960800 2.10025800 -0.00053300
- F 2.79126800 -0.23794000 -0.38805400
- F 1.17671600 -0.90845800 1.03411700
- F -1.17563400 -0.91105000 -1.03175100
- F -2.79207400 -0.23708700 0.38668600

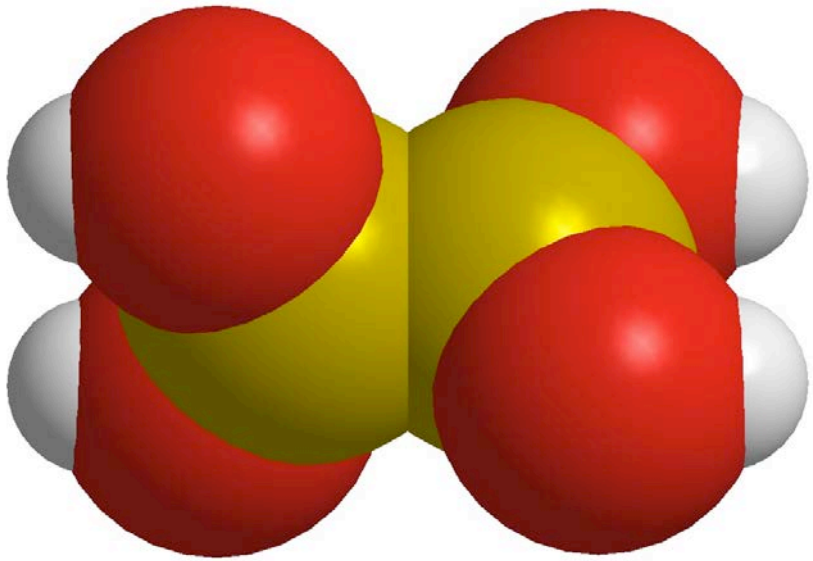


B3LYP $B_2(OH)_4$ 90

- Zero-point correction= 0.067729 (Hartree/Particle)
- Thermal correction to Energy= 0.074781
- Thermal correction to Enthalpy= 0.075725
- Thermal correction to Gibbs Free Energy= 0.035689
- Sum of electronic and zero-point Energies= -353.244516
- Sum of electronic and thermal Energies= -353.237464
- Sum of electronic and thermal Enthalpies= -353.236520
- Sum of electronic and thermal Free Energies= -353.276556

- B2OH490

- 0 1
- B -0.85570600 -0.00001600 0.00000500
- B 0.85568500 -0.00005000 -0.00006800
- O 1.51106600 0.84022900 -0.86317100
- O 1.51099100 -0.84037600 0.86304000
- O -1.51094500 0.86362300 0.83984800
- O -1.51110000 -0.86361700 -0.83973500
- H 2.47352300 0.80212400 -0.82309300
- H 2.47345200 -0.80134700 0.82386300
- H -2.47341200 0.82420900 0.80128100
- H -2.47355700 -0.82352900 -0.80159800

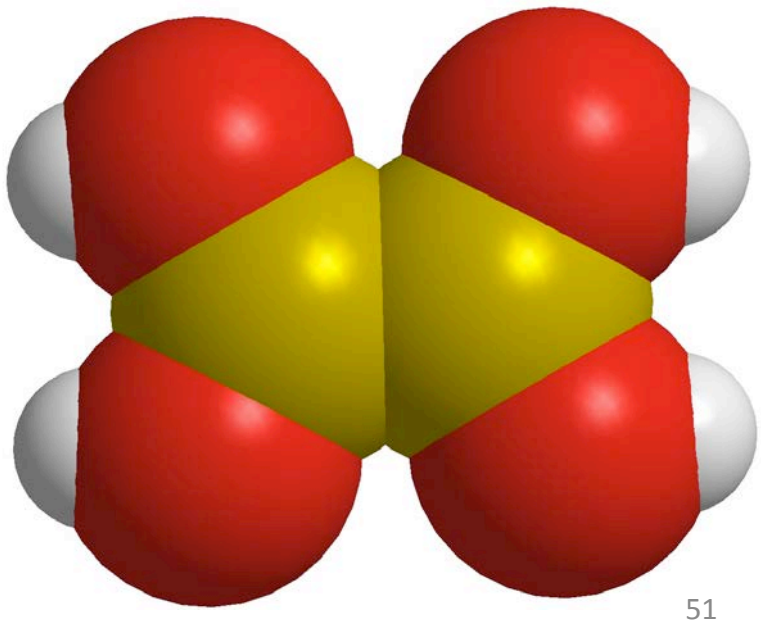


B3LYP $B_2(OH)_4$ 0

Zero-point correction= 0.067873 (Hartree/Particle)
Thermal correction to Energy= 0.073921
Thermal correction to Enthalpy= 0.074865
Thermal correction to Gibbs Free Energy= 0.038373
Sum of electronic and zero-point Energies= -353.243870
Sum of electronic and thermal Energies= -353.237823
Sum of electronic and thermal Enthalpies= -353.236878
Sum of electronic and thermal Free Energies= -353.273371

0 1

B	0.85768400	-0.00026800	-0.00003200
B	-0.85768300	-0.00026300	-0.00002400
O	-1.51232300	1.20383400	0.00081600
O	-1.51339900	-1.20376100	-0.00071300
O	1.51234400	1.20382200	-0.00083300
O	1.51337700	-1.20377600	0.00074400
H	-2.47440600	1.14715700	0.00053000
H	-2.47542900	-1.14628200	-0.00091800
H	2.47442700	1.14713900	-0.00024600
H	2.47540800	-1.14630800	0.00080300

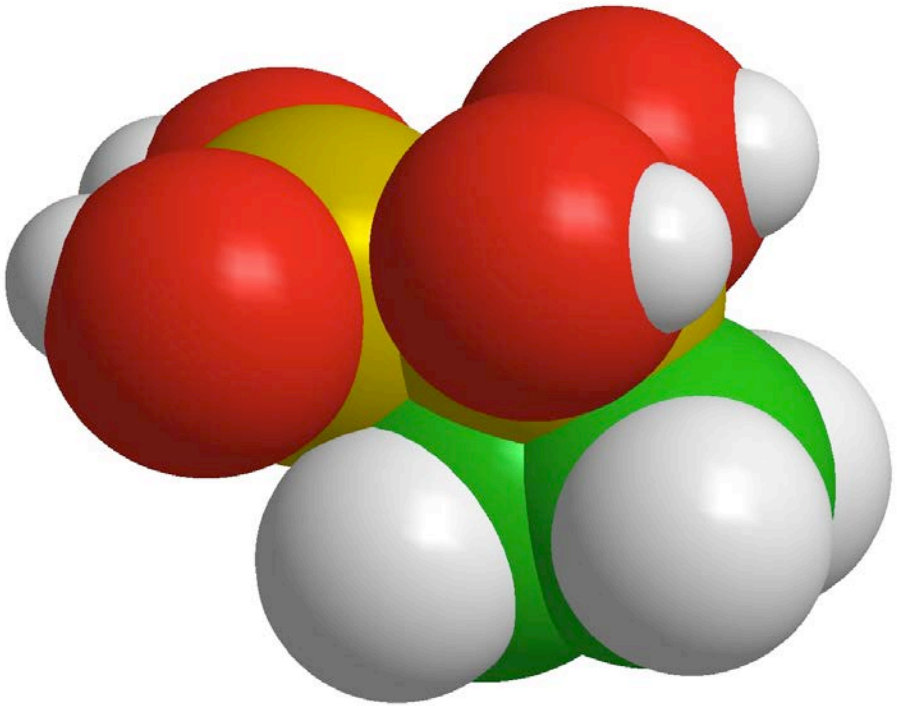


TS ethylene $B_2(OH)_4$ B3LYP

Zero-point correction= 0.120027 (Hartree/Particle)
Thermal correction to Energy= 0.128970
Thermal correction to Enthalpy= 0.129914
Thermal correction to Gibbs Free Energy= 0.086752
Sum of electronic and zero-point Energies= -431.743484
Sum of electronic and thermal Energies= -431.734541
Sum of electronic and thermal Enthalpies= -431.733597
Sum of electronic and thermal Free Energies= -431.776759

0 1

C	-1.81578200	-0.00009500	1.05367800
C	-0.47475600	-0.00010400	1.46124400
B	1.11179400	0.00000500	0.00660800
B	-0.68606000	0.00002800	-0.37723300
O	1.74824500	1.20635200	0.02784800
O	1.74826600	-1.20633400	0.02773000
O	-0.84234600	1.26366000	-1.04665000
O	-0.84228800	-1.26351300	-1.04683900
H	-2.37403700	-0.92622500	1.06987400
H	-0.02778700	0.91927900	1.82067800
H	-0.02776100	-0.91951900	1.82056300
H	-2.37407100	0.92601200	1.07001200
H	2.70951000	1.16365600	-0.01522200
H	2.70953000	-1.16361600	-0.01532100
H	-1.74794700	1.38488200	-1.34176900
H	-1.74789600	-1.38476100	-1.34192600

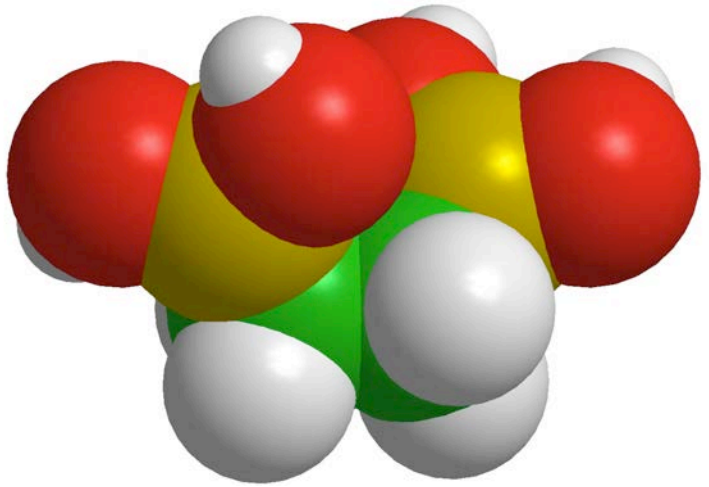


$B_2(OH)_4$ gauche product B3LYP

Zero-point correction= 0.124087 (Hartree/Particle)
Thermal correction to Energy= 0.133650
Thermal correction to Enthalpy= 0.134594
Thermal correction to Gibbs Free Energy= 0.087865
Sum of electronic and zero-point Energies= -431.869678
Sum of electronic and thermal Energies= -431.860115
Sum of electronic and thermal Enthalpies= -431.859170
Sum of electronic and thermal Free Energies= -431.905900

0 1

C	-0.72520600	1.22156000	0.22593200
C	0.70938600	1.21174200	-0.33911400
B	1.60053400	0.00794700	0.14314300
B	-1.59567900	-0.03675900	-0.15823900
O	-2.78201100	-0.35939000	0.45951400
O	-1.19064800	-0.85300900	-1.17743600
O	2.76171400	-0.26025200	-0.53756800
O	1.19572400	-0.70905100	1.24428800
H	-0.69314400	1.31074300	1.31939800
H	0.68611200	1.19912100	-1.43374100
H	1.22910200	2.14332200	-0.07501600
H	-1.25766900	2.12000100	-0.11955100
H	-3.00524400	0.23805300	1.17751900
H	-1.81161100	-1.57559200	-1.31998300
H	3.27846400	-0.99559500	-0.19613700
H	1.76640200	-1.44219000	1.49171200

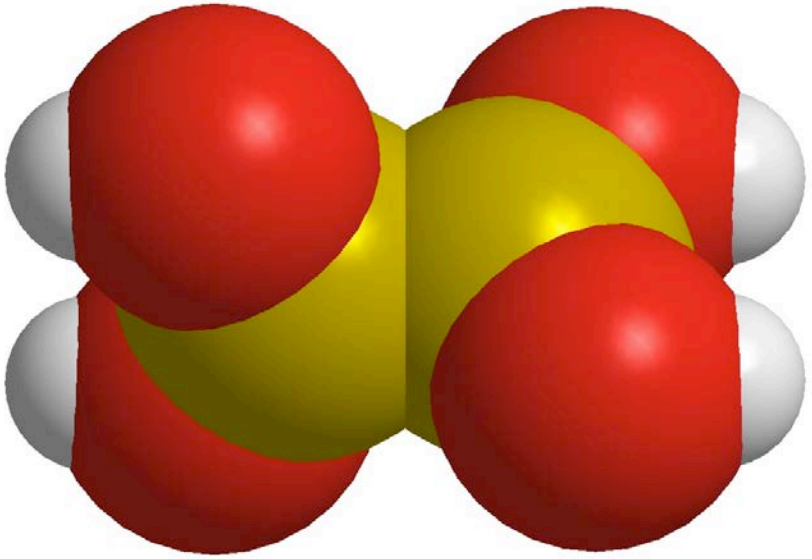


ωB97x-D B_2OH_4 90

- Zero-point correction= 0.068875 (Hartree/Particle)
- Thermal correction to Energy= 0.075898
- Thermal correction to Enthalpy= 0.076842
- Thermal correction to Gibbs Free Energy= 0.036941
- Sum of electronic and zero-point Energies= -353.122784
- Sum of electronic and thermal Energies= -353.115760
- Sum of electronic and thermal Enthalpies= -353.114816
- Sum of electronic and thermal Free Energies= -353.154717
-

- B2OH490WR

- 0 1
- B(Iso=11) 0.85600600 -0.00016400 -0.00024100
- B(Iso=11) -0.85600600 0.00008500 -0.00017400
- O -1.51278400 0.85323200 0.84748500
- O -1.51335800 -0.85301000 -0.84740400
- O 1.51284200 -0.85321400 0.84746900
- O 1.51330100 0.85302200 -0.84742600
- H -2.47007200 0.81291800 0.80775300
- H -2.47061400 -0.81248100 -0.80719000
- H 2.47012600 -0.81286800 0.80770000
- H 2.47055900 0.81258900 -0.80718600

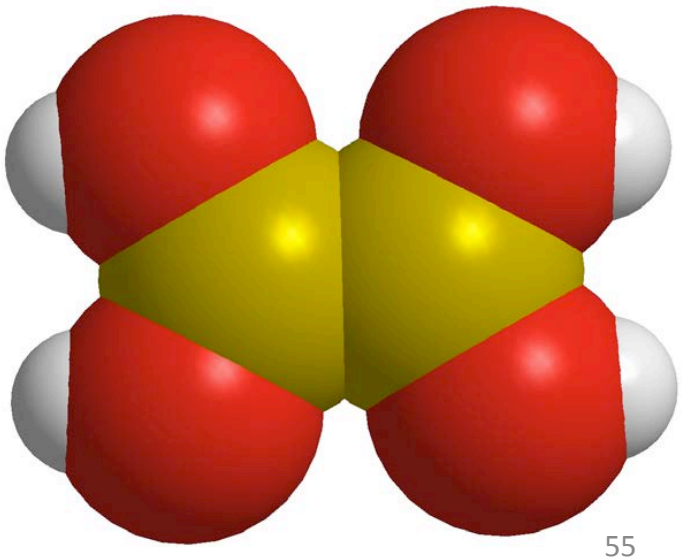


ωB97x-D B_2OH_4 0

- Zero-point correction= 0.069026 (Hartree/Particle)
- Thermal correction to Energy= 0.075048
- Thermal correction to Enthalpy= 0.075992
- Thermal correction to Gibbs Free Energy= 0.039548
- Sum of electronic and zero-point Energies= -353.122191
- Sum of electronic and thermal Energies= -353.116169
- Sum of electronic and thermal Enthalpies= -353.115225
- Sum of electronic and thermal Free Energies= -353.151668

- B2OH40W

- 0 1
- B 0.85855000 -0.00012000 0.00004400
- B -0.85855000 -0.00012000 -0.00007800
- O -1.51443000 1.20171500 0.00091200
- O -1.51488300 -1.20168800 -0.00103000
- O 1.51443200 1.20171400 -0.00085500
- O 1.51488200 -1.20168900 0.00098500
- H -2.47143500 1.14369400 0.00078200
- H -2.47186400 -1.14330100 -0.00105700
- H 2.47143600 1.14369200 -0.00062400
- H 2.47186200 -1.14330300 0.00097600



$B_2(OH)_4$ TS ωB97x-D

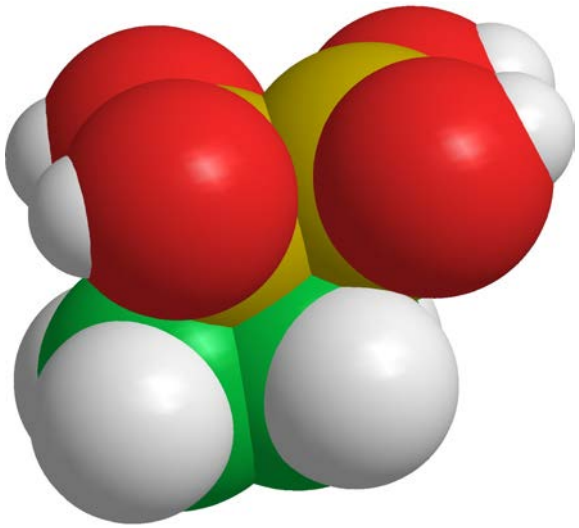
Zero-point correction= 0.122246 (Hartree/Particle)
Thermal correction to Energy= 0.131710
Thermal correction to Enthalpy= 0.132654
Thermal correction to Gibbs Free Energy= 0.088588
Sum of electronic and zero-point Energies= -431.597372
Sum of electronic and thermal Energies= -431.587908
Sum of electronic and thermal Enthalpies= -431.586964
Sum of electronic and thermal Free Energies= -431.631030

rwb97xd/6-311g(d,p)

B2OH4ETSW1

0 1

C	-1.81444600	-0.00000100	1.05520900
C	-0.48429500	-0.00000500	1.46408400
B	1.11109300	0.00000000	-0.00662800
B	-0.66419000	0.00000100	-0.37808300
O	1.75224400	1.20378700	0.02645600
O	1.75224500	-1.20378500	0.02645200
O	-0.84952200	1.26089700	-1.04151800
O	-0.84952200	-1.26089400	-1.04152100
H	-2.36908900	-0.92839900	1.05080500
H	-0.03065000	0.92148600	1.81157900
H	-0.03065300	-0.92150000	1.81157000
H	-2.36908600	0.92840000	1.05081200
H	2.70885400	1.15609800	0.00300700
H	2.70885500	-1.15609600	0.00300200
H	-1.75193100	1.35781000	-1.34096000
H	-1.75192800	-1.35780200	-1.34097200



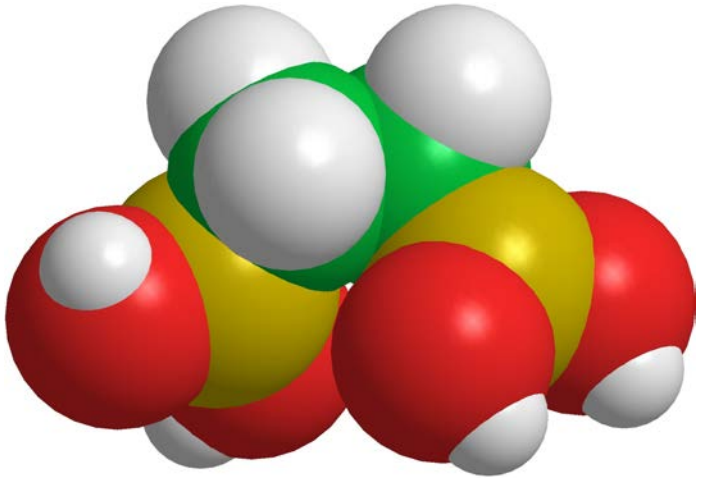
$B_2(OH)_4$ product ωB97x-D

Zero-point correction= 0.125554 (Hartree/Particle)
Thermal correction to Energy= 0.135080
Thermal correction to Enthalpy= 0.136024
Thermal correction to Gibbs Free Energy= 0.089587
Sum of electronic and zero-point Energies= -431.726360
Sum of electronic and thermal Energies= -431.716835
Sum of electronic and thermal Enthalpies= -431.715891
Sum of electronic and thermal Free Energies= -431.762327

B2OH4EPW

0 1

C	-0.71948300	1.23490100	0.28021400
C	0.71725100	1.24703000	-0.26354300
B	1.57011700	-0.00681200	0.15117400
B	-1.56315500	-0.01970900	-0.16762300
O	-2.73070900	-0.40811400	0.44248100
O	-1.15114400	-0.75851300	-1.23935900
O	2.75489100	-0.24076300	-0.49625800
O	1.10253100	-0.80505100	1.16655400
H	-0.70342500	1.28176100	1.37632500
H	0.70837800	1.30062200	-1.35710900
H	1.24715000	2.15008200	0.06608900
H	-1.25357800	2.13959300	-0.04221400
H	-2.94932200	0.13662300	1.19714100
H	-1.75146800	-1.48529500	-1.41389600
H	3.23871300	-1.01049700	-0.19831700
H	1.63758700	-1.57235400	1.36685800

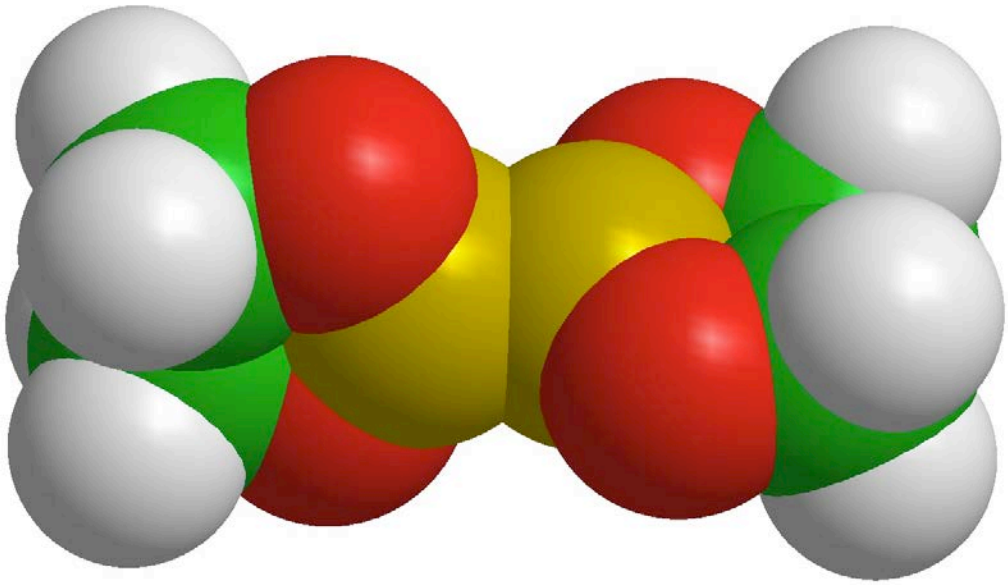


B3LYP $B_2(EG)_2$ 90

Zero-point correction= 0.139971 (Hartree/Particle)
Thermal correction to Energy= 0.149612
Thermal correction to Enthalpy= 0.150556
Thermal correction to Gibbs Free Energy= 0.101327
Sum of electronic and zero-point Energies= -508.000918
Sum of electronic and thermal Energies= -507.991277
Sum of electronic and thermal Enthalpies= -507.990333
Sum of electronic and thermal Free Energies= -508.039562

0 1

B	0.84842600	-0.00013800	0.00006900
B	-0.84842600	-0.00013900	0.00009300
O	-1.60593200	-0.80840800	0.80802800
O	-1.60563700	0.80830500	-0.80798300
O	1.60574100	0.80818100	0.80815900
O	1.60582800	-0.80830900	-0.80807600
C	-2.99964100	0.54704700	-0.54715800
C	-2.99984600	-0.54683700	0.54699300
C	2.99977300	-0.54702600	-0.54693800
C	2.99971400	0.54717200	0.54689900
H	-3.47414300	-0.21822300	1.47442000
H	-3.47470100	-1.47413800	0.21884800
H	-3.47434700	1.47444800	-0.21907900
H	-3.47388200	0.21853700	-1.47465100
H	3.47429200	-0.21883100	-1.47439600
H	3.47433600	-1.47435400	-0.21843500
H	3.47406800	1.47459200	0.21835900
H	3.47437800	0.21906400	1.47431500

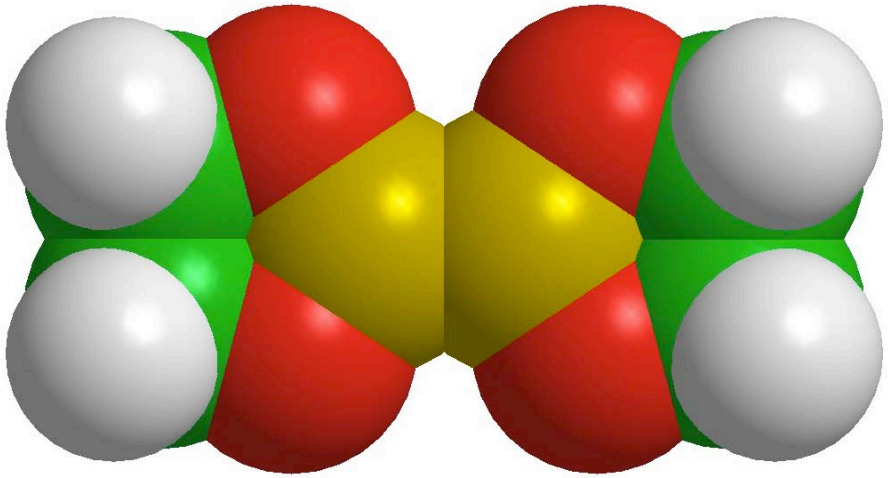


B3LYP $B_2(EG)_2$ 0

- Zero-point correction= 0.139962 (Hartree/Particle)
- Thermal correction to Energy= 0.148635
- Thermal correction to Enthalpy= 0.149579
- Thermal correction to Gibbs Free Energy= 0.104106
- Sum of electronic and zero-point Energies= -508.000498
- Sum of electronic and thermal Energies= -507.991824
- Sum of electronic and thermal Enthalpies= -507.990880
- Sum of electronic and thermal Free Energies= -508.036353

- B2EG20

- 0 1
- B 0.84894000 -0.00006800 0.00004300
- B -0.84894000 -0.00006000 -0.00000900
- O -1.60595500 -1.14285900 0.00004900
- O -1.60585400 1.14281000 -0.00002200
- O 1.60584700 1.14280800 0.00005800
- O 1.60595800 -1.14286200 -0.00007200
- C -2.99910700 0.77396000 -0.00250800
- C -2.99917900 -0.77388400 0.00248900
- C 2.99918400 -0.77387700 -0.00247100
- C 2.99910600 0.77396200 0.00246100
- H -3.47139300 -1.19511100 0.89291900
- H -3.47634000 -1.20107600 -0.88237800
- H -3.47626600 1.20119500 0.88233900
- H -3.47125100 1.19522700 -0.89295800
- H 3.47143100 -1.19513900 -0.89286700
- H 3.47631200 -1.20103600 0.88243100
- H 3.47619700 1.20116100 -0.88244200
- H 3.47131200 1.19527400 0.89285600

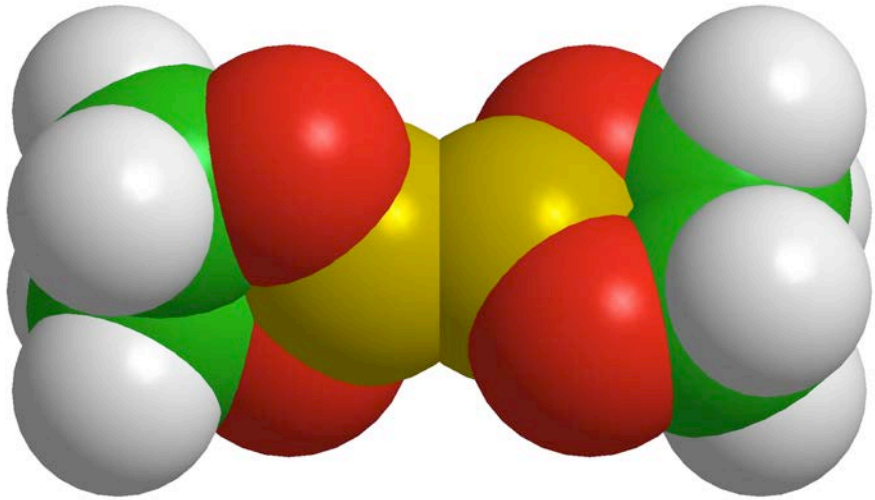


B_2EG_2 90 ωB97xD

- Zero-point correction= 0.142363 (Hartree/Particle)
- Thermal correction to Energy= 0.151652
- Thermal correction to Enthalpy= 0.152596
- Thermal correction to Gibbs Free Energy= 0.105557
- Sum of electronic and zero-point Energies= -507.827098
- Sum of electronic and thermal Energies= -507.817809
- Sum of electronic and thermal Enthalpies= -507.816865
- Sum of electronic and thermal Free Energies= -507.863904

- B2EG290W

- 0 1
- B -0.84899200 0.00005700 -0.00000400
- B 0.84899200 0.00004600 0.00001800
- O 1.60607800 0.88532600 -0.71802400
- O 1.60602800 -0.88528800 0.71804300
- O -1.60601400 -0.88528700 -0.71803700
- O -1.60609200 0.88532600 0.71803100
- C 2.98631100 -0.61675700 0.46392100
- C 2.98635000 0.61670200 -0.46391600
- C -2.98635900 0.61669700 0.46390500
- C -2.98630300 -0.61676400 -0.46393000
- H 3.43508600 1.49519500 0.00569100
- H 3.49175200 0.43005600 -1.41368100
- H 3.49173700 -0.43015000 1.41368100
- H 3.43498700 -1.49527600 -0.00569600
- H -3.43509400 1.49518800 -0.00570400
- H -3.49177000 0.43004400 1.41366400
- H -3.49172300 -0.43016700 -1.41369500
- H -3.43497600 -1.49528400 0.00568800

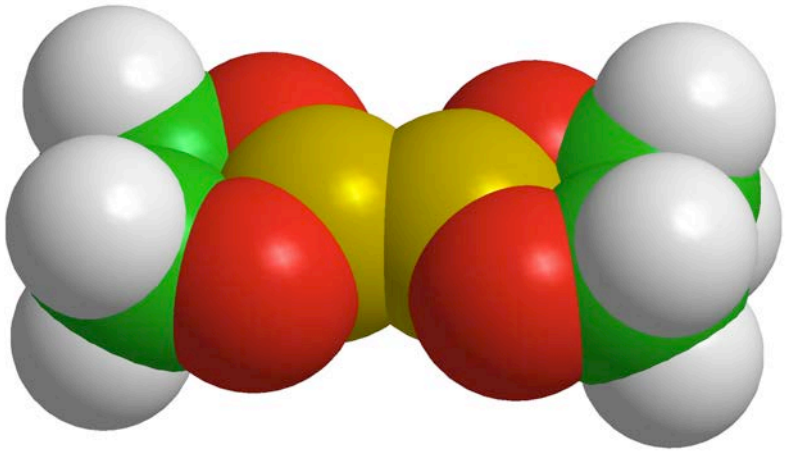


ωB97x-D B_2EG_2 0

- Zero-point correction= 0.142200 (Hartree/Particle)
- Thermal correction to Energy= 0.151633
- Thermal correction to Enthalpy= 0.152577
- Thermal correction to Gibbs Free Energy= 0.104459
- Sum of electronic and zero-point Energies= -507.826744
- Sum of electronic and thermal Energies= -507.817311
- Sum of electronic and thermal Enthalpies= -507.816367
- Sum of electronic and thermal Free Energies= -507.864486

- B2EG20W

- 0 1
- B -0.84988900 -0.00002300 0.00004100
- B 0.84988900 -0.00002200 -0.00003200
- O 1.60606300 -1.13945100 0.00179500
- O 1.60602600 1.13943400 -0.00178000
- O -1.60602500 1.13943300 0.00176300
- O -1.60606400 -1.13945200 -0.00177500
- C 2.98599000 0.77227900 0.00087700
- C 2.98601600 -0.77225200 -0.00086900
- C -2.98601600 -0.77225100 0.00083500
- C -2.98599000 0.77228000 -0.00085000
- H 3.46165800 -1.19255000 -0.88989200
- H 3.46584000 -1.19471500 0.88481500
- H 3.46579800 1.19476600 -0.88480500
- H 3.46162300 1.19258500 0.88990200
- H -3.46170500 -1.19258700 0.88981400
- H -3.46579400 -1.19467700 -0.88489300
- H -3.46575700 1.19473000 0.88487200
- H -3.46166200 1.19262300 -0.88983500



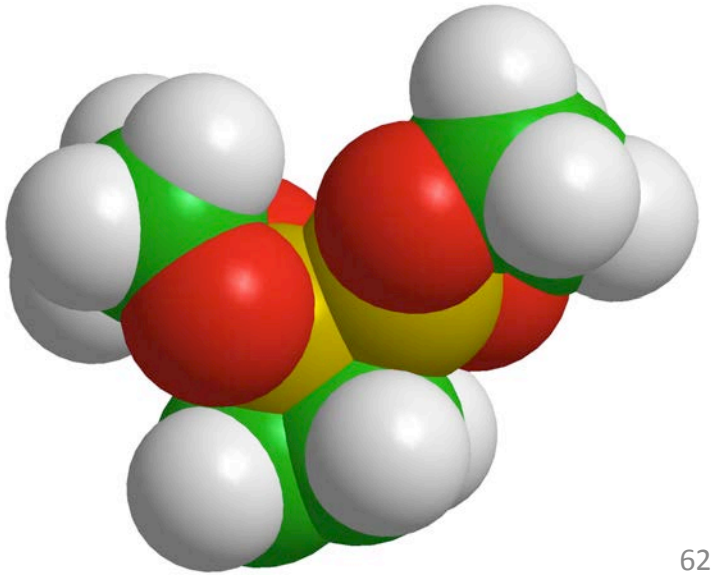
B_2EG_2 C_2H_4 TSWB97xD

- Zero-point correction= 0.195434 (Hartree/Particle)
- Thermal correction to Energy= 0.206855
- Thermal correction to Enthalpy= 0.207800
- Thermal correction to Gibbs Free Energy= 0.157001
- Sum of electronic and zero-point Energies= -586.296498
- Sum of electronic and thermal Energies= -586.285077
- Sum of electronic and thermal Enthalpies= -586.284133
- Sum of electronic and thermal Free Energies= -586.334931

- B2EG2TSW

- 0 1

C	-1.74256800	1.99885400	-0.23311100
C	-0.36859400	2.08120700	-0.45854300
B	0.83804000	0.24803500	-0.09766500
B	-0.94055400	0.41299500	-0.07852200
O	1.35557500	-0.72930500	-0.89743400
O	1.75449600	0.76453900	0.77987000
O	-1.51393500	-0.43787300	-1.09838200
O	-1.15731300	-0.17081200	1.23901700
C	-2.13401400	-1.17213200	1.01648900
C	-1.89195000	-1.62002900	-0.42833900
C	2.73621800	-0.89138200	-0.56272100
C	2.93312200	-0.03929500	0.70573400
H	-2.13789500	2.26497200	0.73760400
H	0.00983000	2.11426500	-1.47601100
H	0.28979600	2.49284700	0.29663400
H	-2.42700200	1.92061300	-1.06487700
H	-2.00767500	-1.97272300	1.74924500
H	-3.14357200	-0.74601100	1.12030100
H	-1.08220600	-2.36270000	-0.47074600
H	-2.78475700	-2.04285000	-0.89734900
H	3.34304300	-0.53914300	-1.40142700
H	2.94249000	-1.94989900	-0.39790700
H	3.80901700	0.60961800	0.65358500
H	2.99763200	-0.64986300	1.61025600



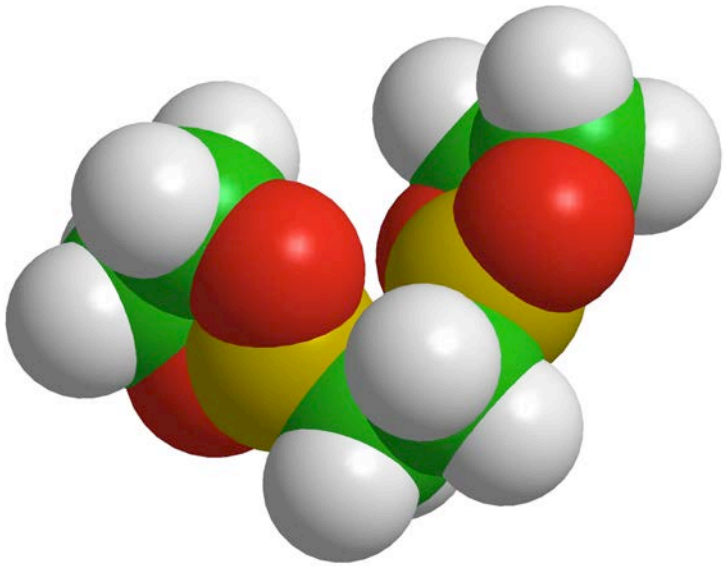
B_2EG_2 C_2H_4 gauche-P WB97xD

- Zero-point correction= 0.198558 (Hartree/Particle)
- Thermal correction to Energy= 0.210338
- Thermal correction to Enthalpy= 0.211282
- Thermal correction to Gibbs Free Energy= 0.158290
- Sum of electronic and zero-point Energies= -586.424387
- Sum of electronic and thermal Energies= -586.412608
- Sum of electronic and thermal Enthalpies= -586.411664
- Sum of electronic and thermal Free Energies= -586.464656

- B2EG2PW

- 0 1

C	-0.67206100	1.89806300	0.37357900
C	0.67206100	1.89806400	-0.37352200
B	1.53828200	0.62897600	-0.08475200
B	-1.53828900	0.62899000	0.08476700
O	-2.63475600	0.25530400	0.81652200
O	-1.27711700	-0.23404000	-0.95240400
O	2.63485500	0.25541300	-0.81640700
O	1.27700800	-0.23417600	0.95229000
C	-3.20290900	-0.90439400	0.21497800
C	-2.18200600	-1.33010800	-0.86079100
C	3.20292300	-0.90439300	-0.21499700
C	2.18200200	-1.33016100	0.86074600
H	-0.50983500	1.95360800	1.45536400
H	0.50982400	1.95362000	-1.45530500
H	1.25602900	2.79187800	-0.12140500
H	-1.25602000	2.79188300	0.12146100
H	-3.35419800	-1.66958300	0.97890800
H	-4.17356800	-0.64301300	-0.21610900
H	-2.64180900	-1.50315300	-1.83573800
H	-1.62523400	-2.22580400	-0.57051500
H	3.35413600	-1.66951000	-0.97901500
H	4.17361200	-0.64314200	0.21609900
H	1.62532700	-2.22592200	0.57049400
H	2.64178600	-1.50312100	1.83571900

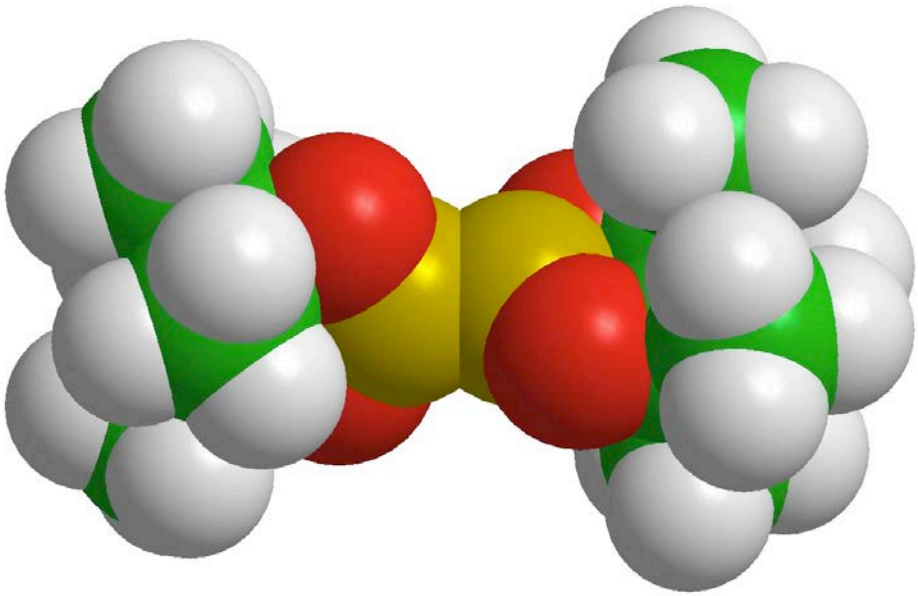


B3LYP $B_2(pin)_2$ 90

Zero-point correction= 0.361353 (Hartree/Particle)
Thermal correction to Energy= 0.381378
Thermal correction to Enthalpy= 0.382322
Thermal correction to Gibbs Free Energy= 0.313597
Sum of electronic and zero-point Energies= -822.403299
Sum of electronic and thermal Energies= -822.383274
Sum of electronic and thermal Enthalpies= -822.382330
Sum of electronic and thermal Free Energies= -822.451055

0 1

B	-0.84873100	-0.00280900	-0.00206900
B	0.84795900	-0.00411900	-0.00108900
O	1.61152900	0.44721100	-1.04980900
O	1.61132000	-0.45590900	1.04670100
O	-1.60965100	1.05010100	0.44063100
O	-1.61430000	-1.05251900	-0.44519900
C	3.00358900	0.49970100	-0.61012900
C	3.00483000	-0.49871900	0.61001100
C	-3.00666000	-0.61283900	-0.49506900
C	-3.00289100	0.61411100	0.49497100
C	-3.27977100	0.22472100	1.95185100
C	-3.88891100	1.78787100	0.08694100
C	-3.89305000	-1.78401900	-0.08140900
C	-3.28626100	-0.22517900	-1.95182900
C	3.88831900	-0.09275900	1.78570100
C	3.28958000	-1.95154900	0.21094100
C	3.89367900	0.09769100	-1.78235900
C	3.27822900	1.95493100	-0.21179900
H	-3.05598100	1.08078100	2.59131100
H	-4.32468100	-0.05687900	2.10450100
H	-2.64490000	-0.60515900	2.26809100
H	-4.94102100	1.49028100	0.05676100
H	-3.78592100	2.59306100	0.81717100
H	-3.60780100	2.18248100	-0.88879900
H	-4.94490000	-1.48534900	-0.05025900
H	-3.79155000	-2.59069900	-0.81028900
H	-3.61133000	-2.17670900	0.89496100
H	-3.05951000	-1.08010900	-2.59161900
H	-4.33257100	0.05068100	-2.10302900
H	-2.65546100	0.60741100	-2.26898900
H	3.79150000	-0.83032900	2.58500100
H	4.93996900	-0.05165900	1.48738100
H	3.59959900	0.87792100	2.18690100
H	4.33638000	-2.09759900	-0.06607900
H	3.06477000	-2.59773900	1.06149100
H	2.65953000	-2.26465900	-0.62380900
H	3.79459900	0.83333100	-2.58304900
H	4.94440900	0.06404100	-1.48011900
H	3.61309000	-0.87567900	-2.18294900
H	4.32354900	2.10726100	0.06743100
H	3.05161900	2.59956100	-1.06322900
H	2.64517900	2.26560100	0.62153100

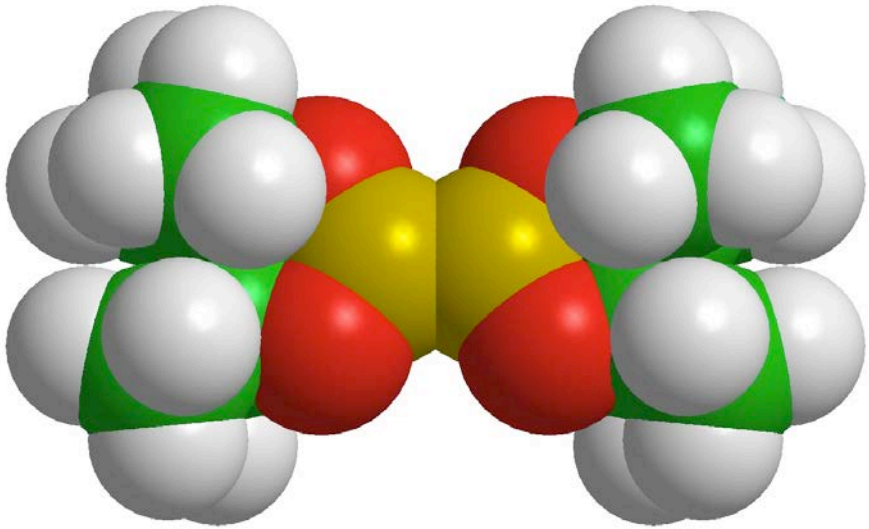


$B_2(pin)_2$ 0 B3LYP

Zero-point correction= 0.361301 (Hartree/Particle)
Thermal correction to Energy= 0.381301
Thermal correction to Enthalpy= 0.382246
Thermal correction to Gibbs Free Energy= 0.313953
Sum of electronic and zero-point Energies= -822.402700
Sum of electronic and thermal Energies= -822.382700
Sum of electronic and thermal Enthalpies= -822.381755
Sum of electronic and thermal Free Energies= -822.450048

0 1

B	-0.84961000	-0.00001000	-0.00004000
B	0.84963000	0.00001000	0.00003000
O	1.61245100	-1.08066900	0.36408000
O	1.61246000	1.08073100	-0.36394000
O	- 1.61243900	-1.08075100	0.36384000
O	-1.61245000	1.08068900	-0.36400000
C	3.00554000	0.78782100	-0.04476000
C	3.00551000	-0.78783900	0.04475000
C	-3.00550000	0.78783900	-0.04470000
C	-3.00552000	-0.78783100	0.04475000
C	3.88413000	1.38016100	-1.14277000
C	3.29841000	1.47763100	1.29268000
C	3.29822100	-1.47766900	-1.29272000
C	3.88419100	-1.38020900	1.14267000
C	-3.88408900	-1.38022100	1.14274000
C	-3.29848900	-1.47752100	-1.29273000
C	-3.88416000	1.38019900	-1.14264000
C	-3.29826000	1.47763900	1.29278000
H	3.77797900	2.46706100	-1.14384000
H	4.93792000	1.14170200	-0.97209000
H	3.59782000	1.01427100	-2.12842000
H	4.34605000	1.36698100	1.58300000
H	3.07732900	2.54219100	1.19352000
H	2.67153000	1.07690100	2.09159000
H	4.34581100	-1.36700900	-1.58318000
H	3.07716100	-2.54222900	-1.19350000
H	2.67123100	-1.07695900	-2.09156000
H	3.77802100	-2.46710900	1.14373000
H	4.93796100	-1.14176800	0.97191000
H	3.59797100	-1.01432900	2.12836000
H	-4.93787900	-1.14172200	0.97213000
H	-3.77796900	-2.46713100	1.14371000
H	-3.59772900	-1.01443100	2.12842000
H	-3.07740900	-2.54210100	-1.19366000
H	-4.34612900	-1.36683100	-1.58300000
H	-2.67163900	-1.07675100	-2.09165000
H	-4.93795000	1.14184800	-0.97183000
H	-3.77791100	2.46708900	-1.14379000
H	-3.59799000	1.01421900	-2.12830000
H	-3.07728100	2.54221900	1.19356000
H	-4.34584000	1.36689900	1.58325000
H	-2.67122000	1.07698900	2.09161

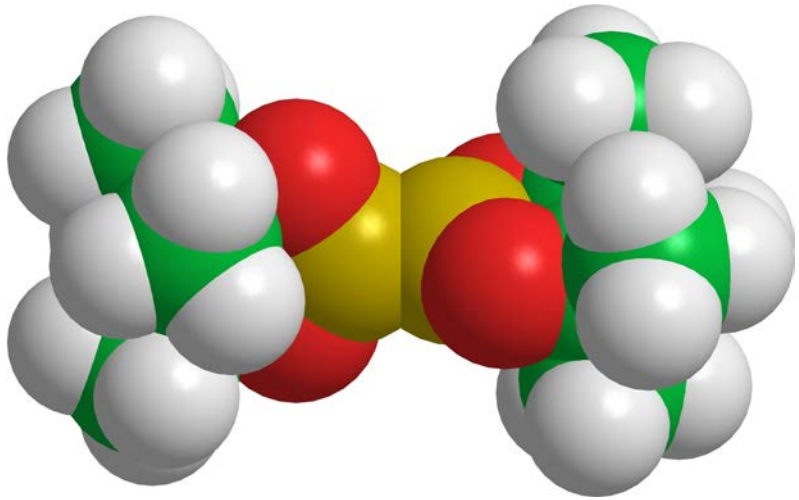


B_2pin_2 90 ωB97x-D

- Zero-point correction= 0.365322 (Hartree/Particle)
- Thermal correction to Energy= 0.384950
- Thermal correction to Enthalpy= 0.385895
- Thermal correction to Gibbs Free Energy= 0.317800
- Sum of electronic and zero-point Energies= -822.148401
- Sum of electronic and thermal Energies= -822.128773
- Sum of electronic and thermal Enthalpies= -822.127828
- Sum of electronic and thermal Free Energies= -822.195922

- B2pin290

B	-0.84801300	-0.00067300	-0.00004700
B	0.84802200	-0.00064700	-0.00004900
O	1.61085100	0.50130700	-1.02203200
O	1.61114900	-0.50216700	1.02189800
O	-1.61064500	1.02188800	0.50103600
O	-1.61133900	-1.02274200	-0.50100400
C	2.98410300	0.53532500	-0.57095900
C	2.98445000	-0.53524500	0.57087500
C	-2.98446900	-0.57124800	-0.53482900
C	-2.98406300	0.57133000	0.53492200
C	-3.24654100	0.06684500	1.95305700
C	-3.89484800	1.74614300	0.21791200
C	-3.89605400	-1.74544500	-0.21784500
C	-3.24663200	-0.06654200	-1.95294100
C	3.89547500	-0.21875200	1.74563500
C	3.24723900	-1.95294400	0.06533700
C	3.89543500	0.21951300	-1.74566600
C	3.24589900	1.95318600	-0.06535900
H	-3.02258500	0.86985200	2.65791300
H	-4.28917600	-0.23238000	2.08557700
H	-2.60388900	-0.78283800	2.19417800
H	-4.93508000	1.41560600	0.14335200
H	-3.82794200	2.48681500	1.01738800
H	-3.61233700	2.22955800	-0.71701100
H	-4.93606100	-1.41418200	-0.14333500
H	-3.82962400	-2.48615900	-1.01732100
H	-3.61393200	-2.22905800	0.71709100
H	-3.02330800	-0.86969600	-2.65782800
H	-4.28904800	0.23347000	-2.08540500
H	-2.60335200	0.78266500	-2.19406400
H	3.82907500	-1.01878000	2.48575400
H	4.93557700	-0.14359100	1.41482100
H	3.61279500	0.71572600	2.22980700
H	4.28980100	-2.08490600	-0.23439200
H	3.02384800	-2.65842100	0.86795400
H	2.60433100	-2.19372500	-0.78424700
H	3.82850400	1.01951100	-2.48577100
H	4.93556700	0.14511900	-1.41477300
H	3.61349900	-0.71516200	-2.22988900
H	4.28836200	2.08584800	0.23440800
H	3.02204600	2.65853700	-0.86795800
H	2.60279500	2.19349400	0.78421100

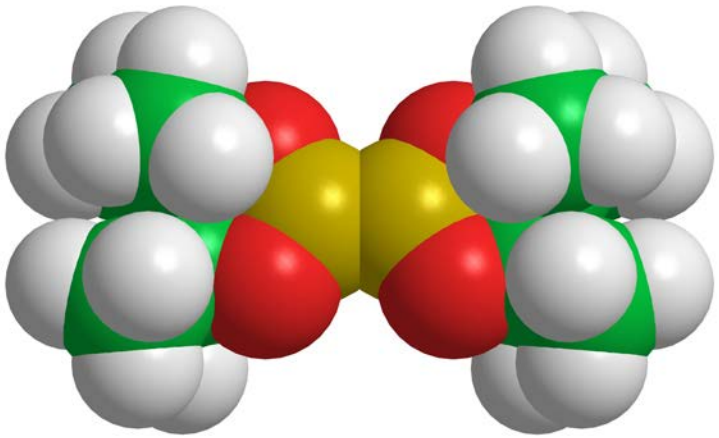


B_2pin_2 0 ωB97x-D

- Zero-point correction= 0.366173 (Hartree/Particle)
- Thermal correction to Energy= 0.385433
- Thermal correction to Enthalpy= 0.386377
- Thermal correction to Gibbs Free Energy= 0.319898
- Sum of electronic and zero-point Energies= -822.146959
- Sum of electronic and thermal Energies= -822.127699
- Sum of electronic and thermal Enthalpies= -822.126755
- Sum of electronic and thermal Free Energies= -822.193233

- B2pin20

- 0 1
- B -0.84955500 0.00000100 -0.00000400
- B 0.84955400 -0.00000100 -0.00000400
- O 1.61172900 -1.06487700 0.40143200
- O 1.61172900 1.06487500 -0.40143800
- O -1.61172900 -1.06487600 0.40143000
- O -1.61173000 1.06487900 -0.40143400
- C 2.98473500 0.78136500 -0.05334200
- C 2.98473600 -0.78136400 0.05334400
- C -2.98473700 0.78136500 -0.05334500
- C -2.98473500 -0.78136600 0.05333700
- C 3.89390400 1.35210700 -1.12964400
- C 3.25139300 1.47453800 1.28222500
- C 3.25140200 -1.47453300 -1.28222300
- C 3.89390100 -1.35210700 1.12964900
- C -3.89389900 -1.35210400 1.12964700
- C -3.25139600 -1.47454800 -1.28222400
- C -3.89390500 1.35212100 -1.12964200
- C -3.25139800 1.47452500 1.28222600
- H 3.80441400 2.44030900 -1.14130800
- H 4.93798200 1.09575500 -0.92753000
- H 3.62597000 0.98027000 -2.11845100
- H 4.29199600 1.35543600 1.59360800
- H 3.03976600 2.53986300 1.17259200
- H 2.60338800 1.07867100 2.06747800
- H 4.29200500 -1.35542600 -1.59360200
- H 3.03977900 -2.53985900 -1.17259300
- H 2.60339800 -1.07866800 -2.06747800
- H 3.80441400 -2.44030900 1.14130900
- H 4.93797900 -1.09575100 0.92754100
- H 3.62596100 -0.98027400 2.11845600
- H -4.93797800 -1.09575800 0.92753400
- H -3.80440300 -2.44030500 1.14131900
- H -3.62596200 -0.98025700 2.11845000
- H -3.03978000 -2.53987400 -1.17258200
- H -4.29199700 -1.35543800 -1.59361100
- H -2.60338500 -1.07869600 -2.06748000
- H -4.93798300 1.09576400 -0.92753500
- H -3.80441600 2.44032200 -1.14128900
- H -3.62596800 0.98030200 -2.11845500
- H -3.03977100 2.53985100 1.17260500
- H -4.29200200 1.35541900 1.59360600
- H -2.60339500 1.07864900 2.06747700



B_2Cat_2 90˚ ωB97X-D

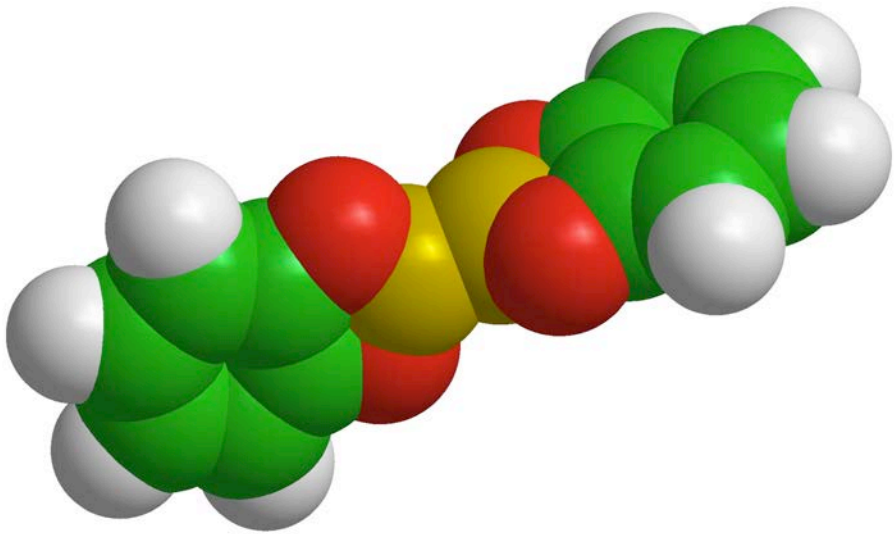
- Zero-point correction= 0.189526 (Hartree/Particle)
- Thermal correction to Energy= 0.202130
- Thermal correction to Enthalpy= 0.203075
- Thermal correction to Gibbs Free Energy= 0.148209
- Sum of electronic and zero-point Energies= -812.600913
- Sum of electronic and thermal Energies= -812.588308
- Sum of electronic and thermal Enthalpies= -812.587364
- Sum of electronic and thermal Free Energies= -812.642229

- B2Cat29W

- 0 1

C	-5.28623800	0.49290500	-0.49257100
C	-4.09623600	1.00810700	-1.00744500
C	-2.92850400	0.49045700	-0.49013000
C	-2.92850200	-0.49046300	0.49012400
C	-4.09623300	-1.00809900	1.00745600
C	-5.28623600	-0.49288800	0.49259500
H	-6.23001100	0.86928400	-0.86871100
H	-4.08216800	1.77351200	-1.77238200
H	-4.08216200	-1.77350200	1.77239600
H	-6.23000800	-0.86925600	0.86875000
O	-1.63181900	-0.80619100	0.80557600
O	-1.63182200	0.80618000	-0.80559200
B	-0.84510700	-0.00002300	-0.00002700
B	0.84510700	-0.00001600	-0.00002200
O	1.63180800	0.80616800	0.80557700
O	1.63183300	-0.80619200	-0.80560200

C	2.92849500	0.49045500	0.49012800
C	2.92851100	-0.49045800	-0.49013200
C	4.09621900	1.00810300	1.00746500
C	4.09625100	-1.00808900	-1.00744900
C	5.28622900	0.49290900	0.49260400
H	4.08213700	1.77350200	1.77240900
C	5.28624500	-0.49287700	-0.49256900
H	4.08219300	-1.77348800	-1.77239300
H	6.22999500	0.86928700	0.86876200
H	6.23002300	-0.86924200	-0.86871100

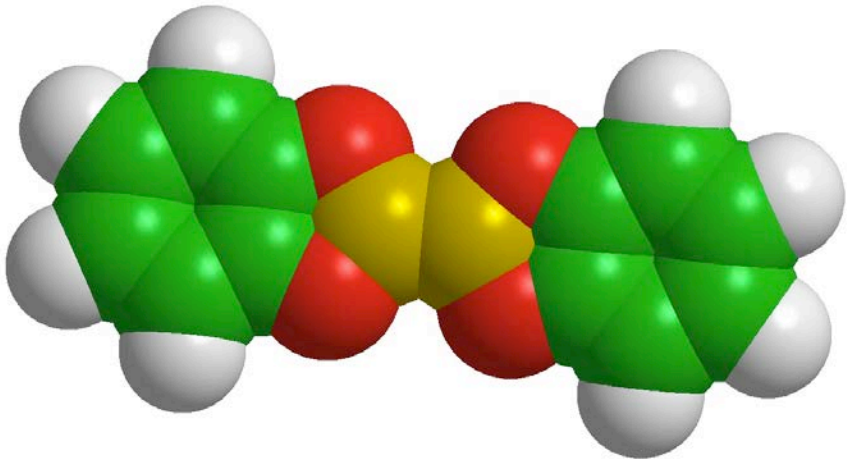


$B_2(catechol)_2$ 0˚ ωB97-xD

- Zero-point correction= 0.189181 (Hartree/Particle)
- Thermal correction to Energy= 0.201864
- Thermal correction to Enthalpy= 0.202808
- Thermal correction to Gibbs Free Energy= 0.147363
- Sum of electronic and zero-point Energies= -812.602529
- Sum of electronic and thermal Energies= -812.589846
- Sum of electronic and thermal Enthalpies= -812.588902
- Sum of electronic and thermal Free Energies= -812.644347

- B2Cat2W

- 0 1
- C -5.28209000 -0.69474800 0.05792300
- C -4.09276800 -1.42079100 0.11752100
- C -2.92430800 -0.69148600 0.05645900
- C -2.92424000 0.69147500 -0.05646700
- C -4.09265700 1.42085800 -0.11752100
- C -5.28203100 0.69490600 -0.05791900
- H -6.22683700 -1.22318100 0.10275100
- H -4.07823400 -2.49920900 0.20819800
- H -4.07803900 2.49927600 -0.20819700
- H -6.22673900 1.22341000 -0.10274100
- O -1.62930500 1.13603400 -0.09130400
- O -1.62938900 -1.13615300 0.09129100
- B -0.84244600 -0.00008000 -0.00000600
- B 0.84245600 -0.00013000 0.00000000
- O 1.62929200 1.13600900 0.09131300
- O 1.62940200 -1.13618300 -0.09130500
- C 2.92423700 0.69145300 0.05646100
- C 2.92430600 -0.69150900 -0.05645500
- C 4.09263500 1.42086600 0.11751700
- C 4.09279400 -1.42078300 -0.11751200
- C 5.28202100 0.69493400 0.05792000
- H 4.07800900 2.49928200 0.20819300
- C 5.28209400 -0.69472500 -0.05791700
- H 4.07825400 -2.49920300 -0.20819000
- H 6.22672300 1.22344900 0.10274300
- H 6.22685500 -1.22313300 -0.10274400



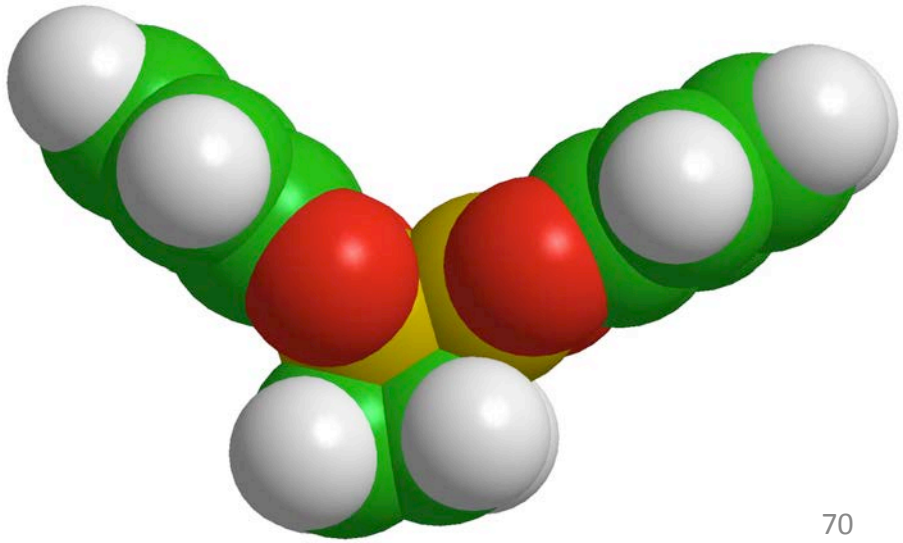
B_2cat_2 C_2H_4 TS WB97xD

- Zero-point correction= 0.242116 (Hartree/Particle)
- Thermal correction to Energy= 0.257381
- Thermal correction to Enthalpy= 0.258325
- Thermal correction to Gibbs Free Energy= 0.197634
- Sum of electronic and zero-point Energies= -891.074793
- Sum of electronic and thermal Energies= -891.059529
- Sum of electronic and thermal Enthalpies= -891.058584
- Sum of electronic and thermal Free Energies= -891.119275

- B2Cat2TSW

- 0 1

C	-1.37201700	2.90189900	0.02633400
C	0.01925100	2.72669400	0.02610200
B	0.78345300	0.75335000	0.00602600
B	-0.94603300	1.19871900	0.00970200
H	-1.88026300	3.11248800	0.95662500
H	0.58121900	2.87431900	-0.89105900
H	0.57921500	2.85515500	0.94748800
H	-1.87785800	3.13165400	-0.90076400
C	-2.49690100	-0.23343500	0.69634300
C	-3.40657800	-0.98550200	1.40605300
C	-2.49677300	-0.22095900	-0.70305000
C	-4.33684500	-1.73670800	0.67670000
H	-3.39121100	-0.98948400	2.48895600
C	-3.40629700	-0.96041500	-1.42609700
C	-4.33677400	-1.72430700	-0.71024900
H	-5.06572600	-2.33666900	1.20912100
H	-3.39100800	-0.94482500	-2.50889400
H	-5.06552700	-2.31478000	-1.25333600
C	2.64269100	-0.17370600	0.69301200
C	2.65162500	-0.14575100	-0.69444100
C	3.67851300	-0.71671800	1.42102700
C	3.69737300	-0.65832600	-1.43028200
C	4.74587900	-1.23716100	0.68818800
H	3.65523100	-0.73816900	2.50283100
C	4.75521400	-1.20842200	-0.70526500
H	3.68895300	-0.63451800	-2.51225900
H	5.58444600	-1.67608000	1.21523000
H	5.60092300	-1.62537400	-1.23868000
O	-1.50382300	0.54957600	1.19876900
O	-1.50332200	0.57092600	-1.19126200
O	1.48172500	0.40220300	1.14461700
O	1.49596400	0.44765100	-1.13714400



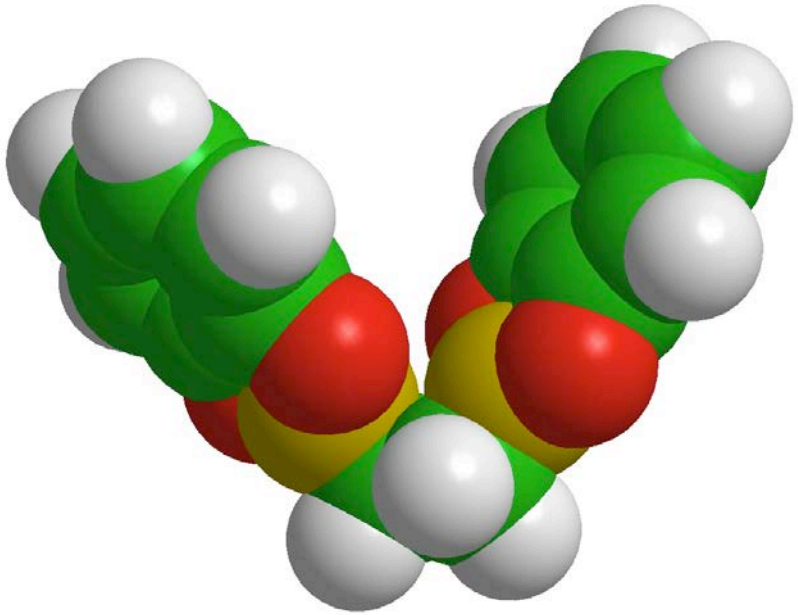
B_2Cat_2 Gproduct WB97xD

- Zero-point correction= 0.245258 (Hartree/Particle)
- Thermal correction to Energy= 0.259600
- Thermal correction to Enthalpy= 0.260544
- Thermal correction to Gibbs Free Energy= 0.202043
- Sum of electronic and zero-point Energies= -891.199184
- Sum of electronic and thermal Energies= -891.184842
- Sum of electronic and thermal Enthalpies= -891.183897
- Sum of electronic and thermal Free Energies= -891.242399

- B2Cat2PW

- 0 1

C	0.63457700	2.84513900	-0.43496400
C	-0.63338200	2.84489700	0.43766500
B	-1.52410700	1.58438100	0.22568800
B	1.52484000	1.58408000	-0.22433500
O	2.57119800	1.18819000	-1.04367500
O	1.36620600	0.69649600	0.83398100
O	-2.56703400	1.18522200	1.04786400
O	-1.36955300	0.70077200	-0.83649700
H	0.37190000	2.90141200	-1.49669800
H	-0.37076100	2.90002200	1.49945700
H	-1.23388900	3.74103200	0.24075300
H	1.23541900	3.74087900	-0.23729800
C	-2.32270900	-0.26586700	-0.65241600
C	-3.05178400	0.03077100	0.49172800
C	-2.58825000	-1.37846300	-1.41935700
C	-4.08452700	-0.77002200	0.92650500
C	-3.63302000	-2.19916100	-0.98907900
H	-2.01155700	-1.59894300	-2.30841900
C	-4.36463400	-1.90167800	0.15781100
H	-4.64375900	-0.52823200	1.82119200
H	-3.87688400	-3.08701600	-1.56023200
H	-5.16737400	-2.56237400	0.46284500
C	2.32031300	-0.26925100	0.65023400
C	3.05404000	0.03181400	-0.48977400
C	2.58297900	-1.38465800	1.41408900
C	4.08887800	-0.76700800	-0.92320400
C	3.62979000	-2.20342600	0.98512000
H	2.00256900	-1.60870900	2.29983500
C	4.36613800	-1.90142700	-0.15756300
H	4.65179200	-0.52165000	-1.81460400
H	3.87148400	-3.09338900	1.55391000
H	5.17037600	-2.56073400	-0.46166200

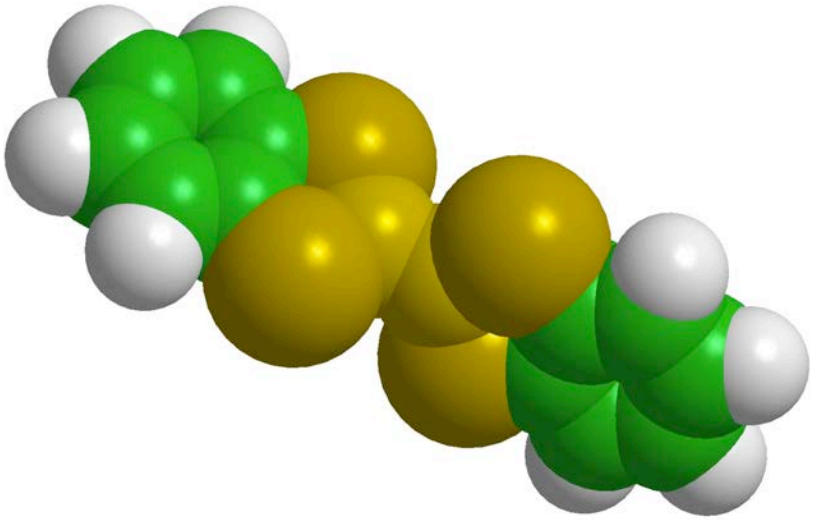


B_2(dithiocatechol)$_2$ 90˚ ωB97X-D

- Zero-point correction= 0.177114 (Hartree/Particle)
- Thermal correction to Energy= 0.191299
- Thermal correction to Enthalpy= 0.192243
- Thermal correction to Gibbs Free Energy= 0.134247
- Sum of electronic and zero-point Energies= -2104.484849
- Sum of electronic and thermal Energies= -2104.470664
- Sum of electronic and thermal Enthalpies= -2104.469719
- Sum of electronic and thermal Free Energies= -2104.527716

- B2SC290W

- 0 1
- B -0.84077600 -0.00002000 -0.00010200
- C -3.40658800 -0.54201500 0.44040400
- C -3.40662200 0.54197600 -0.44040200
- C -4.61237200 -1.08380600 0.88418600
- C -4.61243900 1.08379100 -0.88406500
- C -5.80603600 -0.54029600 0.44122600
- H -4.60950400 -1.92268900 1.57022500
- C -5.80607000 0.54030700 -0.44098400
- H -4.60962300 1.92267600 -1.57010100
- H -6.74445200 -0.95947000 0.78435000
- H -6.74451300 0.95950200 -0.78400700
- S -1.83265800 -1.16334200 0.94050200
- S -1.83273100 1.16329900 -0.94063100
- B 0.84077100 0.00000200 -0.00010300
- S 1.83274200 -1.16330500 -0.94064700
- S 1.83264600 1.16333500 0.94049300
- C 3.40662800 -0.54198600 -0.44039600
- C 4.61245200 -1.08379400 -0.88404600
- C 3.40658400 0.54201200 0.44040000
- C 5.80607600 -0.54029400 -0.44096700
- H 4.60964600 -1.92268500 -1.57007600
- C 4.61236000 1.08382100 0.88418100
- C 5.80603200 0.54032100 0.44122900
- H 6.74452300 -0.95948400 -0.78398400
- H 4.60948100 1.92271100 1.57021100
- H 6.74444300 0.95950700 0.78434900

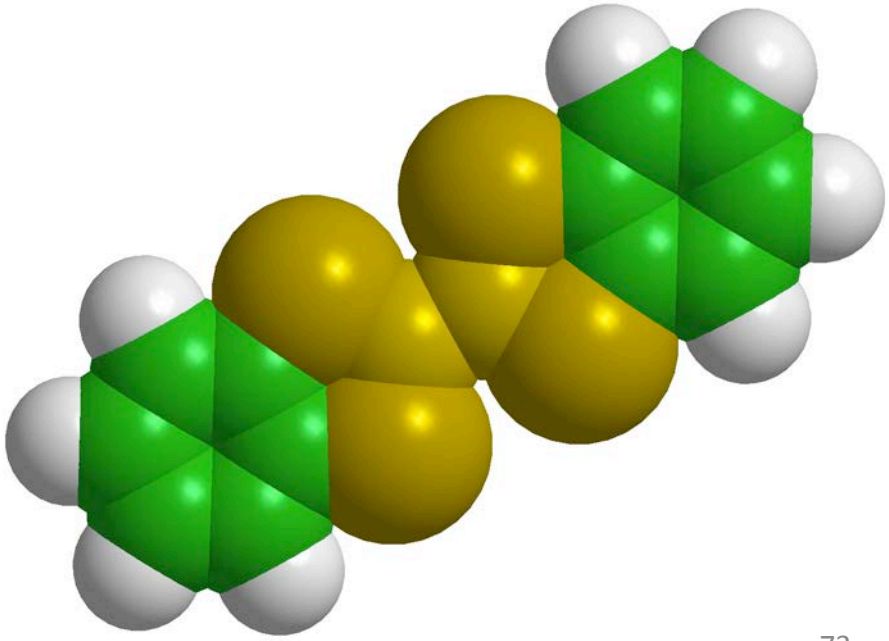


B_2(dithiocatechol)$_2$ 0˚ ωB97-xD

- Zero-point correction= 0.176971 (Hartree/Particle)
- Thermal correction to Energy= 0.191174
- Thermal correction to Enthalpy= 0.192118
- Thermal correction to Gibbs Free Energy= 0.134377
- Sum of electronic and zero-point Energies= -2104.484074
- Sum of electronic and thermal Energies= -2104.469871
- Sum of electronic and thermal Enthalpies= -2104.468927
- Sum of electronic and thermal Free Energies= -2104.526668

- B2SC20W

- 0 1
- B -0.84345900 -0.00005400 -0.00000100
- C -3.41345300 -0.69873100 -0.00002100
- C -3.41342400 0.69872500 0.00001300
- C -4.61993100 -1.39877800 -0.00004500
- C -4.61987000 1.39882500 0.00005300
- C -5.81296000 -0.69777100 -0.00001900
- H -4.61680300 -2.48248600 -0.00009100
- C -5.81293000 0.69787100 0.00003800
- H -4.61669300 2.48253300 0.00010600
- H -6.75215100 -1.23813000 -0.00004300
- H -6.75209600 1.23827300 0.00007100
- S -1.84204400 -1.49441100 -0.00003500
- S -1.84198300 1.49434000 0.00001900
- B 0.84345500 -0.00002900 0.00000900
- S 1.84201000 -1.49436600 0.00002400
- S 1.84201100 1.49439400 -0.00003200
- C 3.41344300 -0.69872400 0.00002600
- C 4.61990100 -1.39880100 0.00005500
- C 3.41344100 0.69873200 -0.00000400
- C 5.81294700 -0.69782000 0.00002700
- H 4.61674900 -2.48250800 0.00010000
- C 4.61990400 1.39880300 -0.00004200
- C 5.81294700 0.69782200 -0.00002800
- H 6.75212400 -1.23820200 0.00004500
- H 4.61675200 2.48251100 -0.00008900
- H 6.75212700 1.23819900 -0.00006700

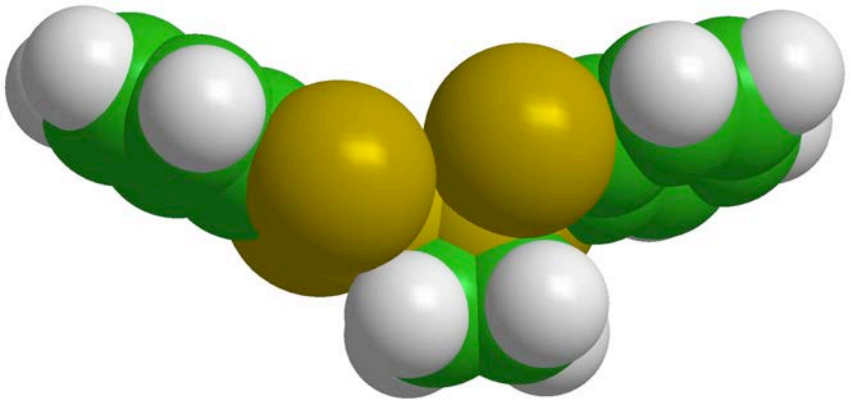


B_2(dithiocatechol)$_2$ C_2H_4 TS WB97-xD

- Zero-point correction= 0.231157 (Hartree/Particle)
- Thermal correction to Energy= 0.248578
- Thermal correction to Enthalpy= 0.249522
- Thermal correction to Gibbs Free Energy= 0.184161
- Sum of electronic and zero-point Energies= -2182.966966
- Sum of electronic and thermal Energies= -2182.949545
- Sum of electronic and thermal Enthalpies= -2182.948600
- Sum of electronic and thermal Free Energies= -2183.013961

- B2SC2TSW

- 0 1
- C -1.53165500 0.23004500 -2.47014400
- C -0.10599400 -0.00514600 -2.51315800
- B 0.86861600 0.01032600 -0.78529700
- B -0.96705600 0.01524400 -0.94559700
- H -1.86915200 1.23655400 -2.68119300
- H 0.23824000 -0.99351600 -2.79767200
- H 0.53536200 0.80692300 -2.83314500
- H -2.18190200 -0.56954600 -2.79749500
- C -2.99923900 0.69074700 0.51922700
- C -4.10077200 1.41740200 0.95805700
- C -3.10225200 -0.69915900 0.34662800
- C -5.29633100 0.76739900 1.23776700
- H -4.01900900 2.49106100 1.08220300
- C -4.30750900 -1.33892000 0.61566300
- C -5.39939200 -0.60754700 1.06642900
- H -6.14979600 1.33932600 1.58307200
- H -4.38937100 -2.40992300 0.47054000
- H -6.33450700 -1.11412600 1.27555900
- C 3.27413900 0.67306900 0.14217500
- C 3.19813200 -0.71575800 0.26825400
- C 4.42063800 1.35232800 0.55087900
- C 4.26714000 -1.42938300 0.80804900
- C 5.48120700 0.63705400 1.08029100
- H 4.47640800 2.43002000 0.45292800
- C 5.40437000 -0.74962400 1.20934600
- H 4.20129000 -2.50584300 0.91294100
- H 6.37453100 1.16128500 1.39809800
- H 6.23776300 -1.30054100 1.62850900
- S -1.42064200 1.45797000 0.22219900
- S -1.65212800 -1.58900300 -0.16875300
- S 1.87494100 1.49563100 -0.54092700
- S 1.70767000 -1.49175800 -0.25981100



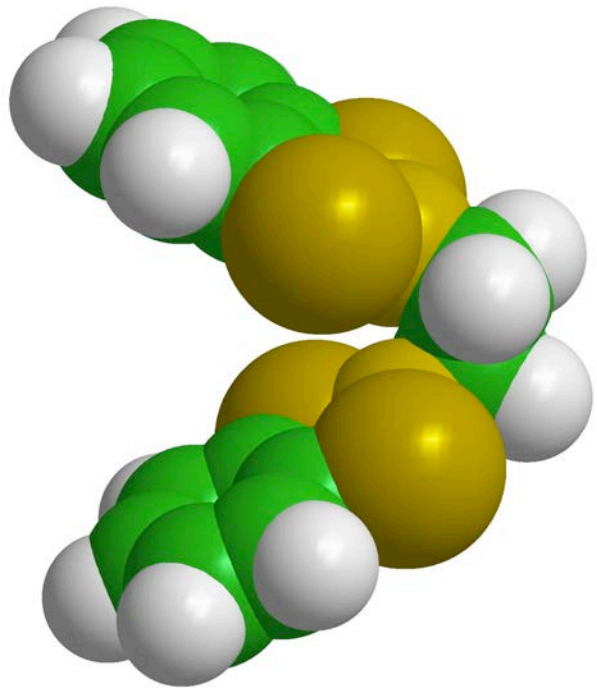
B_2Scat_2 gauche product wB97x-D

- Zero-point correction= 0.233752 (Hartree/Particle)
- Thermal correction to Energy= 0.251334
- Thermal correction to Enthalpy= 0.252279
- Thermal correction to Gibbs Free Energy= 0.185468
- Sum of electronic and zero-point Energies= -2183.066616
- Sum of electronic and thermal Energies= -2183.049033
- Sum of electronic and thermal Enthalpies= -2183.048089
- Sum of electronic and thermal Free Energies= -2183.114900

- B2SC2PW

- 0 1
- C 0.55554600 0.54592000 -2.95088000
- C -0.55554600 -0.54592000 -2.95088000
- B -0.47163200 -1.47617000 -1.68411300
- B 0.47163200 1.47617000 -1.68411300
- H 1.53622900 0.06321300 -3.00418800
- H -1.53622900 -0.06321300 -3.00418800
- H -0.45591200 -1.14798300 -3.86044500
- H 0.45591200 1.14798300 -3.86044500
- C 0.79576800 2.59575200 0.70740300
- C 1.24361200 2.95531400 1.97733000
- C -0.33312300 3.21450000 0.16270900
- C 0.56280200 3.92707800 2.69208000
- H 2.11868500 2.47418500 2.39826200
- C -1.01297000 4.19207400 0.88649100
- C -0.56280200 4.54396700 2.14805800
- H 0.90997400 4.20636300 3.67988100
- H -1.88774800 4.66929200 0.46053900
- H -1.09087700 5.30321800 2.71276500

- C 0.33312300 -3.21450000 0.16270900
- C -0.79576800 -2.59575200 0.70740300
- C 1.01297000 -4.19207400 0.88649100
- C -1.24361200 -2.95531400 1.97733000
- C 0.56280200 -4.54396700 2.14805800
- H 1.88774800 -4.66929200 0.46053900
- C -0.56280200 -3.92707800 2.69208000
- H -2.11868500 -2.47418500 2.39826200
- H 1.09087700 -5.30321800 2.71276500
- H -0.90997400 -4.20636300 3.67988100
- S 1.59544800 1.37183800 -0.28061700
- S -0.82913400 2.70394700 -1.45097100
- S 0.82913400 -2.70394700 -1.45097100
- S -1.59544800 -1.37183800 -0.28061700

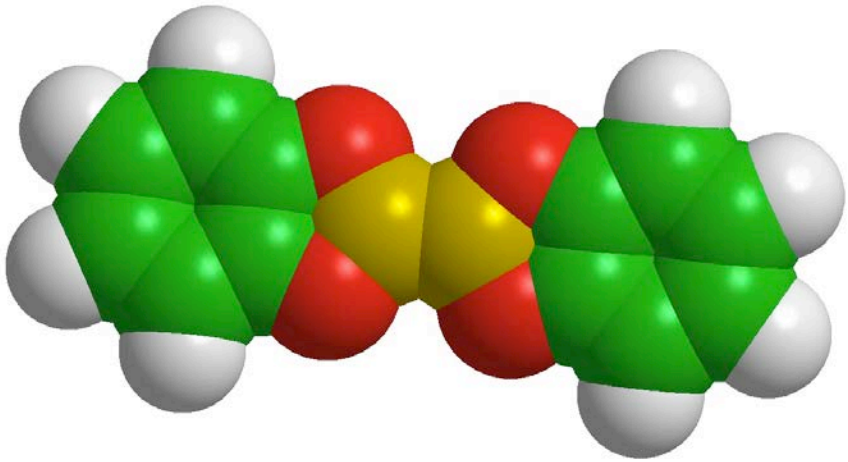


$B_2(catechol)_2$ 0˚ WB97-xD

- Zero-point correction= 0.189181 (Hartree/Particle)
- Thermal correction to Energy= 0.201864
- Thermal correction to Enthalpy= 0.202808
- Thermal correction to Gibbs Free Energy= 0.147363
- Sum of electronic and zero-point Energies= -812.602529
- Sum of electronic and thermal Energies= -812.589846
- Sum of electronic and thermal Enthalpies= -812.588902
- Sum of electronic and thermal Free Energies= -812.644347

- B2Cat2W

- 0 1
- C -5.28209000 -0.69474800 0.05792300
- C -4.09276800 -1.42079100 0.11752100
- C -2.92430800 -0.69148600 0.05645900
- C -2.92424000 0.69147500 -0.05646700
- C -4.09265700 1.42085800 -0.11752100
- C -5.28203100 0.69490600 -0.05791900
- H -6.22683700 -1.22318100 0.10275100
- H -4.07823400 -2.49920900 0.20819800
- H -4.07803900 2.49927600 -0.20819700
- H -6.22673900 1.22341000 -0.10274100
- O -1.62930500 1.13603400 -0.09130400
- O -1.62938900 -1.13615300 0.09129100
- B -0.84244600 -0.00008000 -0.00000600
- B 0.84245600 -0.00013000 0.00000000
- O 1.62929200 1.13600900 0.09131300
- O 1.62940200 -1.13618300 -0.09130500
- C 2.92423700 0.69145300 0.05646100
- C 2.92430600 -0.69150900 -0.05645500
- C 4.09263500 1.42086600 0.11751700
- C 4.09279400 -1.42078300 -0.11751200
- C 5.28202100 0.69493400 0.05792000
- H 4.07800900 2.49928200 0.20819300
- C 5.28209400 -0.69472500 -0.05791700
- H 4.07825400 -2.49920300 -0.20819000
- H 6.22672300 1.22344900 0.10274300
- H 6.22685500 -1.22313300 -0.10274400



B_2Cat_2 90˚ WB97xD

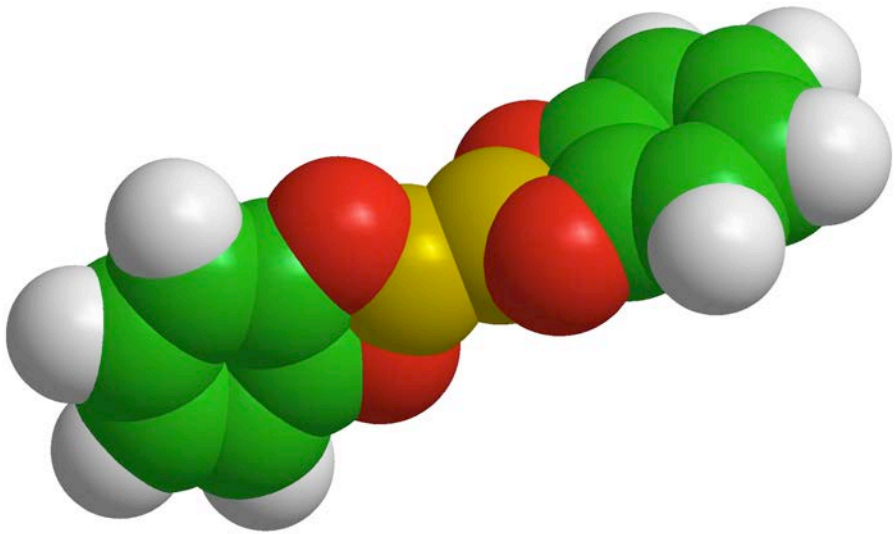
- Zero-point correction= 0.189526 (Hartree/Particle)
- Thermal correction to Energy= 0.202130
- Thermal correction to Enthalpy= 0.203075
- Thermal correction to Gibbs Free Energy= 0.148209
- Sum of electronic and zero-point Energies= -812.600913
- Sum of electronic and thermal Energies= -812.588308
- Sum of electronic and thermal Enthalpies= -812.587364
- Sum of electronic and thermal Free Energies= -812.642229

- B2Cat29W

- 0 1

C	-5.28623800	0.49290500	-0.49257100
C	-4.09623600	1.00810700	-1.00744500
C	-2.92850400	0.49045700	-0.49013000
C	-2.92850200	-0.49046300	0.49012400
C	-4.09623300	-1.00809900	1.00745600
C	-5.28623600	-0.49288800	0.49259500
H	-6.23001100	0.86928400	-0.86871100
H	-4.08216800	1.77351200	-1.77238200
H	-4.08216200	-1.77350200	1.77239600
H	-6.23000800	-0.86925600	0.86875000
O	-1.63181900	-0.80619100	0.80557600
O	-1.63182200	0.80618000	-0.80559200
B	-0.84510700	-0.00002300	-0.00002700
B	0.84510700	-0.00001600	-0.00002200
O	1.63180800	0.80616800	0.80557700
O	1.63183300	-0.80619200	-0.80560200

C	2.92849500	0.49045500	0.49012800
C	2.92851100	-0.49045800	-0.49013200
C	4.09621900	1.00810300	1.00746500
C	4.09625100	-1.00808900	-1.00744900
C	5.28622900	0.49290900	0.49260400
H	4.08213700	1.77350200	1.77240900
C	5.28624500	-0.49287700	-0.49256900
H	4.08219300	-1.77348800	-1.77239300
H	6.22999500	0.86928700	0.86876200
H	6.23002300	-0.86924200	-0.86871100



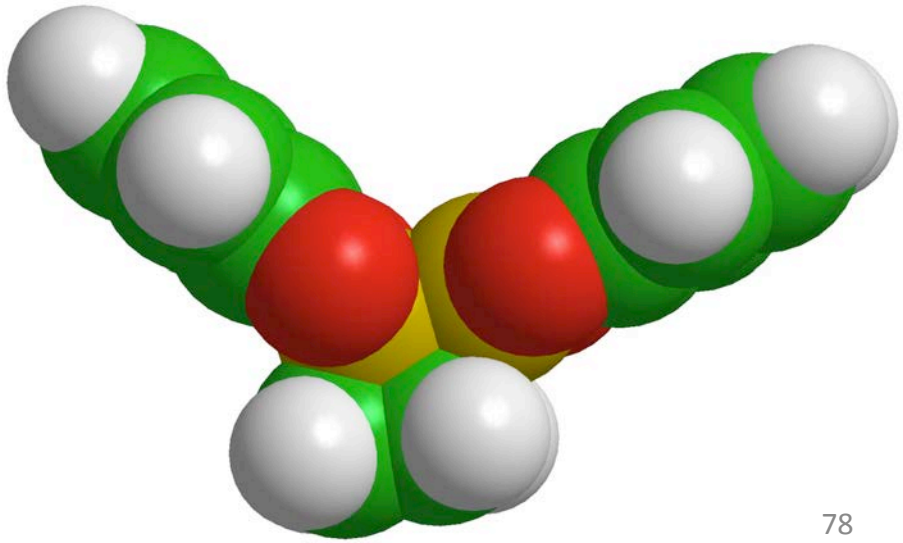
B_2cat_2 C_2H_4 TS WB97xD

- Zero-point correction= 0.242116 (Hartree/Particle)
- Thermal correction to Energy= 0.257381
- Thermal correction to Enthalpy= 0.258325
- Thermal correction to Gibbs Free Energy= 0.197634
- Sum of electronic and zero-point Energies= -891.074793
- Sum of electronic and thermal Energies= -891.059529
- Sum of electronic and thermal Enthalpies= -891.058584
- Sum of electronic and thermal Free Energies= -891.119275

- B2Cat2TSW

- 0 1

C	-1.37201700	2.90189900	0.02633400
C	0.01925100	2.72669400	0.02610200
B	0.78345300	0.75335000	0.00602600
B	-0.94603300	1.19871900	0.00970200
H	-1.88026300	3.11248800	0.95662500
H	0.58121900	2.87431900	-0.89105900
H	0.57921500	2.85515500	0.94748800
H	-1.87785800	3.13165400	-0.90076400
C	-2.49690100	-0.23343500	0.69634300
C	-3.40657800	-0.98550200	1.40605300
C	-2.49677300	-0.22095900	-0.70305000
C	-4.33684500	-1.73670800	0.67670000
H	-3.39121100	-0.98948400	2.48895600
C	-3.40629700	-0.96041500	-1.42609700
C	-4.33677400	-1.72430700	-0.71024900
H	-5.06572600	-2.33666900	1.20912100
H	-3.39100800	-0.94482500	-2.50889400
H	-5.06552700	-2.31478000	-1.25333600
C	2.64269100	-0.17370600	0.69301200
C	2.65162500	-0.14575100	-0.69444100
C	3.67851300	-0.71671800	1.42102700
C	3.69737300	-0.65832600	-1.43028200
C	4.74587900	-1.23716100	0.68818800
H	3.65523100	-0.73816900	2.50283100
C	4.75521400	-1.20842200	-0.70526500
H	3.68895300	-0.63451800	-2.51225900
H	5.58444600	-1.67608000	1.21523000
H	5.60092300	-1.62537400	-1.23868000
O	-1.50382300	0.54957600	1.19876900
O	-1.50332200	0.57092600	-1.19126200
O	1.48172500	0.40220300	1.14461700
O	1.49596400	0.44765100	-1.13714400



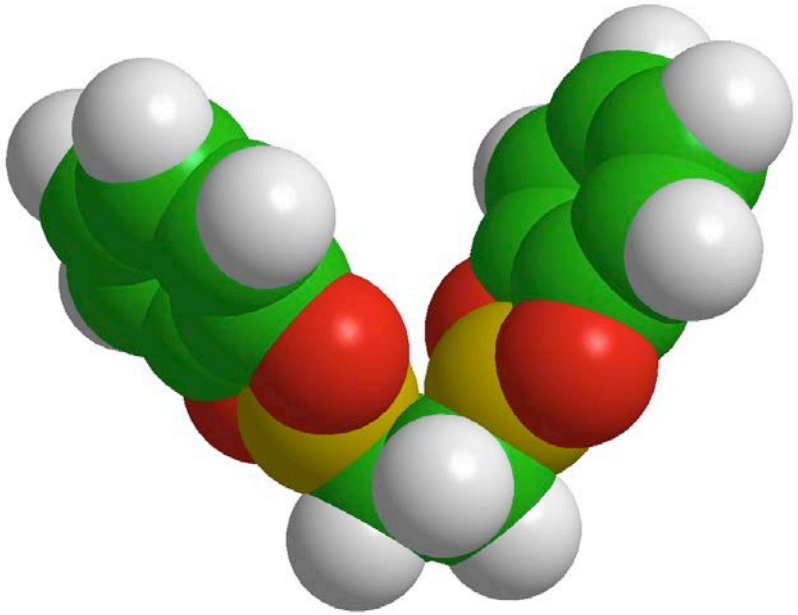
B_2Cat_2 Gproduct WB97xD

- Zero-point correction= 0.245258 (Hartree/Particle)
- Thermal correction to Energy= 0.259600
- Thermal correction to Enthalpy= 0.260544
- Thermal correction to Gibbs Free Energy= 0.202043
- Sum of electronic and zero-point Energies= -891.199184
- Sum of electronic and thermal Energies= -891.184842
- Sum of electronic and thermal Enthalpies= -891.183897
- Sum of electronic and thermal Free Energies= -891.242399

- B2Cat2PW

- 0 1

C	0.63457700	2.84513900	-0.43496400
C	-0.63338200	2.84489700	0.43766500
B	-1.52410700	1.58438100	0.22568800
B	1.52484000	1.58408000	-0.22433500
O	2.57119800	1.18819000	-1.04367500
O	1.36620600	0.69649600	0.83398100
O	-2.56703400	1.18522200	1.04786400
O	-1.36955300	0.70077200	-0.83649700
H	0.37190000	2.90141200	-1.49669800
H	-0.37076100	2.90002200	1.49945700
H	-1.23388900	3.74103200	0.24075300
H	1.23541900	3.74087900	-0.23729800
C	-2.32270900	-0.26586700	-0.65241600
C	-3.05178400	0.03077100	0.49172800
C	-2.58825000	-1.37846300	-1.41935700
C	-4.08452700	-0.77002200	0.92650500
C	-3.63302000	-2.19916100	-0.98907900
H	-2.01155700	-1.59894300	-2.30841900
C	-4.36463400	-1.90167800	0.15781100
H	-4.64375900	-0.52823200	1.82119200
H	-3.87688400	-3.08701600	-1.56023200
H	-5.16737400	-2.56237400	0.46284500
C	2.32031300	-0.26925100	0.65023400
C	3.05404000	0.03181400	-0.48977400
C	2.58297900	-1.38465800	1.41408900
C	4.08887800	-0.76700800	-0.92320400
C	3.62979000	-2.20342600	0.98512000
H	2.00256900	-1.60870900	2.29983500
C	4.36613800	-1.90142700	-0.15756300
H	4.65179200	-0.52165000	-1.81460400
H	3.87148400	-3.09338900	1.55391000
H	5.17037600	-2.56073400	-0.46166200



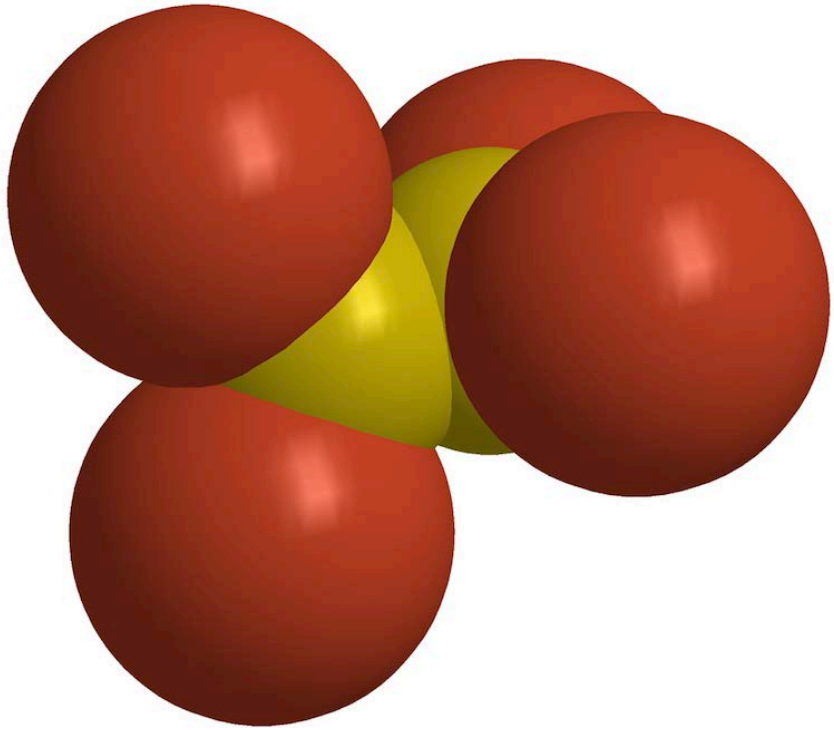
B_2Br_4 90˚

- Zero-point correction= 0.011146 (Hartree/Particle)
- Thermal correction to Energy= 0.019178
- Thermal correction to Enthalpy= 0.020122
- Thermal correction to Gibbs Free Energy= -0.027391
- Sum of electronic and zero-point Energies= -10346.516244

- Sum of electronic and thermal Energies= -10346.508211
- Sum of electronic and thermal Enthalpies= -10346.507267
- Sum of electronic and thermal Free Energies= -10346.554781

- B2Br490

- 0 1
- B 0.00000000 0.00000000 -0.84093000
- B 0.00000000 0.00000000 0.84093000
- Br 0.00000000 1.65632300 1.78761600
- Br 0.00000000 -1.65632300 1.78761600
- Br 1.65632300 -0.00000700 -1.78761600
- Br -1.65632300 0.00000700 -1.78761600

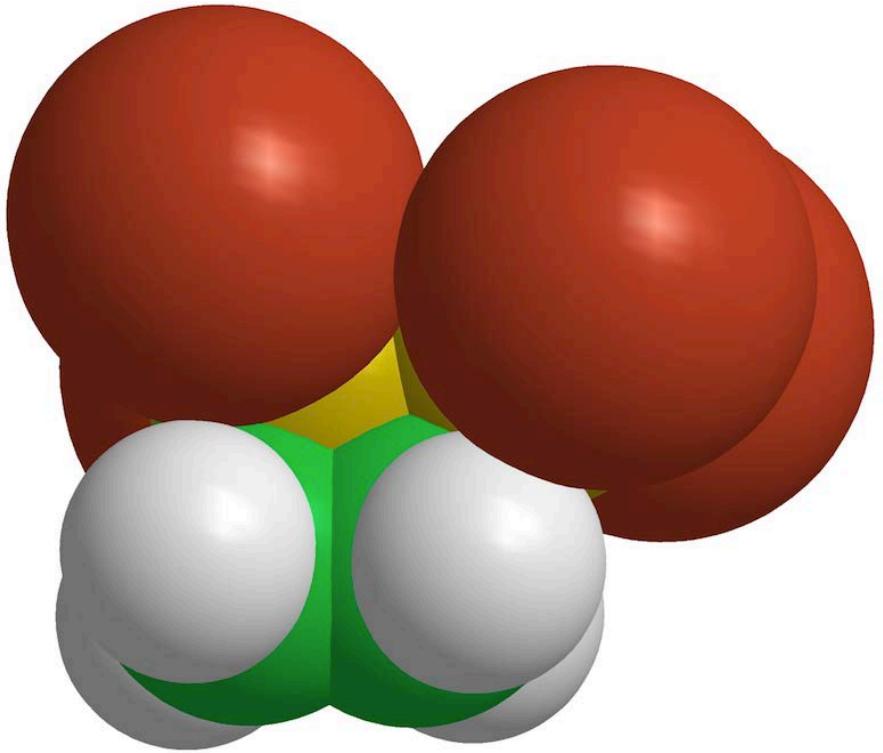


B_2Br_4 ethene TS

- Zero-point correction= 0.065691 (Hartree/Particle)
- Thermal correction to Energy= 0.075913
- Thermal correction to Enthalpy= 0.076857
- Thermal correction to Gibbs Free Energy= 0.024996
- Sum of electronic and zero-point Energies= -10425.026153
- Sum of electronic and thermal Energies= -10425.015931
- Sum of electronic and thermal Enthalpies= -10425.014987
- Sum of electronic and thermal Free Energies= -10425.066848

- B2Br4ETSW

- 0 1
- C -1.33150600 0.75851900 2.05849500
- H -2.25041900 0.26580200 2.34276600
- C -0.12264900 0.01778900 2.06598800
- B 0.80222800 -0.25556500 0.18737200
- H 0.80444300 0.52492300 2.30817600
- H -0.16115900 -1.05021800 2.25650100
- B -0.92103800 0.34827200 0.46403000
- H -1.27464800 1.82327100 2.24081200
- Br 1.11820900 -2.06991300 -0.32373600
- Br 2.33556000 0.90885600 0.06975200
- Br -2.20710800 -1.05290500 -0.16528800
- Br -0.89806800 2.02295700 -0.64221800

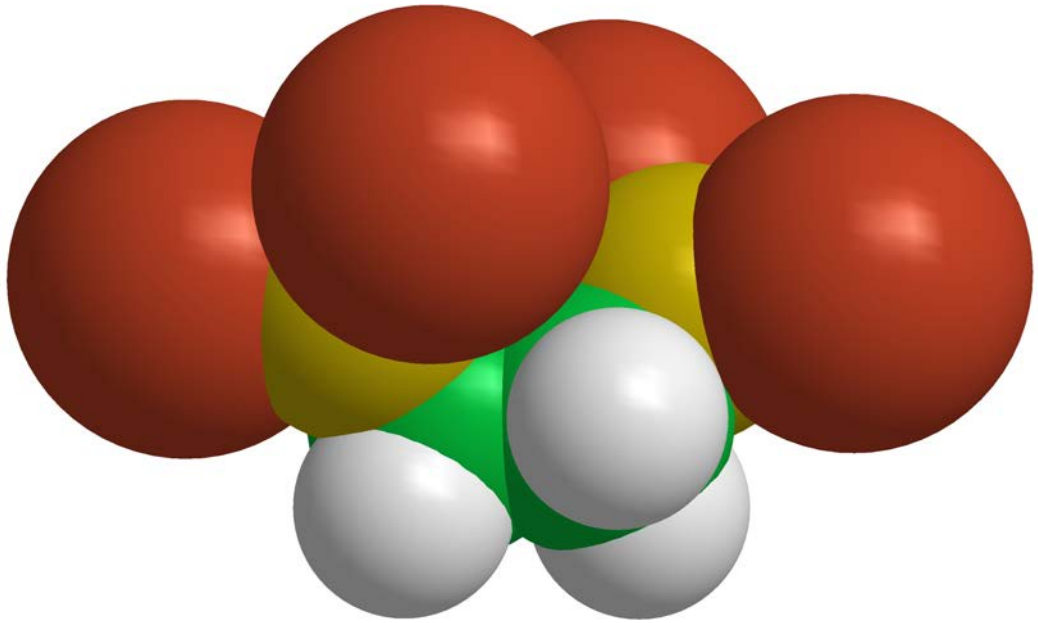


B_2Br_4 ethene gauche product

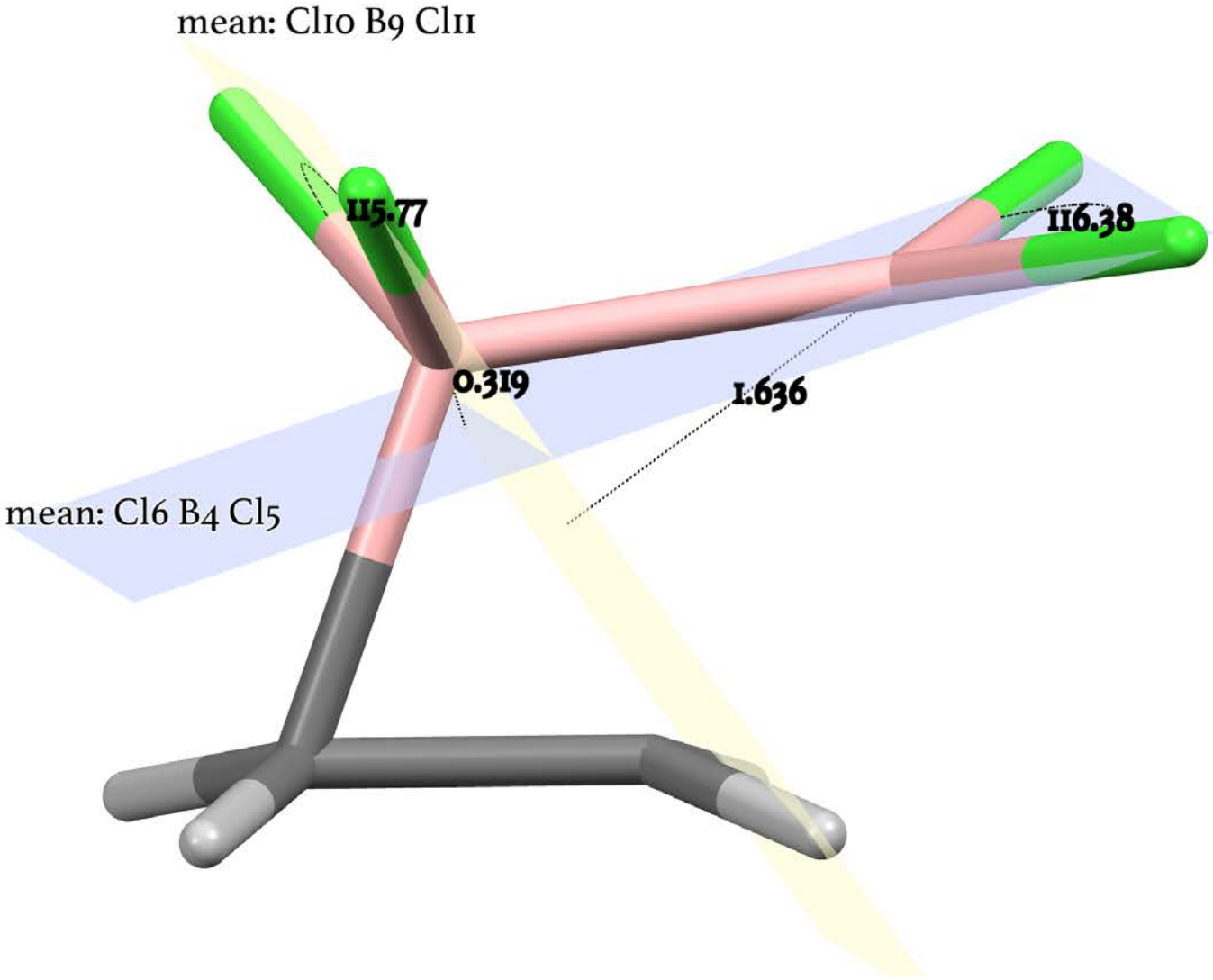
- Zero-point correction= 0.066955 (Hartree/Particle)
- Thermal correction to Energy= 0.077507
- Thermal correction to Enthalpy= 0.078451
- Thermal correction to Gibbs Free Energy= 0.024040
- Sum of electronic and zero-point Energies= -10425.110396
- Sum of electronic and thermal Energies= -10425.099845
- Sum of electronic and thermal Enthalpies= -10425.098901
- Sum of electronic and thermal Free Energies= -10425.153312

- B2Br4EPW

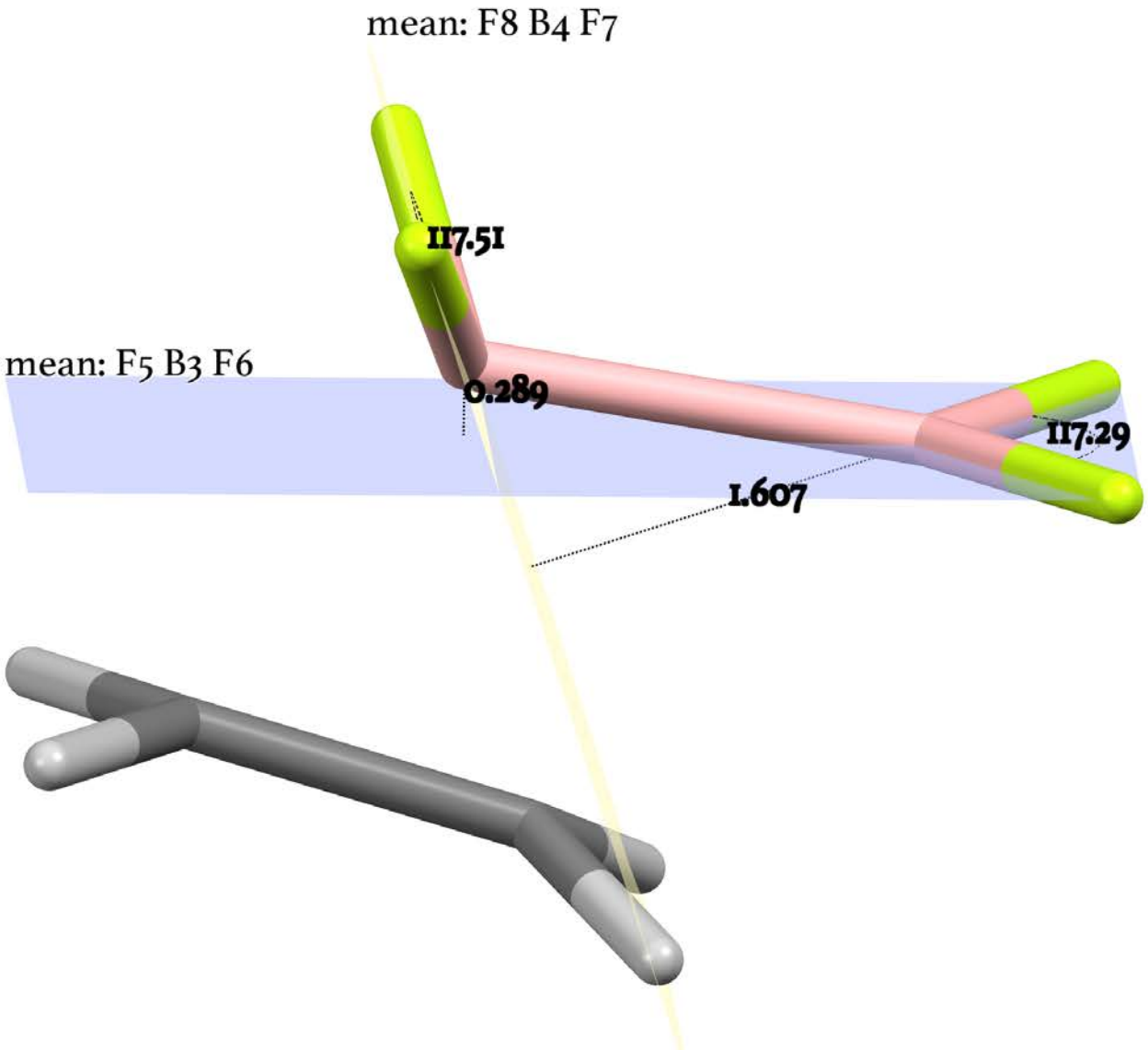
- 0 1
- C -0.72970200 -0.23450900 1.64300100
- H -1.22955100 0.12230400 2.55650200
- B -1.65076700 0.24073200 0.47100100
- C 0.72970500 0.23476200 1.64289700
- H 1.22964500 -0.12181200 2.55644100
- B 1.65070000 -0.24070400 0.47093600
- H -0.79161200 -1.32586000 1.70655400
- H 0.79160900 1.32612900 1.70620600
- Br -1.17482400 1.71265700 -0.66732000
- Br -3.35174700 -0.60082100 0.19660600
- Br 1.17467700 -1.71258800 -0.66731100
- Br 3.35190000 0.60068300 0.19657500

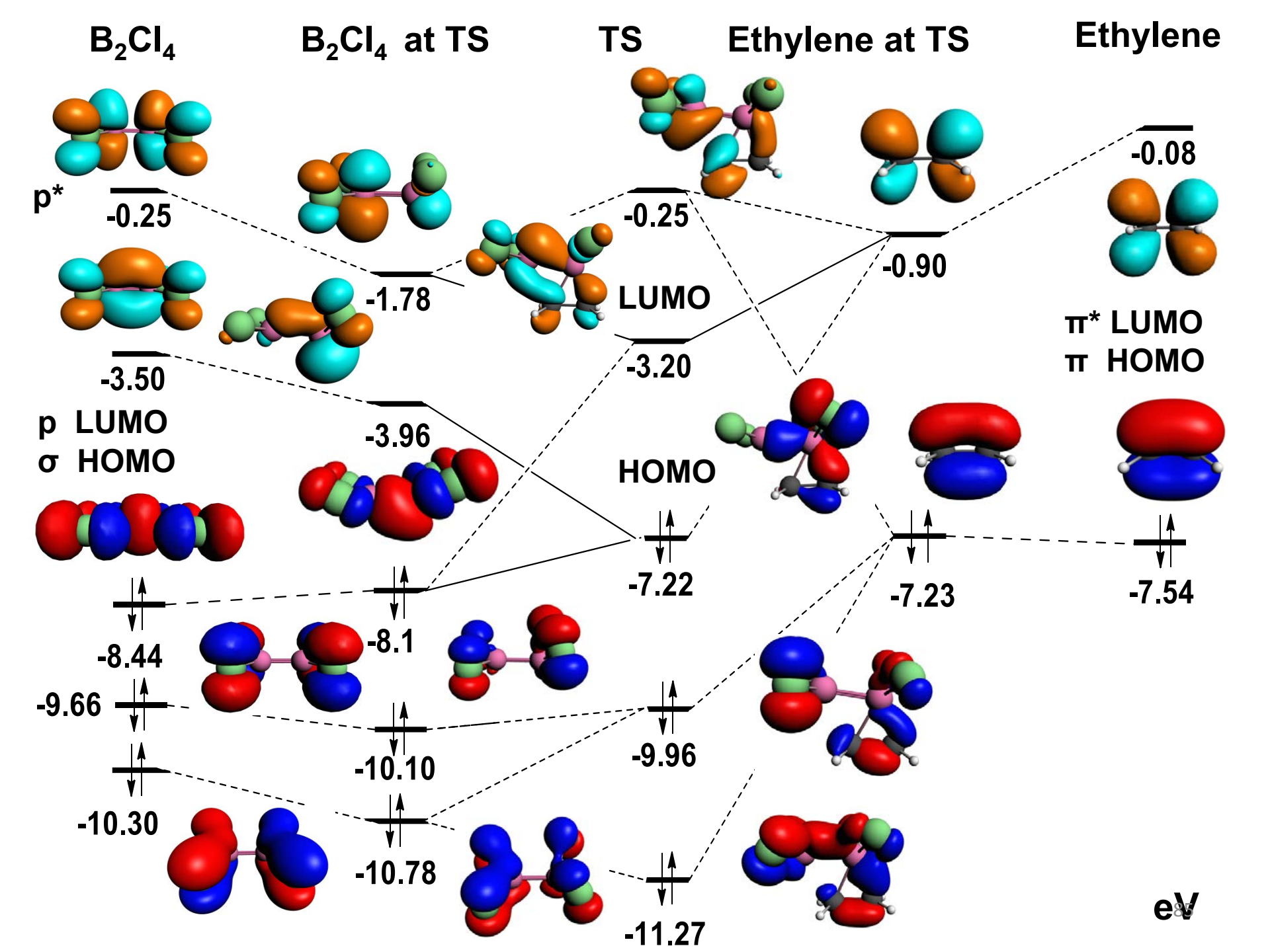


Geometry of TS for B_2Cl_4/ethene ωB97x-D



Geometry of TS for B_2F_4/ethene ωB97x-D



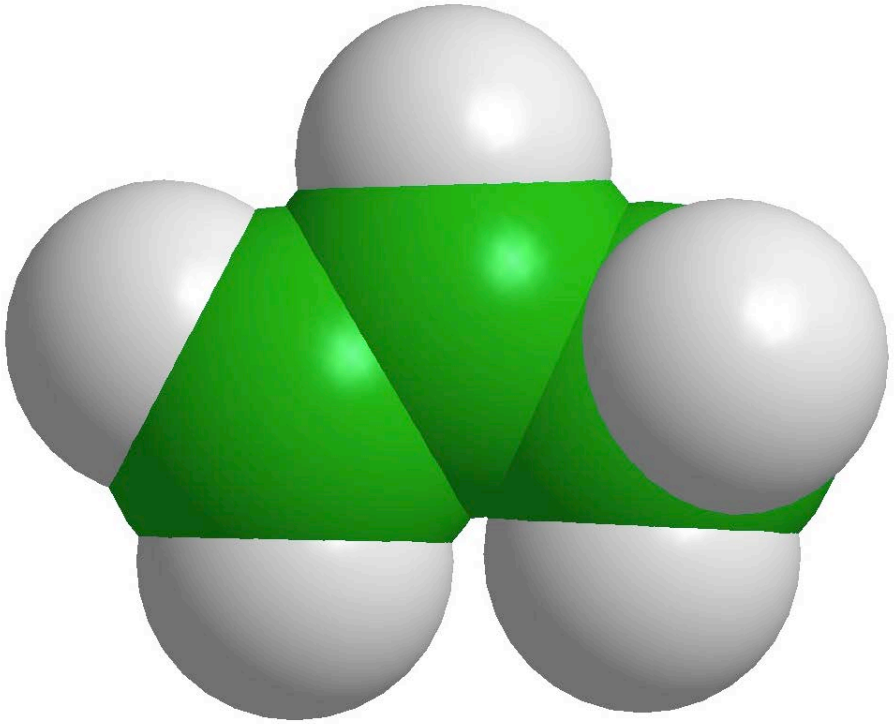

B2Cl4
B2Cl4 at TS
TS
Ethylene at TS
Ethylene
p*
-0.25
-1.78
-0.25
LUMO
-0.90
-0.08
π* LUMO
π HOMO
-3.50
p LUMO
σ HOMO
-3.96
HOMO
-3.20
-7.22
-7.23
-7.54
-8.44
-8.1
-9.66
-10.10
-9.96
-10.30
-10.78
-11.27
eV

Propene B3LYP

- Zero-point correction= 0.079309 (Hartree/Particle)
- Thermal correction to Energy= 0.083395
- Thermal correction to Enthalpy= 0.084339
- Thermal correction to Gibbs Free Energy= 0.054305
- Sum of electronic and zero-point Energies= -117.864739
- Sum of electronic and thermal Energies= -117.860653
- Sum of electronic and thermal Enthalpies= -117.859709
- Sum of electronic and thermal Free Energies= -117.889743

- Propene

- 0 1
- C -1.28041800 -0.22047500 -0.00001500
- H -1.30061000 -1.30658500 0.00004800
- H -2.23921600 0.28574700 -0.00000300
- C -0.13476500 0.45381100 0.00000100
- H -0.16672900 1.54232600 0.00002200
- C 1.23346100 -0.16231400 -0.00002000
- H 1.18155700 -1.25381100 -0.00043200
- H 1.80790800 0.15346100 -0.87820900
- H 1.80742400 0.15273000 0.87878000

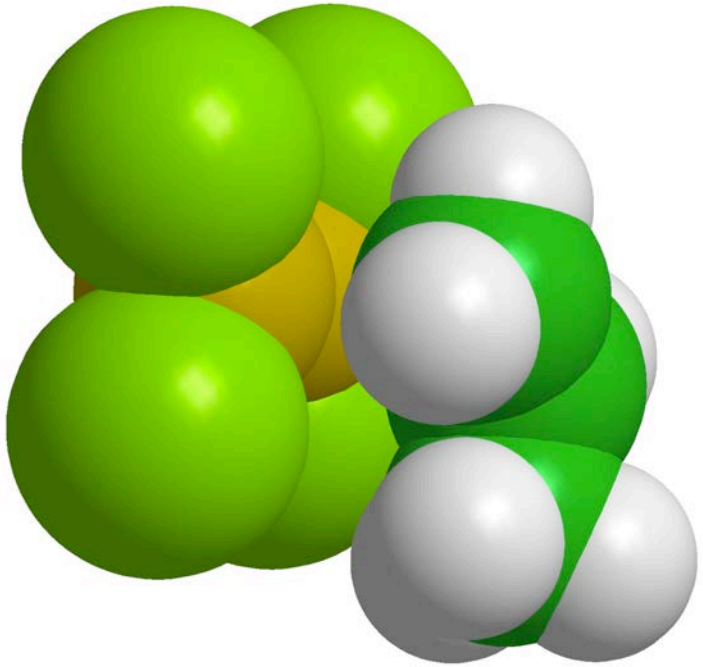


Propene B_2Cl_4 vdW B3LYP

- Zero-point correction= 0.093374 (Hartree/Particle)
- Thermal correction to Energy= 0.106546
- Thermal correction to Enthalpy= 0.107491
- Thermal correction to Gibbs Free Energy= 0.049267
- Sum of electronic and zero-point Energies= -2008.620095
- Sum of electronic and thermal Energies= -2008.606922
- Sum of electronic and thermal Enthalpies= -2008.605978
- Sum of electronic and thermal Free Energies= -2008.664201

- B2Cl4PV

- 0 1
- C -2.20580300 -0.23624900 -1.36932500
- H -2.36760500 0.82888400 -1.52608800
- B 0.35581100 0.99986700 0.36352100
- Cl -0.74246000 1.52584200 1.63673000
- Cl 0.88878300 2.19987300 -0.80823100
- C -1.19934800 -0.83089500 -2.01440700
- H -0.55710200 -0.28265700 -2.69367700
- B 0.95649800 -0.60041800 0.33428600
- C -3.16361600 -0.91709800 -0.44114600
- H -3.13818800 -0.45763800 0.55281100
- H -2.93849400 -1.98019100 -0.33566500
- H -4.19125400 -0.81573300 -0.80691100
- Cl 0.29965000 -1.83804600 1.39983500
- Cl 2.32180200 -1.03412400 -0.68838800
- H -1.00847700 -1.89471800 -1.90933000

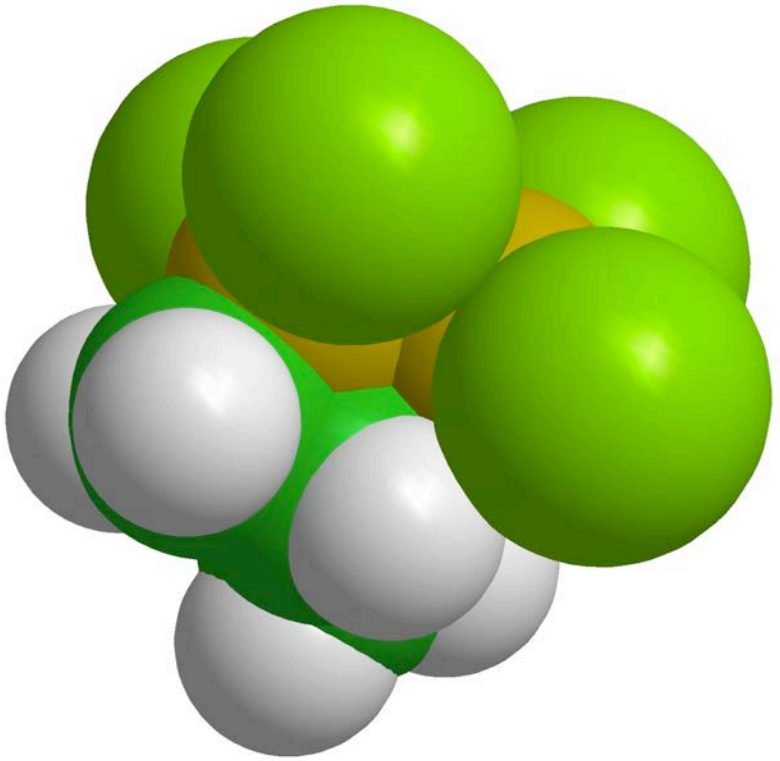


Propene B_2Cl_4 TS1 B3LYP

- Zero-point correction= 0.095019 (Hartree/Particle)
- Thermal correction to Energy= 0.105826
- Thermal correction to Enthalpy= 0.106770
- Thermal correction to Gibbs Free Energy= 0.056947
- Sum of electronic and zero-point Energies= -2008.586123
- Sum of electronic and thermal Energies= -2008.575316
- Sum of electronic and thermal Enthalpies= -2008.574371
- Sum of electronic and thermal Free Energies= -2008.624195

- B2Cl4PTS1

- 0 1
- C -0.37844300 -0.72446500 1.57960500
- H 0.53468000 -0.48783200 2.10976000
- B 0.86716800 -0.15838300 -0.16340400
- Cl 1.04185200 -1.03369200 -1.67253100
- Cl 2.38834600 0.28917200 0.64119600
- C -1.44673400 0.23735200 1.71059600
- H -1.26473700 1.07332700 2.37646400
- B -0.85951900 0.46076100 0.20407000
- C -0.63198600 -2.18660500 1.33381000
- H 0.25214000 -2.71332900 0.97267500
- H -1.45739800 -2.34692700 0.64077500
- H -0.91150000 -2.62104200 2.30115600
- Cl -2.03999200 -0.15597500 -1.06772100
- Cl -0.21276300 2.18046400 -0.13932400
- H -2.46496700 -0.13326700 1.70422200

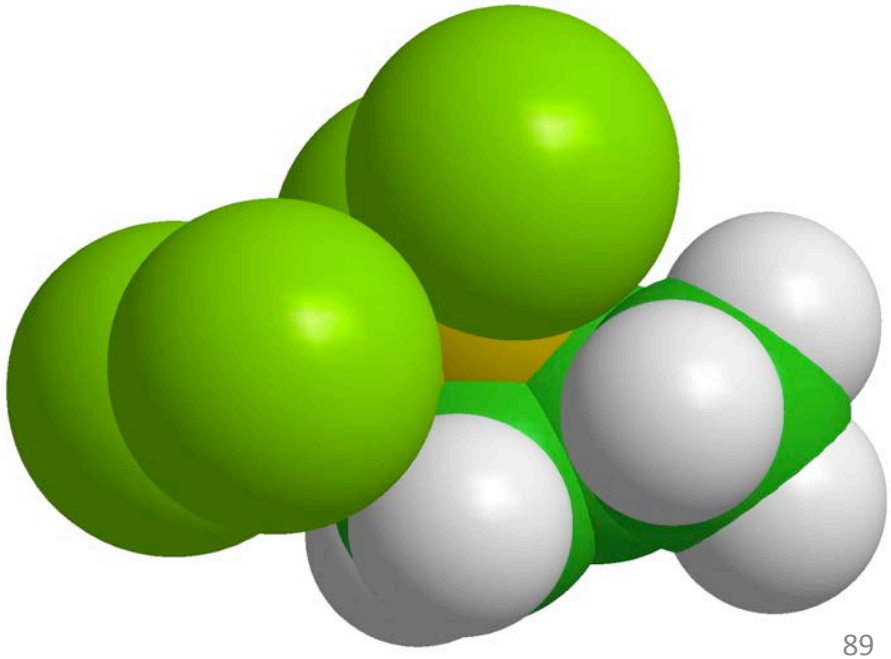


Propene B_2Cl_4 TS2 B3LYP

- Zero-point correction= 0.095131 (Hartree/Particle)
- Thermal correction to Energy= 0.105907
- Thermal correction to Enthalpy= 0.106851
- Thermal correction to Gibbs Free Energy= 0.057251
- Sum of electronic and zero-point Energies= -2008.583995
- Sum of electronic and thermal Energies= -2008.573219
- Sum of electronic and thermal Enthalpies= -2008.572275
- Sum of electronic and thermal Free Energies= -2008.621875

- B2Cl4PTS2

- 0 1
- C 0.39102100 0.13353300 1.58194800
- H -0.16507200 -0.63053200 2.11474200
- B -1.08462200 0.24661000 0.15111400
- Cl -1.56099900 1.92048800 -0.14577100
- Cl -2.39019600 -0.90962800 0.35525900
- C 1.73339500 -0.15393600 1.17216800
- H 2.10041500 -1.13898900 1.43560200
- B 0.66170200 -0.36393300 -0.13902500
- C 2.78353400 0.93035300 1.09873700
- H 2.35206600 1.90929100 0.88462500
- H 3.51297700 0.71063700 0.31678700
- H 3.31801000 0.99053700 2.05236300
- Cl 1.15335400 0.69276600 -1.56770100
- Cl 0.52767400 -2.16703100 -0.51215900
- H 0.14134900 1.16386000 1.81464000

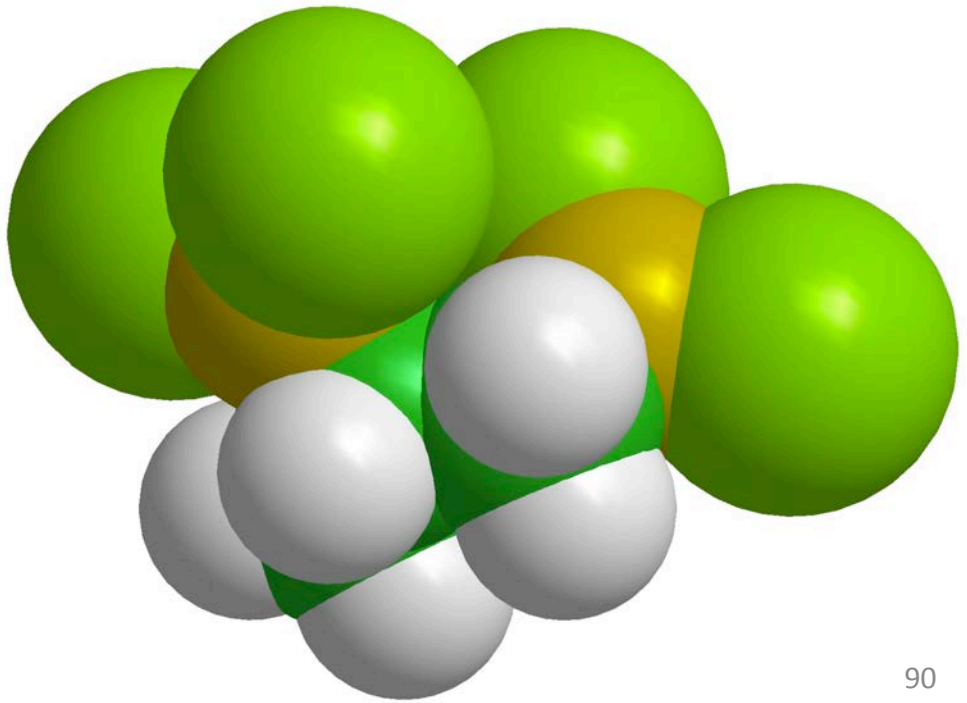


Propene B_2Cl_4 product gauche B3LYP

- Zero-point correction= 0.096649 (Hartree/Particle)
- Thermal correction to Energy= 0.107754
- Thermal correction to Enthalpy= 0.108698
- Thermal correction to Gibbs Free Energy= 0.056853
- Sum of electronic and zero-point Energies= -2008.666651
- Sum of electronic and thermal Energies= -2008.655546
- Sum of electronic and thermal Enthalpies= -2008.654602
- Sum of electronic and thermal Free Energies= -2008.706447

- B2Cl4PPG

- 0 1
- C 0.84780300 0.24116200 -1.27424700
- H 0.79721800 -0.74254300 -1.76535800
- B 1.72638900 0.00295300 -0.00366300
- Cl 1.02858600 -0.17004900 1.61046900
- Cl 3.47593900 -0.17216300 -0.15662900
- C -0.53927900 2.28974700 -0.63289000
- H -0.15014700 2.38063600 0.38422200
- H -1.53180700 2.74263100 -0.64316500
- H 0.10360600 2.87905700 -1.29299100
- C -0.58003700 0.82192000 -1.09580500
- H -1.02816800 0.81729700 -2.10602400
- B -1.58006300 -0.11037000 -0.31723400
- Cl -1.60717300 -1.85540000 -0.63050200
- Cl -2.82117800 0.51981900 0.76619800
- H 1.41180100 0.86551700 -1.97666700

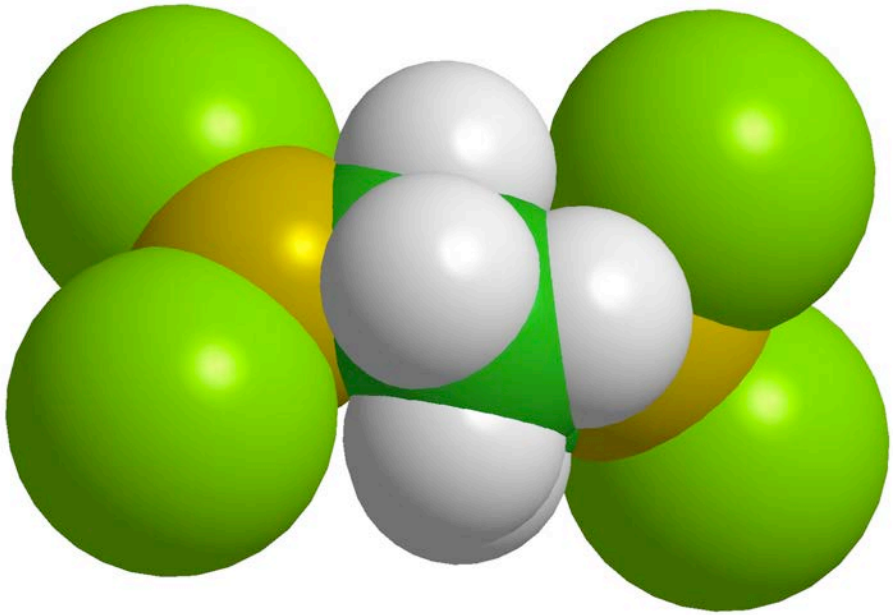


Propene B_2Cl_4 product trans B3LYP

- Zero-point correction= 0.096860 (Hartree/Particle)
- Thermal correction to Energy= 0.108124
- Thermal correction to Enthalpy= 0.109068
- Thermal correction to Gibbs Free Energy= 0.055652
- Sum of electronic and zero-point Energies= -2008.666947
- Sum of electronic and thermal Energies= -2008.655684
- Sum of electronic and thermal Enthalpies= -2008.654739
- Sum of electronic and thermal Free Energies= -2008.708155

- B2Cl4PPT

- 0 1
- C 0.47452000 -0.27011300 -0.49224600
- H 0.32275100 -1.30452000 -0.81789300
- B 1.99600100 -0.02683800 -0.21186700
- Cl 3.21572700 -1.00671600 -1.02871800
- Cl 2.56355300 1.27599700 0.83375000
- C -0.36501000 -0.84759600 1.85181900
- H -0.53213200 -1.89010600 1.57011400
- H -1.07159400 -0.60406800 2.64896900
- H 0.64170000 -0.76815000 2.27134300
- C -0.53163900 0.09302400 0.64525500
- H -0.30814200 1.11743600 0.96292400
- B -1.97214900 0.10998800 0.02044400
- Cl -2.56285300 1.54915300 -0.82036900
- Cl -3.03479800 -1.29853600 0.05529200
- H 0.27323200 0.34349200 -1.38655100

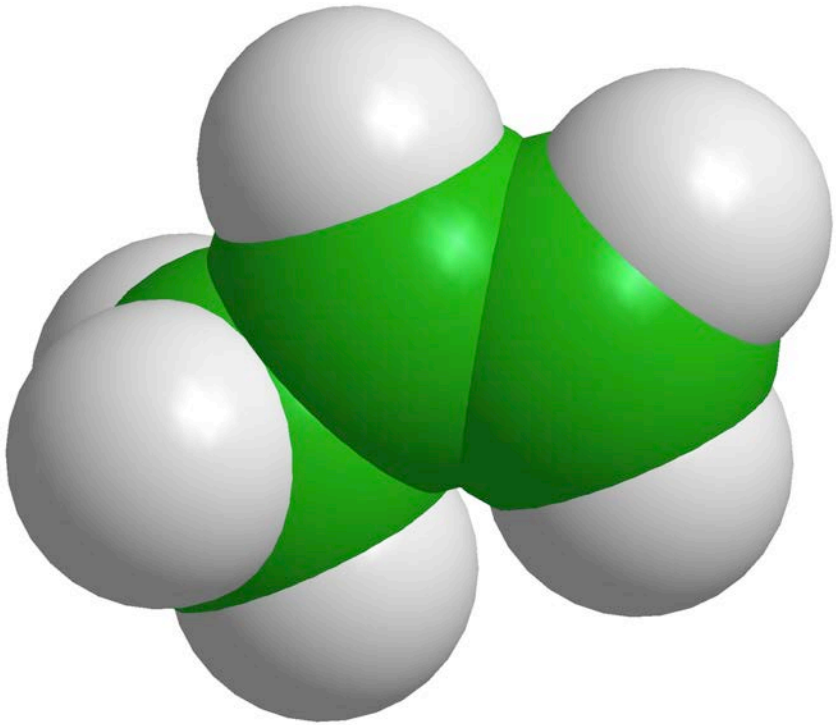


Propene ωB97X-D

- Zero-point correction= 0.079846 (Hartree/Particle)
- Thermal correction to Energy= 0.083965
- Thermal correction to Enthalpy= 0.084910
- Thermal correction to Gibbs Free Energy= 0.054776
- Sum of electronic and zero-point Energies= -117.816761
- Sum of electronic and thermal Energies= -117.812642
- Sum of electronic and thermal Enthalpies= -117.811698
- Sum of electronic and thermal Free Energies= -117.841831

- PropeneW

- 0 1
- C 1.27622300 0.22096300 -0.00004200
- H 1.29206800 1.30746200 -0.00012800
- H 2.23535400 -0.28472800 -0.00001400
- C 0.13459900 -0.45427700 0.00001700
- H 0.16868900 -1.54238100 0.00009000
- C -1.23053600 0.16217100 0.00001800
- H -1.17530900 1.25320600 -0.00031800
- H -1.80139700 -0.15362300 -0.87914300
- H -1.80112500 -0.15308000 0.87955700

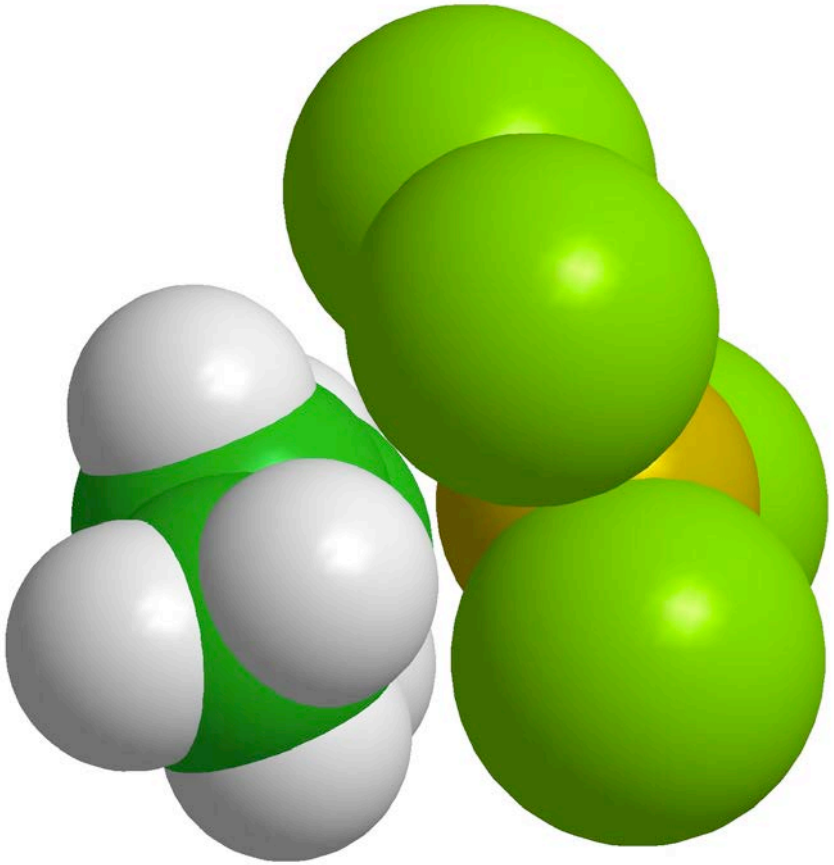


Propene B_2Cl_4 vdW ωB97X-D

- Zero-point correction= 0.094985 (Hartree/Particle)
- Thermal correction to Energy= 0.107635
- Thermal correction to Enthalpy= 0.108580
- Thermal correction to Gibbs Free Energy= 0.053283
- Sum of electronic and zero-point Energies= -2008.494004
- Sum of electronic and thermal Energies= -2008.481354
- Sum of electronic and thermal Enthalpies= -2008.480409
- Sum of electronic and thermal Free Energies= -2008.535706

- B2Cl4PVW

- 0 1
- C -1.86513500 -0.42274300 -1.51985700
- H -2.17527600 0.61253800 -1.65381100
- B 0.14343600 1.01736200 0.39829000
- Cl -1.13564800 1.36021100 1.55364300
- Cl 0.64948400 2.31434300 -0.67130100
- C -0.73428000 -0.82936800 -2.09553800
- H -0.12884900 -0.15928300 -2.69544600
- B 0.93164700 -0.50459200 0.39092200
- C -2.76847300 -1.28389900 -0.69752800
- H -2.90354900 -0.85868400 0.30198700
- H -2.37326000 -2.29618400 -0.59328100
- H -3.76029900 -1.34245600 -1.15624300
- Cl 0.29907300 -1.85596500 1.31813300
- Cl 2.45575800 -0.72718300 -0.45136900
- H -0.39419800 -1.85761600 -2.00654200

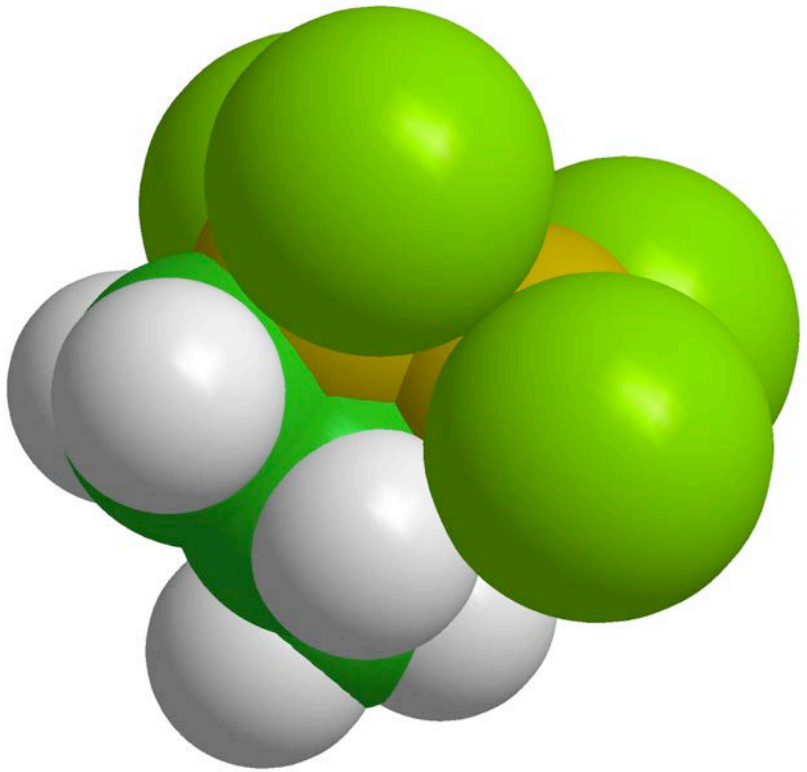


Propene B_2Cl_4 TS1 ωB97X-D

- Zero-point correction= 0.096395 (Hartree/Particle)
- Thermal correction to Energy= 0.107028
- Thermal correction to Enthalpy= 0.107972
- Thermal correction to Gibbs Free Energy= 0.058413
- Sum of electronic and zero-point Energies= -2008.468794
- Sum of electronic and thermal Energies= -2008.458162
- Sum of electronic and thermal Enthalpies= -2008.457217
- Sum of electronic and thermal Free Energies= -2008.506777

- B2Cl4P1TSWa

- 0 1
- C -0.35434500 -0.45740000 1.67178800
- H 0.52992200 -0.05422700 2.15039700
- B 0.87174900 -0.14759400 -0.14714600
- Cl 1.11235000 -1.28594000 -1.45277800
- Cl 2.35016500 0.53460300 0.54889800
- C -1.49446700 0.40381500 1.63912700
- H -1.40696500 1.35655900 2.14719700
- B -0.86278800 0.44034700 0.11307300
- C -0.47390800 -1.95433300 1.65408700
- H 0.46740600 -2.44742400 1.40930000
- H -1.24924600 -2.28736000 0.96373600
- H -0.76368900 -2.25434800 2.66642400
- Cl -1.98453800 -0.43093400 -1.05000200
- Cl -0.37257300 2.14233600 -0.43474000
- H -2.47778200 -0.05055900 1.64989800

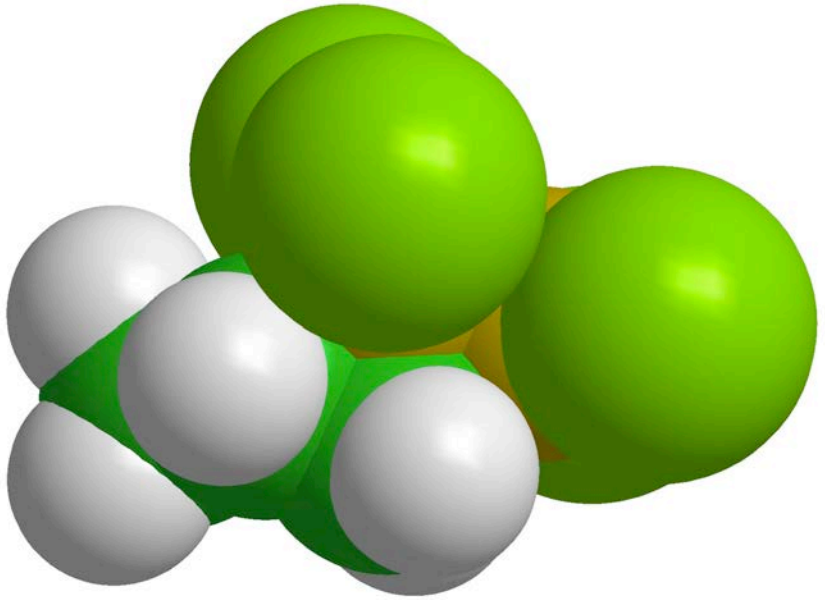


Propene B_2Cl_4 TS2 ωB97X-D

- Zero-point correction= 0.096460 (Hartree/Particle)
- Thermal correction to Energy= 0.107027
- Thermal correction to Enthalpy= 0.107971
- Thermal correction to Gibbs Free Energy= 0.058839
- Sum of electronic and zero-point Energies= -2008.465954
- Sum of electronic and thermal Energies= -2008.455387
- Sum of electronic and thermal Enthalpies= -2008.454443
- Sum of electronic and thermal Free Energies= -2008.503575

- B2Cl4P2TSW

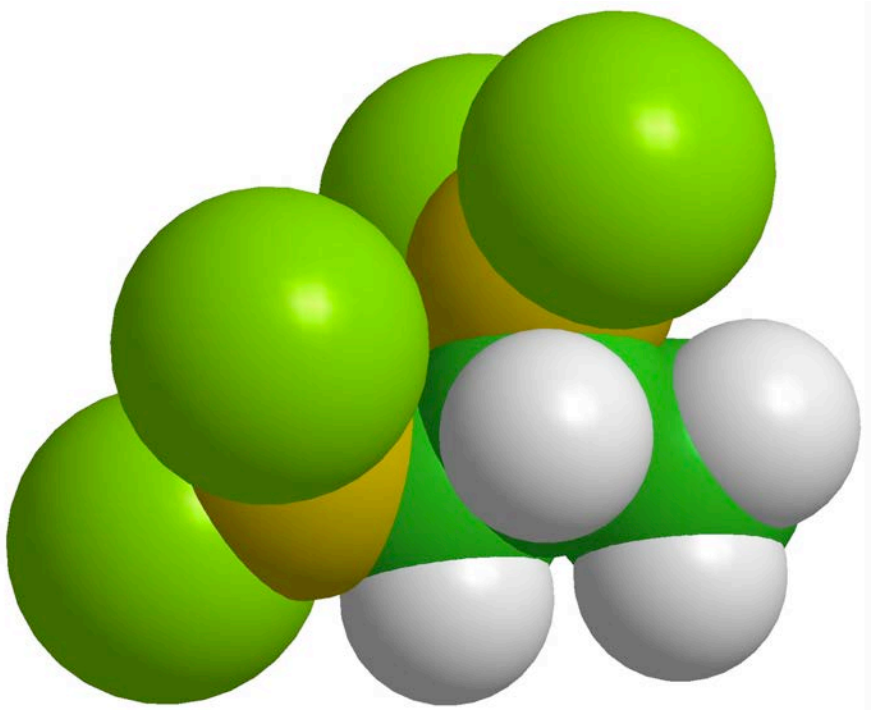
- 0 1
- C -0.40056600 -0.11426300 1.58335800
- H 0.15698600 0.66152600 2.09922500
- B 1.08015500 -0.24846000 0.13774400
- Cl 1.53185600 -1.92720000 -0.14431900
- Cl 2.39681100 0.88707300 0.34550700
- C -1.73384800 0.15688200 1.17217600
- H -2.11393600 1.14253400 1.41337700
- B -0.64375600 0.37034600 -0.13931300
- C -2.76236900 -0.93977700 1.07906600
- H -2.30659200 -1.91001900 0.87414500
- H -3.47913600 -0.73123800 0.28306900
- H -3.30956200 -1.00680400 2.02384500
- Cl -1.15603200 -0.67137300 -1.55938600
- Cl -0.51452600 2.16794200 -0.49533000
- H -0.13691300 -1.14201300 1.81655800



Propene B_2Cl_4 product ωB97X-D

- Zero-point correction= 0.097833 (Hartree/Particle)
- Thermal correction to Energy= 0.108938
- Thermal correction to Enthalpy= 0.109882
- Thermal correction to Gibbs Free Energy= 0.057921
- Sum of electronic and zero-point Energies= -2008.549526
- Sum of electronic and thermal Energies= -2008.538421
- Sum of electronic and thermal Enthalpies= -2008.537477
- Sum of electronic and thermal Free Energies= -2008.589439
- B2Cl4PPGW

- 0 1
- C -0.77396200 1.26093300 -0.25476300
- H -0.78351300 1.71054600 0.74736900
- B -1.74735300 0.03958300 -0.22457700
- Cl -1.24642800 -1.57134700 -0.73530800
- Cl -3.40968100 0.24670500 0.31134200
- C 0.66687400 1.02222600 -0.72833800
- B 1.49507200 0.01093900 0.14230900
- Cl 1.23132400 -0.14595700 1.87917000
- Cl 2.81408100 -0.91198400 -0.56604200
- H -1.24819500 2.02191800 -0.89174500
- H 0.64299900 0.62780900 -1.75012500
- C 1.45566800 2.35219200 -0.76391100
- H 0.93848500 3.07401000 -1.40180700
- H 1.53814000 2.78969100 0.23557900
- H 2.46395500 2.21521400 -1.16161100

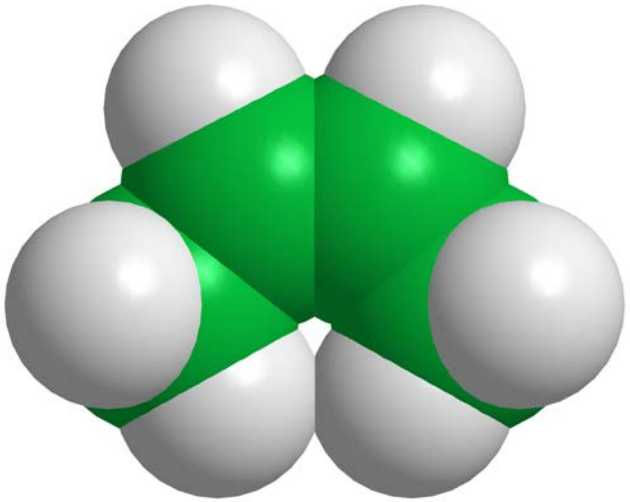


Z-butene B3LYP

- Zero-point correction= 0.107528 (Hartree/Particle)
- Thermal correction to Energy= 0.113063
- Thermal correction to Enthalpy= 0.114007
- Thermal correction to Gibbs Free Energy= 0.079646
- Sum of electronic and zero-point Energies= -157.163588
- Sum of electronic and thermal Energies= -157.158054
- Sum of electronic and thermal Enthalpies= -157.157110
- Sum of electronic and thermal Free Energies= -157.191471

- C2B

- 0 1
- C 0.66717900 0.66371400 0.00000100
- H 1.16520600 1.63140300 -0.00002700
- C -0.66718300 0.66371500 0.00000900
- H -1.16520600 1.63140600 -0.00001000
- C -1.58946900 -0.52189800 -0.00000300
- H -2.24485500 -0.50383300 0.87816500
- H -2.24510400 -0.50361700 -0.87798300
- H -1.05873500 -1.47486200 -0.00019500
- C 1.58947200 -0.52189800 -0.00000300
- H 2.24484700 -0.50380800 0.87817500
- H 1.05874300 -1.47486500 -0.00017500
- H 2.24511200 -0.50362500 -0.87797500

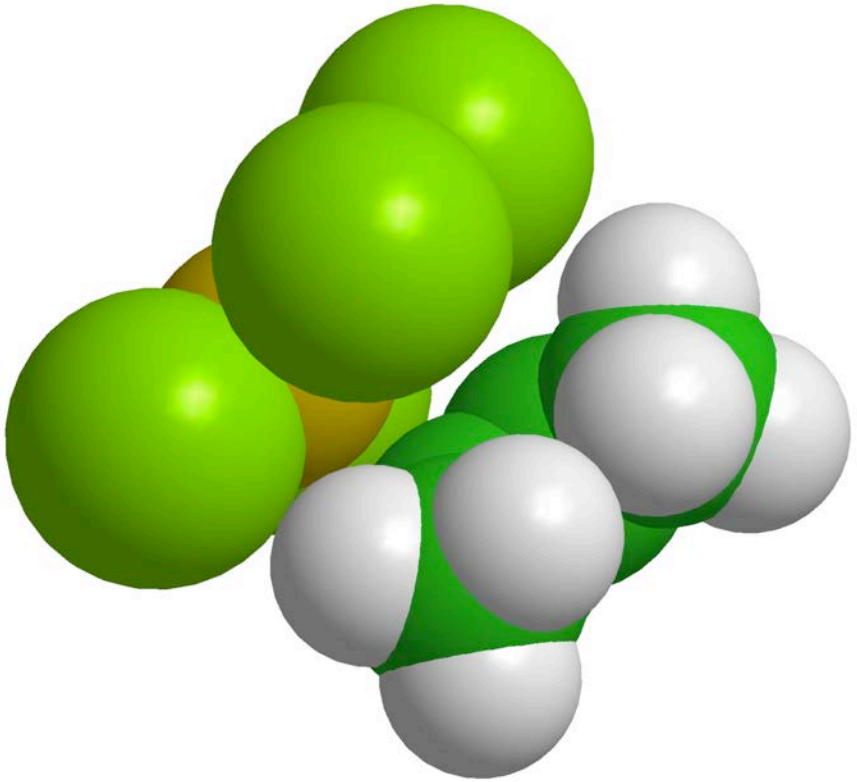


Z-butene B_2Cl_4 vdW B3LYP

- Zero-point correction= 0.121706 (Hartree/Particle)
- Thermal correction to Energy= 0.136271
- Thermal correction to Enthalpy= 0.137215
- Thermal correction to Gibbs Free Energy= 0.076402
- Sum of electronic and zero-point Energies= -2047.919465
- Sum of electronic and thermal Energies= -2047.904900
- Sum of electronic and thermal Enthalpies= -2047.903956
- Sum of electronic and thermal Free Energies= -2047.964769

- B2Cl4MV

- 0 1
- C 1.35300200 -1.61759900 -0.90974800
- H 0.48114400 -2.03524300 -1.40901300
- B -1.38065200 -0.14053600 -0.05783500
- Cl -1.99025600 -1.48248000 0.90776000
- Cl -2.04488100 0.07431600 -1.67489900
- C 1.84516200 -0.46955500 -1.39986900
- H 1.32736400 -0.03151400 -2.25034500
- B -0.25966200 0.96660600 0.59725400
- C 3.06750000 0.27248400 -0.94801000
- H 3.52664400 -0.15847000 -0.05817000
- H 2.83167500 1.32062900 -0.73620600
- H 3.81927100 0.27948300 -1.74544300
- C 1.89152200 -2.44133900 0.22153200
- H 1.11344200 -2.62988900 0.96846300
- H 2.73749700 -1.97446400 0.72604500
- H 2.21586600 -3.42175600 -0.14526800
- Cl 0.57225500 0.64049600 2.11459600
- Cl 0.00438500 2.53572300 -0.16102100

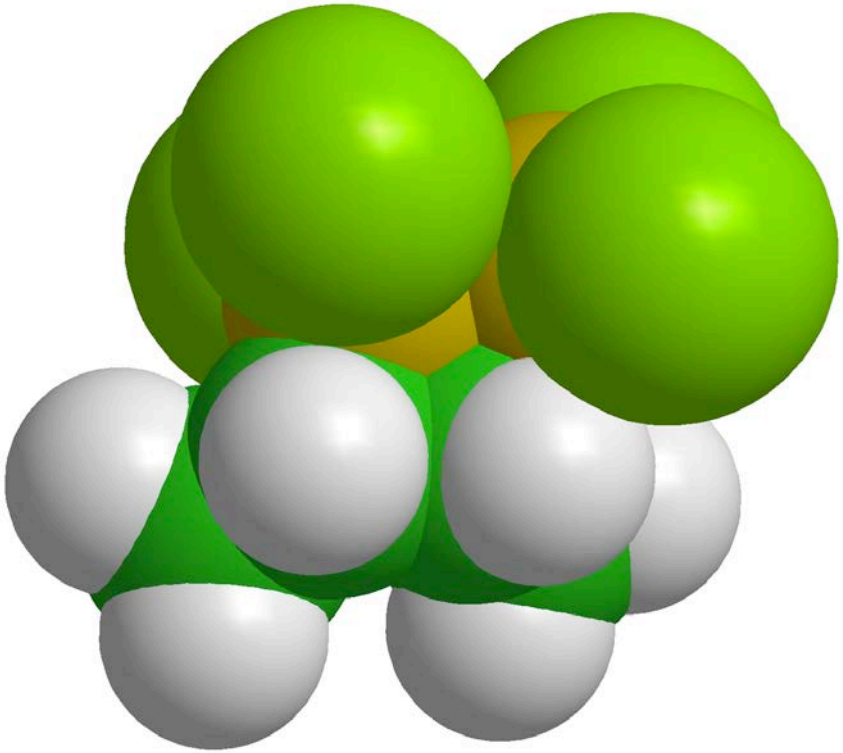


Z-butene B_2Cl_4 TS B3LYP

- Zero-point correction= 0.123115 (Hartree/Particle)
- Thermal correction to Energy= 0.135423
- Thermal correction to Enthalpy= 0.136367
- Thermal correction to Gibbs Free Energy= 0.083527
- Sum of electronic and zero-point Energies= -2047.881218
- Sum of electronic and thermal Energies= -2047.868910
- Sum of electronic and thermal Enthalpies= -2047.867966
- Sum of electronic and thermal Free Energies= -2047.920806

- BCscan2101TSfreq

- 0 1
- C 0.53417400 -0.57990900 -1.35508500
- H -0.17444200 -0.25964200 -2.10912600
- B -1.12493300 -0.17734100 -0.05424100
- Cl -1.70066200 -1.30876300 1.15534800
- Cl -2.37093900 0.49891600 -1.12121500
- C 1.62860800 0.34644900 -1.11192100
- H 1.55031400 1.24886000 -1.71316300
- B 0.62475400 0.49633600 0.18055000
- C 3.06161600 -0.11570300 -0.92092600
- H 3.13708800 -1.03472800 -0.34174500
- H 3.63365300 0.64976700 -0.39301400
- H 3.53687800 -0.28031600 -1.89339000
- C 0.68491600 -2.07229600 -1.19867900
- H -0.26658700 -2.59554800 -1.29208700
- H 1.14845400 -2.34563600 -0.25134700
- H 1.34294300 -2.41403500 -2.00608500
- Cl 1.32730500 -0.24614500 1.71093100
- Cl -0.01236700 2.23040800 0.42482300

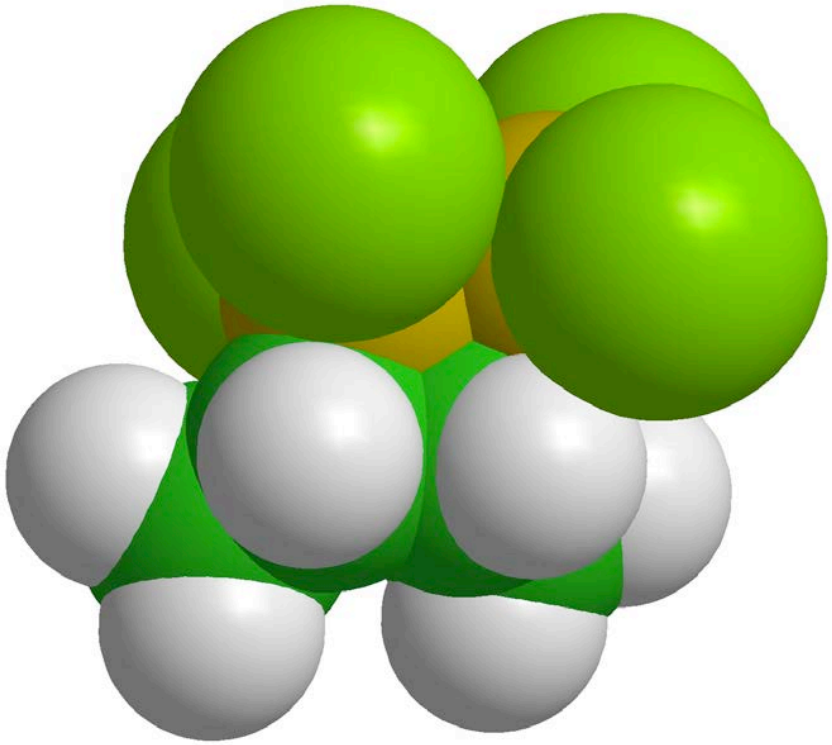


Z-butene B_2Cl_4 gauche product B3LYP

- Zero-point correction= 0.124808 (Hartree/Particle)
- Thermal correction to Energy= 0.137369
- Thermal correction to Enthalpy= 0.138313
- Thermal correction to Gibbs Free Energy= 0.083181
- Sum of electronic and zero-point Energies= -2047.957634
- Sum of electronic and thermal Energies= -2047.945073
- Sum of electronic and thermal Enthalpies= -2047.944129
- Sum of electronic and thermal Free Energies= -2047.999261

- B2Cl4SRPG

- 0 1
- C 0.83037100 0.98178200 -0.45457500
- H 0.49506500 0.87080800 -1.49784400
- B 1.56671400 -0.37845000 -0.17174400
- Cl 0.65324600 -1.89632800 -0.14272200
- Cl 3.30825900 -0.49722500 0.07431300
- C -0.17220300 1.12690000 1.92601400
- H 0.13272200 0.13023900 2.25767600
- H -1.05253400 1.40267500 2.50880700
- H 0.62512800 1.82687700 2.18514400
- C 1.73072900 2.23020500 -0.40741000
- H 2.57050000 2.13764800 -1.09884100
- H 2.14941700 2.40036500 0.58668500
- H 1.16176400 3.11990300 -0.69125800
- C -0.46749100 1.15561200 0.41482500
- H -0.83234500 2.16920200 0.17124000
- B -1.68903500 0.27194500 -0.04206100
- Cl -2.14918400 0.19349500 -1.75282200
- Cl -2.76329400 -0.53477700 1.10207200

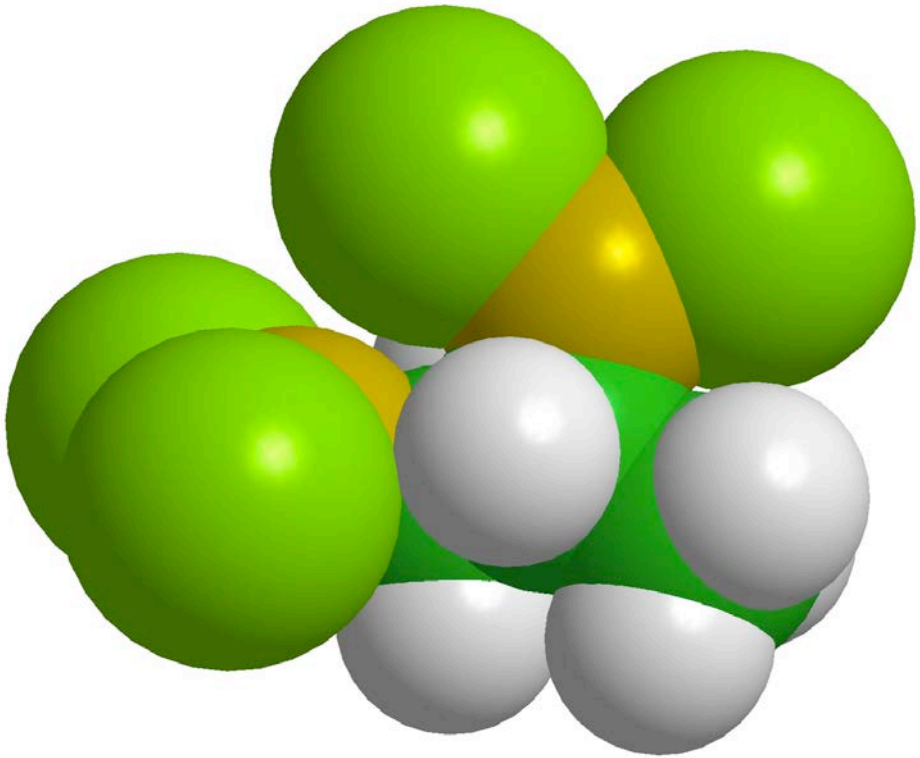


Z-butene B_2Cl_4 trans-product B3LYP

- Zero-point correction= 0.125016 (Hartree/Particle)
- Thermal correction to Energy= 0.137827
- Thermal correction to Enthalpy= 0.138771
- Thermal correction to Gibbs Free Energy= 0.082573
- Sum of electronic and zero-point Energies= -2047.959578
- Sum of electronic and thermal Energies= -2047.946767
- Sum of electronic and thermal Enthalpies= -2047.945822
- Sum of electronic and thermal Free Energies= -2048.002021

- B2CL4SRPT

- 0 1
- C 0.52839900 -0.42827600 -0.37637300
- H 0.39930100 -1.47426800 -0.07941300
- B 2.01481200 -0.02124700 -0.06952300
- Cl 3.25386100 -1.24410100 0.22231100
- Cl 2.53797300 1.66790400 -0.09953700
- C -0.33863700 0.35099400 1.91700000
- H -0.41443300 -0.67971900 2.27277300
- H -1.08583100 0.94716100 2.44727700
- H 0.64331900 0.73779700 2.20425500
- C 0.33869000 -0.35087100 -1.91706300
- H 1.08589600 -0.94702700 -2.44733600
- H 0.41452300 0.67985800 -2.27278300
- H -0.64326000 -0.73764100 -2.20438100
- C -0.52841400 0.42832200 0.37631500
- H -0.39935700 1.47430400 0.07930400
- B -2.01483000 0.02123600 0.06954800
- Cl -3.25390200 1.24403900 -0.22240100
- Cl -2.53795000 -1.66792600 0.09968000

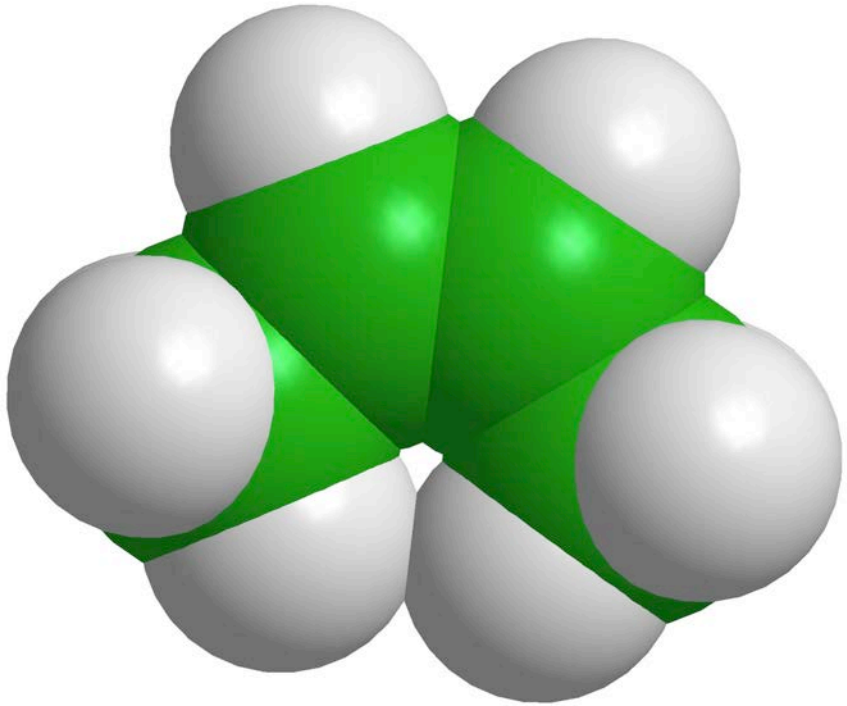


Z-butene ωB97X-D

- Zero-point correction= 0.108417 (Hartree/Particle)
- Thermal correction to Energy= 0.114058
- Thermal correction to Enthalpy= 0.115002
- Thermal correction to Gibbs Free Energy= 0.080020
- Sum of electronic and zero-point Energies= -157.103034
- Sum of electronic and thermal Energies= -157.097393
- Sum of electronic and thermal Enthalpies= -157.096449
- Sum of electronic and thermal Free Energies= -157.131431

- B2Cl4ZW

- 0 1
- C 1.58163000 -0.52261800 0.00000800
- H 1.04697200 -1.47351100 -0.00023300
- H 2.23430800 -0.50455700 0.87898900
- H 2.23464300 -0.50430300 -0.87871600
- C 0.66539200 0.66447200 0.00000300
- H 1.16471000 1.63125200 0.00001900
- C -0.66539000 0.66446900 -0.00000200
- H -1.16471200 1.63124800 0.00000100
- C -1.58163100 -0.52261700 -0.00001200
- H -2.23455800 -0.50436500 0.87877800
- H -2.23439300 -0.50448400 -0.87892800
- H -1.04697900 -1.47351300 0.00010800

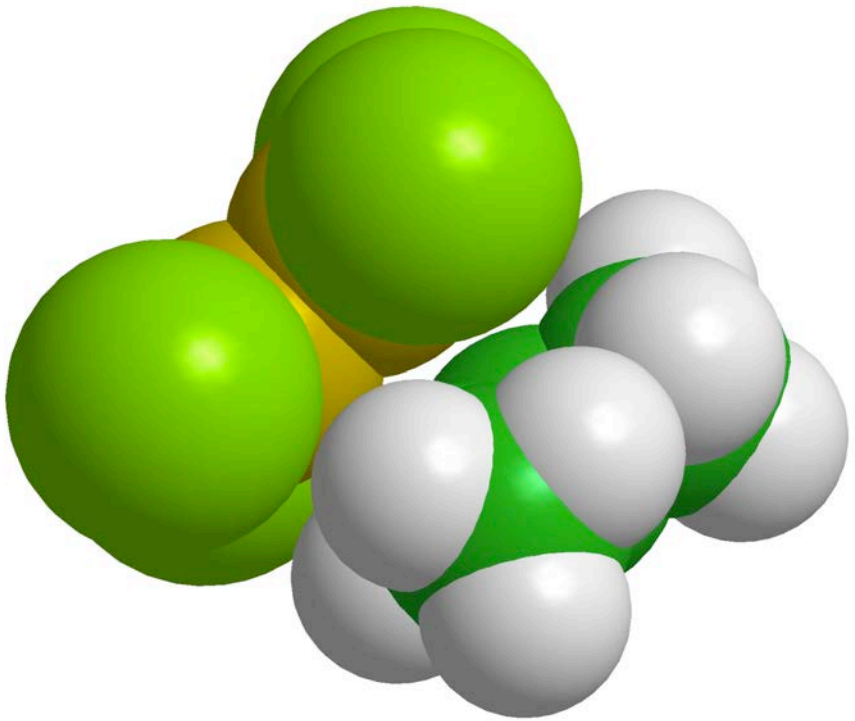


Z-butene B_2Cl_4 vdW ωB97X-D

- Zero-point correction= 0.124044 (Hartree/Particle)
- Thermal correction to Energy= 0.137835
- Thermal correction to Enthalpy= 0.138780
- Thermal correction to Gibbs Free Energy= 0.081530
- Sum of electronic and zero-point Energies= -2047.782462
- Sum of electronic and thermal Energies= -2047.768670
- Sum of electronic and thermal Enthalpies= -2047.767726
- Sum of electronic and thermal Free Energies= -2047.824976

- B2Cl4ZVW

- 0 1
- C 0.92106400 -1.64413900 -1.09958400
- H -0.02087600 -1.89403400 -1.58460300
- B -1.34869800 0.04152700 0.02434700
- Cl -2.08397800 -1.27044900 0.93367700
- Cl -2.09696600 0.50393400 -1.49663000
- C 1.55630100 -0.54730100 -1.52945400
- H 1.07733400 0.02625400 -2.32033300
- B -0.01203700 0.90290300 0.65470200
- C 2.89144300 -0.03726500 -1.08235600
- H 3.26280900 -0.54026700 -0.18920000
- H 2.84700000 1.03596400 -0.87578000
- H 3.62935200 -0.17414300 -1.87963900
- C 1.37936200 -2.61464100 -0.05683100
- H 0.60946400 -2.74772900 0.70945800
- H 2.29996200 -2.30519300 0.43807100
- H 1.54995500 -3.59640300 -0.50979500
- Cl 0.90036100 0.30580700 2.03212500
- Cl 0.40174000 2.49209000 0.02647100



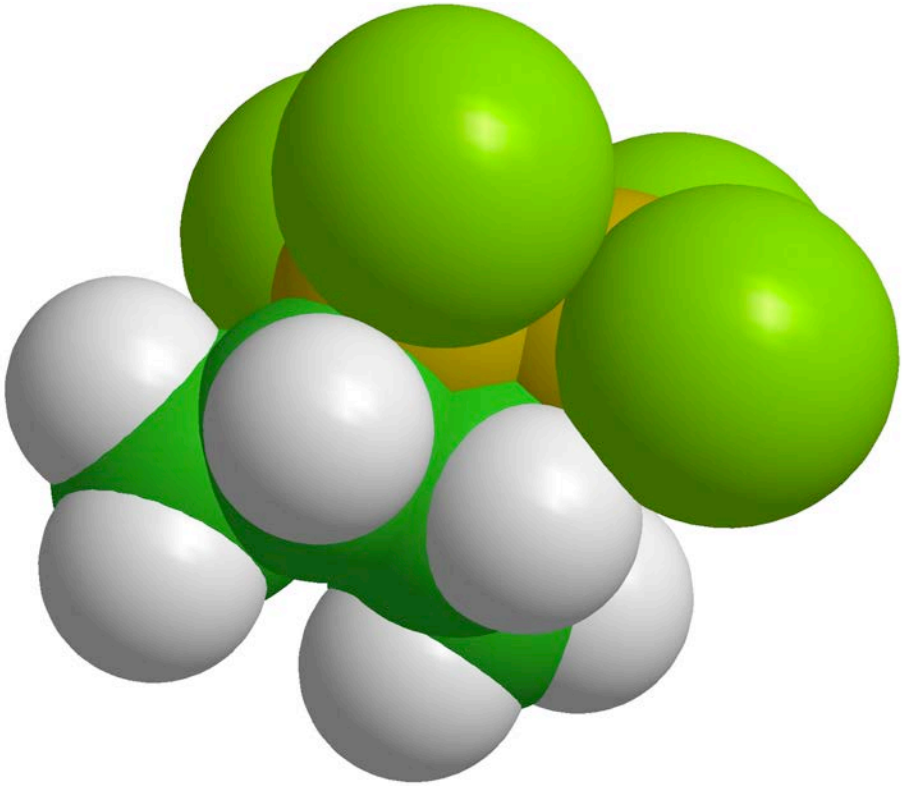
Z-butene B_2Cl_4 TS ωB97X-D

- Zero-point correction= 0.125149 (Hartree/Particle)
- Thermal correction to Energy= 0.137051
- Thermal correction to Enthalpy= 0.137995
- Thermal correction to Gibbs Free Energy= 0.086298
- Sum of electronic and zero-point Energies= -2047.753945
- Sum of electronic and thermal Energies= -2047.742043
- Sum of electronic and thermal Enthalpies= -2047.741099
- Sum of electronic and thermal Free Energies= -2047.792795

- B2Cl4ZTSW

- 0 1

C	0.51054600	-0.49710100	-1.38147800
H	-0.19271700	-0.10006600	-2.10503400
B	-1.12304900	-0.16534700	-0.04008200
Cl	-1.68701700	-1.38890700	1.07664400
Cl	-2.37540900	0.59772800	-1.02607300
C	1.64174100	0.34907500	-1.09927900
H	1.62167800	1.28885200	-1.64344300
B	0.61325800	0.49123500	0.19509400
C	3.03347800	-0.20222100	-0.89023000
H	3.03405900	-1.16578300	-0.38212800
H	3.62259100	0.48730600	-0.28326200
H	3.53343700	-0.32071300	-1.85611600
C	0.59779200	-1.99882300	-1.30195200
H	-0.36809900	-2.47639200	-1.46441000
H	1.00355000	-2.33526700	-0.34729000
H	1.28388000	-2.32082600	-2.09179500
Cl	1.30081400	-0.30769700	1.69471900
Cl	0.07392000	2.24051500	0.45683100

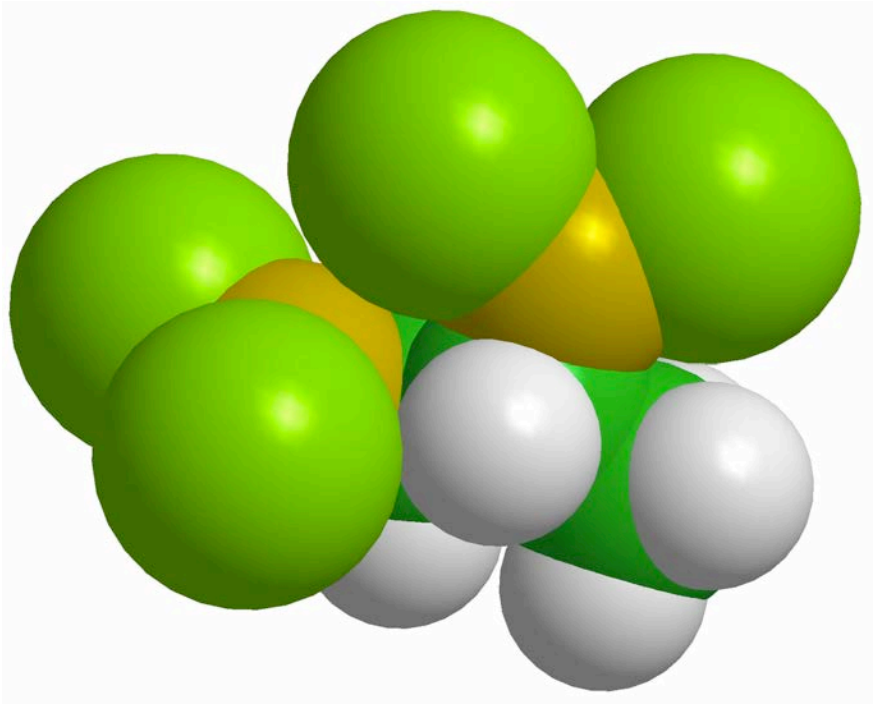


Z-butene B_2Cl_4 gauche product ωB97X-D

- Zero-point correction= 0.126340 (Hartree/Particle)
- Thermal correction to Energy= 0.138695
- Thermal correction to Enthalpy= 0.139640
- Thermal correction to Gibbs Free Energy= 0.085181
- Sum of electronic and zero-point Energies= -2047.830166
- Sum of electronic and thermal Energies= -2047.817810
- Sum of electronic and thermal Enthalpies= -2047.816866
- Sum of electronic and thermal Free Energies= -2047.871325

- B2Cl4ZPW

- 0 1
- C 0.81910500 1.00105000 -0.46509200
- H 0.45394700 0.93255000 -1.50062100
- B 1.54260800 -0.37486400 -0.22810400
- Cl 0.62368600 -1.88109700 -0.31982600
- Cl 3.26064500 -0.51008900 0.11085800
- C -0.07867700 1.01915700 1.94291400
- H 0.21380100 -0.00381500 2.20068300
- H -0.92565100 1.27991600 2.57964700
- H 0.74773700 1.68330000 2.20537500
- C 1.73305000 2.22969000 -0.38851900
- H 2.55272700 2.15646000 -1.10633900
- H 2.18027900 2.34974300 0.60095600
- H 1.16816200 3.13745800 -0.61741800
- C -0.43476600 1.14182600 0.45556100
- H -0.80343700 2.16815200 0.28467000
- B -1.67591100 0.28409500 0.00161700
- Cl -2.20272900 0.29899200 -1.68482400
- Cl -2.69062100 -0.59017400 1.14180900

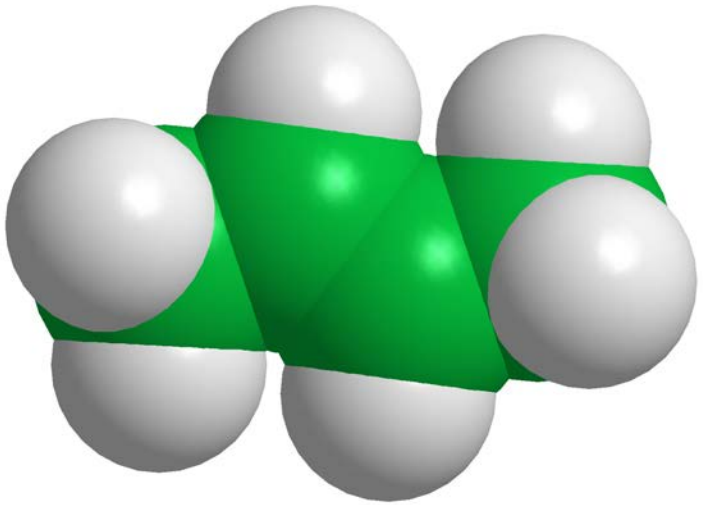


E-butene B3LYP

- Zero-point correction= 0.107435 (Hartree/Particle)
- Thermal correction to Energy= 0.112913
- Thermal correction to Enthalpy= 0.113857
- Thermal correction to Gibbs Free Energy= 0.080043
- Sum of electronic and zero-point Energies= -157.165726
- Sum of electronic and thermal Energies= -157.160248
- Sum of electronic and thermal Enthalpies= -157.159304
- Sum of electronic and thermal Free Energies= -157.193118

- E2B

- 0 1
- C 0.53645000 -0.39412900 -0.00010100
- H 0.39034200 -1.47429200 -0.00015900
- C -0.53647100 0.39409300 -0.00011000
- H -0.39010400 1.47422900 -0.00015500
- C -1.96090100 -0.07908100 0.00005800
- H -2.50164100 0.28896900 0.87942800
- H -2.50262600 0.29121000 -0.87772600
- H -2.02075200 -1.17026900 -0.00125800
- C 1.96089800 0.07912000 0.00006200
- H 2.50241100 -0.29067000 -0.87808100
- H 2.02074500 1.17029200 -0.00061800
- H 2.50176500 -0.28948900 0.87911700

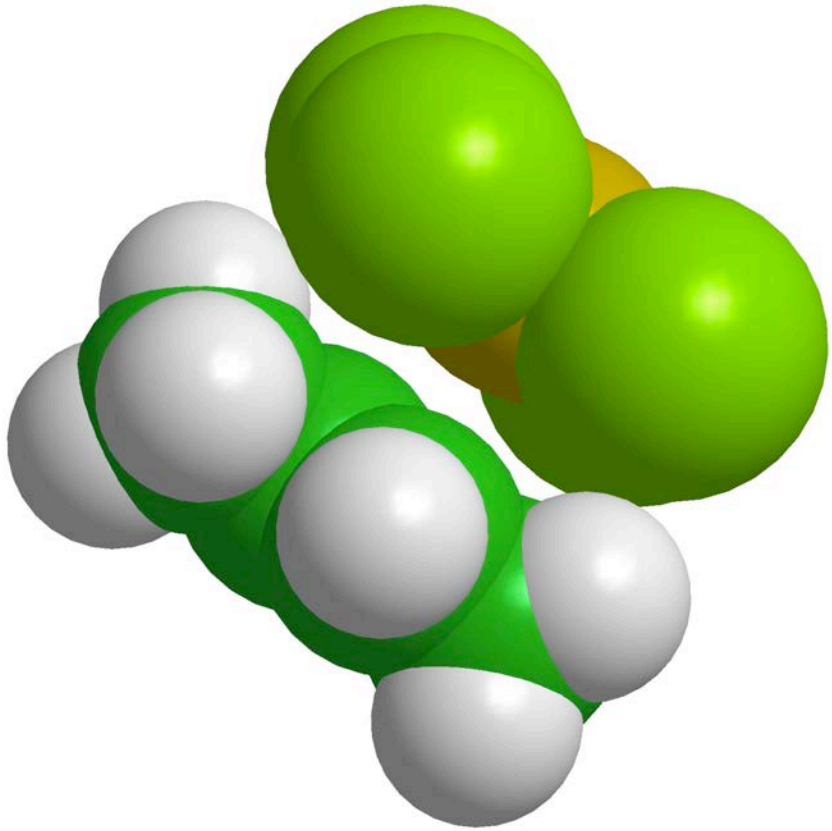


E-butene B_2Cl_4 vdW B3LYP

- Zero-point correction= 0.121485 (Hartree/Particle)
- Thermal correction to Energy= 0.136061
- Thermal correction to Enthalpy= 0.137006
- Thermal correction to Gibbs Free Energy= 0.076007
- Sum of electronic and zero-point Energies= -2047.920989
- Sum of electronic and thermal Energies= -2047.906412
- Sum of electronic and thermal Enthalpies= -2047.905468
- Sum of electronic and thermal Free Energies= -2047.966467

- B2Cl4TV

- 0 1
- C -2.32174600 0.70266700 -0.22001200
- H -2.30100500 0.92206300 -1.28732800
- B 0.95001800 0.31132900 -0.77463500
- Cl 1.17053300 2.04266200 -1.01103200
- Cl 0.88223500 -0.71028600 -2.20539400
- C -2.37220400 -0.57804600 0.16513300
- B 0.90930000 -0.36064300 0.79641000
- C -2.36013500 1.88744700 0.69847100
- H -1.50526800 2.55157500 0.53548900
- H -2.36424900 1.58491700 1.74767100
- H -3.26013500 2.48462500 0.51323100
- Cl 0.86274400 0.66457700 2.22548300
- Cl 1.02386200 -2.10160900 1.03709100
- H -2.41179100 -0.79636900 1.23214400
- C -2.44658900 -1.75975400 -0.75483600
- H -2.38728700 -1.46005400 -1.80311000
- H -1.64284600 -2.47604300 -0.55605500
- H -3.38932800 -2.29888100 -0.60797200

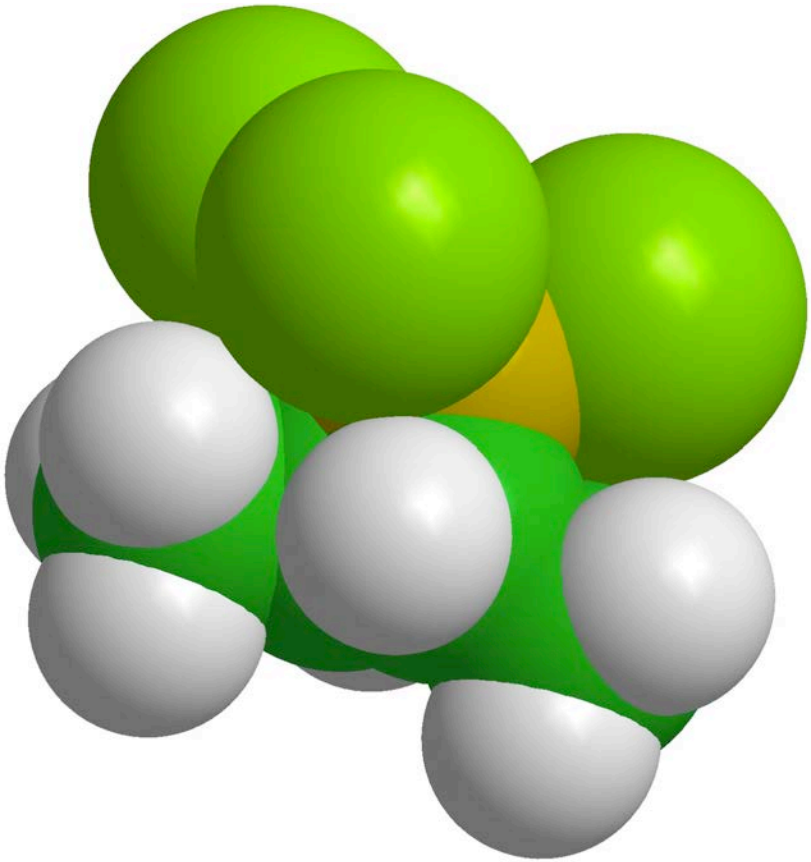


E-butene B_2Cl_4 TS B3LYP

- Zero-point correction= 0.123061 (Hartree/Particle)
- Thermal correction to Energy= 0.135384
- Thermal correction to Enthalpy= 0.136328
- Thermal correction to Gibbs Free Energy= 0.083556
- Sum of electronic and zero-point Energies= -2047.883497
- Sum of electronic and thermal Energies= -2047.871174
- Sum of electronic and thermal Enthalpies= -2047.870229
- Sum of electronic and thermal Free Energies= -2047.923002

- B2Cl4TTSF

- 0 1
- C 1.88263200 -0.13075900 0.75177700
- H 2.47185900 0.74960600 0.99286000
- C 0.61800100 -0.22150400 1.45654700
- B -1.03705000 -0.24046000 0.05125300
- C 2.70315700 -1.38791300 0.51738400
- H 3.36113300 -1.26214800 -0.34476800
- H 2.07182000 -2.25727100 0.32442200
- H 3.32636900 -1.60516800 1.39044600
- Cl -1.66368900 -1.89631900 0.20805000
- Cl -2.25160600 1.01369500 -0.11034400
- H 0.28260200 -1.23272700 1.65535900
- B 0.72630300 0.28881700 -0.33307100
- Cl 0.77118800 2.09654100 -0.68867700
- Cl 0.64779000 -0.76352900 -1.86886500
- C 0.16913700 0.82127300 2.44846800
- H -0.88667000 0.73399000 2.70734800
- H 0.37042600 1.83239700 2.09591400
- H 0.75602400 0.65637000 3.35966100

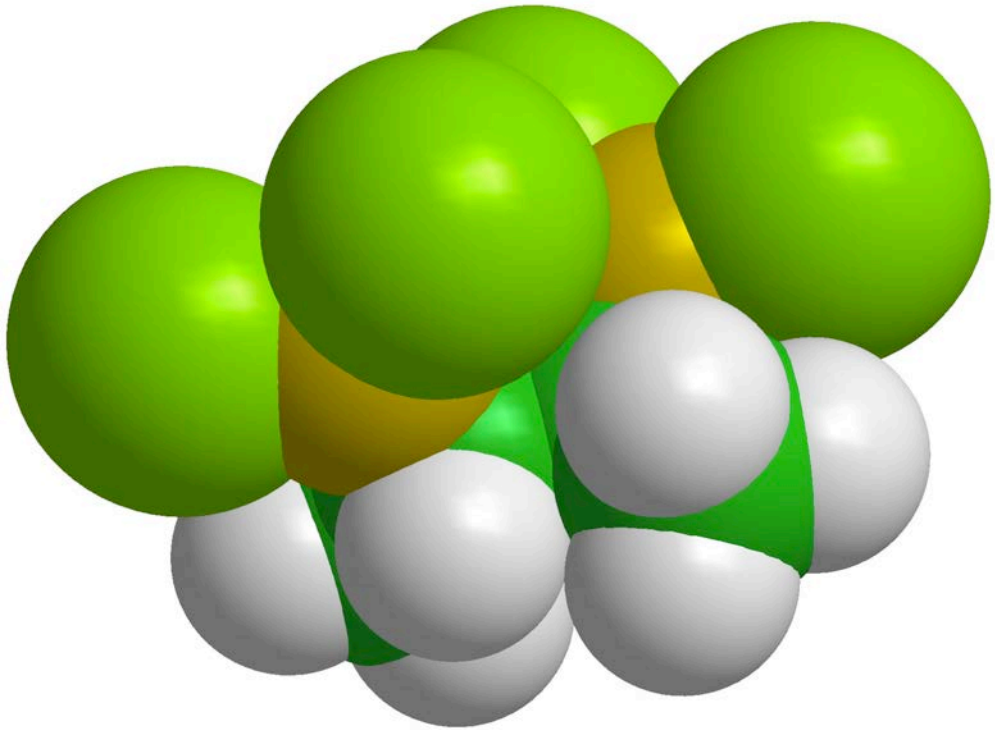


E-butene B_2Cl_4 gauche product B3LYP

- Zero-point correction= 0.124694 (Hartree/Particle)
- Thermal correction to Energy= 0.137283
- Thermal correction to Enthalpy= 0.138228
- Thermal correction to Gibbs Free Energy= 0.082623
- Sum of electronic and zero-point Energies= -2047.955016
- Sum of electronic and thermal Energies= -2047.942426
- Sum of electronic and thermal Enthalpies= -2047.941482
- Sum of electronic and thermal Free Energies= -2047.997087

- B2Cl4SSPG

- 0 1
- C 0.77919800 0.09191800 1.26403000
- H 1.15556700 -0.63671800 2.00584300
- B 1.53202700 -0.39186300 -0.02955100
- Cl 3.15246000 0.18024200 -0.43454300
- Cl 0.85931300 -1.64446200 -1.08984400
- C -1.21392600 -1.47170300 1.79139700
- H -0.90500500 -2.27309800 1.11790400
- H -2.29650900 -1.53537700 1.90777100
- H -0.76186800 -1.66040300 2.76930200
- C 1.21426800 1.47838700 1.78565000
- H 2.29686000 1.54238300 1.90175100
- H 0.76225200 1.67086200 2.76282700
- H 0.90544700 2.27723600 1.10913400
- C -0.77897900 -0.08720700 1.26447600
- H -1.15527800 0.64420900 2.00358500
- B -1.53201600 0.39171500 -0.03077200
- Cl -0.85990500 1.64106800 -1.09529500
- Cl -3.15215600 -0.18253700 -0.43383600

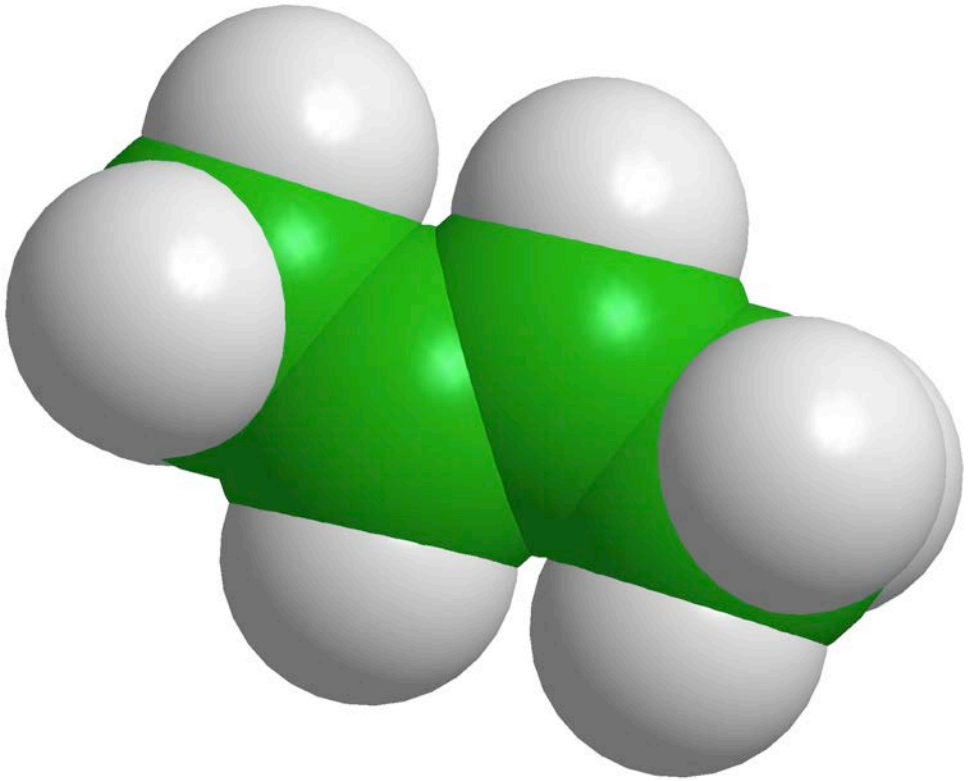


E-butene ωB97X-D

- Zero-point correction= 0.108232 (Hartree/Particle)
- Thermal correction to Energy= 0.113759
- Thermal correction to Enthalpy= 0.114703
- Thermal correction to Gibbs Free Energy= 0.080741
- Sum of electronic and zero-point Energies= -157.104732
- Sum of electronic and thermal Energies= -157.099205
- Sum of electronic and thermal Enthalpies= -157.098261
- Sum of electronic and thermal Free Energies= -157.132222

- EBW

- 0 1
- C 1.95589200 -0.07885100 0.00002500
- H 2.01337900 -1.17012200 -0.00004200
- H 2.49311100 0.29045800 0.87969900
- H 2.49316800 0.29057000 -0.87956700
- C 0.53404500 0.39454400 0.00000900
- H 0.38555900 1.47431300 0.00002100
- C -0.53404500 -0.39454400 -0.00001400
- H -0.38555900 -1.47431200 -0.00002900
- C -1.95589200 0.07885100 -0.00002200
- H -2.49314000 -0.29053100 -0.87964700
- H -2.49313800 -0.29049800 0.87961900
- H -2.01337900 1.17012200 -0.00004200

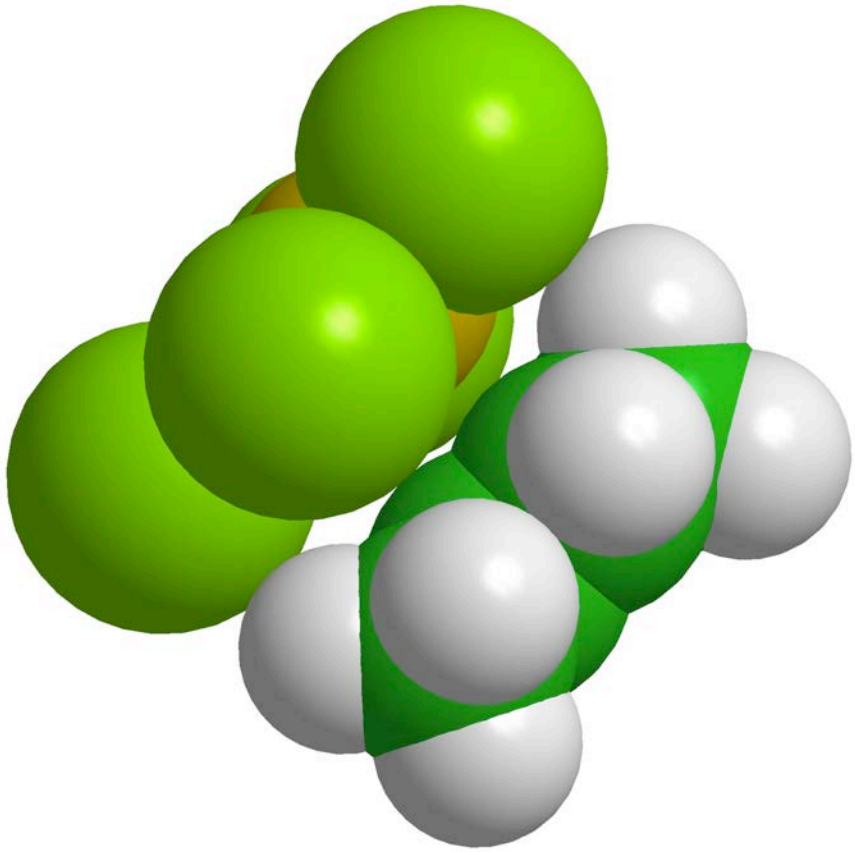


E-butene B_2Cl_4 vdW ωB97X-D

- Zero-point correction= 0.123644 (Hartree/Particle)
- Thermal correction to Energy= 0.137675
- Thermal correction to Enthalpy= 0.138620
- Thermal correction to Gibbs Free Energy= 0.079095
- Sum of electronic and zero-point Energies= -2047.782209
- Sum of electronic and thermal Energies= -2047.768177
- Sum of electronic and thermal Enthalpies= -2047.767233
- Sum of electronic and thermal Free Energies= -2047.826758

- EBNVW

- 0 1
- C 0.51295700 2.27229600 -0.42930000
- C -0.51491500 2.26932300 0.42161000
- H -0.30424500 2.26603900 1.49092300
- C -1.95729400 2.36664700 0.02796200
- H -2.08390400 2.30524900 -1.05484800
- H -2.56346200 1.58369100 0.49301700
- H -2.37048700 3.32297600 0.36481400
- B -0.85440800 -0.90957600 -0.04352500
- Cl -1.68408400 -0.81187200 -1.58488300
- Cl -1.82495600 -1.11713500 1.40415300
- C 1.95550500 2.36474500 -0.03515500
- H 2.36918800 3.32437200 -0.36178800
- H 2.08275200 2.29100500 1.04680600
- H 2.56063700 1.58621000 -0.50896600
- H 0.30220200 2.27788800 -1.49858700
- B 0.85509300 -0.90848000 0.04620400
- Cl 1.82598300 -1.12281700 -1.40016900
- Cl 1.68460900 -0.80142400 1.58704800

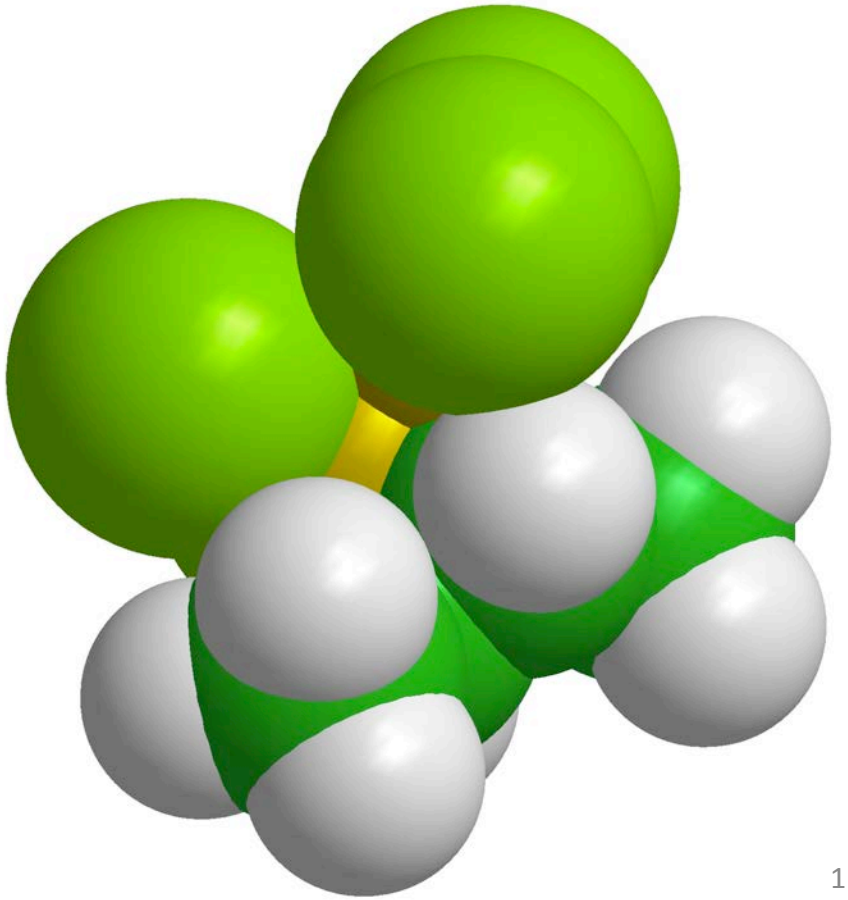


E-butene B_2Cl_4 TS ωB97X-D

- Zero-point correction= 0.124460 (Hartree/Particle)
- Thermal correction to Energy= 0.136672
- Thermal correction to Enthalpy= 0.137616
- Thermal correction to Gibbs Free Energy= 0.084734
- Sum of electronic and zero-point Energies= -2047.756259
- Sum of electronic and thermal Energies= -2047.744047
- Sum of electronic and thermal Enthalpies= -2047.743103
- Sum of electronic and thermal Free Energies= -2047.795985

- B2Cl4EBTSW

- 0 1
- C 1.90200200 -0.14250600 0.72914400
- H 2.48844700 0.73967600 0.96872100
- C 0.65958700 -0.26261100 1.44132700
- B -1.02886800 -0.24230300 0.03974900
- C 2.70875900 -1.38274500 0.41059800
- H 3.30980400 -1.22975300 -0.48764400
- H 2.06590700 -2.24772000 0.23352600
- H 3.38308700 -1.61949100 1.23821400
- Cl -1.63755400 -1.89974700 0.20780500
- Cl -2.25717800 0.99653800 -0.10191100
- H 0.32407400 -1.28050700 1.60622200
- B 0.70147400 0.30315800 -0.31749000
- Cl 0.74807600 2.11220000 -0.61929400
- Cl 0.61564900 -0.70326500 -1.87220500
- C 0.19526500 0.74814700 2.45281900
- H 0.76670400 0.55892000 3.36722600
- H 0.39752600 1.76836200 2.12697000
- H -0.86514600 0.64718400 2.68741400

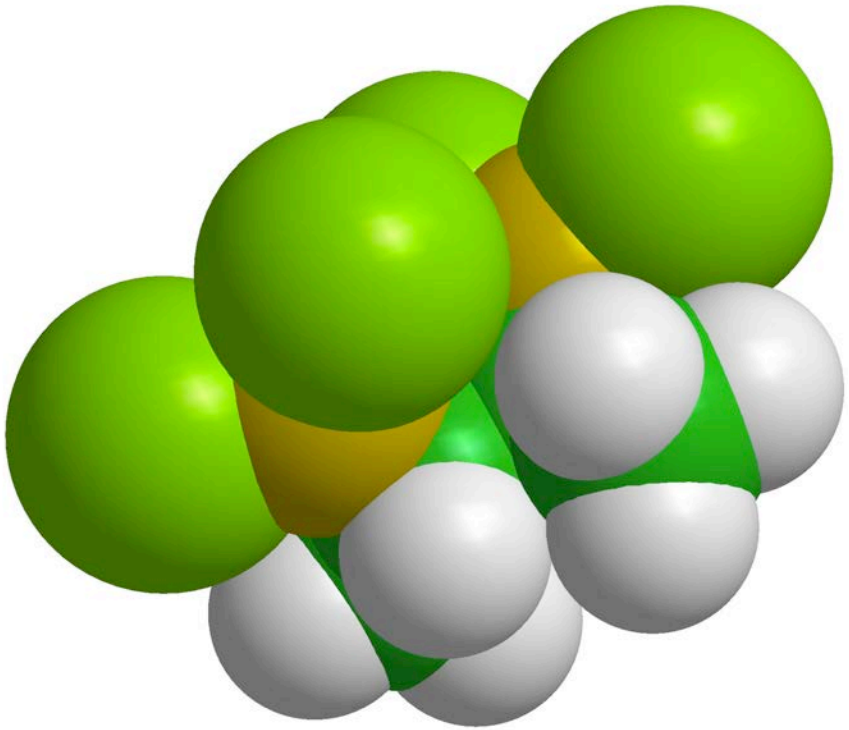


E-butene B_2Cl_4 gaucheP ωB97X-D

- Zero-point correction= 0.126269 (Hartree/Particle)
- Thermal correction to Energy= 0.138627
- Thermal correction to Enthalpy= 0.139571
- Thermal correction to Gibbs Free Energy= 0.085253
- Sum of electronic and zero-point Energies= -2047.827523
- Sum of electronic and thermal Energies= -2047.815165
- Sum of electronic and thermal Enthalpies= -2047.814221
- Sum of electronic and thermal Free Energies= -2047.868539

- B2Cl4EPW

- 0 1
- C -0.77769900 0.05496900 -1.28713900
- H -1.13367800 -0.70537400 -2.00566400
- B -1.49034900 -0.42216000 0.03079300
- Cl -3.08572400 0.15528800 0.49286900
- Cl -0.77510500 -1.66683700 1.06550100
- C 1.26392500 -1.42307500 -1.81581600
- H 0.97888200 -2.23682000 -1.14579600
- H 2.34885800 -1.44834100 -1.92735700
- H 0.82204400 -1.62170300 -2.79612500
- C -1.26349000 1.40925500 -1.82696500
- H -2.34836300 1.43354200 -1.93929900
- H -0.82107900 1.60043200 -2.80850500
- H -0.97891700 2.22810500 -1.16301200
- C 0.77800600 -0.06467300 -1.28656100
- H 1.13410000 0.69012300 -2.01085600
- B 1.49043700 0.42251400 0.02779300
- Cl 0.77436600 1.67409500 1.05354900
- Cl 3.08606700 -0.15081700 0.49411500

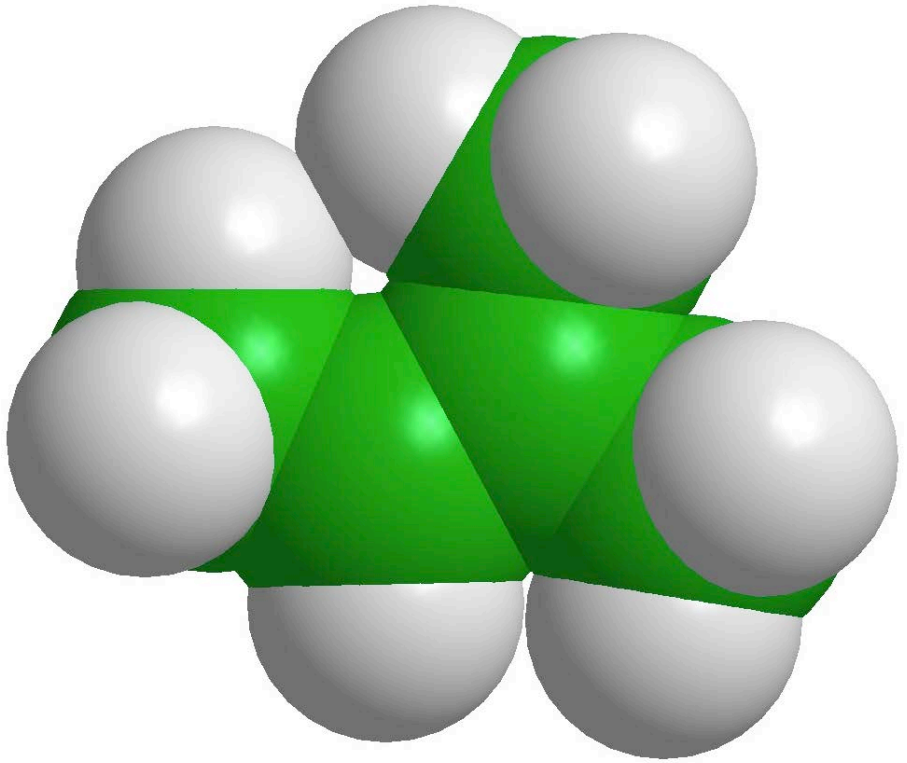


Trimethylethylene B3LYP

- Zero-point correction= 0.135361 (Hartree/Particle)
- Thermal correction to Energy= 0.142280
- Thermal correction to Enthalpy= 0.143224
- Thermal correction to Gibbs Free Energy= 0.105479
- Sum of electronic and zero-point Energies= -196.464155
- Sum of electronic and thermal Energies= -196.457235
- Sum of electronic and thermal Enthalpies= -196.456291
- Sum of electronic and thermal Free Energies= -196.494036

- TriMe

- 0 1
- C 0.44826500 -0.04104100 -0.00002100
- C -0.73123600 -0.67240900 -0.00003200
- H -0.70840100 -1.76133800 -0.00006300
- C -2.11095900 -0.07916700 0.00002100
- H -2.11108400 1.01138800 0.00040000
- H -2.67693000 -0.41121600 -0.87808500
- H -2.67706900 -0.41185800 0.87778500
- C 0.62456400 1.45659000 0.00000100
- H -0.31836800 2.00249400 0.00016100
- H 1.19816000 1.77633400 0.87805500
- H 1.19784300 1.77634700 -0.87825800
- C 1.74124300 -0.82013700 0.00001000
- H 2.34957000 -0.57360500 -0.87859900
- H 2.34935400 -0.57385400 0.87886100
- H 1.56566500 -1.89770800 -0.00013800

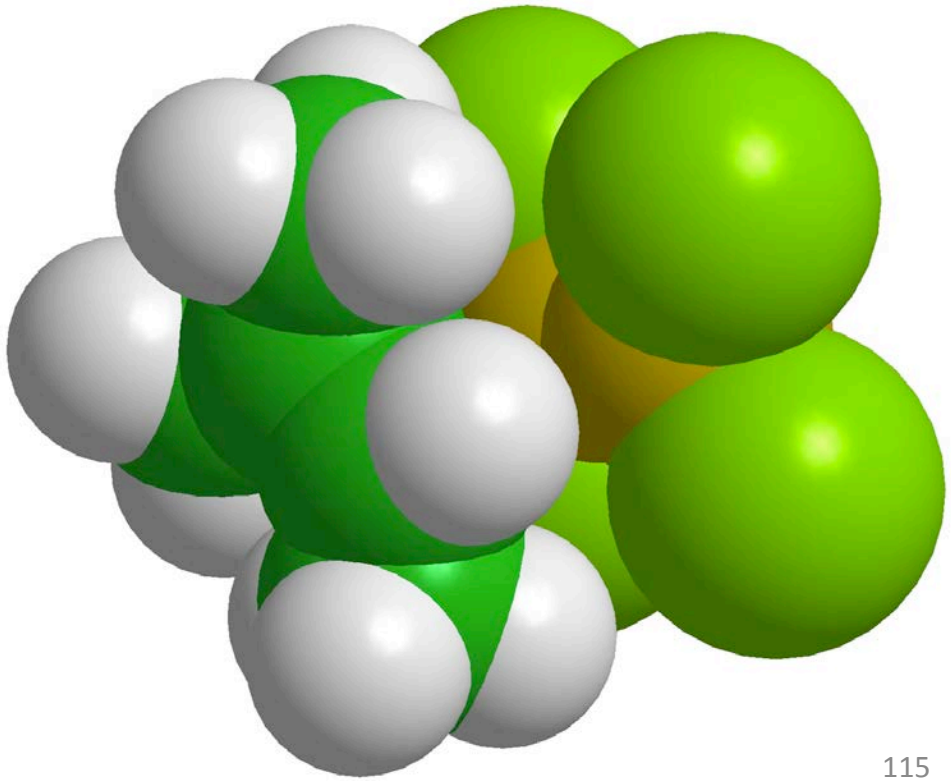


TME B_2Cl_4 vdW B3LYP

- Zero-point correction= 0.149489 (Hartree/Particle)
- Thermal correction to Energy= 0.165460
- Thermal correction to Enthalpy= 0.166405
- Thermal correction to Gibbs Free Energy= 0.102787
- Sum of electronic and zero-point Energies= -2087.219843
- Sum of electronic and thermal Energies= -2087.203871
- Sum of electronic and thermal Enthalpies= -2087.202927
- Sum of electronic and thermal Free Energies= -2087.266545

- B2Cl4TriV

- 0 1
- C -2.13580500 0.02749300 0.92336400
- B 0.51862100 0.25275300 -1.13466000
- Cl -0.10455600 1.80698400 -1.68679900
- Cl 0.22435500 -1.15295600 -2.15311200
- C -1.36676500 -0.98023200 1.37866200
- B 1.48996600 0.14891300 0.26510800
- Cl 1.73277400 1.54154800 1.31506900
- Cl 2.37252500 -1.32724900 0.64774600
- H -0.71970600 -0.75894900 2.22610700
- C -3.13561400 -0.10037600 -0.19575100
- H -2.96363100 0.67044200 -0.95505400
- H -3.11435500 -1.07138600 -0.68816500
- H -4.15002600 0.06233600 0.18681400
- C -2.09326400 1.38688100 1.57374100
- H -1.85377100 2.16862900 0.84466400
- H -3.07559300 1.63827300 1.99067400
- H -1.35997200 1.43312400 2.37989900
- C -1.36296600 -2.41654700 0.94278300
- H -0.34468000 -2.76915100 0.75348600
- H -1.76924600 -3.05093100 1.73947600
- H -1.95212300 -2.59558800 0.04370100

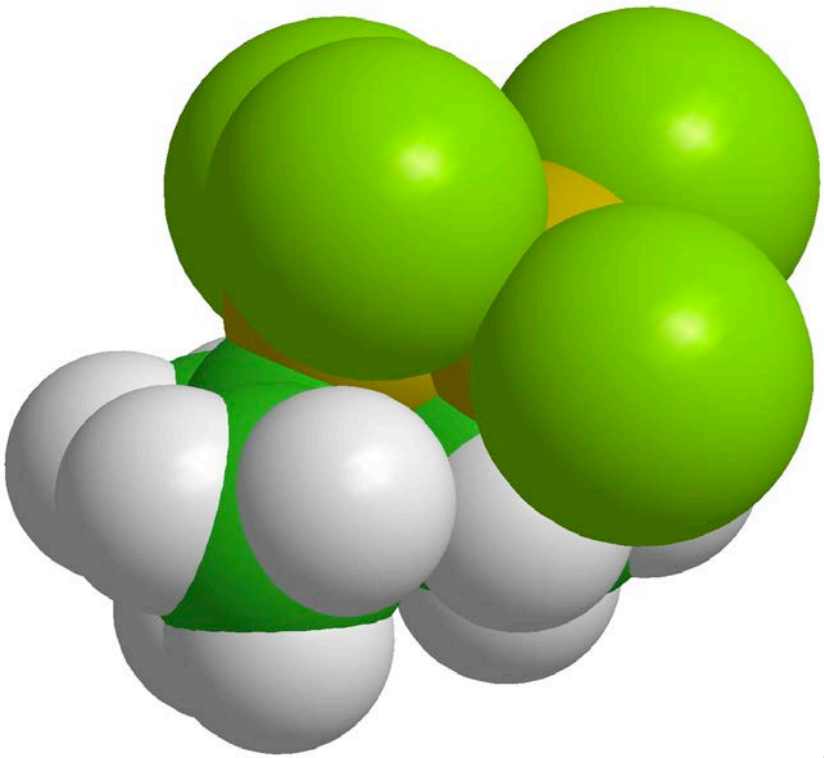


TME B_2Cl_4 TS1 B3LYP

- Zero-point correction= 0.151492 (Hartree/Particle)
- Thermal correction to Energy= 0.164895
- Thermal correction to Enthalpy= 0.165839
- Thermal correction to Gibbs Free Energy= 0.112015
- Sum of electronic and zero-point Energies= -2087.176177
- Sum of electronic and thermal Energies= -2087.162774
- Sum of electronic and thermal Enthalpies= -2087.161830
- Sum of electronic and thermal Free Energies= -2087.215654

- B2Cl4TriSF

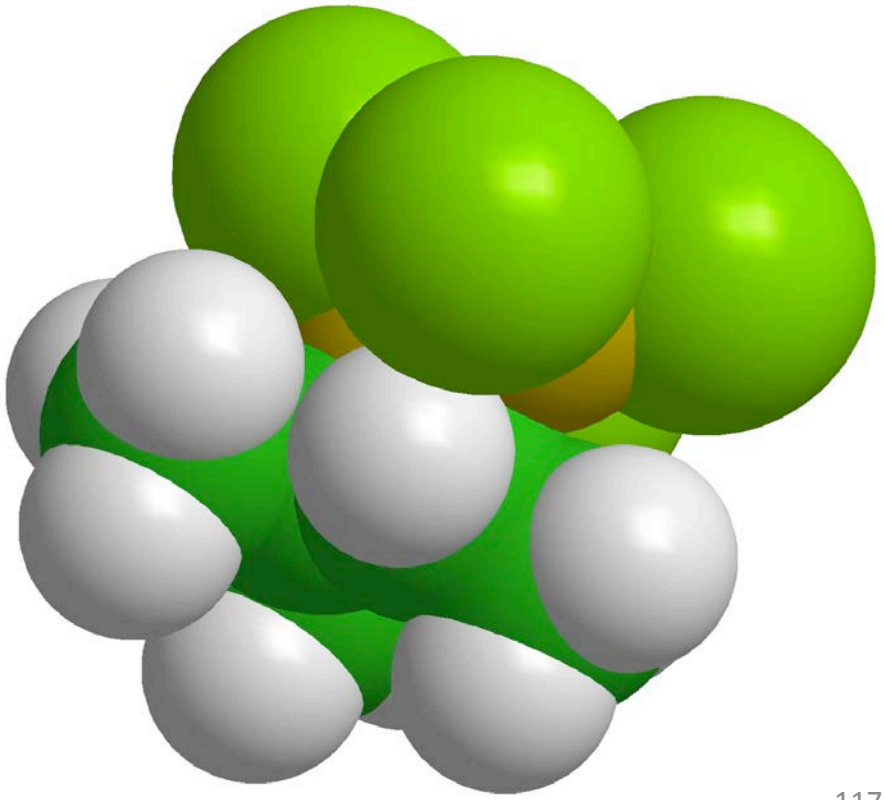
- 0 1
- C -1.64773200 0.74868900 0.12612600
- C -0.49077600 0.46722200 1.11462400
- B 1.05057700 0.07959200 0.16840600
- C -1.69734100 2.20917200 -0.32632800
- H -2.30820600 2.29865700 -1.22875900
- H -0.71197300 2.61802800 -0.55503200
- H -2.15209200 2.83713300 0.44759200
- Cl 2.13957700 1.53516600 0.40893500
- Cl 1.94236700 -1.44355400 0.44820100
- H -0.04902000 1.41168100 1.40500800
- B -0.59827800 -0.20326300 -0.51620100
- Cl -1.03998000 -1.96178300 -0.70065300
- Cl 0.51065600 0.35434400 -1.92326500
- C -0.65443000 -0.47975400 2.29232800
- H -1.42996400 -0.06935500 2.94552400
- H -0.95424200 -1.48237300 1.99289800
- H 0.26989400 -0.55404700 2.86636400
- C -3.03119900 0.22485700 0.49059100
- H -3.49548500 0.86001200 1.25291900
- H -3.67499400 0.24671500 -0.39274800
- H -3.02107700 -0.80015500 0.85646000



TME B_2Cl_4 TS2 B3LYP

- Zero-point correction= 0.150758 (Hartree/Particle)
- Thermal correction to Energy= 0.164495
- Thermal correction to Enthalpy= 0.165440
- Thermal correction to Gibbs Free Energy= 0.109840
- Sum of electronic and zero-point Energies= -2087.176668
- Sum of electronic and thermal Energies= -2087.162931
- Sum of electronic and thermal Enthalpies= -2087.161987
- Sum of electronic and thermal Free Energies= -2087.217587

- 0 1
- C -1.72277800 0.46948100 0.47427100
- C -0.58121400 0.18499400 1.33725500
- B 1.24583600 0.05910900 0.18087100
- C -2.06456800 1.95114200 0.31027300
- H -2.60280700 2.11870900 -0.62515900
- H -1.17946000 2.58795000 0.29763200
- H -2.70978800 2.27623800 1.13356500
- Cl 2.11252800 1.54844800 0.62094000
- Cl 2.23984700 -1.38062900 0.05621600
- H -0.08972100 1.06822100 1.72707900
- B -0.49540000 -0.07731700 -0.50234200
- Cl -0.76933800 -1.79022500 -1.12272700
- Cl 0.01148300 1.08223200 -1.87781700
- C -0.47915700 -1.03638800 2.21666100
- H -1.22260300 -0.92026000 3.01376200
- H -0.70115900 -1.95858400 1.68187800
- H 0.50349800 -1.12483000 2.68084000
- C -2.97460400 -0.39653100 0.56740500
- H -3.61751400 -0.02630700 1.37368300
- H -3.54056600 -0.33565900 -0.36462900
- H -2.76497200 -1.44765800 0.75110300

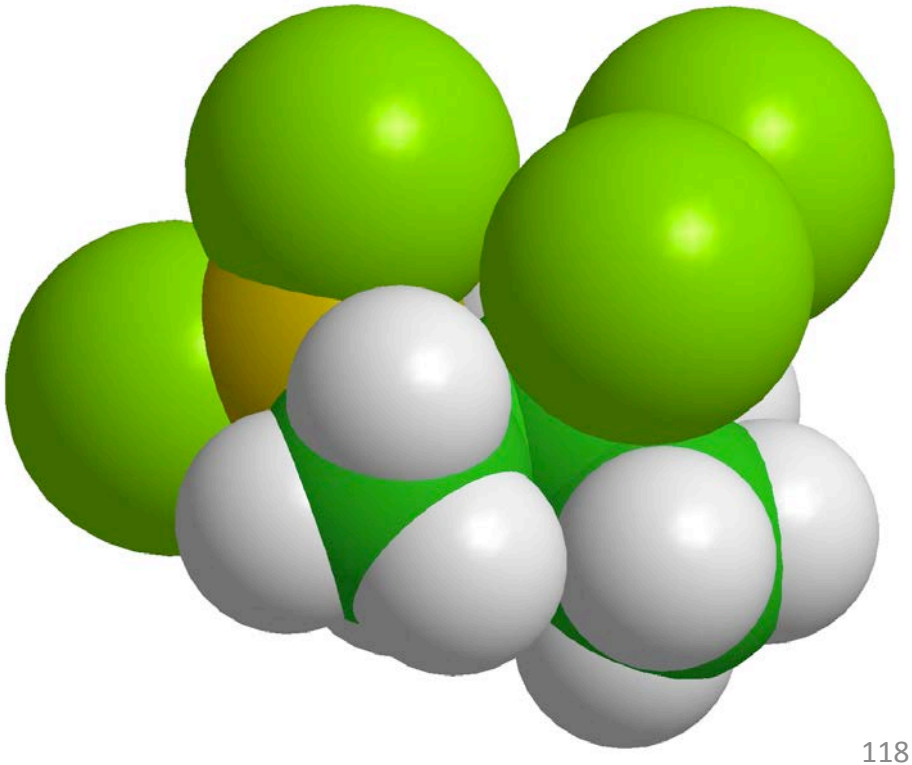


TME B_2Cl_4 gauche product B3LYP

- Zero-point correction= 0.152872 (Hartree/Particle)
- Thermal correction to Energy= 0.166808
- Thermal correction to Enthalpy= 0.167752
- Thermal correction to Gibbs Free Energy= 0.110388
- Sum of electronic and zero-point Energies= -2087.246227
- Sum of electronic and thermal Energies= -2087.232290
- Sum of electronic and thermal Enthalpies= -2087.231346
- Sum of electronic and thermal Free Energies= -2087.288710

- B2Cl4TriPF

- 0 1
- C 0.53327800 0.88583400 0.72994400
- C -0.85693700 1.08998700 0.01472400
- B -1.75077000 -0.19769200 -0.07841400
- C 0.22145100 0.42726300 2.17546600
- H 1.12571600 0.35976200 2.78261300
- H -0.25861000 -0.55492800 2.20503400
- H -0.45081700 1.14494300 2.65597300
- Cl -3.48139800 -0.13100300 0.26447400
- Cl -1.09855600 -1.74472900 -0.63466300
- H -1.39202800 1.80011500 0.65758500
- B 1.55434200 -0.09773100 0.01098400
- Cl 2.12496600 0.16881600 -1.64631800
- Cl 2.35762200 -1.41676800 0.87573500
- C -0.85613300 1.72818300 -1.40348500
- H -0.27902100 2.65471700 -1.41540100
- H -0.44498000 1.06639900 -2.16512100
- H -1.87903800 1.98162100 -1.69478100
- C 1.26908600 2.25555800 0.83106500
- H 0.62467800 2.97825300 1.34275100
- H 2.18768500 2.16213700 1.41750300
- H 1.53931500 2.66577200 -0.14217300

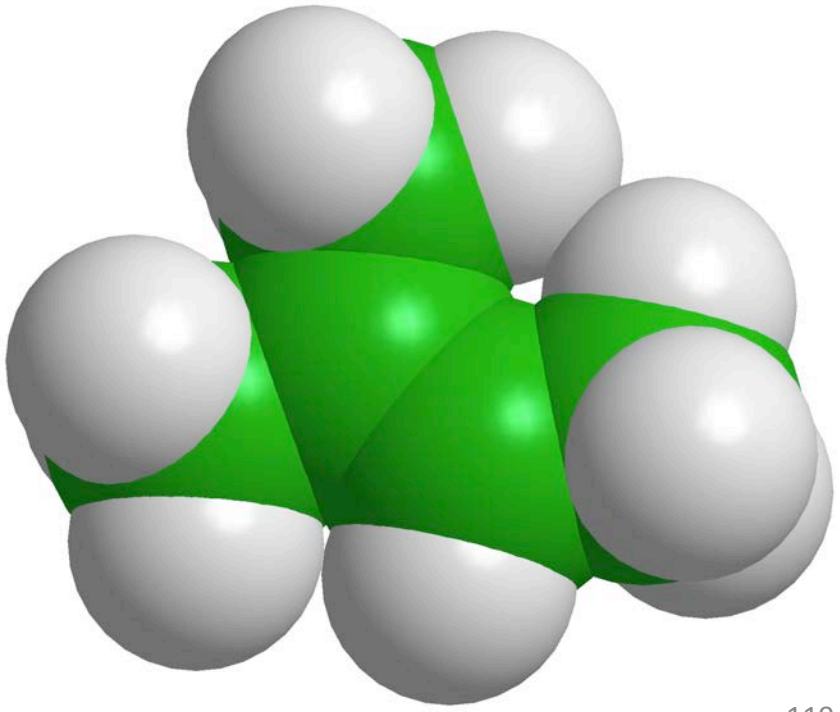


Trimethylethylene ωB97X-D

- Zero-point correction= 0.136078 (Hartree/Particle)
- Thermal correction to Energy= 0.143223
- Thermal correction to Enthalpy= 0.144167
- Thermal correction to Gibbs Free Energy= 0.105403
- Sum of electronic and zero-point Energies= -196.392057
- Sum of electronic and thermal Energies= -196.384912
- Sum of electronic and thermal Enthalpies= -196.383967
- Sum of electronic and thermal Free Energies= -196.422732

- TrimeW

- 0 1
- C -1.73735900 -0.81702900 -0.00001100
- H -1.56514800 -1.89505400 0.00122900
- H -2.34058700 -0.56700400 -0.88025800
- H -2.34172800 -0.56519400 0.87893700
- C -0.44564400 -0.04217600 0.00000000
- C 0.72988900 -0.67207300 0.00000800
- H 0.70717700 -1.76106200 0.00010400
- C 2.10614100 -0.07730600 -0.00002200
- H 2.66838000 -0.40884300 0.87928200
- H 2.66885300 -0.40998400 -0.87857800
- H 2.10419200 1.01324200 -0.00069400
- C -0.62367900 1.45207700 0.00000000
- H -1.19611300 1.76618800 0.87984000
- H 0.31757700 2.00084900 -0.00146200
- H -1.19868800 1.76590900 -0.87824800

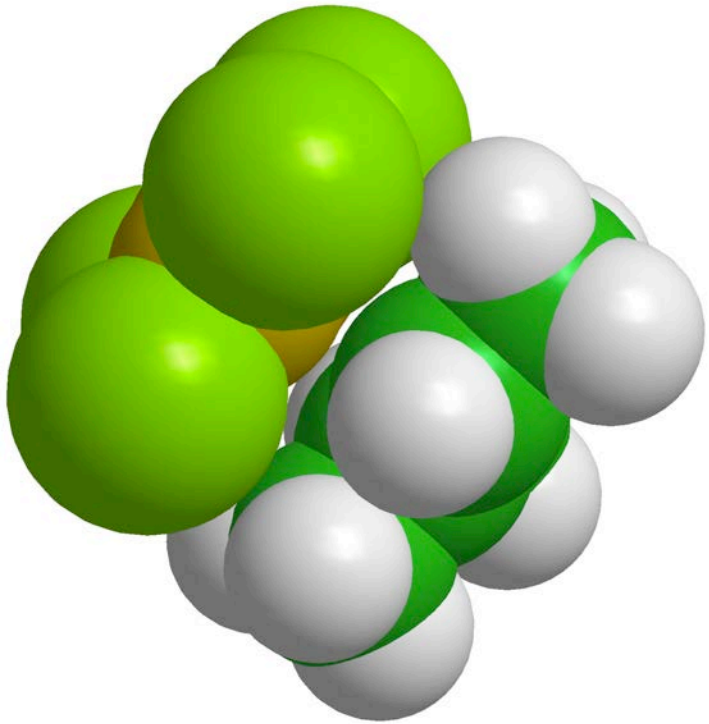


Trimethylethylene B_2Cl_4 vdW ωB97X-D

- Zero-point correction= 0.152360 (Hartree/Particle)
- Thermal correction to Energy= 0.167408
- Thermal correction to Enthalpy= 0.168352
- Thermal correction to Gibbs Free Energy= 0.108448
- Sum of electronic and zero-point Energies= -2087.072972
- Sum of electronic and thermal Energies= -2087.057924
- Sum of electronic and thermal Enthalpies= -2087.056980
- Sum of electronic and thermal Free Energies= -2087.116884

- B2Cl4TriVW

- 0 1
- C -1.86788700 -0.18362300 -1.10610300
- B 0.27971500 -0.01677200 1.17390900
- Cl -0.44211800 -1.41338900 1.96423200
- Cl -0.09737700 1.56926400 1.82858100
- C -1.00847200 0.69478400 -1.64835800
- B 1.43755100 -0.22211000 -0.06832900
- Cl 1.73397400 -1.79897300 -0.78396000
- Cl 2.45926900 1.11131200 -0.58549900
- H -0.27602400 0.29827500 -2.35099700
- C -2.98615400 0.18819300 -0.17264700
- H -3.01491500 -0.49932900 0.67868700
- H -2.90941500 1.20339100 0.21472400
- H -3.94766200 0.09213400 -0.68853400
- C -1.81892100 -1.64138400 -1.47125600
- H -1.66731000 -2.26407200 -0.58333900
- H -2.77360700 -1.94633900 -1.91327300
- H -1.02529300 -1.86054600 -2.18666800
- C -1.00293400 2.18574000 -1.50674300
- H -0.00759500 2.55327600 -1.24174700
- H -1.26530700 2.64658300 -2.46480200
- H -1.70673000 2.54914300 -0.75833500

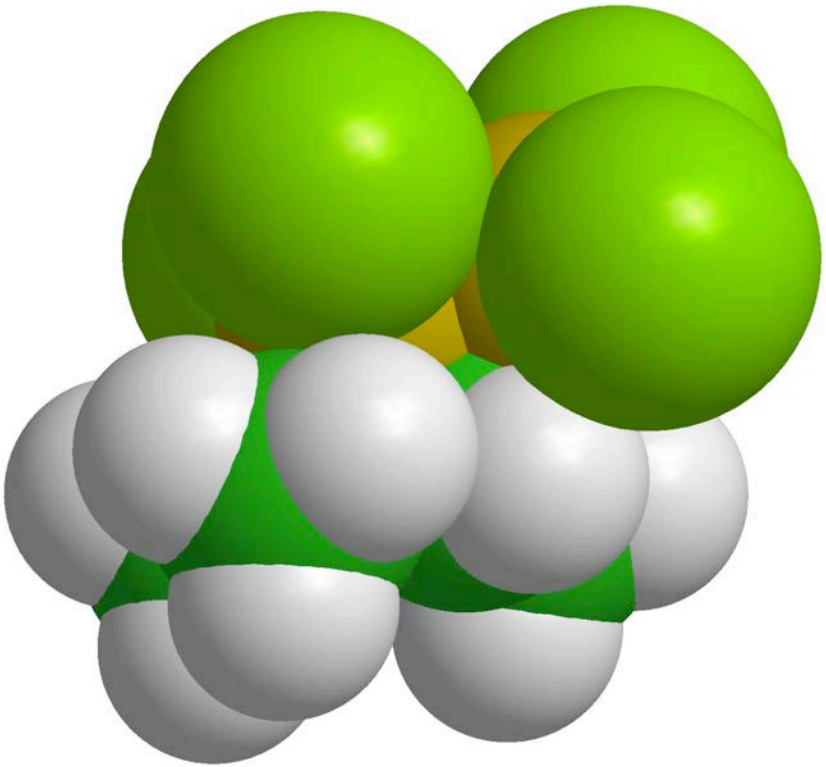


Trimethylethylene B_2Cl_4 TS(tert) ωB97X-D

- Zero-point correction= 0.152807 (Hartree/Particle)
- Thermal correction to Energy= 0.166228
- Thermal correction to Enthalpy= 0.167172
- Thermal correction to Gibbs Free Energy= 0.112423
- Sum of electronic and zero-point Energies= -2087.040761
- Sum of electronic and thermal Energies= -2087.027340
- Sum of electronic and thermal Enthalpies= -2087.026396
- Sum of electronic and thermal Free Energies= -2087.081146

- B2Cl4TriTSW

- 0 1
- C -1.71644300 0.39641800 0.54512400
- C -0.55494400 0.09036500 1.34660300
- B 1.25062500 0.05724900 0.16209500
- C -2.10557700 1.86642700 0.47790600
- H -2.64736800 2.07569200 -0.44700600
- H -1.24043300 2.53052700 0.50969900
- H -2.76096900 2.11121300 1.31999100
- Cl 2.09997900 1.53330500 0.65098500
- Cl 2.25522700 -1.36350800 -0.02235700
- H -0.06821000 0.95806200 1.77842100
- B -0.47712900 -0.03958900 -0.49933700
- Cl -0.73672600 -1.69886200 -1.23875300
- Cl -0.09275600 1.23991100 -1.78370100
- C -0.39776200 -1.18646800 2.12828100
- H -1.15109700 -1.16682200 2.92238800
- H -0.57343200 -2.07225100 1.51844300
- H 0.58756100 -1.26355900 2.58818000
- C -2.92613200 -0.52069700 0.57644500
- H -3.59688000 -0.20562600 1.38258900
- H -3.47289600 -0.44753400 -0.36596300
- H -2.67593100 -1.56864300 0.72833200



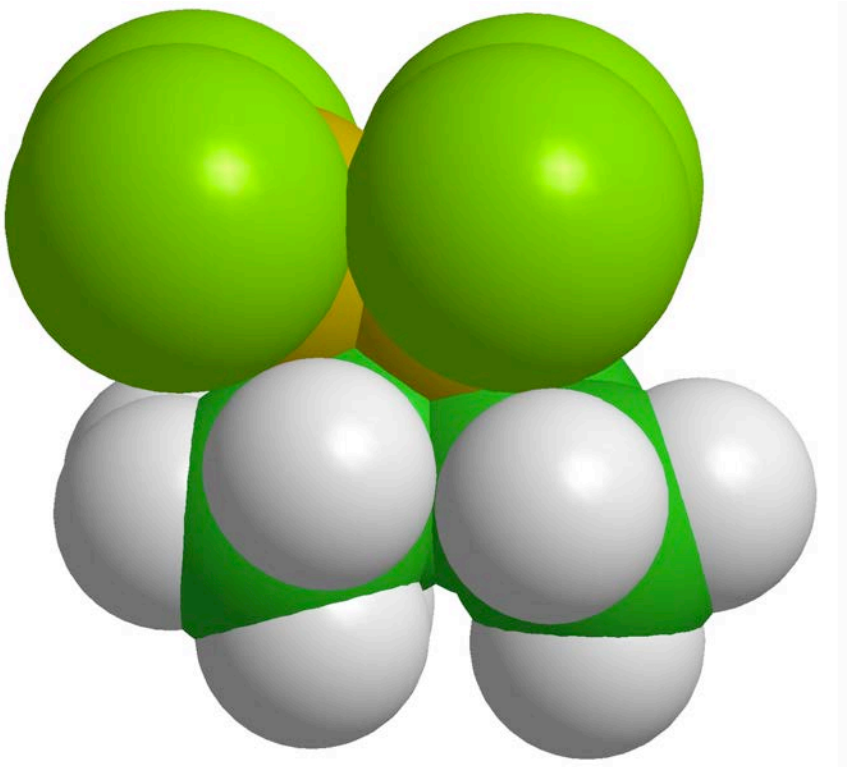
Trimethylethylene B_2Cl_4 TS(sec) ωB97X-D

- Zero-point correction= 0.153081 (Hartree/Particle)
- Thermal correction to Energy= 0.166261
- Thermal correction to Enthalpy= 0.167205
- Thermal correction to Gibbs Free Energy= 0.113020
- Sum of electronic and zero-point Energies= -2087.038956
- Sum of electronic and thermal Energies= -2087.025776
- Sum of electronic and thermal Enthalpies= -2087.024832
- Sum of electronic and thermal Free Energies= -2087.079018

- B2Cl4TTSW

- 0 1

C	1.71939700	0.12546700	-0.85699400
C	0.52614800	-0.65706500	-1.19384600
B	-1.09214700	-0.20814600	0.15527800
Cl	-2.44166900	0.68621400	-0.52824100
Cl	-1.56771800	-1.52603800	1.21782000
B	0.67359700	0.60706800	0.27577200
Cl	1.13491800	0.10185600	1.97826300
Cl	0.23994800	2.38615900	0.10640500
C	0.58338800	-2.14650800	-0.93904300
H	-0.36382500	-2.64257600	-1.14731100
H	1.33847700	-2.53696500	-1.63044500
H	0.90143300	-2.39063100	0.07320500
C	3.01806600	-0.54891800	-0.46499700
H	3.49366600	-1.00593400	-1.33872900
H	3.70423400	0.19655800	-0.05917800
H	2.88769700	-1.31549300	0.29825400
C	-0.17979800	-0.24245700	-2.46755500
H	-1.13760000	-0.74092300	-2.61451900
H	-0.31794800	0.83726000	-2.52655600
H	0.49273500	-0.54033200	-3.27952300
H	1.87751800	0.94207100	-1.55804400

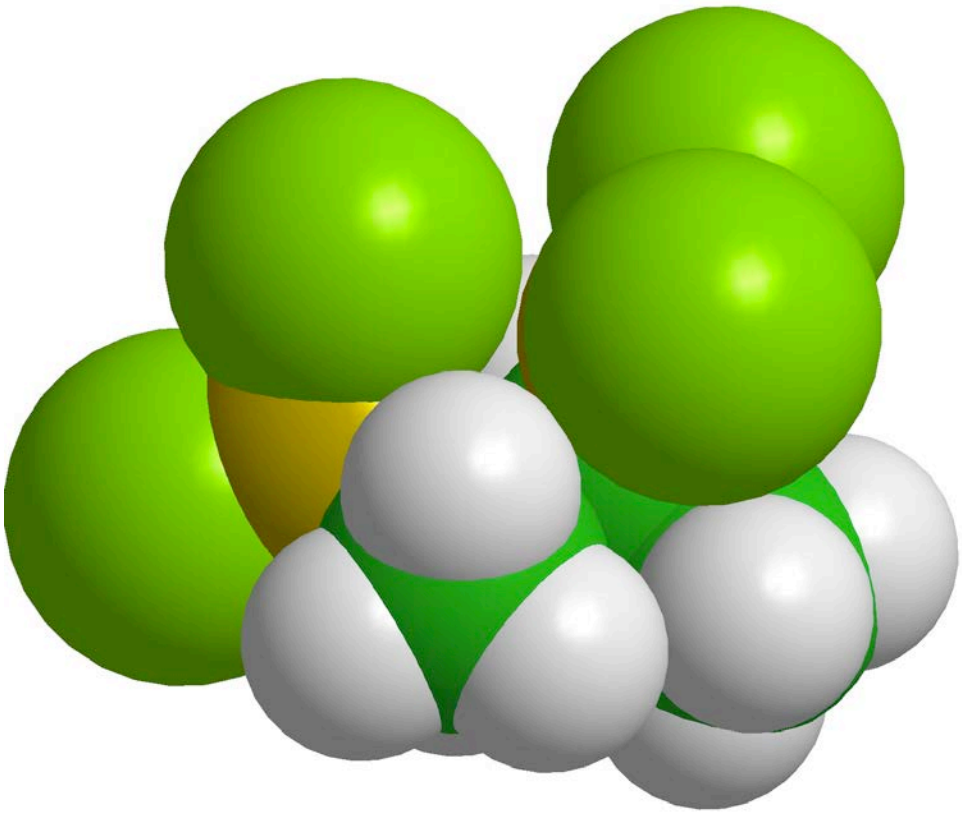


Trimethylethylene B_2Cl_4 gaucheP ωB97X-D

- Zero-point correction= 0.154627 (Hartree/Particle)
- Thermal correction to Energy= 0.168330
- Thermal correction to Enthalpy= 0.169275
- Thermal correction to Gibbs Free Energy= 0.112492
- Sum of electronic and zero-point Energies= -2087.110612
- Sum of electronic and thermal Energies= -2087.096908
- Sum of electronic and thermal Enthalpies= -2087.095964
- Sum of electronic and thermal Free Energies= -2087.152747

- B2Cl4TriPFW

- 0 1
- C 0.51397800 0.87371700 0.74180000
- C -0.84243700 1.10415800 -0.00573100
- B -1.74249800 -0.17821900 -0.10863100
- C 0.15609100 0.38704100 2.16026600
- H 1.03901700 0.31118100 2.79786400
- H -0.32124600 -0.59797500 2.15316800
- H -0.53603100 1.09343300 2.62964100
- Cl -3.45833200 -0.12438000 0.27194400
- Cl -1.09559000 -1.70532500 -0.71174000
- H -1.38432000 1.82512400 0.61931500
- B 1.54346300 -0.10571800 0.03121800
- Cl 2.17516400 0.20136900 -1.59022300
- Cl 2.28897300 -1.45813200 0.88406700
- C -0.79068700 1.72295400 -1.42245100
- H -0.18344600 2.63025400 -1.43239600
- H -0.38391300 1.03787700 -2.16687300
- H -1.79890600 2.00398900 -1.73915900
- C 1.25756900 2.22543100 0.88955200
- H 0.61363900 2.93727400 1.41652700
- H 2.17141600 2.10707200 1.47961200
- H 1.53821800 2.66159500 -0.07006100

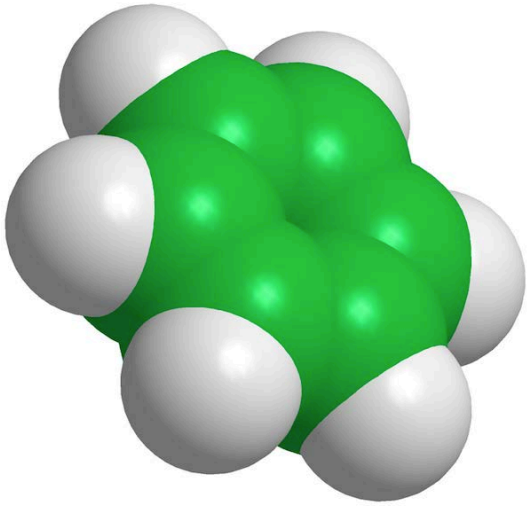


Benzene ωB97x-D

- Zero-point correction= 0.101138 (Hartree/Particle)
- Thermal correction to Energy= 0.105506
- Thermal correction to Enthalpy= 0.106450
- Thermal correction to Gibbs Free Energy= 0.073694
- Sum of electronic and zero-point Energies= -232.117707
- Sum of electronic and thermal Energies= -232.113338
- Sum of electronic and thermal Enthalpies= -232.112394
- Sum of electronic and thermal Free Energies= -232.145151

- BzW

- 0 1
- C -1.37908800 0.17601800 0.00000100
- C -0.84187000 -1.10634800 0.00000900
- C 0.53705300 -1.28232100 0.00000100
- C 1.37909500 -0.17595800 0.00000200
- C 0.84191900 1.10631000 0.00000200
- C -0.53710900 1.28229700 -0.00000600
- H -2.45460700 0.31308700 -0.00000600
- H -1.49907900 -1.96879500 -0.00002000
- H 0.95645800 -2.28223000 -0.00002400
- H 2.45459800 -0.31316000 -0.00001000
- H 1.49901800 1.96884000 0.00000600
- H -0.95638600 2.28226000 -0.00000100

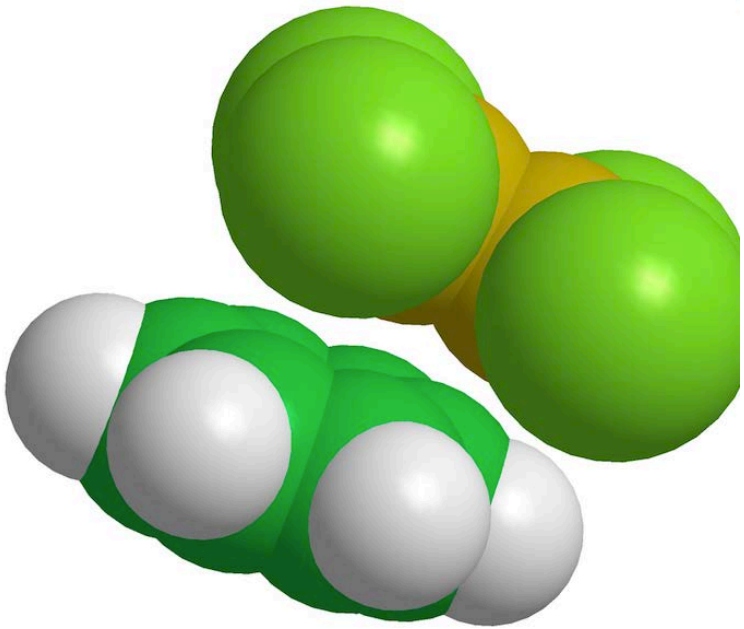


Benzene B_2Cl_4 vdW ωB97x-D

- Zero-point correction= 0.115460 (Hartree/Particle)
- Thermal correction to Energy= 0.128063
- Thermal correction to Enthalpy= 0.129008
- Thermal correction to Gibbs Free Energy= 0.072717
- Sum of electronic and zero-point Energies= -2122.795390
- Sum of electronic and thermal Energies= -2122.782787
- Sum of electronic and thermal Enthalpies= -2122.781843
- Sum of electronic and thermal Free Energies= -2122.838133

- BzVW

- 0 1
- C -1.07329600 -1.95825500 -0.00003500
- C -1.56786900 -1.46936300 -1.20587400
- C -2.55641400 -0.49268400 -1.20482200
- C -3.04943000 -0.00365200 -0.00009400
- C -2.55654100 -0.49274100 1.20466400
- C -1.56799700 -1.46942100 1.20577400
- H -0.30763500 -2.72655000 -0.00001300
- H -1.17631600 -1.84699800 -2.14347300
- H -2.93744500 -0.10560100 -2.14281000
- H -2.93767200 -0.10570300 2.14263000
- H -1.17654400 -1.84710100 2.14339600
- H -3.81519800 0.76343500 -0.00011600
- B 0.56339800 1.19746500 0.00006600
- B 1.57424100 -0.19590600 -0.00000300
- Cl 2.15558500 -0.89023600 -1.50269600
- Cl 2.15548800 -0.89046400 1.50262500
- Cl 0.07655600 1.95445700 -1.50131700
- Cl 0.07660000 1.95432700 1.50152900

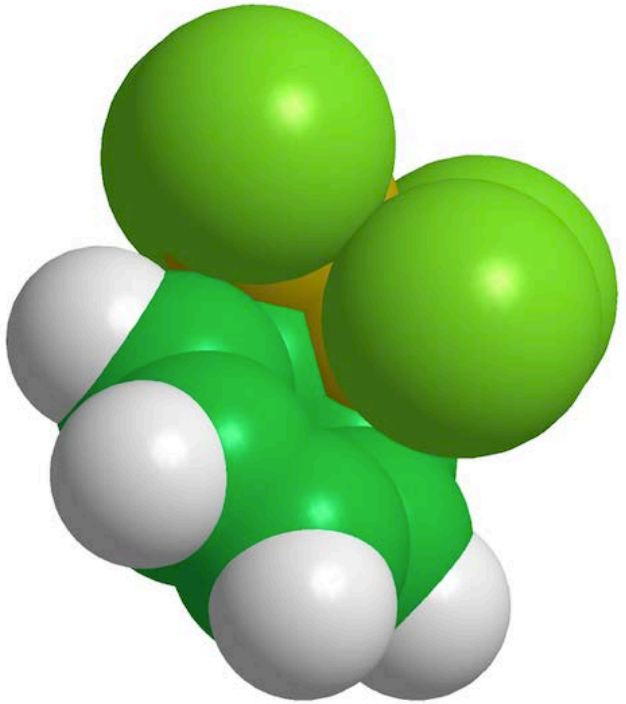


Benzene B_2Cl_4 TS ωB97x-D

- Zero-point correction= 0.115470 (Hartree/Particle)
- Thermal correction to Energy= 0.127092
- Thermal correction to Enthalpy= 0.128036
- Thermal correction to Gibbs Free Energy= 0.076102
- Sum of electronic and zero-point Energies= -2122.727564
- Sum of electronic and thermal Energies= -2122.715942
- Sum of electronic and thermal Enthalpies= -2122.714998
- Sum of electronic and thermal Free Energies= -2122.766932

- B2Cl4BzTSW

- 0 1
- C 0.41278900 -0.35537500 -1.17061400
- H -0.29017700 -0.36906100 -1.99941800
- B -1.16531800 -0.56680500 -0.05550700
- Cl -1.19473100 -1.81659600 1.17749700
- Cl -2.64377800 -0.43256800 -1.01810500
- C 1.17976200 0.91891600 -1.04108900
- H 0.92979700 1.68700600 -1.76458000
- B 0.07296600 0.93569400 0.16359600
- Cl 0.74120700 0.70599100 1.83257800
- Cl -1.11966500 2.31111300 -0.03772000
- C 1.14622200 -1.59262000 -0.90655000
- C 2.42827400 -1.56229900 -0.48808700
- H 2.94183000 -2.50126300 -0.31319300
- H 0.64427500 -2.53454300 -1.08688600
- C 3.17043500 -0.33534900 -0.35627800
- C 2.58940100 0.83277600 -0.68220400
- H 4.21011000 -0.37612500 -0.05787400
- H 3.15307700 1.75828700 -0.67180600

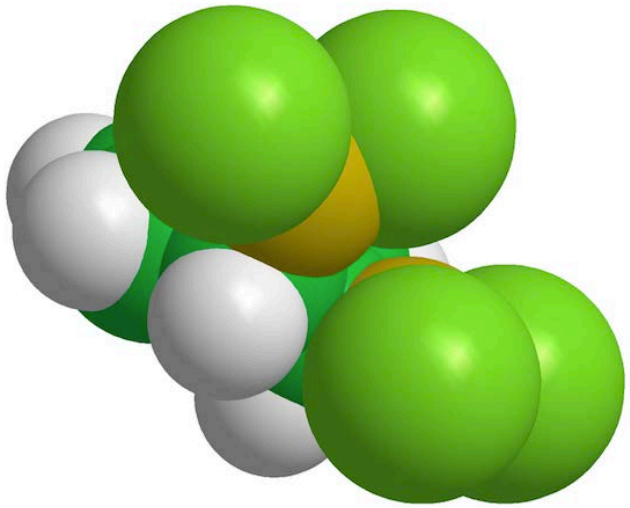


Benzene B_2Cl_4 product

- Zero-point correction= 0.116512 (Hartree/Particle)
- Thermal correction to Energy= 0.128686
- Thermal correction to Enthalpy= 0.129630
- Thermal correction to Gibbs Free Energy= 0.075154
- Sum of electronic and zero-point Energies= -2122.790104
- Sum of electronic and thermal Energies= -2122.777930
- Sum of electronic and thermal Enthalpies= -2122.776986
- Sum of electronic and thermal Free Energies= -2122.831461

- B2Cl4BzPW

- 0 1
- C -1.68358900 2.55788300 -0.48569000
- C -1.82317200 1.37821700 -1.09404000
- H -0.52976600 3.69930700 1.00302900
- C -0.51176100 2.83740200 0.34574000
- C -0.78879200 0.27927700 -0.90403200
- C 0.61622400 0.87645200 -0.65714500
- C 0.56883600 2.05795100 0.28776600
- H 1.44270800 2.28403900 0.88724600
- H -0.76799700 -0.32579600 -1.81590400
- H 0.95637300 1.28841600 -1.63189400
- B 1.74326200 -0.18401900 -0.38826200
- B -1.36613300 -0.64821000 0.23445100
- Cl 1.62858500 -1.80696900 -1.07249800
- Cl 3.22367200 0.21862000 0.46810400
- Cl -0.61907100 -0.78074700 1.82226700
- Cl -2.82799100 -1.58295700 -0.06136400
- H -2.70019900 1.15217200 -1.68985000
- H -2.44156700 3.32480300 -0.59982100

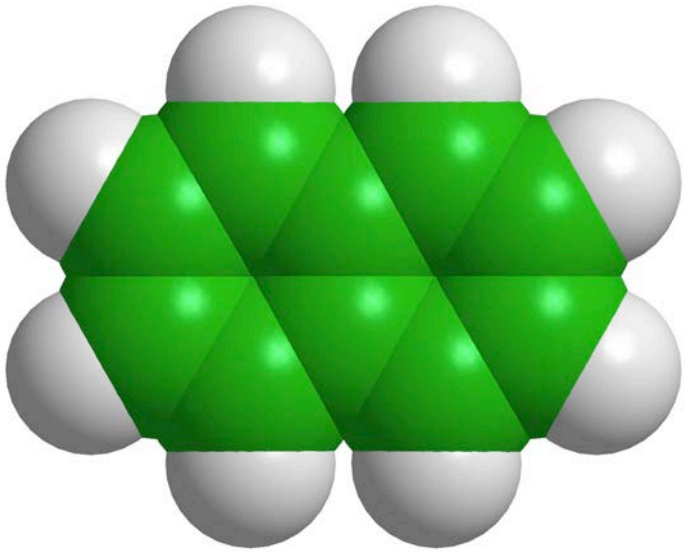


Naphthalene ωB97X-D

- Zero-point correction= 0.148369 (Hartree/Particle)
- Thermal correction to Energy= 0.155163
- Thermal correction to Enthalpy= 0.156107
- Thermal correction to Gibbs Free Energy= 0.117161
- Sum of electronic and zero-point Energies= -385.691517
- Sum of electronic and thermal Energies= -385.684723
- Sum of electronic and thermal Enthalpies= -385.683779
- Sum of electronic and thermal Free Energies= -385.722724

- Np

- 0 1
- C 2.42196000 -0.70692900 0.00000300
- C 1.24121100 -1.39656700 0.00000200
- C -0.00002400 -0.71004000 -0.00000400
- C 0.00005800 0.71007300 -0.00000300
- C 1.24126500 1.39655800 -0.00000300
- C 2.42200200 0.70687400 0.00000000
- H -1.23743000 -2.48173700 -0.00001400
- H 3.36544200 -1.24082700 0.00001100
- H 1.23740500 -2.48175700 0.00000700
- C -1.24127500 -1.39654700 -0.00000600
- C -1.24124200 1.39656200 0.00000100
- H 1.23748300 2.48174700 -0.00000300
- H 3.36549200 1.24075500 0.00000500
- C -2.42195700 0.70693900 0.00000600
- C -2.42199800 -0.70692400 0.00000200
- H -1.23745400 2.48175800 -0.00001300
- H -3.36543300 1.24084200 0.00001100
- H -3.36550600 -1.24076800 0.00000500

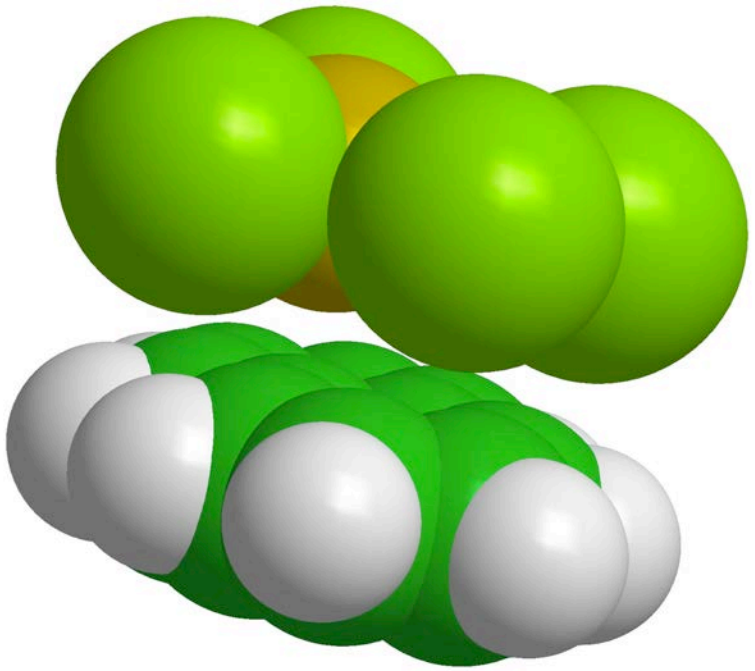


B_2Cl_4 Np vdW ωB97X-D

- Zero-point correction= 0.162673 (Hartree/Particle)
- Thermal correction to Energy= 0.178573
- Thermal correction to Enthalpy= 0.179517
- Thermal correction to Gibbs Free Energy= 0.115847
- Sum of electronic and zero-point Energies= -2276.372283
- Sum of electronic and thermal Energies= -2276.356383
- Sum of electronic and thermal Enthalpies= -2276.355438
- Sum of electronic and thermal Free Energies= -2276.419108

- NpBVW

- 0 1
- H 3.56824400 -0.36165500 1.86100200
- C 2.52178200 -0.07952300 1.85428900
- H 1.81929900 -2.09420800 1.84236800
- C 1.55190900 -1.04273500 1.84355100
- C 0.85352400 1.66302800 1.83142900
- C 0.17741000 -0.68808900 1.83170800
- C 2.16851100 1.28972800 1.84561100
- C -0.17741000 0.68808900 1.83170800
- C -0.85352400 -1.66302800 1.83142900
- H 2.94732700 2.04330700 1.84382400
- H -1.81929900 2.09420800 1.84236800
- H 0.57973500 2.71272300 1.81983100
- C -2.16851100 -1.28972800 1.84561100
- H -0.57973500 -2.71272300 1.81983100
- H -2.94732700 -2.04330700 1.84382400
- C -2.52178200 0.07952300 1.85428900
- H -3.56824400 0.36165500 1.86100200
- C -1.55190900 1.04273500 1.84355100
- B -0.73703600 0.44382600 -1.55154900
- B 0.73703600 -0.44382600 -1.55154900
- Cl -0.73703600 2.19750800 -1.55056100
- Cl -2.27318000 -0.38339200 -1.67583900
- Cl 2.27318000 0.38339200 -1.67583900
- Cl 0.73703600 -2.19750800 -1.55056100

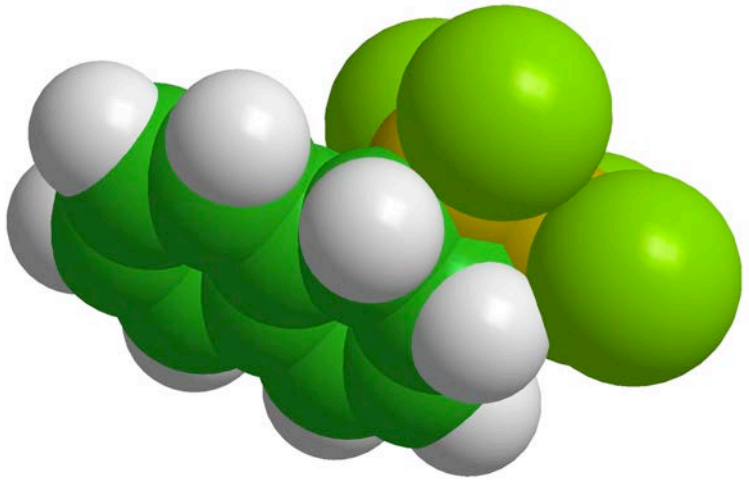


B2Cl4 Np TS ωB97X-D

- Zero-point correction= 0.162971 (Hartree/Particle)
- Thermal correction to Energy= 0.177183
- Thermal correction to Enthalpy= 0.178127
- Thermal correction to Gibbs Free Energy= 0.120200
- Sum of electronic and zero-point Energies= -2276.317520
- Sum of electronic and thermal Energies= -2276.303309
- Sum of electronic and thermal Enthalpies= -2276.302364
- Sum of electronic and thermal Free Energies= -2276.360292

- B2Cl4NpTSFW

- 0 1
- C -0.45900900 -0.39819400 -1.21579400
- H -1.15885500 -0.22970200 -2.02833200
- B -2.09951800 -0.38958600 -0.06114600
- Cl -2.36275800 -1.67961100 1.09764200
- Cl -3.50610300 0.03048900 -1.04707800
- C 0.49100200 0.70261000 -0.97371600
- H 0.39372800 1.54554900 -1.64971900
- B -0.61636400 0.82883800 0.22458600
- Cl 0.01547100 0.39094600 1.87050000
- Cl -1.54815800 2.40812200 0.12753500
- C 0.01239900 -1.76792900 -1.01541300
- C 1.26632100 -2.00792800 -0.59530900
- H 1.59174400 -3.03616100 -0.47141400
- H -0.66357800 -2.58322000 -1.23903800
- C 2.24181800 -0.96336800 -0.36353600
- C 1.87788100 0.37121000 -0.60104900
- C 3.54972100 -1.26606500 0.03220200
- H 3.82095600 -2.30014700 0.21717600
- C 2.83237800 1.37583500 -0.45495900
- H 2.55105000 2.40759200 -0.63540300
- C 4.48440800 -0.26062100 0.18633200
- H 5.49484200 -0.49843600 0.49667900
- C 4.12316700 1.06363300 -0.06341600
- H 4.85533000 1.85407600 0.05461300



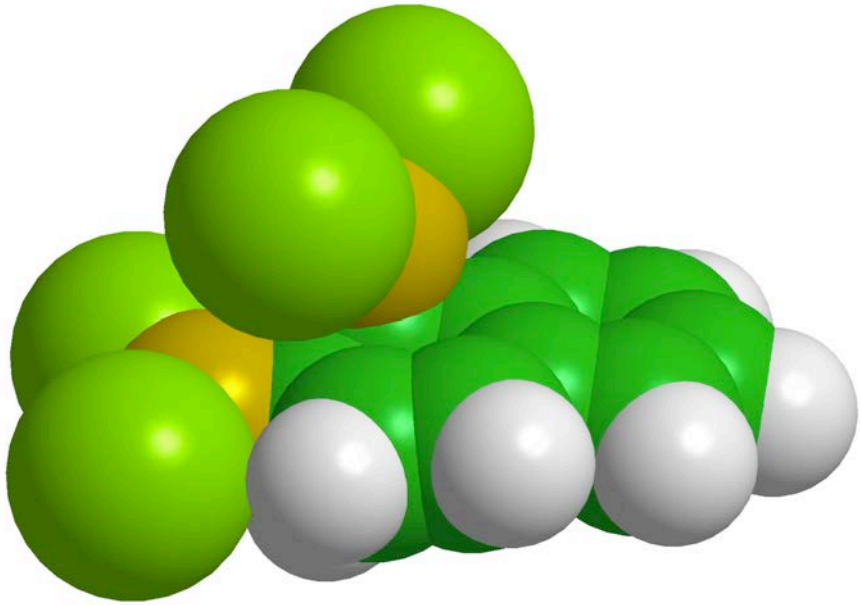
B_2Cl_4Np gauche product ωB97X-D

- Zero-point correction= 0.164115 (Hartree/Particle)
- Thermal correction to Energy= 0.178803
- Thermal correction to Enthalpy= 0.179747
- Thermal correction to Gibbs Free Energy= 0.119162
- Sum of electronic and zero-point Energies= -2276.383298
- Sum of electronic and thermal Energies= -2276.368610
- Sum of electronic and thermal Enthalpies= -2276.367666
- Sum of electronic and thermal Free Energies= -2276.428251

- B2Cl4NpP

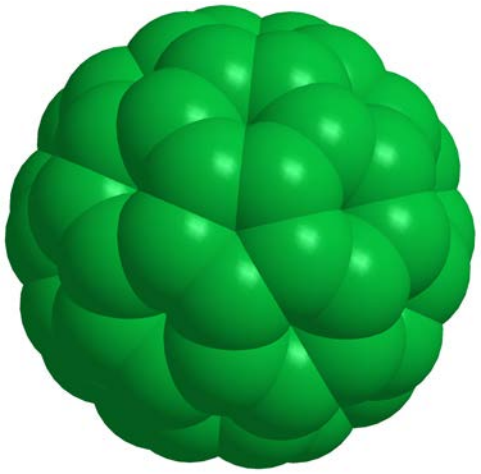
- 0 1

C	4.31323000	-1.08659200	-0.24306900
C	3.31019000	-1.69916400	0.49481800
C	1.98238200	-1.29388300	0.36563200
C	1.66579900	-0.24574500	-0.51132800
C	2.67448300	0.35717200	-1.25222900
C	3.99371300	-0.06068600	-1.12325300
H	1.16877700	-2.61298200	1.92147600
H	5.34151000	-1.41130700	-0.13389800
H	3.55298700	-2.50772700	1.17669000
C	0.90016300	-1.96467400	1.09369500
C	0.22035800	0.23097800	-0.57779600
H	2.42806700	1.16621100	-1.93183000
H	4.77057600	0.41847000	-1.70768900
C	-0.75413500	-0.96049000	-0.44691400
C	-0.37406700	-1.83511700	0.72663700
H	-1.15158400	-2.37872200	1.25013300
H	0.07511500	0.71306200	-1.55123900
H	-0.61149600	-1.58234600	-1.35595400
B	-2.27637100	-0.60101600	-0.58696200
B	0.00610900	1.38012300	0.49173800
Cl	-2.78848800	0.74700800	-1.60528600
Cl	-3.54200000	-1.60031600	0.11111800
Cl	-1.19456600	1.26657600	1.77556300
Cl	0.94768100	2.86020400	0.40397400



C60

- Zero-point correction= 0.382920 (Hartree/Particle)
- Thermal correction to Energy= 0.403159
- Thermal correction to Enthalpy= 0.404103
- Thermal correction to Gibbs Free Energy= 0.340114
- Sum of electronic and zero-point Energies= -2285.072477
- Sum of electronic and thermal Energies= -2285.052238
- Sum of electronic and thermal Enthalpies= -2285.051294
- Sum of electronic and thermal Free Energies= -2285.115284
- C60
- 0 1
- C 0.81670900 1.46545600 3.11318400
- C -0.10845800 0.42162800 3.50957800
- C 0.26325400 -0.90985800 3.40698700
- C 1.57757900 -1.25885400 2.90371000
- C 2.46197100 -0.26106100 2.52467400
- C 2.07314200 1.13177200 2.63199700
- C -1.44292000 0.83359500 3.11916700
- C 1.86349500 2.95257500 -0.56073900
- C 1.89639300 2.85022600 0.88529300
- C 0.05436200 2.52258600 2.47759500
- C 0.58219400 3.19907500 1.38892900
- C -0.26266500 3.51733700 0.25424000
- C -1.59773100 3.14413800 0.25799700
- C -2.14954200 2.43609200 1.39666900
- C -1.34198900 2.13187800 2.48157700
- C 3.35494500 0.88443900 0.68222100
- C 0.52915900 3.36464200 -0.95086600
- C 3.25395200 -0.41382600 1.31980400
- C 3.12716100 -1.55770200 0.54700200
- C -2.20205200 2.60139900 -0.94329400
- C 1.44486000 -2.45520100 2.09525100
- C -3.09482000 1.45560400 0.89909300
- C 1.95788500 1.49648100 -2.53667200
- C 2.56187000 2.03974300 -1.33568400
- C 3.32413700 0.98244200 -0.70019100
- C -3.19127600 0.21424200 1.50852300
- C -2.34693800 -0.10368900 2.64361900
- C 2.62499500 1.83949000 1.49306000
- C -0.68209200 -1.89032200 2.90972800
- C -0.04824100 2.84549400 -2.09917600
- C -1.95788500 -1.49648100 2.53667200
- C -2.56187000 -2.03974300 1.33568400
- C -1.86349500 -2.95257500 0.56073900
- C -1.89639300 -2.85022600 -0.88529300
- C -0.58219400 -3.19907500 -1.38892900
- C -0.05436200 -2.52258600 -2.47759500
- C -0.81670900 -1.46545600 -3.11318400
- C 0.10845800 -0.42162800 -3.50957800
- C -0.26325400 0.90985800 -3.40698700
- C -1.57757900 1.25885400 -2.90371000
- C -2.46197100 0.26106100 -2.52467400
- C -2.07314200 -1.13177200 -2.63199700
- C -2.62499500 -1.83949000 -1.49306000
- C -3.35494500 -0.88443900 -0.68222100
- C -3.25395200 0.41382600 -1.31980400
- C -3.12716100 1.55770200 -0.54700200
- C -1.44486000 2.45520100 -2.09525100
- C 0.68209200 1.89032200 -2.90972800
- C 2.20205200 -2.60139900 0.94329400
- C 1.59773100 -3.14413800 -0.25799700
- C 0.26266500 -3.51733700 -0.25424000
- C -0.52915900 -3.36464200 0.95086600
- C 0.04824100 -2.84549400 2.09917600
- C 2.14954200 -2.43609200 -1.39666900
- C 1.34198900 -2.13187800 -2.48157700
- C 1.44292000 -0.83359500 -3.11916700
- C 2.34693800 0.10368900 -2.64361900
- C 3.19127600 -0.21424200 -1.50852300
- C 3.09482000 -1.45560400 -0.89909300
- C -3.32413700 -0.98244200 0.70019100

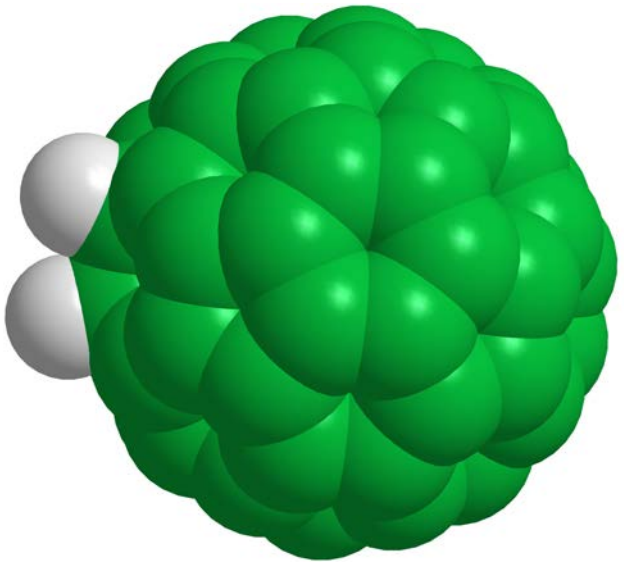


$C_{60}H_2(6,6)$

- Zero-point correction= 0.406663 (Hartree/ Particle)
- Thermal correction to Energy= 0.427253
- Thermal correction to Enthalpy= 0.428197
- Thermal correction to Gibbs Free Energy= 0.363642
- Sum of electronic and zero-point Energies= -2286.271168
- Sum of electronic and thermal Energies= -2286.250578
- Sum of electronic and thermal Enthalpies= -2286.249634
- Sum of electronic and thermal Free Energies= -2286.314189

- C60H266

- 0 1
- C -1.38795200 -1.17316700 -2.98963500
- C -0.66416200 0.00005000 -3.43417500
- C 0.72102500 0.00004900 -3.45294600
- C 1.45075900 -1.17407300 -3.01355300
- C 0.76118800 -2.29962500 -2.58907600
- C -0.68744800 -2.30451700 -2.58516400
- C -1.38795300 1.17325500 -2.98960100
- C -2.24393100 -2.56949900 0.72402800
- C -2.24393100 -2.56947600 -0.72410200
- C -2.56114800 -0.74060000 -2.27448500
- C -2.98955200 -1.42966000 -1.17191600
- C -3.72900600 -0.78939900 -0.00001200
- C -3.72900600 0.78940000 0.00001300
- C -2.98955500 1.42969700 -1.17187400
- C -2.56115000 0.74066900 -2.27446300
- C 0.04342100 -3.47390400 -0.69233900
- C -2.98955500 -1.42969700 1.17187400
- C 1.21393300 -3.02564300 -1.41824300
- C 2.33515500 -2.59409600 -0.72503200
- C -2.98955000 1.42966100 1.17191500
- C 2.62163500 -0.72577100 -2.29206700
- C -2.24393100 2.56949900 -0.72402800
- C -0.68744800 -2.30459400 2.58509900
- C -1.12798700 -3.02144100 1.41990600
- C 0.04342000 -3.47392500 0.69223900
- C -1.12798600 3.02144200 -1.41990600
- C -0.68744700 2.30459400 -2.58510000
- C -1.12798700 -3.02140000 -1.41999300
- C 1.45076000 1.17416000 -3.01352000
- C -2.56115000 -0.74066800 2.27446200
- C 0.76118900 2.29970000 -2.58901100
- C 1.21393100 3.02568200 -1.41815600
- C 2.33515500 2.59411900 -0.72495700
- C 2.33515600 2.59409600 0.72503200
- C 3.05504900 1.41942000 1.17206000
- C 2.62163400 0.72577000 2.29206600
- C 1.45076000 1.17407300 3.01355400
- C 0.72102500 -0.00005000 3.45294500
- C -0.66416200 -0.00005000 3.43417700
- C -1.38795200 1.17316700 2.98963400
- C -0.68744800 2.30451900 2.58516500
- C 0.76118800 2.29962400 2.58907500
- C 1.21393300 3.02564200 1.41824300
- C 0.04342100 3.47390400 0.69233900
- C -1.12798700 3.02140100 1.41999300
- C -2.24393000 2.56947600 0.72410200
- C -2.56114900 0.74060000 2.27448600
- C -1.38795300 -1.17325400 2.98960100
- C 3.05504800 -1.41942000 -1.17205900
- C 3.50165800 -0.69308900 -0.00001000
- C 3.50165700 0.69308800 0.00001000
- C 3.05504800 1.41945500 -1.17201800
- C 2.62163600 0.72583700 -2.29204600
- C 3.05504700 -1.41945500 1.17201700
- C 2.62163700 -0.72583800 2.29204700
- C 1.45076000 -1.17416000 3.01352000
- C 0.76118800 -2.29970100 2.58901100
- C 1.21393100 -3.02568300 1.41815600
- C 2.33515500 -2.59411900 0.72495700
- C 0.04342100 3.47392500 -0.69223900
- H -4.77451600 -1.11415100 -0.00002400
- H -4.77451600 1.11415100 0.00002600

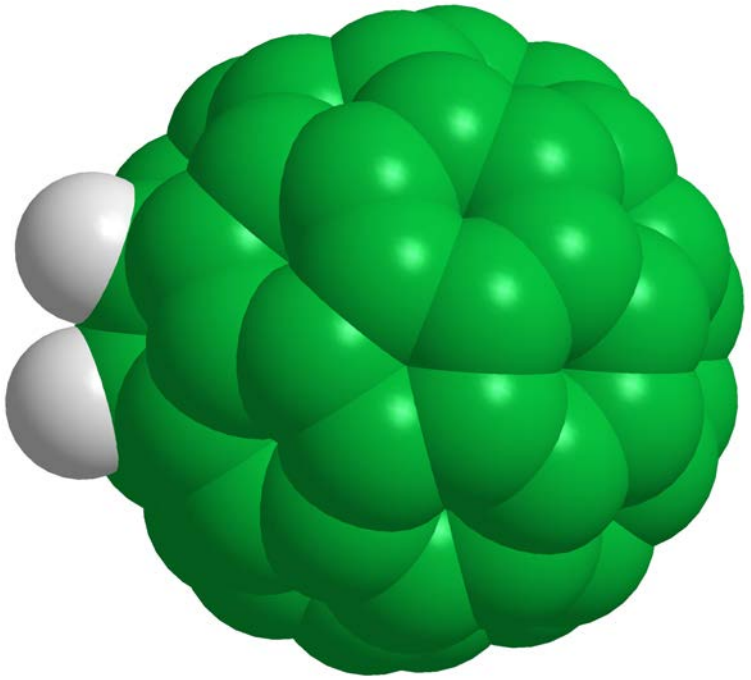


$C_{60}H_2(6,5)$

- Zero-point correction= 0.405420 (Hartree/Particle)
- Thermal correction to Energy= 0.426223
- Thermal correction to Enthalpy= 0.427167
- Thermal correction to Gibbs Free Energy= 0.362268
- Sum of electronic and zero-point Energies= -2286.236784
- Sum of electronic and thermal Energies= -2286.215981
- Sum of electronic and thermal Enthalpies= -2286.215036
- Sum of electronic and thermal Free Energies= -2286.279936

- C60H2

- 0 1
- C 2.16592500 -2.60087800 0.95815100
- C 1.21691300 -2.61197500 2.04693100
- C -0.09056800 -3.04330100 1.84516300
- C -0.50181600 -3.48461600 0.53255900
- C 0.41450500 -3.46641700 -0.51178700
- C 1.77288200 -3.02370900 -0.28758600
- C 1.47765400 -1.43326400 2.82792400
- C 2.73314400 0.00028800 -2.13097200
- C 3.01442200 -1.16634200 -1.35246200
- C 3.03217900 -1.42540300 1.10858200
- C 3.75226400 -0.80184800 -0.06350000
- C 3.75229400 0.80172700 -0.06324900
- C 3.03223000 1.42493700 1.10902700
- C 2.61164900 0.72493600 2.20338200
- C 2.61162200 -0.72573900 2.20315200
- C 1.10703300 -2.27054100 -2.40823500
- C 3.01447300 1.16666000 -1.35209800
- C 0.00374300 -3.00678300 -1.82225600
- C -1.29837100 -2.58849000 -2.04090900
- C 2.16602400 2.60049100 0.95896600
- C -1.86122100 -3.02945500 0.30784800
- C 1.47770700 1.43230100 2.82837600
- C 0.85804100 1.16608900 -3.20949100
- C 1.68650800 0.00045300 -3.06195300
- C 0.85799400 -1.16510300 -3.20984800
- C 0.43461500 0.73641900 3.38998400
- C 0.43458700 -0.73752200 3.38975000
- C 2.20569000 -2.26894300 -1.47902400
- C -1.18617700 -2.31068400 2.43426000
- C 2.20578200 2.26932900 -1.47831600
- C -0.92450900 -1.17769900 3.19650900
- C -1.76152200 -0.00046000 3.06530200
- C -2.81832200 -0.00029700 2.17066700
- C -3.08028800 1.17432700 1.36078700
- C -3.49497900 0.72354900 0.04575800
- C -3.08827700 1.41854200 -1.08339800
- C -2.25076900 2.59590000 -0.94686900
- C -1.29826700 2.58919000 -2.04009400
- C 0.00386700 3.00736000 -1.82131300
- C 0.41464800 3.46656400 -0.51070000
- C -0.50166900 3.48446500 0.53365600
- C -1.86109500 3.02943200 0.30880600
- C -2.28673100 2.30181300 1.49041500
- C -1.18608100 2.30994800 2.43498400
- C -0.09044600 3.04271600 1.84612200
- C 1.21701500 2.61127400 2.04775600
- C 1.77300200 3.02373400 -0.28663800
- C 1.10712600 2.27126400 -2.40753300
- C -2.25087600 -2.59550600 -0.94768900
- C -3.08833400 -1.41806900 -1.08384900
- C -3.49500500 -0.72341600 0.04552800
- C -3.08033800 -1.17464000 1.36041000
- C -2.28682500 -2.30219800 1.48968500
- C -2.66080100 -0.69495500 -2.26181000
- C -2.66077500 0.69578300 -2.26159000
- C -1.55840300 1.41821400 -2.85790300
- C -0.50366100 0.72581700 -3.43221000
- C -0.50368900 -0.72470800 -3.43243700
- C -1.55845800 -1.41724300 -2.85834700
- C -0.92446200 1.17670600 3.19687400
- H 4.79157000 -1.14347600 -0.09992400
- H 4.79161200 1.14333200 -0.09955500



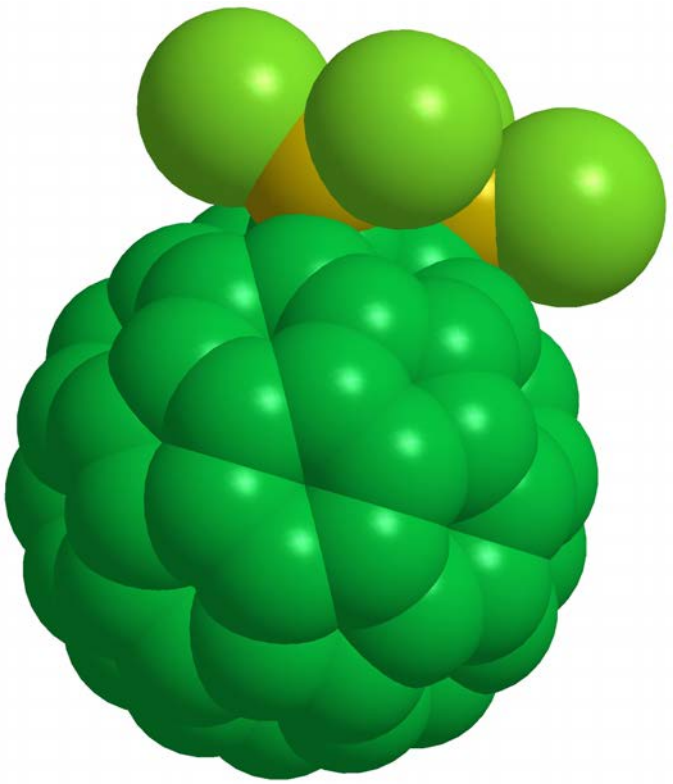
$C_{60}P1(6,6)$

- Zero-point correction= 0.398168 (Hartree/Particle)
- Thermal correction to Energy= 0.426854
- Thermal correction to Enthalpy= 0.427798
- Thermal correction to Gibbs Free Energy= 0.344296
- Sum of electronic and zero-point Energies= -4175.663889
- Sum of electronic and thermal Energies= -4175.635203
- Sum of electronic and thermal Enthalpies= -4175.634259
- Sum of electronic and thermal Free Energies= -4175.717761

- C60P1

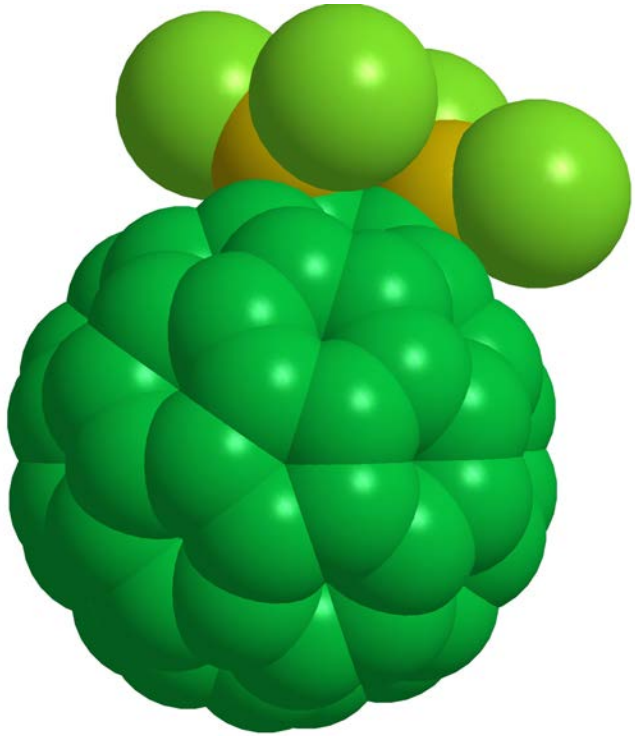
- 0 1

C	2.23369100	3.04017200	1.38798400
C	1.78073300	2.32627000	2.56621700
C	2.47035700	1.20536100	3.00167300
C	3.64163400	0.74945500	2.28479400
C	4.07479600	1.43120900	1.15773500
C	3.35474400	2.60157900	0.69893500
C	0.33197800	2.33021900	2.56216600
C	1.78249300	2.27308100	-2.61223100
C	2.23554200	3.01223400	-1.44953400
C	1.06348900	3.48009600	0.65698900
C	1.06574100	3.46788900	-0.72732100
C	-0.10432500	3.00550900	-1.44874800
C	-1.21639800	2.56097300	-0.74504500
C	-1.22414400	2.57528300	0.70005000
C	-0.10836100	3.03348300	1.38894300
C	4.07449600	1.40724200	-1.18622500
C	0.33376400	2.27477000	-2.60538100
C	4.52121300	0.69304700	-0.00700200
C	4.52121500	-0.69303900	0.00695300
C	-1.95225200	1.41492300	-1.18482700
C	3.64167400	-0.70186900	2.29925800
C	-1.97931800	1.44279400	1.15873000
C	1.74000400	-0.03655300	-3.45235000
C	2.47018400	1.14242400	-3.02441900
C	3.64163900	0.70187400	-2.29929500
C	-1.54710300	0.76587800	2.26812500
C	-0.37020400	1.20506500	2.97745200
C	3.35552400	2.58691900	-0.75112600
C	1.74005300	0.03655200	3.45234100
C	-0.36685100	1.14031100	-3.00172600
C	0.35504800	0.03735100	3.43485000
C	-0.36680400	-1.14031800	3.00174600
C	0.33380900	-2.27477600	2.60539300
C	-0.10429400	-3.00551400	1.44876400
C	1.06576200	-3.46789100	0.72732200
C	1.06349000	-3.48009800	-0.65698900
C	-0.10837200	-3.03349000	-1.38892600
C	0.33194900	-2.33022300	-2.56215600
C	-0.37024300	-1.20507100	-2.97743300
C	-1.54713300	-0.76588800	-2.26808600
C	-1.97932700	-1.44280600	-1.15868500
C	-1.22414600	-2.57529500	-0.70001700
C	-1.21637900	-2.56098300	0.74507800
C	-1.95222600	-1.41493000	1.18486600
C	-2.73408700	-0.80024500	0.00694300
C	-1.53809800	0.71254900	-2.28337200
C	0.35499900	-0.03735600	-3.43484000
C	4.07451700	-1.40723600	1.18618200
C	3.35554300	-2.58691500	0.75109400
C	2.23557200	-3.01223200	1.44951800
C	1.78253700	-2.27308100	2.61222200
C	2.47023200	-1.14242300	3.02440000
C	3.35474300	-2.60157400	-0.69896800
C	2.23368000	-3.04017100	-1.38800000
C	1.78070400	-2.32627100	-2.56622800
C	2.47031800	-1.20535900	-3.00169300
C	3.64160400	-0.74945000	-2.28483100
C	4.07478400	-1.43120300	-1.15777800
C	-1.53806400	-0.71256000	2.28340900
B	-4.16178300	1.44307400	-0.31148400
B	-4.16181000	-1.44306100	0.31150600
Cl	-5.15090600	-0.74060100	1.59624200
Cl	-4.70248600	-2.92745200	-0.43861500
Cl	-5.15089100	0.74058000	-1.59620700
Cl	-4.70243800	2.92750100	0.43856600
C	-2.73408700	0.80022300	-0.00688100



$C_{60}P2(6,5)$

1.	Zero-point correction=	0.397263 (Hartree/Particle)		
2.	Thermal correction to Energy=	0.426095		
3.	Thermal correction to Enthalpy=	0.427040		
4.	Thermal correction to Gibbs Free Energy=	0.343375		
5.	Sum of electronic and zero-point Energies=	-4175.632848		
6.	Sum of electronic and thermal Energies=	-4175.604016		
7.	Sum of electronic and thermal Enthalpies=	-4175.603071		
8.	Sum of electronic and thermal Free Energies= -4175.686736			
9.	C60B2I			
10.	0 1			
11.	C	-1.12707600	-2.61133600	-0.97053300
12.	C	-0.16568900	-2.62709600	-2.04682000
13.	C	1.13956500	-3.05430500	-1.82453500
14.	C	1.53530300	-3.48759700	-0.50400200
15.	C	0.60650000	-3.46943900	0.52813000
16.	C	-0.74879900	-3.02963200	0.28095500
17.	C	-0.41927200	-1.45609200	-2.84057200
18.	C	-1.74560100	0.01177000	2.08974100
19.	C	-1.99544900	-1.16264000	1.31565300
20.	C	-1.99539000	-1.43976100	-1.13908600
21.	C	-2.75685200	0.79815300	0.01137200
22.	C	-1.98755400	1.40556400	-1.15514600
23.	C	-1.55892000	0.69738800	-2.24414600
24.	C	-1.56393700	-0.74783300	-2.23777200
25.	C	-0.11236700	-2.26089700	2.40650800
26.	C	-2.02882100	1.17222900	1.30507200
27.	C	0.99880200	-3.00057200	1.84145100
28.	C	2.29577200	-2.57531600	2.07435400
29.	C	-1.13391400	2.58556100	-0.99967800
30.	C	2.89097600	-3.02852800	-0.26429800
31.	C	-0.42420200	1.40827200	-2.85747700
32.	C	0.11220100	1.18297000	3.18739500
33.	C	-0.71083300	0.01622300	3.03277800
34.	C	0.11956500	-1.14731900	3.19964900
35.	C	0.62875000	0.71073500	-3.39977400
36.	C	0.63083200	-0.76186700	-3.39219200
37.	C	-1.19448700	-2.26667200	1.45864200
38.	C	2.24194400	-2.32402500	-2.40388500
39.	C	-1.21577100	2.27396500	1.43275800
40.	C	1.98843700	-1.19729900	-3.17735800
41.	C	2.82141400	-0.01731800	-3.04241600
42.	C	3.86479500	-0.00858300	-2.13258700
43.	C	4.11250100	1.17175800	-1.32608300
44.	C	4.51057200	0.73023000	-0.00291700
45.	C	4.08631100	1.43113000	1.11608700
46.	C	3.24816800	2.60583400	0.96103500
47.	C	2.28041900	2.60395700	2.04092800
48.	C	0.98101900	3.01951700	1.80319200
49.	C	0.58813300	3.47145400	0.48502600
50.	C	1.51789200	3.48120900	-0.54793900
51.	C	2.87523500	3.03070900	-0.30242400
52.	C	3.31894700	2.29672800	-1.47338600
53.	C	2.23049800	2.29489200	-2.43222500
54.	C	1.12632800	3.02939200	-1.86268900
55.	C	-0.17616600	2.59010700	-2.07787300
56.	C	-0.76576800	3.02434200	0.24695100
57.	C	-0.12948400	2.28266600	2.37655800
58.	C	3.26266300	-2.58583300	0.99370500
59.	C	4.09502300	-1.40548100	1.13432100
60.	C	4.51439400	-0.71670900	0.00613900
61.	C	4.11869300	-1.17705800	-1.31144800
62.	C	3.32998900	-2.30751500	-1.44472200
63.	C	3.64892900	-0.67600100	2.30159900
64.	C	3.64449400	0.71454800	2.29261600
65.	C	2.53214100	1.43805100	2.86903000
66.	C	1.47198400	0.74707900	3.43341600
67.	C	1.47612500	-0.70297500	3.44225500
68.	C	2.54003400	-1.39728300	2.88708500
69.	C	1.98325800	1.15691200	-3.19240100
70.	B	-4.14988200	1.49186800	-0.29393700
71.	B	-4.17613500	-1.48723900	0.30257600
72.	Cl	-4.66810900	-2.98188300	-0.45985200
73.	Cl	-5.20305500	-0.80829400	1.56718000
74.	Cl	-5.18568300	0.81555400	-1.55527300
75.	Cl	-4.60880300	3.00385500	0.45851800
76.	C	-2.75456200	-0.82704500	0.01483100



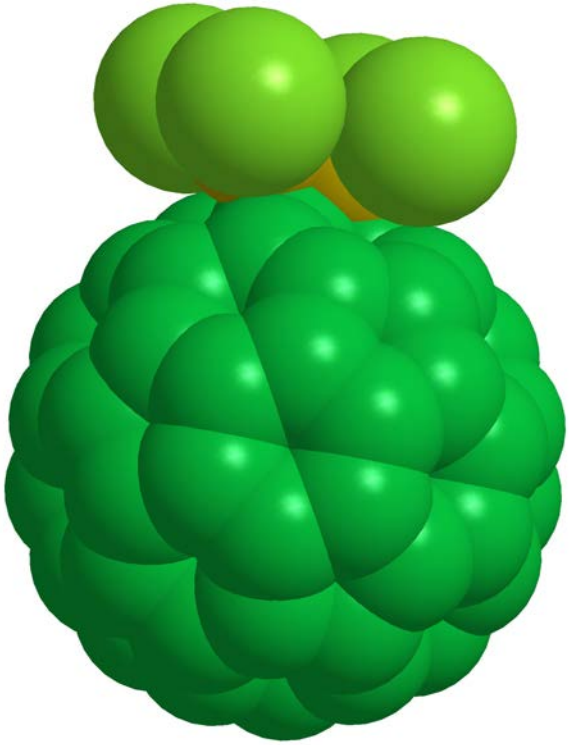
C_{60} B_2Cl_4 TS [6,6]

- Zero-point correction= 0.396574 (Hartree/Particle)
- Thermal correction to Energy= 0.424783
- Thermal correction to Enthalpy= 0.425727
- Thermal correction to Gibbs Free Energy= 0.343607
- Sum of electronic and zero-point Energies= -4175.598372
- Sum of electronic and thermal Energies= -4175.570163
- Sum of electronic and thermal Enthalpies= -4175.569219
- Sum of electronic + thermal Free Energies= -4175.651339

- C60TS

- 0 1

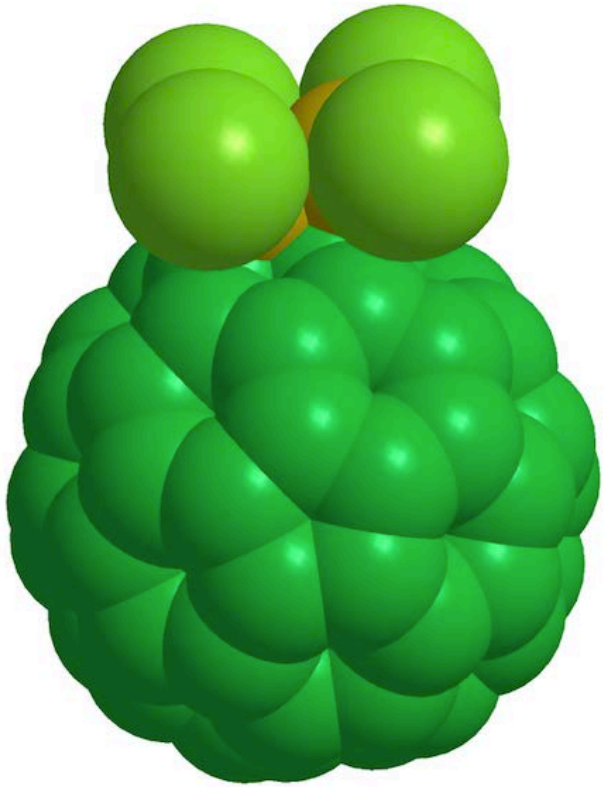
C	1.79014300	3.17434500	1.41822100
C	1.45084300	2.39069100	2.58926100
C	2.29674800	1.37769500	3.01355100
C	3.52250900	1.10669300	2.29322000
C	3.84686400	1.85524100	1.17212900
C	2.96164600	2.91172800	0.72488900
C	0.01803100	2.17631200	2.58254300
C	1.45083200	2.39069900	-2.58924900
C	1.79013600	3.17434900	-1.41820800
C	0.56568500	3.44631100	0.69228600
C	0.56568100	3.44631100	-0.69226600
C	-0.52836200	2.82799900	-1.41565600
C	-1.57196200	2.23181200	-0.72435100
C	-1.57195800	2.23180700	0.72437500
C	-0.52835600	2.82799400	1.41567800
C	3.84685600	1.85524800	-1.17212900
C	0.01801900	2.17632100	-2.58252900
C	4.39683100	1.20401900	-0.00000200
C	4.59772900	-0.16720100	-0.00000400
C	-2.13162100	0.98729300	-1.18443800
C	3.73432000	-0.32843400	2.29365600
C	-2.13161400	0.98728700	1.18445900
C	1.75046200	0.10999500	-3.46067900
C	2.29673700	1.37770700	-3.01355200
C	3.52249700	1.10670300	-2.29322200
C	-1.59368700	0.35151700	2.27900200
C	-0.50500500	0.96252700	3.00537600
C	2.96164300	2.91173100	-0.72488100
C	1.75047500	0.10998400	3.46068000
C	-0.50501500	0.96253500	-3.00535800
C	0.38083600	-0.09240700	3.45347100
C	-0.16443800	-1.35991600	3.00762000
C	0.68996700	-2.37098300	2.59016500
C	0.35510600	-3.14303300	1.41926700
C	1.57860100	-3.41920200	0.69283600
C	1.57859800	-3.41920300	-0.69284500
C	0.35510000	-3.14303100	-1.41927000
C	0.68995600	-2.37097600	-2.59016600
C	-0.16444800	-1.35990600	-3.00761100
C	-1.38863800	-1.09869100	-2.28971400
C	-1.70551400	-1.83388400	-1.17331100
C	-0.81528100	-2.86628700	-0.72329500
C	-0.81527800	-2.86628700	0.72329900
C	-1.70551300	-1.83388400	1.17332000
C	-2.41051400	-1.24679400	0.00000200
C	-1.59369900	0.35152600	-2.27898600
C	0.38082400	-0.09239700	-3.45346100
C	4.26261700	-0.95066100	1.17298300
C	3.71983700	-2.21685000	0.72508500
C	2.67416700	-2.80697700	1.41810400
C	2.12329100	-2.15651600	2.59060200
C	2.64246000	-0.94444900	3.01786200
C	3.71983400	-2.21684700	-0.72509900
C	2.67416000	-2.80697300	-1.41811400
C	2.12328100	-2.15650900	-2.59060800
C	2.64244800	-0.94443900	-3.01786500
C	3.73430700	-0.32842400	-2.29365800
C	4.26261200	-0.95065700	-1.17299200
C	-1.38863100	-1.09870000	2.28972800
B	-4.68308000	0.79039800	0.00001900
B	-4.09020200	-0.99800000	-0.00002500
Cl	-4.80146900	-1.65919600	1.55001100
Cl	-4.80138000	-1.65904900	-1.55017100
Cl	-5.18663100	1.57430300	-1.48786600
Cl	-5.18673400	1.57415500	1.48797200
C	-2.59281300	0.22019600	0.00001100



C_{60} B_2Cl_4 TS [6,5]

- Zero-point correction= 0.395614 (Hartree/Particle)
- Thermal correction to Energy= 0.423919
- Thermal correction to Enthalpy= 0.424863
- Thermal correction to Gibbs Free Energy= 0.342726
- Sum of electronic and zero-point Energies= -4175.577425
- Sum of electronic and thermal Energies= -4175.549120
- Sum of electronic and thermal Enthalpies= -4175.548176
- Sum of electronic and thermal Free Energies= -4175.63031
- C60ITSc

- 0 1
- C -0.73235900 -2.94896500 -0.66569100
- C 0.20679200 -2.93977400 -1.76408800
- C 1.55668900 -3.15640000 -1.53010900
- C 2.02069100 -3.39494300 -0.17797400
- C 1.11679700 -3.41282400 0.87383000
- C -0.28833400 -3.17489000 0.61873300
- C -0.21800700 -1.90664300 -2.67750500
- C -1.69758400 -0.17415200 2.16658900
- C -1.78803900 -1.43868500 1.49763200
- C -1.73213000 -1.92639800 -0.91514300
- C -2.66604600 0.26175700 0.00953400
- C -2.16206000 0.86082000 -1.20723000
- C -1.62150100 0.09464800 -2.24943400
- C -1.43684700 -1.30291200 -2.13429600
- C 0.25027500 -2.15141800 2.65296600
- C -2.13105400 0.85954200 1.27239000
- C 1.45149900 -2.77448000 2.12928100
- C 2.67788500 -2.15067400 2.28577200
- C -1.48107900 2.14365300 -1.18446500
- C 3.30349800 -2.73852100 -0.01825200
- C -0.62590300 0.90351300 -2.95605400
- C -0.00696100 1.35164100 3.08141100
- C -0.66380000 0.07101800 3.07313100
- C 0.33062000 -0.94392800 3.32627200
- C 0.51455400 0.31021100 -3.45449800
- C 0.72505600 -1.13094500 -3.31676500
- C -0.83200100 -2.39905400 1.73009000
- C 2.54470300 -2.34349400 -2.20299600
- C -1.48355500 2.07732300 1.26157500
- C 2.13403700 -1.34918200 -3.08050700
- C 2.79446600 -0.05777400 -3.07462800
- C 3.83103500 0.18557300 -2.18882700
- C 3.91356600 1.46111200 -1.50247100
- C 4.38390900 1.21314100 -0.15373300
- C 3.87338900 1.95186300 0.90273400
- C 2.87568700 2.97600500 0.65777300
- C 1.92978700 2.94592700 1.75580800
- C 0.58300100 3.15377100 1.51362100
- C 0.11493800 3.41172100 0.16714600
- C 1.02032900 3.44462100 -0.88432900
- C 2.43015200 3.21520400 -0.63165300
- C 2.96342400 2.44144200 -1.73682400
- C 1.87830500 2.18733600 -2.66396900
- C 0.68252500 2.80974900 -2.13908900
- C -0.54343700 2.17567000 -2.28558100
- C -1.16632200 2.75793900 0.00734400
- C -0.40646600 2.33036800 2.18245200
- C 3.62116300 -2.12813500 1.18409000
- C 4.28404500 -0.83840000 1.19194500
- C 4.59071200 -0.21221800 -0.00609900
- C 4.25284400 -0.84901200 -1.26477400
- C 3.62621100 -2.08406900 -1.27162600
- C 3.74991700 -0.06737400 2.29565000
- C 3.55037400 1.29926200 2.15441600
- C 2.34998600 1.91155700 2.68382200
- C 1.40502500 1.13658200 3.33607400
- C 1.61434200 -0.28921000 3.48506500
- C 2.76134700 -0.87773100 2.97600900
- C 1.79556900 0.96475900 -3.31614200
- B -4.55571500 0.82925400 -0.05374700
- B -4.09579900 -1.04598200 0.08903000
- Cl -4.78693500 -1.76000200 -1.43245200
- Cl -4.89362900 -1.53845400 1.65012500
- Cl -5.15698400 1.45413300 -1.59118300
- Cl -5.05888500 1.74165300 1.36891200
- C -2.44283800 -1.27401700 0.16522300



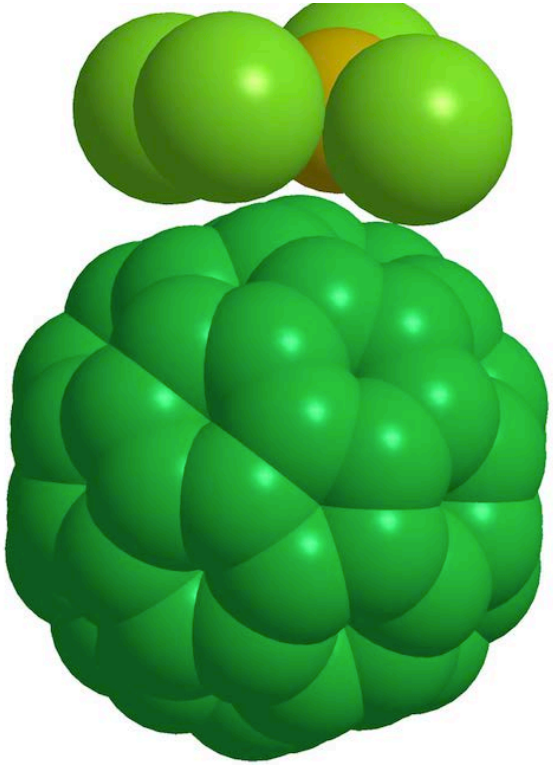
C_{60} VDW

- Zero-point correction= 0.397219 (Hartree/ Particle)
- Thermal correction to Energy= 0.426807
- Thermal correction to Enthalpy= 0.427751
- Thermal correction to Gibbs Free Energy= 0.338105
- Sum of electronic and zero-point Energies= -4175.633621
- Sum of electronic and thermal Energies= -4175.604034
- Sum of electronic and thermal Enthalpies= -4175.603090
- Sum of electronic + thermal Free Energies= -4175.692735

- wb97xd/6-31g(d,p)
- C60ITSb

- 0 1

C	1.85847800	-0.05235900	-1.84167900
C	1.13661500	-1.16282200	-2.42843200
C	0.01477100	-0.92269800	-3.20614900
C	-0.43326500	0.43737000	-3.43248900
C	0.25918400	1.49919600	-2.87198100
C	1.43046800	1.24752300	-2.05676100
C	1.13592200	-2.25369000	-1.47304800
C	1.13569600	2.25393600	1.47306100
C	1.85634600	1.81843000	0.29489300
C	2.30000100	-0.45705800	-0.52236600
C	1.85842400	0.05267100	1.84168900
C	1.43059500	-1.24726900	2.05677200
C	1.43016100	-2.20263000	0.96553100
C	1.85654100	-1.81813600	-0.29488100
C	0.25933900	3.04483900	-1.10657800
C	1.13649700	1.16307500	2.42845800
C	-0.46531600	2.60883900	-2.28394900
C	-1.85093400	2.60832700	-2.28351400
C	0.25933400	-1.49905500	2.87199000
C	-1.88296000	0.43735800	-3.43270600
C	0.25965000	-3.04469500	1.10658700
C	-1.15849900	2.80546100	2.15226000
C	0.01419000	3.05693400	1.33833600
C	-0.43360500	3.46028600	0.01977100
C	-0.43325300	-3.46020700	-0.01976200
C	0.01449600	-3.05680100	-1.33832600
C	1.42993100	2.20289100	-0.96551500
C	-1.15814100	-1.76264200	-3.06519100
C	0.01467800	0.92282300	3.20616700
C	-1.15821800	-2.80545100	-2.15224600
C	-2.33082300	-3.05603700	-1.33762000
C	-3.45189200	-2.25230600	-1.47132300
C	-4.17649300	-1.81653500	-0.29401900
C	-4.62444900	-0.45676400	-0.52124500
C	-4.62449700	0.45642300	0.52125200
C	-4.17635900	0.05175200	1.83905900
C	-3.45225100	1.16155900	2.42646900
C	-2.33101300	0.92218500	3.20519600
C	-1.88291800	-0.43742000	3.43271700
C	-2.57506300	-1.49845500	2.87070100
C	-3.74790600	-1.24817800	2.05661200
C	-3.74821500	-2.20323100	0.96608200
C	-2.57559600	-3.04354900	1.10599800
C	-1.85067100	-2.60838700	2.28352900
C	-0.46505200	-2.60877100	2.28396100
C	-0.43322300	-0.43729500	3.43249800
C	-1.15831700	1.76265300	3.06520600
C	-2.57521100	1.49832200	-2.87068700
C	-3.74802800	1.24792300	-2.05660300
C	-4.17635200	-0.05205000	-1.83905000
C	-3.45213300	-1.16178300	-2.42645700
C	-2.33092100	-0.92229000	-3.20518500
C	-3.74844400	2.20297600	-0.96607600
C	-4.17667800	1.81623600	0.29402700
C	-3.45212000	2.25207900	1.47133400
C	-2.33113100	3.05592300	1.33763600
C	-1.88325000	3.46055800	0.01972200
C	-2.57590800	3.04341500	-1.10598200
C	-1.88289800	-3.46062400	-0.01970700
B	5.31596000	0.86130500	0.00086000
B	5.31585800	-0.86130800	-0.00098200
Cl	5.16034200	-1.76206900	1.49662900
Cl	5.54436900	-1.75640800	-1.49351600
Cl	5.54481500	1.75621300	1.49344700
Cl	5.16020400	1.76220000	-1.49665300
C	2.29993400	0.45740600	0.52237400

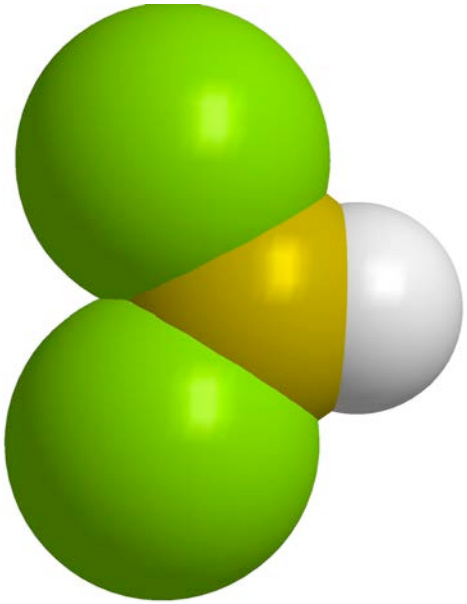


$HBCl_2$ B3LYP

- Zero-point correction= 0.014795 (Hartree/Particle)
- Thermal correction to Energy= 0.018324
- Thermal correction to Enthalpy= 0.019268
- Thermal correction to Gibbs Free Energy= -0.011160
- Sum of electronic and zero-point Energies= -945.968644
- Sum of electronic and thermal Energies= -945.965115
- Sum of electronic and thermal Enthalpies= -945.964171
- Sum of electronic and thermal Free Energies= -945.994599

- HBCl2

- 0 1
- B 0.00000000 0.00000000 0.70547800
- H 0.00000000 0.00000000 1.88568100
- Cl 0.00000000 1.51926400 -0.15920800
- Cl 0.00000000 -1.51926400 -0.15920800

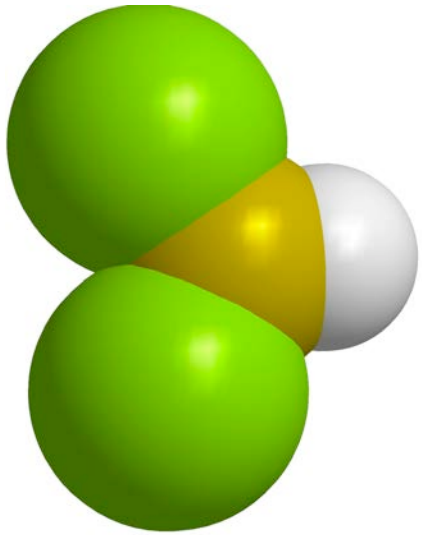


$HBCl_2$ ωB97X-D

- Zero-point correction= 0.014839 (Hartree/Particle)
- Thermal correction to Energy= 0.018358
- Thermal correction to Enthalpy= 0.019302
- Thermal correction to Gibbs Free Energy= -0.011104
- Sum of electronic and zero-point Energies= -945.921527
- Sum of electronic and thermal Energies= -945.918009
- Sum of electronic and thermal Enthalpies= -945.917065
- Sum of electronic and thermal Free Energies= -945.947471

- HBCl2W

- 0 1
- B 0.00000000 0.00000000 0.70586400
- H 0.00000000 0.00000000 1.88968400
- Cl 0.00000000 1.51482000 -0.15938300
- Cl 0.00000000 -1.51482000 -0.15938300

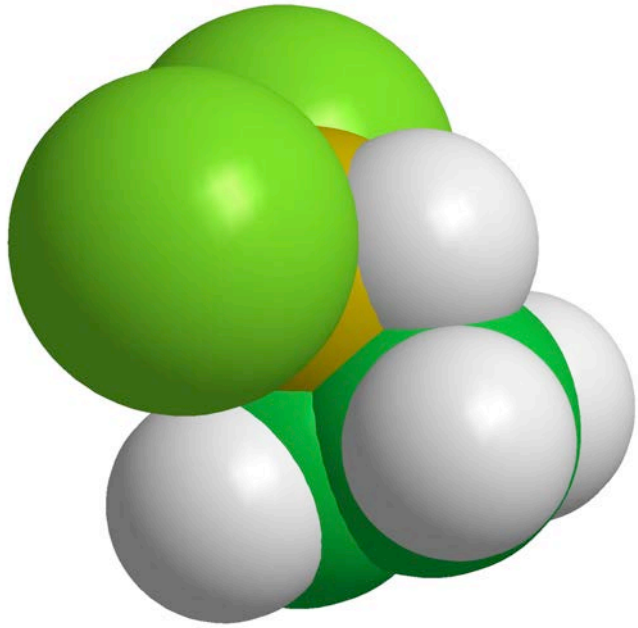


$HBCl_2$ C_2H_4 TS B3LYP

- Zero-point correction= 0.069435 (Hartree/Particle)
- Thermal correction to Energy= 0.075101
- Thermal correction to Enthalpy= 0.076046
- Thermal correction to Gibbs Free Energy= 0.039280
- Sum of electronic and zero-point Energies= -1024.506548
- Sum of electronic and thermal Energies= -1024.500882
- Sum of electronic and thermal Enthalpies= -1024.499938
- Sum of electronic and thermal Free Energies= -1024.536704

- HBEtTSF

- 0 1
- C 0.00092800 1.92954800 -0.51723800
- C 0.00029400 1.49167300 0.80547900
- B 0.00001000 0.06363400 -0.24565400
- Cl 1.58017000 -0.84460100 0.00621100
- Cl -1.58076000 -0.84362700 0.00611400
- H 0.00002100 0.41447000 -1.42295700
- H -0.92188400 1.50345900 1.36917700
- H 0.92076200 2.21647600 -1.01307900
- H -0.91835000 2.21724900 -1.01364900
- H 0.92210900 1.50273000 1.36979300

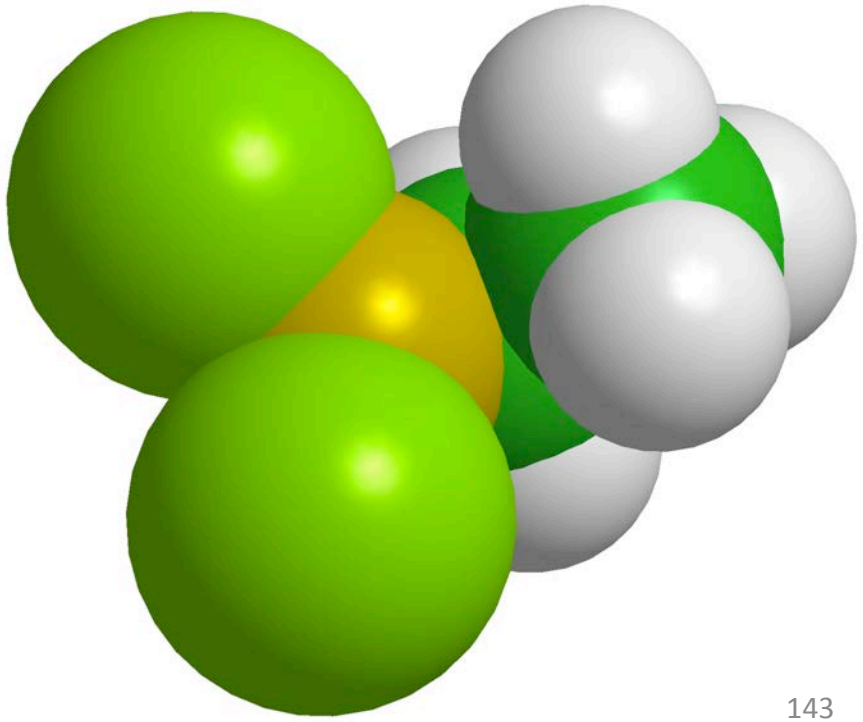


$HBCl_2$ ethylene gauche product B3LYP

- Zero-point correction= 0.072012 (Hartree/Particle)
- Thermal correction to Energy= 0.078495
- Thermal correction to Enthalpy= 0.079439
- Thermal correction to Gibbs Free Energy= 0.039663
- Sum of electronic and zero-point Energies= -1024.577396
- Sum of electronic and thermal Energies= -1024.570913
- Sum of electronic and thermal Enthalpies= -1024.569968
- Sum of electronic and thermal Free Energies= -1024.609744

- HBCl2EtP

- 0 1
- C 2.35376400 -0.00666300 -0.49961100
- H 2.21370800 0.87995800 -1.12256600
- C 1.38181000 -0.00701300 0.71029700
- B -0.10409400 -0.00037900 0.23582700
- Cl -0.95979900 1.51412700 -0.07861300
- Cl -0.97330800 -1.50691400 -0.07956400
- H 1.57647400 -0.89285100 1.32237000
- H 3.38962600 -0.01150300 -0.15320900
- H 1.58253200 0.87400900 1.32741200
- H 2.20751200 -0.88829100 -1.12824700



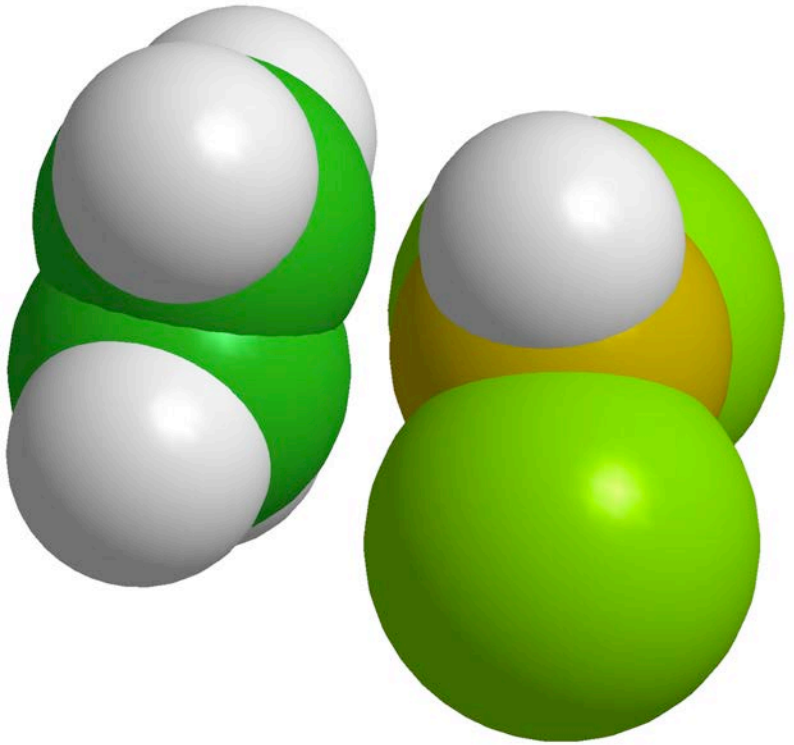
Ethene $HBCl_2$ vdW ωB97X-D

Zero-point correction= 0.067428 (Hartree/Particle)
Thermal correction to Energy= 0.075612
Thermal correction to Enthalpy= 0.076556
Thermal correction to Gibbs Free Energy= 0.032046
Sum of electronic and zero-point Energies= -1024.454100
Sum of electronic and thermal Energies= -1024.445916
Sum of electronic and thermal Enthalpies= -1024.444972
Sum of electronic and thermal Free Energies= -1024.489482

HBCl2EtVW

0 1

C	-2.57151900	0.15749700	0.47173300
C	-2.27910800	-0.49027700	-0.64808700
H	-2.39627100	-1.56565100	-0.73105900
B	0.64947300	0.06034500	0.67127500
H	0.19015000	0.06245800	1.76066500
Cl	0.87215500	1.57305800	-0.18139800
Cl	1.20836800	-1.43793100	-0.03651900
H	-2.94104900	-0.36200300	1.34977500
H	-1.91120400	0.02971800	-1.52680400
H	-2.45410700	1.23327000	0.55376100

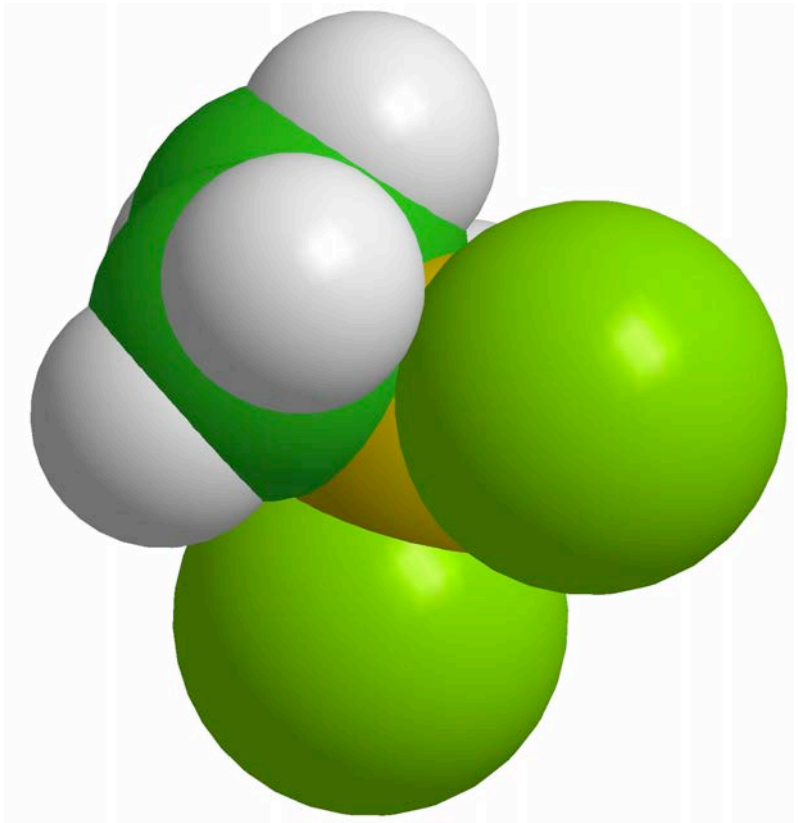


Ethene $HBCl_2$ TS ωB97X-D

- Zero-point correction= 0.070232 (Hartree/Particle)
- Thermal correction to Energy= 0.075862
- Thermal correction to Enthalpy= 0.076806
- Thermal correction to Gibbs Free Energy= 0.040071
- Sum of electronic and zero-point Energies= -1024.435489
- Sum of electronic and thermal Energies= -1024.429859
- Sum of electronic and thermal Enthalpies= -1024.428915
- Sum of electronic and thermal Free Energies= -1024.465649

- HBEtTSFW

- 0 1
- C 0.00004100 1.92282500 -0.50943100
- C 0.00001100 1.48907300 0.80510600
- B -0.00000100 0.05713100 -0.27412100
- Cl 1.57189600 -0.83883300 0.00967300
- Cl -1.57192100 -0.83879200 0.00966800
- H 0.00000700 0.39218900 -1.45283000
- H -0.92400100 1.48013400 1.36621200
- H 0.92154000 2.20506400 -1.00591500
- H -0.92142900 2.20511500 -1.00594100
- H 0.92400600 1.48008600 1.36623900

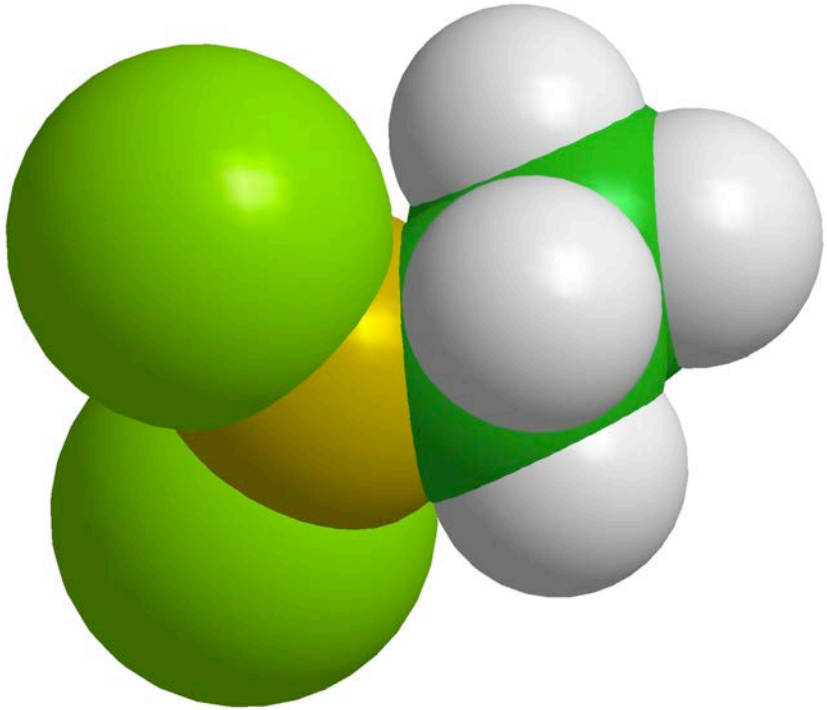


Ethene $HBCl_2$ product ωB97X-D

- Zero-point correction= 0.072424 (Hartree/Particle)
- Thermal correction to Energy= 0.078034
- Thermal correction to Enthalpy= 0.078978
- Thermal correction to Gibbs Free Energy= 0.042178
- Sum of electronic and zero-point Energies= -1024.506225
- Sum of electronic and thermal Energies= -1024.500615
- Sum of electronic and thermal Enthalpies= -1024.499671
- Sum of electronic and thermal Free Energies= -1024.536471

- HBCl2EtPW

- 0 1
- C 2.32679300 -0.00433200 -0.50735800
- H 2.17240300 0.88222600 -1.12736300
- C 1.38268200 -0.00451600 0.71662300
- B -0.10377800 -0.00021900 0.24297500
- Cl -0.95503100 1.50890300 -0.07858700
- Cl -0.96373900 -1.50423900 -0.07918600
- H 1.58403300 -0.89069200 1.32507700
- H 3.36922500 -0.00808700 -0.18283000
- H 1.58803100 0.87850100 1.32836800
- H 2.16741800 -0.88706000 -1.13157600

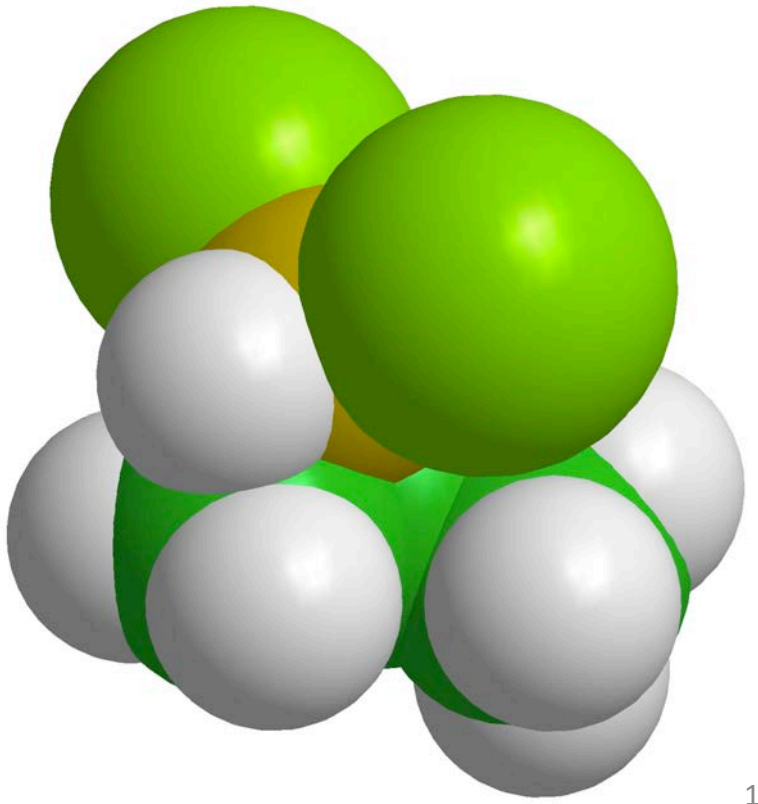


$HBCl_2$ propene sec-TS B3LYP

- Zero-point correction= 0.097528 (Hartree/Particle)
- Thermal correction to Energy= 0.104588
- Thermal correction to Enthalpy= 0.105532
- Thermal correction to Gibbs Free Energy= 0.065666
- Sum of electronic and zero-point Energies= -1063.804714
- Sum of electronic and thermal Energies= -1063.797654
- Sum of electronic and thermal Enthalpies= -1063.796710
- Sum of electronic and thermal Free Energies= -1063.836576

- HBP2TSF

- 0 1
- C 0.75779100 -1.24538600 1.14665000
- C 0.94297900 -1.04915900 -0.23210100
- B -0.33544300 0.02433600 0.34950100
- Cl 0.14146100 1.78365200 0.14217000
- Cl -1.94879400 -0.51732900 -0.35503100
- H -0.44474200 -0.12710400 1.57187200
- H 0.44214900 -1.75617800 -0.88367100
- H 1.44280800 -0.80335800 1.86317400
- C 2.18472900 -0.40226700 -0.80344900
- H 2.89072700 -1.18111900 -1.10808800
- H 1.94563000 0.20022700 -1.68131300
- H 2.67922300 0.24647300 -0.07938800
- H 0.13308600 -2.04724700 1.52194200

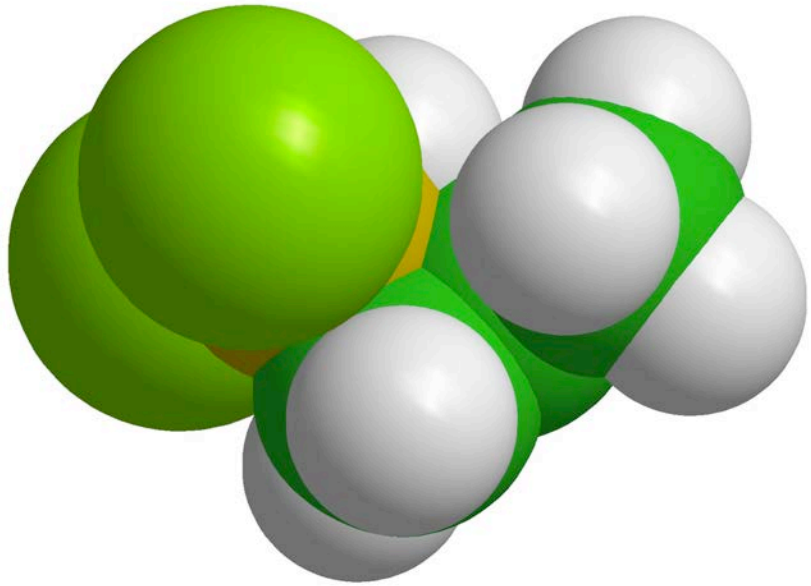


$HBCl_2$ propene prim-TS B3LYP

- Zero-point correction= 0.097307 (Hartree/Particle)
- Thermal correction to Energy= 0.104407
- Thermal correction to Enthalpy= 0.105351
- Thermal correction to Gibbs Free Energy= 0.065248
- Sum of electronic and zero-point Energies= -1063.812102
- Sum of electronic and thermal Energies= -1063.805002
- Sum of electronic and thermal Enthalpies= -1063.804057
- Sum of electronic and thermal Free Energies= -1063.844161

- HBP1TSF

- 0 1
- C 1.36832400 -0.99886000 -0.03968200
- C 0.67422000 -0.69905400 1.14568000
- B -0.28869500 -0.01545800 -0.12150900
- Cl -1.90793000 -0.89276700 -0.21427200
- Cl -0.31442500 1.82327900 0.03498900
- H 0.26643700 -0.24588700 -1.19602500
- C 2.59838500 -0.27281400 -0.48902800
- H 3.45505400 -0.77639200 -0.02596700
- H 2.72721100 -0.30828500 -1.57132700
- H 2.59387800 0.76489600 -0.15426400
- H 1.06225900 0.08317500 1.78628100
- H 1.16495300 -1.95277200 -0.51774700
- H 0.10813400 -1.48178300 1.63258000

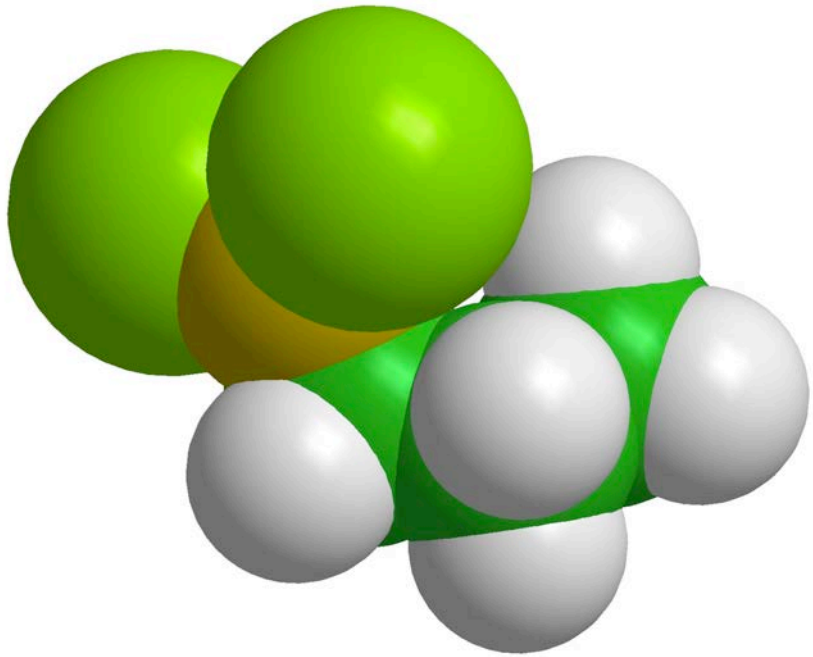


$HBCl_2$ to propene primary product B3LYP

- Zero-point correction= 0.100111 (Hartree/Particle)
- Thermal correction to Energy= 0.107810
- Thermal correction to Enthalpy= 0.108754
- Thermal correction to Gibbs Free Energy= 0.066402
- Sum of electronic and zero-point Energies= -1063.873888
- Sum of electronic and thermal Energies= -1063.866188
- Sum of electronic and thermal Enthalpies= -1063.865244
- Sum of electronic and thermal Free Energies= -1063.907596

- HBCl2P2P

- 0 1
- C -2.09168300 0.30695600 0.55254500
- H -2.11167700 -0.70639400 0.96433500
- C -0.67968200 0.90204400 0.70744000
- B 0.53698700 0.08258100 0.17424400
- Cl 0.50908300 -1.68053500 0.04621400
- Cl 2.05150900 0.89531900 -0.24611000
- H -0.64299200 1.91552000 0.29169100
- H -2.78914400 0.89710900 1.15562000
- C -2.57810400 0.28368100 -0.89972600
- H -2.59421600 1.29175900 -1.32585500
- H -1.93239600 -0.33427500 -1.53069400
- H -3.59058200 -0.12211600 -0.96942000
- H -0.45718300 1.03807400 1.77977900

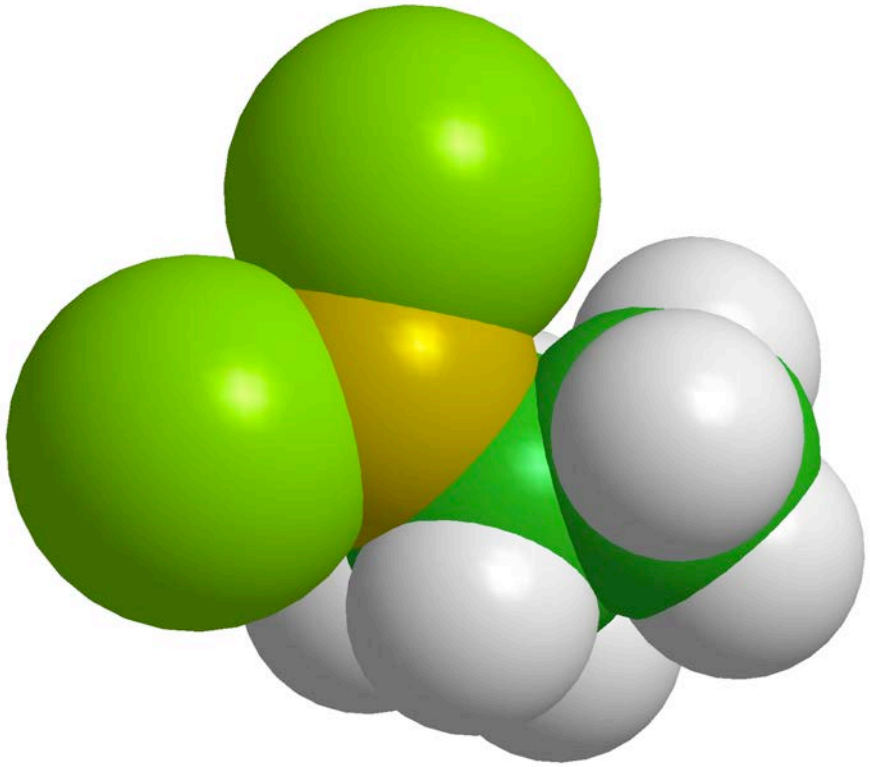


$HBCl_2$ to propene secondary product B3LYP

- Zero-point correction= 0.099987 (Hartree/Particle)
- Thermal correction to Energy= 0.107842
- Thermal correction to Enthalpy= 0.108786
- Thermal correction to Gibbs Free Energy= 0.066134
- Sum of electronic and zero-point Energies= -1063.871832
- Sum of electronic and thermal Energies= -1063.863977
- Sum of electronic and thermal Enthalpies= -1063.863033
- Sum of electronic and thermal Free Energies= -1063.905684

- HBCl2P1P

- 0 1
- C -1.57834600 -1.14473200 1.06119200
- H -1.67297700 -0.35070500 1.80746000
- C -1.10317700 -0.57618300 -0.30493000
- B 0.33949900 0.00565900 -0.11489100
- Cl 0.62696900 1.69520900 0.31644500
- Cl 1.75877500 -1.04222000 -0.25160400
- C -2.13469300 0.41498200 -0.87177600
- H -2.28533400 1.26269800 -0.19876200
- H -1.82543100 0.81297900 -1.84179700
- H -3.10066400 -0.08042600 -1.00709100
- H -1.02014100 -1.42644200 -0.99250300
- H -2.56065400 -1.61156400 0.94531500
- H -0.89263700 -1.90004500 1.45262400

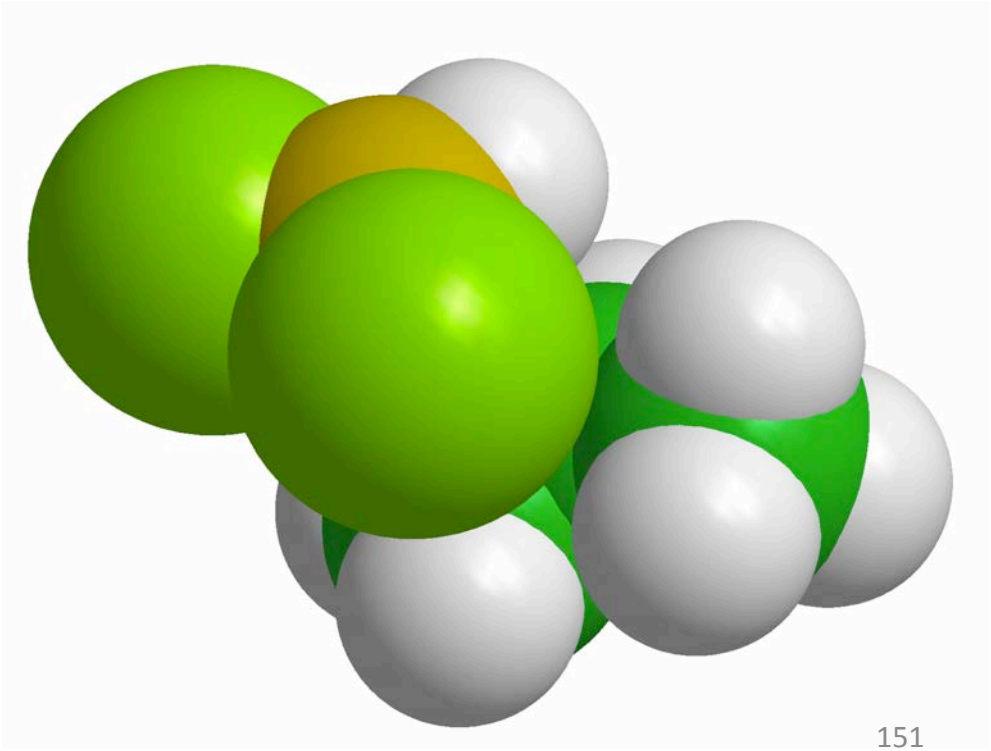


Propene $HBCl_2$ vdW (B-C_1) ωB97X-D

- Zero-point correction= 0.097016 (Hartree/Particle)
- Thermal correction to Energy= 0.105896
- Thermal correction to Enthalpy= 0.106841
- Thermal correction to Gibbs Free Energy= 0.061294
- Sum of electronic and zero-point Energies= -1063.743469
- Sum of electronic and thermal Energies= -1063.734589
- Sum of electronic and thermal Enthalpies= -1063.733645
- Sum of electronic and thermal Free Energies= -1063.779191

- HBCl2PaltVW

- 0 1
- C -2.08879900 -0.86787100 0.19441400
- C -1.46964900 -1.23638300 -0.92257200
- H -1.02556500 -2.21971600 -1.02758700
- B 0.87490300 0.19243600 0.63351400
- H 0.29242700 0.07370200 1.65610200
- Cl 0.72189500 1.67581200 -0.28530500
- Cl 2.00411300 -1.04439100 0.12719800
- H -2.14338000 -1.57610500 1.01928800
- H -1.39096900 -0.56531000 -1.77330300
- C -2.73170800 0.46438100 0.42280100
- H -3.79996600 0.34659600 0.62907100
- H -2.29214400 0.96455400 1.29220200
- H -2.61610300 1.11916600 -0.44338200

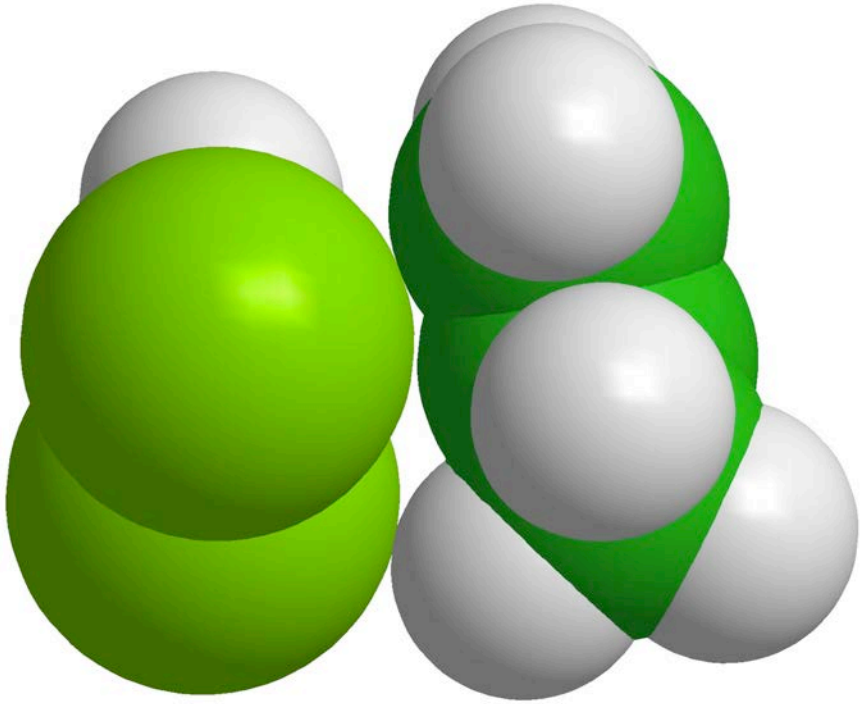


Propene $HBCl_2$ vdW (B-C_2) ωB97X-D

- Zero-point correction= 0.096225 (Hartree/Particle)
- Thermal correction to Energy= 0.105412
- Thermal correction to Enthalpy= 0.106356
- Thermal correction to Gibbs Free Energy= 0.059903
- Sum of electronic and zero-point Energies= -1063.744772
- Sum of electronic and thermal Energies= -1063.735586
- Sum of electronic and thermal Enthalpies= -1063.734641
- Sum of electronic and thermal Free Energies= -1063.781095

- HBCl2PVW

- 0 1
- C -1.97830800 0.11873300 1.27802800
- C -2.02805600 -0.54934600 0.12976700
- H -2.02992000 -1.63742200 0.15823300
- C -2.07288500 0.07464600 -1.22916900
- H -2.06844100 1.16504700 -1.16980900
- H -1.21137800 -0.24154200 -1.82756700
- H -2.97015200 -0.24107600 -1.77005500
- B 1.07486600 0.04143000 0.70268500
- H 0.94708800 0.02386200 1.87753800
- Cl 1.10030700 1.56885200 -0.15318200
- Cl 1.39136700 -1.44823700 -0.16373200
- H -1.97281500 1.20497000 1.30185500
- H -1.95166800 -0.39563900 2.23216100

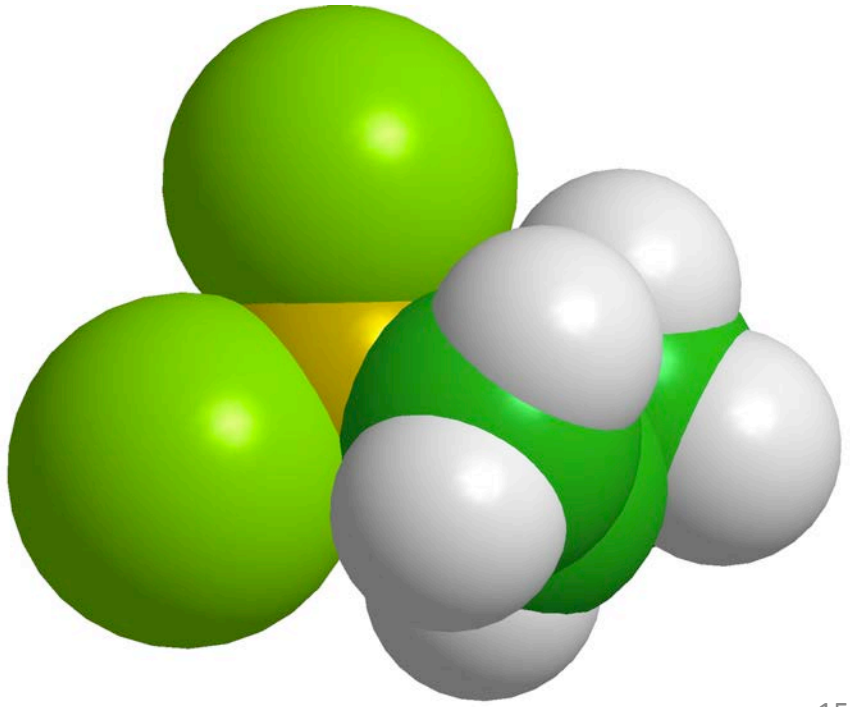


Propene $HBCl_2$ prim-TS ωB97X-D

- Zero-point correction= 0.098532 (Hartree/Particle)
- Thermal correction to Energy= 0.105542
- Thermal correction to Enthalpy= 0.106486
- Thermal correction to Gibbs Free Energy= 0.066601
- Sum of electronic and zero-point Energies= -1063.729592
- Sum of electronic and thermal Energies= -1063.722582
- Sum of electronic and thermal Enthalpies= -1063.721638
- Sum of electronic and thermal Free Energies= -1063.761523

- HBP1TSFW

- 0 1
- C 1.35202600 -1.01207700 -0.03359400
- C 0.66728800 -0.71256400 1.14326100
- B -0.28467400 -0.01447000 -0.15665400
- Cl -1.90712300 -0.86878100 -0.21025600
- Cl -0.28912400 1.81179700 0.04205800
- H 0.25356700 -0.23845800 -1.23591900
- C 2.57439700 -0.27987300 -0.48573200
- H 3.43523300 -0.77564200 -0.02543000
- H 2.69415600 -0.31488500 -1.56848300
- H 2.55782400 0.75820900 -0.15165300
- H 1.04418500 0.07964900 1.77840500
- H 1.14254200 -1.96248200 -0.51689000
- H 0.06979100 -1.47823300 1.61899400

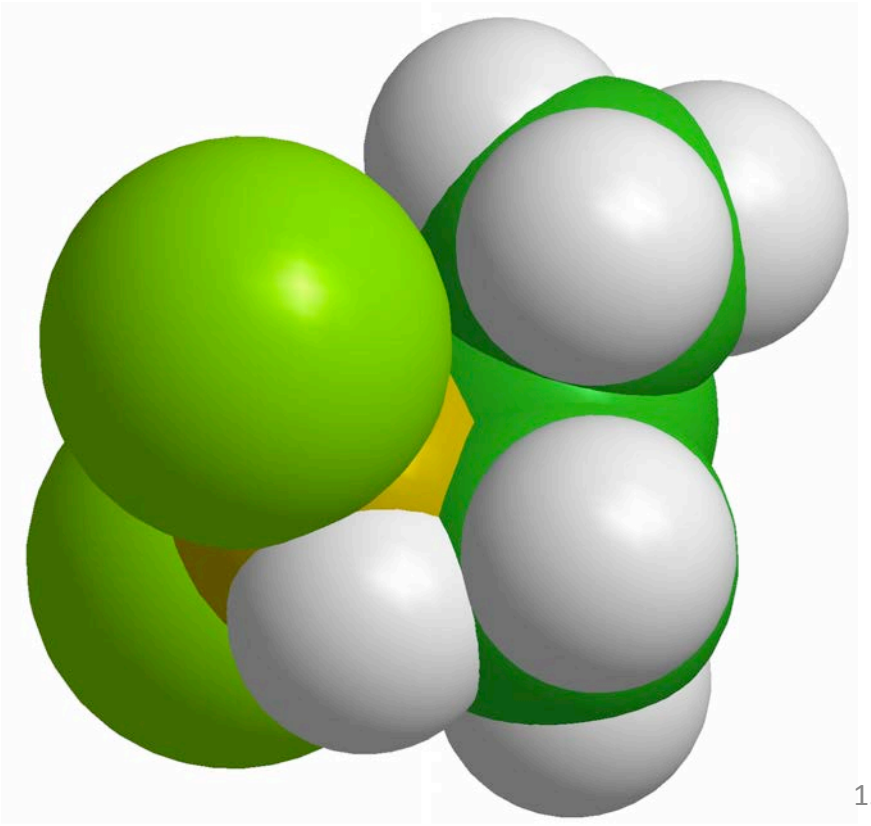


Propene $HBCl_2$ sec-TS ωB97X-D

- Zero-point correction= 0.098741 (Hartree/Particle)
- Thermal correction to Energy= 0.105685
- Thermal correction to Enthalpy= 0.106630
- Thermal correction to Gibbs Free Energy= 0.066976
- Sum of electronic and zero-point Energies= -1063.722767
- Sum of electronic and thermal Energies= -1063.715823
- Sum of electronic and thermal Enthalpies= -1063.714879
- Sum of electronic and thermal Free Energies= -1063.754533

- HBP2TSFW

- 0 1
- C 0.74503500 -1.25172000 1.13805900
- C 0.93208200 -1.05908800 -0.23225200
- B -0.34274500 0.02922600 0.36931800
- Cl 0.16028700 1.76975000 0.14292800
- Cl -1.94056000 -0.49817700 -0.35752200
- H -0.46178100 -0.11613000 1.58900800
- H 0.41442500 -1.74907900 -0.88871800
- H 1.43476100 -0.81455600 1.85398700
- C 2.16336400 -0.40553400 -0.80460700
- H 2.86076100 -1.18103100 -1.13326300
- H 1.91114400 0.21575200 -1.66540300
- H 2.66789500 0.22609800 -0.07208800
- H 0.10828700 -2.04587900 1.51079400



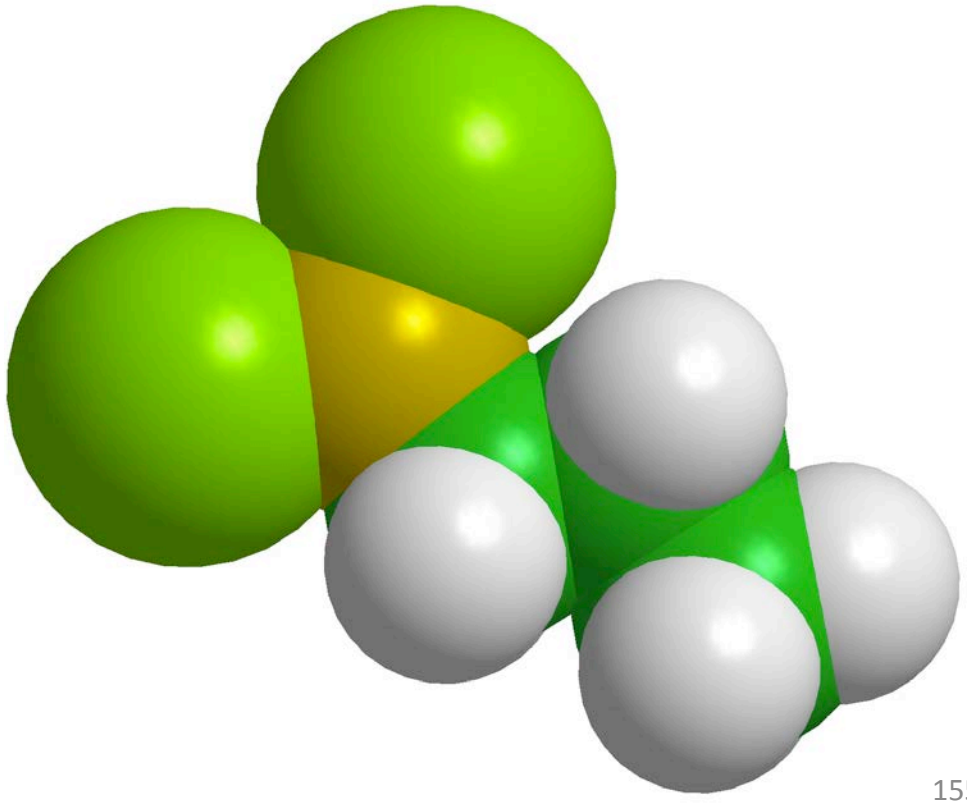
Propene $HBCl_2$ prim-product ωB97X-D

- Zero-point correction= 0.100722 (Hartree/Particle)
- Thermal correction to Energy= 0.107660
- Thermal correction to Enthalpy= 0.108604
- Thermal correction to Gibbs Free Energy= 0.068424
- Sum of electronic and zero-point Energies= -1063.791722
- Sum of electronic and thermal Energies= -1063.784784
- Sum of electronic and thermal Enthalpies= -1063.783840
- Sum of electronic and thermal Free Energies= -1063.824020

- HBCl2P1PWa

- 0 1

C	-0.81186500	-0.68715800	0.02284800
B	0.62726800	-0.08639800	0.00453900
Cl	0.93787800	1.64635200	0.00541000
Cl	2.02931000	-1.15856400	-0.00761700
C	-1.99771000	0.27910600	-0.03169100
H	-1.93558700	0.98312000	0.80402200
H	-1.93153600	0.88554100	-0.94069400
H	-0.87090100	-1.41115300	-0.80247100
H	-0.87526600	-1.31442500	0.92503800
C	-3.34116900	-0.44337600	0.00568500
H	-4.17199300	0.26452500	-0.04273100
H	-3.43962500	-1.13538000	-0.83619500
H	-3.44915100	-1.02406500	0.92681200

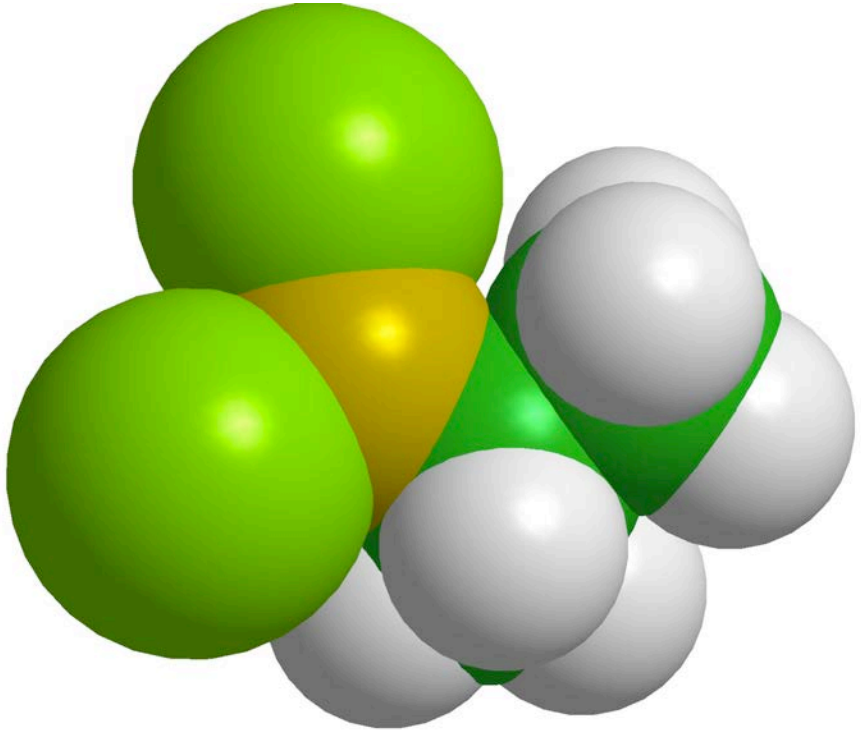


Propene $HBCl_2$ sec-product ωB97X-D

- Zero-point correction= 0.101265 (Hartree/Particle)
- Thermal correction to Energy= 0.108891
- Thermal correction to Enthalpy= 0.109835
- Thermal correction to Gibbs Free Energy= 0.068262
- Sum of electronic and zero-point Energies= -1063.789544
- Sum of electronic and thermal Energies= -1063.781918
- Sum of electronic and thermal Enthalpies= -1063.780974
- Sum of electronic and thermal Free Energies= -1063.822546

- HBCl2P1PW

- 0 1
- C -1.54742900 -1.19305500 1.02480300
- H -1.63146700 -0.42603000 1.80075400
- C -1.10147700 -0.57296100 -0.32056400
- B 0.33857900 0.01187800 -0.12139200
- Cl 0.61637400 1.69524200 0.31729900
- Cl 1.75564500 -1.03057200 -0.25087500
- C -2.14152500 0.43414700 -0.82338400
- H -2.29236300 1.23994000 -0.09990500
- H -1.84331800 0.88961800 -1.77102500
- H -3.10444500 -0.06138700 -0.97651600
- H -1.02208300 -1.39210000 -1.04494600
- H -2.52991800 -1.65873200 0.90919500
- H -0.85104500 -1.95885900 1.37507000



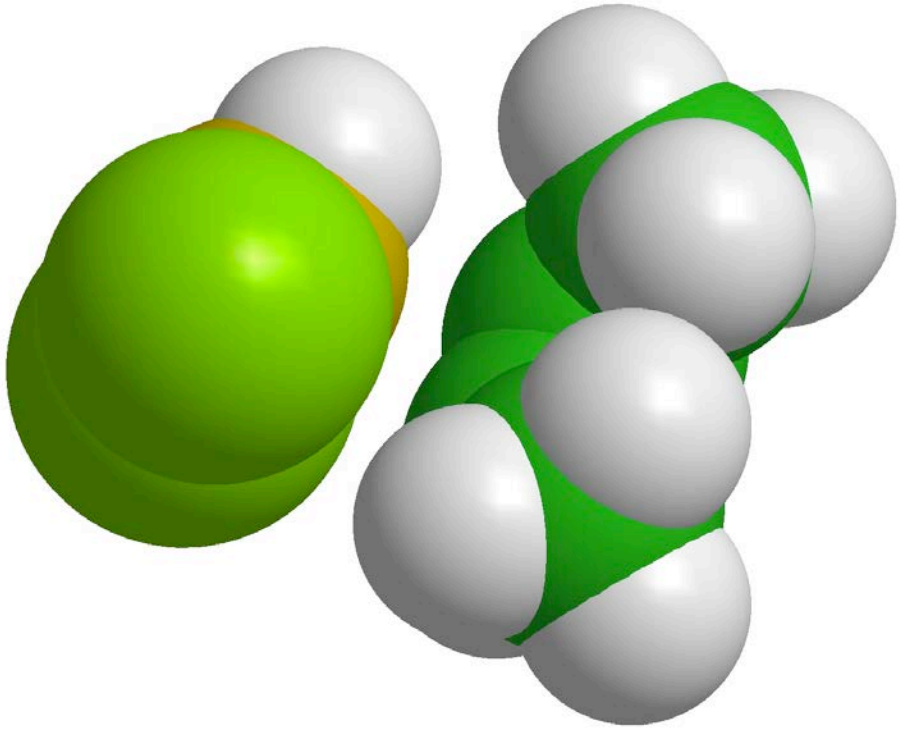
$HBCl_2$ Z-Butene vdW B3LYP

- Zero-point correction= 0.123291 (Hartree/Particle)
- Thermal correction to Energy= 0.134353
- Thermal correction to Enthalpy= 0.135297
- Thermal correction to Gibbs Free Energy= 0.082311
- Sum of electronic and zero-point Energies= -1103.133043
- Sum of electronic and thermal Energies= -1103.121981
- Sum of electronic and thermal Enthalpies= -1103.121037
- Sum of electronic and thermal Free Energies= -1103.174023

- HBCl2V

- 0 1

C	2.61902300	-0.67159000	-1.33501500
H	3.00256800	0.34915800	-1.32959800
H	1.99082500	-0.78982900	-2.22496000
H	3.46984900	-1.35011500	-1.46281800
C	1.85178500	-1.01791600	-0.09172100
H	1.44188600	-2.02577800	-0.07045300
C	1.63679900	-0.24886800	0.98123700
H	1.06336000	-0.68440400	1.79704100
C	2.10418900	1.15752900	1.21681400
H	2.69049600	1.55805600	0.38916500
H	1.25115400	1.82581900	1.37892300
H	2.71926200	1.21053500	2.12191500
B	-1.31477400	-0.16456000	-0.67816400
H	-0.79785300	-0.62223100	-1.63301900
Cl	-1.37697500	1.57580500	-0.47582900
Cl	-2.12469800	-1.22070800	0.46387200

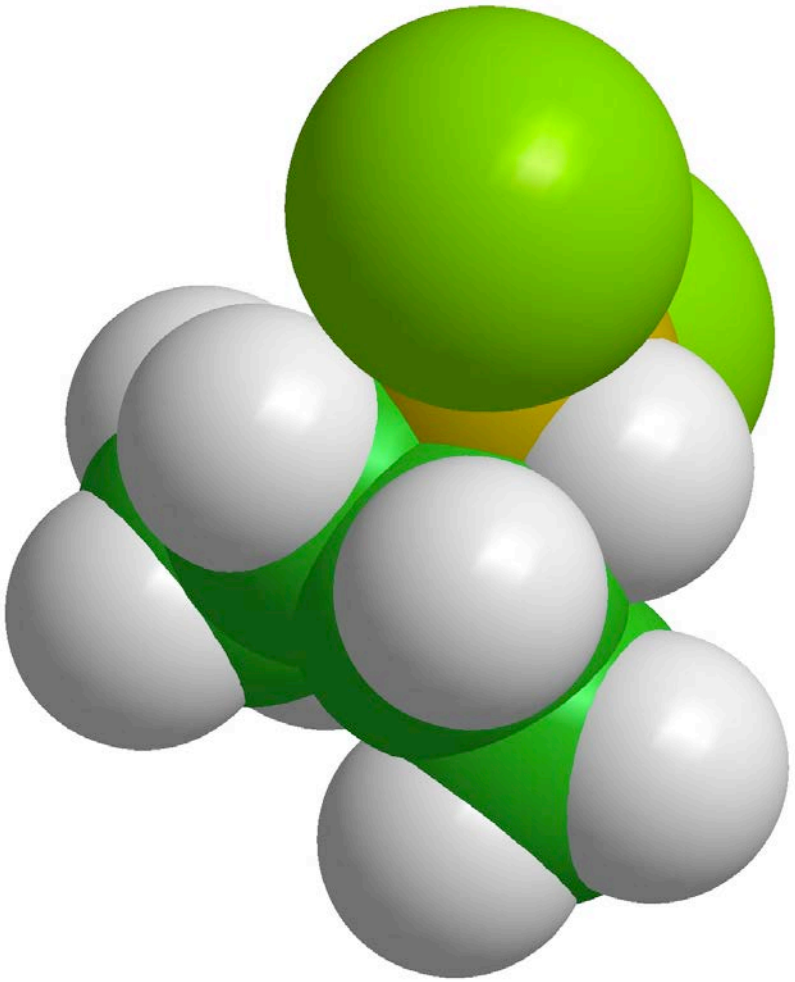


$HBCl_2$ Z-Butene TS

- Zero-point correction= 0.125489 (Hartree/Particle)
- Thermal correction to Energy= 0.134106
- Thermal correction to Enthalpy= 0.135051
- Thermal correction to Gibbs Free Energy= 0.091671
- Sum of electronic and zero-point Energies= -1103.107792
- Sum of electronic and thermal Energies= -1103.099175
- Sum of electronic and thermal Enthalpies= -1103.098230
- Sum of electronic and thermal Free Energies= -1103.141610

- HBCTSF

- 0 1
- C -1.08118700 -1.11866500 -0.40042600
- H -0.72924400 -2.10736600 -0.67952900
- C -0.69307000 -0.64062800 0.87800300
- H -0.17289300 -1.37028200 1.48989500
- B 0.48910600 -0.06137700 -0.24832000
- C -1.48708200 0.37674000 1.67280400
- H -2.01047100 1.09660800 1.04518300
- H -0.82425100 0.94155600 2.33042800
- H -2.22507800 -0.13654800 2.29750300
- C -2.22754900 -0.58308700 -1.20778600
- H -2.13721800 -0.84995900 -2.26123100
- H -2.32176300 0.49864100 -1.12026500
- H -3.14582700 -1.03507800 -0.81579700
- Cl 0.46117500 1.77437100 -0.38481700
- Cl 2.12102800 -0.86120600 0.07134500
- H 0.15709100 -0.46066400 -1.37114700

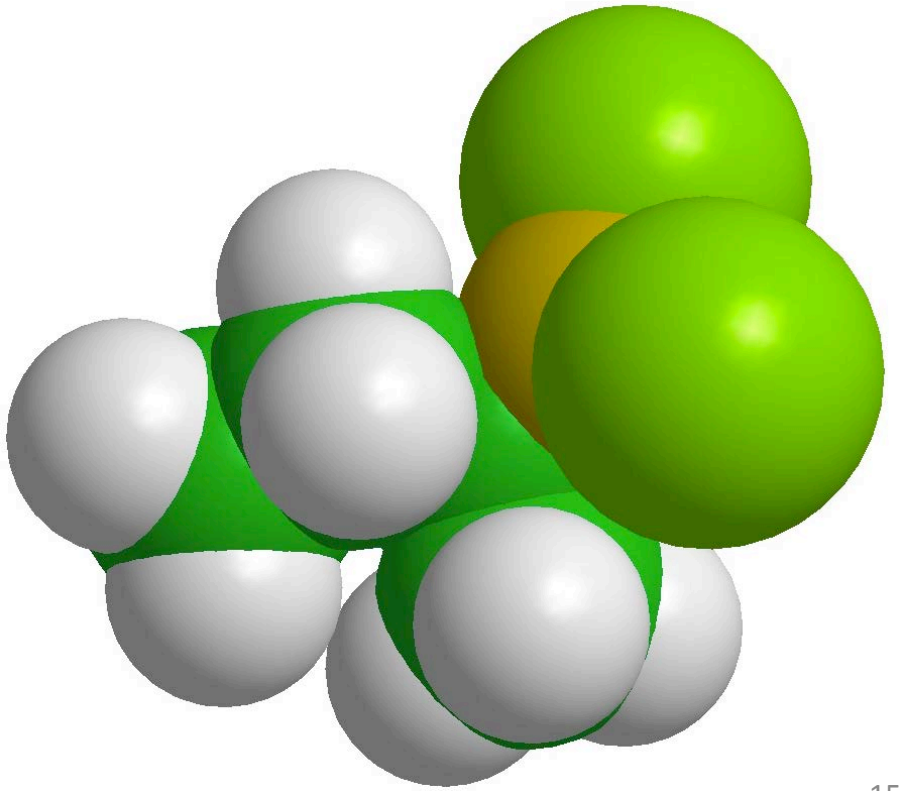


$HBCl_2$ Z-butene product B3LYP

- Zero-point correction= 0.128413 (Hartree/Particle)
- Thermal correction to Energy= 0.137641
- Thermal correction to Enthalpy= 0.138586
- Thermal correction to Gibbs Free Energy= 0.092292
- Sum of electronic and zero-point Energies= -1103.166339
- Sum of electronic and thermal Energies= -1103.157111
- Sum of electronic and thermal Enthalpies= -1103.156167
- Sum of electronic and thermal Free Energies= -1103.202460

- HBCl2P

- 0 1
- C -1.61640900 0.38036800 0.73887300
- H -1.19746400 1.29026600 1.18196300
- C -1.23040000 -1.35332700 -1.12773800
- H -1.16120800 -2.16010700 -0.39340200
- H -0.61038900 -1.63274000 -1.98364000
- H -2.26393200 -1.30395200 -1.47754600
- C -3.10382100 0.61777400 0.45469900
- H -3.62048700 0.93204500 1.36555900
- H -3.60124300 -0.28385900 0.09049600
- H -3.24036700 1.40395200 -0.29395200
- C -0.78426400 -0.00799000 -0.52393600
- H -0.95129200 0.78281400 -1.26644100
- B 0.73079100 0.04507300 -0.12852300
- Cl 1.65006400 1.55160900 -0.26222500
- Cl 1.57987100 -1.35548900 0.53732500
- H -1.50710300 -0.40877300 1.49149000

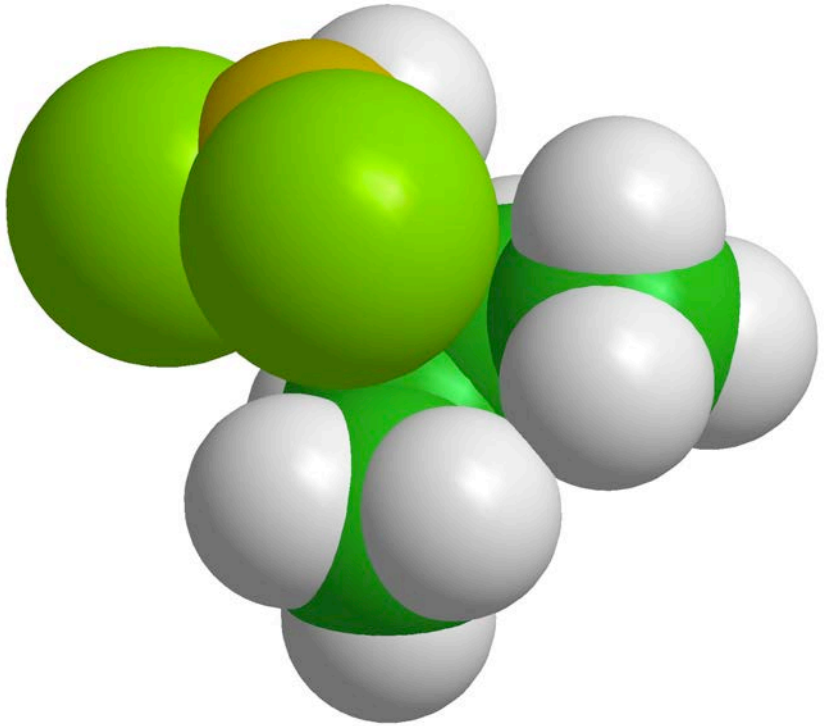


Z-Butene $HBCl_2$ vdW ωB97X-D

- Zero-point correction= 0.125581 (Hartree/Particle)
- Thermal correction to Energy= 0.135816
- Thermal correction to Enthalpy= 0.136760
- Thermal correction to Gibbs Free Energy= 0.088177
- Sum of electronic and zero-point Energies= -1103.032077
- Sum of electronic and thermal Energies= -1103.021843
- Sum of electronic and thermal Enthalpies= -1103.020899
- Sum of electronic and thermal Free Energies= -1103.069481

- HBCl2ZVW

- 0 1
- C -2.40603200 0.84600200 0.88494900
- H -2.50467000 1.26714500 -0.11582100
- H -1.80971200 1.54221100 1.48402900
- H -3.40132800 0.80920800 1.33857600
- C -1.78257000 -0.51629000 0.89069100
- H -1.65051000 -0.95933800 1.87575000
- C -1.38859100 -1.24113200 -0.15856500
- H -0.95961900 -2.21928700 0.04769200
- C -1.46468700 -0.87646400 -1.60879300
- H -1.88228300 0.11633300 -1.77846500
- H -0.46797600 -0.90531800 -2.06192900
- H -2.08052400 -1.60120800 -2.15039800
- B 1.11763000 0.37902900 0.67844600
- H 0.72664000 0.55089000 1.78078800
- Cl 0.87490300 1.62130700 -0.53462500
- Cl 2.10704500 -1.01945200 0.30744000

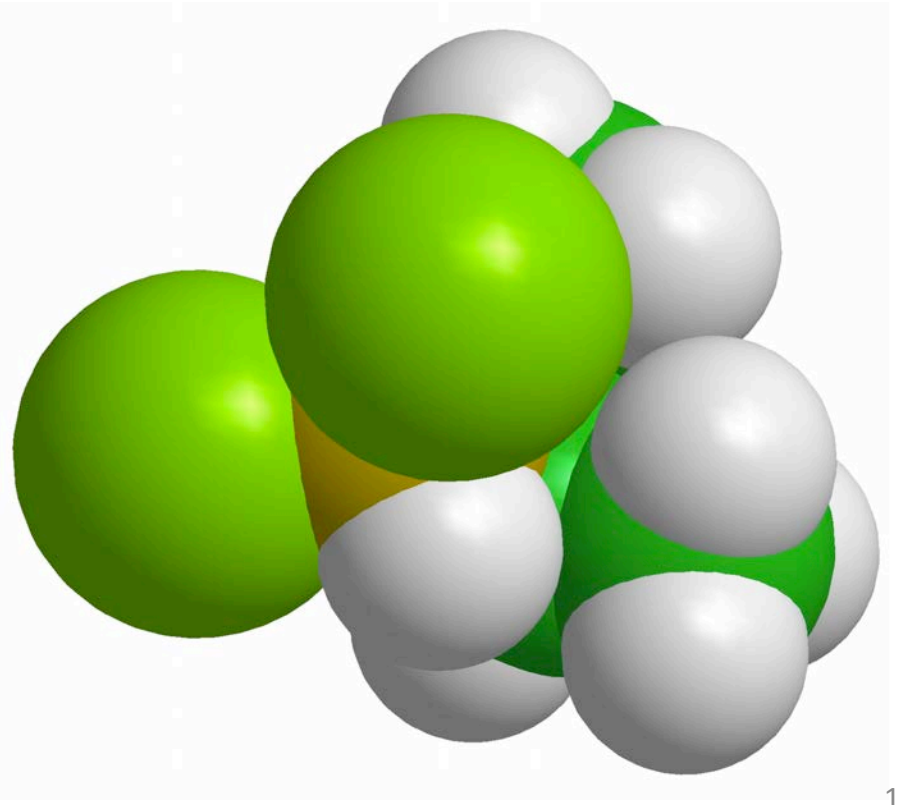


Z-Butene $HBCl_2$ TS ωB97X-D

- Zero-point correction= 0.127390 (Hartree/Particle)
- Thermal correction to Energy= 0.135701
- Thermal correction to Enthalpy= 0.136645
- Thermal correction to Gibbs Free Energy= 0.094049
- Sum of electronic and zero-point Energies= -1103.014987
- Sum of electronic and thermal Energies= -1103.006676
- Sum of electronic and thermal Enthalpies= -1103.005732
- Sum of electronic and thermal Free Energies= -1103.04832

- HBCReTSFW

- 0 1
- C -1.06361700 -1.12747400 -0.39668800
- H -0.70333200 -2.11062000 -0.68617600
- C -0.68512400 -0.65916100 0.87580000
- H -0.13748600 -1.37254100 1.48211500
- B 0.48984000 -0.06240300 -0.27589400
- C -1.47183000 0.35879500 1.66584400
- H -2.03987100 1.04202800 1.03550200
- H -0.80191400 0.96113000 2.28121100
- H -2.17055500 -0.16001800 2.32839200
- C -2.20565600 -0.58152400 -1.19831400
- H -2.11736100 -0.84896000 -2.25109300
- H -2.27964300 0.50223500 -1.11093000
- H -3.12672400 -1.01877600 -0.80005300
- Cl 0.42967700 1.76587900 -0.37348600
- Cl 2.11819300 -0.83486100 0.06891000
- H 0.17126500 -0.45358900 -1.40155200

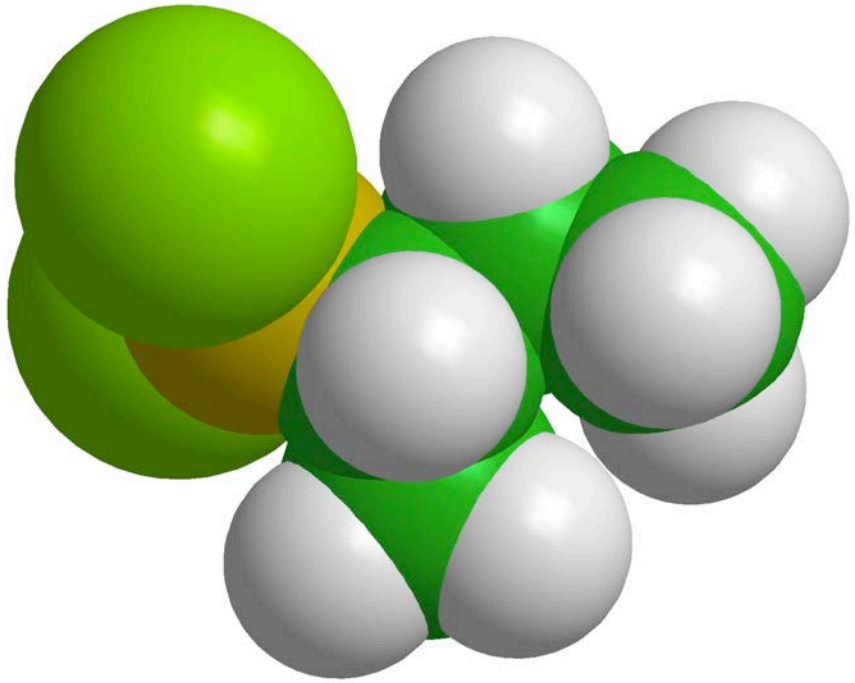


Z-Butene $HBCl_2$ product ωB97X-D

- Zero-point correction= 0.129943 (Hartree/Particle)
- Thermal correction to Energy= 0.138948
- Thermal correction to Enthalpy= 0.139892
- Thermal correction to Gibbs Free Energy= 0.094816
- Sum of electronic and zero-point Energies= -1103.072942
- Sum of electronic and thermal Energies= -1103.063937
- Sum of electronic and thermal Enthalpies= -1103.062993
- Sum of electronic and thermal Free Energies= -1103.108069

- HBCl2ZPW

- 0 1
- C -1.59780800 -0.42457100 -0.72095600
- H -1.19341800 -1.36559800 -1.10928800
- C -1.24514200 1.36746400 1.07385500
- H -1.21762300 2.13421800 0.29465300
- H -0.60919400 1.70733100 1.89516900
- H -2.26732200 1.30897200 1.45411900
- C -3.08831200 -0.60836800 -0.44322000
- H -3.60044600 -0.98048200 -1.33375200
- H -3.56716300 0.33040200 -0.15595800
- H -3.24801900 -1.33072000 0.36281300
- C -0.78331900 0.00997900 0.52826800
- H -0.94615700 -0.75630100 1.29693600
- B 0.73173600 -0.04252700 0.13504400
- Cl 1.64385700 -1.54724200 0.25822200
- Cl 1.57616200 1.35750800 -0.52270400
- H -1.46217100 0.32325800 -1.51139900

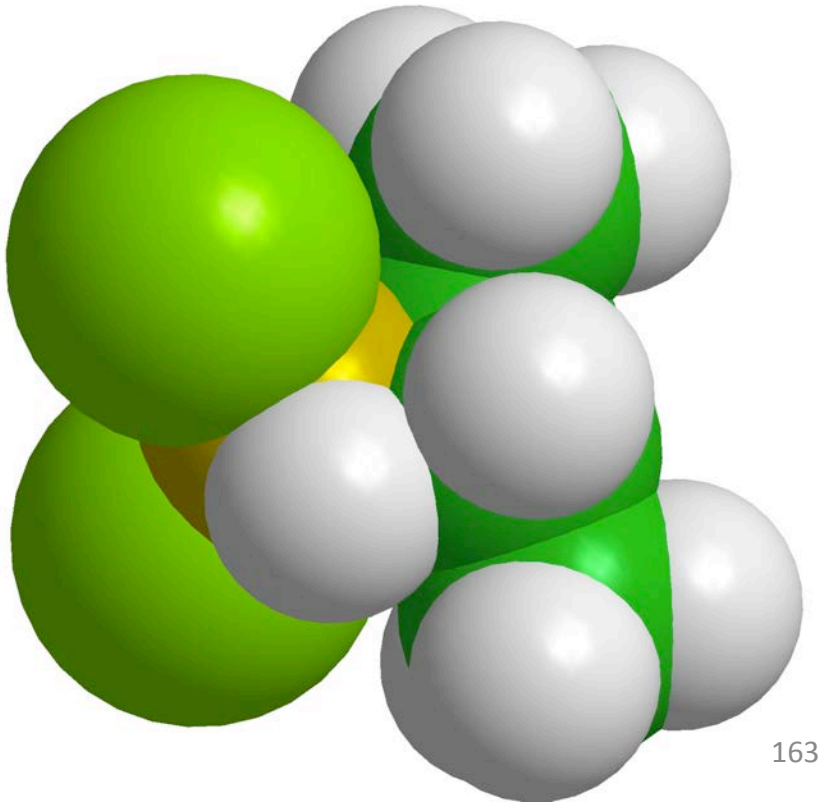


$HBCl_2$ E-Butene TS B3LYP

- Zero-point correction= 0.125352 (Hartree/Particle)
- Thermal correction to Energy= 0.133930
- Thermal correction to Enthalpy= 0.134874
- Thermal correction to Gibbs Free Energy= 0.091681
- Sum of electronic and zero-point Energies= -1103.109081
- Sum of electronic and thermal Energies= -1103.100503
- Sum of electronic and thermal Enthalpies= -1103.099559
- Sum of electronic and thermal Free Energies= -1103.142752

- HBETSF

- 0 1
- C -1.34451300 0.63429100 -0.56128000
- C -0.67680700 0.83869700 0.66784600
- B 0.28214300 -0.29692000 -0.23723500
- C -0.03043000 2.16274000 1.02429300
- H 0.30204200 2.70643300 0.13907900
- H 0.83919400 2.01292900 1.66601600
- H -0.74813000 2.78827300 1.56423300
- Cl 1.93437900 0.38937300 -0.66365500
- Cl 0.25027600 -1.94856800 0.59036000
- H -0.27314900 -0.46768300 -1.32759100
- C -2.57128900 -0.21449000 -0.71814500
- H -3.43407500 0.42304800 -0.49341200
- H -2.68360400 -0.59612000 -1.73395600
- H -2.57326700 -1.04750200 -0.01494500
- H -1.08703900 0.28954000 1.51040000
- H -1.15358100 1.35456900 -1.35390600

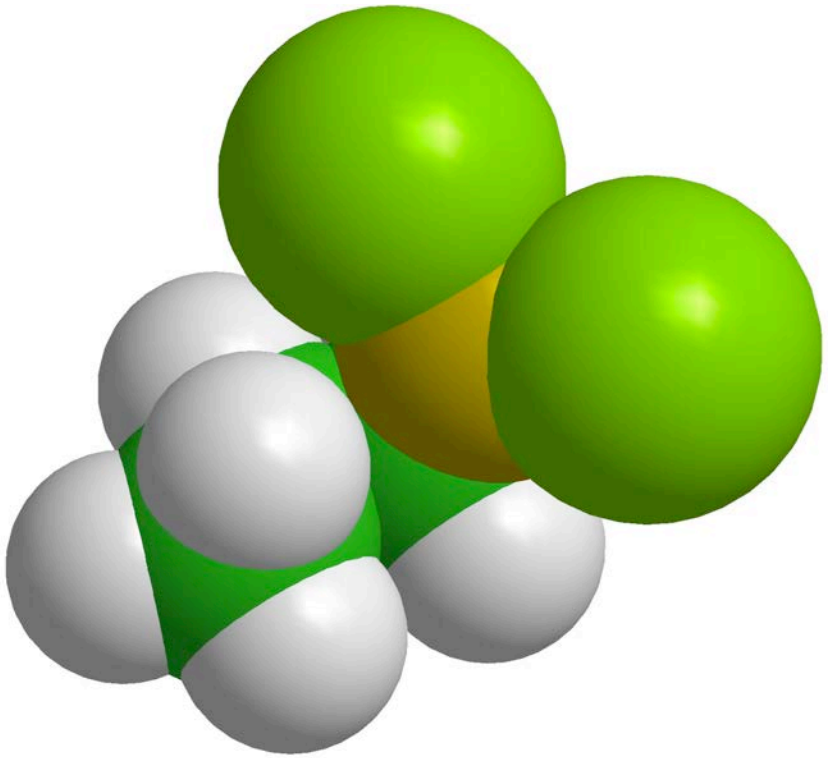


$HBCl_2$ E-butene gauche product B3LYP

- Zero-point correction= 0.128398 (Hartree/Particle)
- Thermal correction to Energy= 0.137573
- Thermal correction to Enthalpy= 0.138517
- Thermal correction to Gibbs Free Energy= 0.092825
- Sum of electronic and zero-point Energies= -1103.167313
- Sum of electronic and thermal Energies= -1103.158139
- Sum of electronic and thermal Enthalpies= -1103.157195
- Sum of electronic and thermal Free Energies= -1103.202887

- HBCl2EP

- 0 1
- C -2.05337100 -0.01313900 -0.03402200
- H -2.07292200 -0.76823500 0.75872300
- C -0.76804200 0.83203200 0.09264500
- B 0.56845100 0.01782700 -0.00355400
- Cl 0.78044000 -1.52544500 0.83577900
- Cl 1.96599300 0.65125500 -0.88243300
- C -0.75026600 1.61583800 1.43406600
- H -0.76241700 0.93550600 2.28986500
- H 0.13020700 2.25745200 1.52342000
- H -1.63565000 2.25448100 1.50076000
- H -0.76499100 1.57254000 -0.71625500
- C -2.21662100 -0.68944600 -1.39856900
- H -2.21598300 0.04743000 -2.20763400
- H -1.41009300 -1.40207700 -1.59763900
- H -3.15860800 -1.24103100 -1.45337700
- H -2.91137200 0.64431200 0.14830200

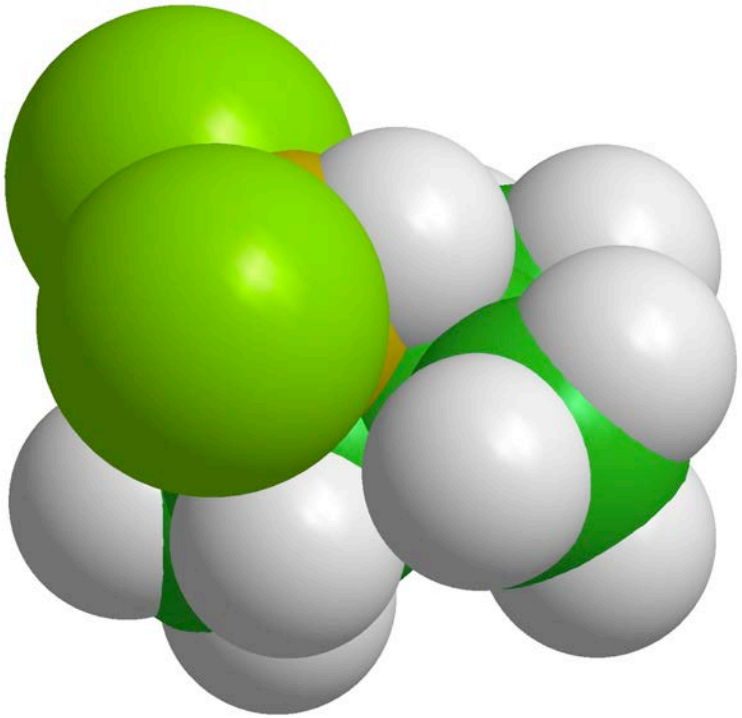


$HBCl_2$ TME sec-TS B3LYP

- Zero-point correction= 0.153021 (Hartree/Particle)
- Thermal correction to Energy= 0.163041
- Thermal correction to Enthalpy= 0.163985
- Thermal correction to Gibbs Free Energy= 0.117927
- Sum of electronic and zero-point Energies= -1142.411184
- Sum of electronic and thermal Energies= -1142.401164
- Sum of electronic and thermal Enthalpies= -1142.400220
- Sum of electronic and thermal Free Energies= -1142.446278

- HBT2TSF

- 0 1
- C 1.34620500 0.37854900 -0.16072300
- C 0.62359300 -0.05113500 1.00071800
- B -0.58202400 0.08971100 -0.19416300
- C 0.83630900 -1.40158600 1.66313600
- H 0.99579000 -2.20885400 0.94987100
- H -0.04018200 -1.66587300 2.25733300
- H 1.69908200 -1.35997000 2.33584700
- C 2.12833500 -0.59444600 -1.00256100
- H 2.31779800 -0.19685500 -2.00051000
- H 1.63283100 -1.55978400 -1.08924100
- H 3.09370800 -0.75333200 -0.50795500
- Cl -1.32534300 -1.53425000 -0.66056600
- Cl -1.77375100 1.44784600 0.20625700
- H -0.00061400 0.47023400 -1.22239000
- C 1.72056500 1.83096900 -0.29951300
- H 2.67921300 1.96403900 0.21584600
- H 1.85027600 2.12499100 -1.34239500
- H 0.98851800 2.48378700 0.17457400
- H 0.44826800 0.74783000 1.71675500

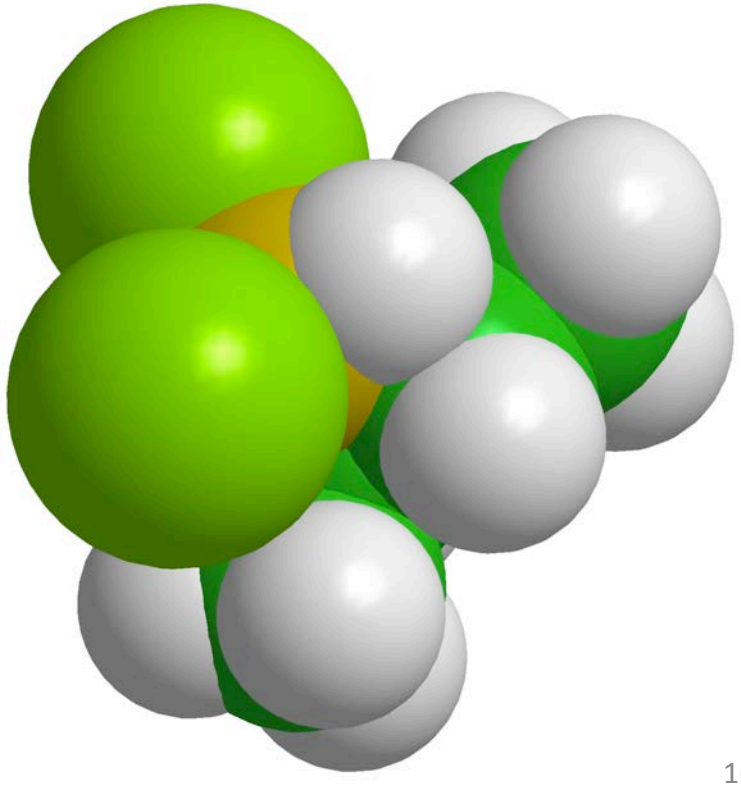


$HBCl_2$ TME tert-TS B3LYP

- Zero-point correction= 0.153259 (Hartree/Particle)
- Thermal correction to Energy= 0.163241
- Thermal correction to Enthalpy= 0.164185
- Thermal correction to Gibbs Free Energy= 0.118155
- Sum of electronic and zero-point Energies= -1142.402153
- Sum of electronic and thermal Energies= -1142.392171
- Sum of electronic and thermal Enthalpies= -1142.391227
- Sum of electronic and thermal Free Energies= -1142.437256

- HBT1TSF

- 0 1
- C -1.08681200 -0.41964400 -1.00759600
- H -0.80336400 -1.14811000 -1.76327600
- C -0.76090900 -0.75708900 0.33636100
- B 0.52318300 0.27178100 -0.30204200
- C -1.53839900 -0.15260100 1.49852600
- H -1.91489100 0.84843900 1.30175200
- H -0.90254400 -0.09048800 2.38398400
- H -2.38818700 -0.79951100 1.74182600
- C -2.13421200 0.56938000 -1.43528200
- H -1.99285000 0.87812900 -2.47190900
- H -2.15106900 1.45467500 -0.80140300
- H -3.10854000 0.07465200 -1.35248100
- Cl 0.57327300 1.91788500 0.52754200
- Cl 2.13523600 -0.60921300 -0.42335200
- H 0.22734300 0.52707100 -1.47521900
- C -0.31362500 -2.18809900 0.61934700
- H 0.16663600 -2.65580200 -0.23976500
- H 0.39554100 -2.21694500 1.44875600
- H -1.18490100 -2.79012700 0.89857100



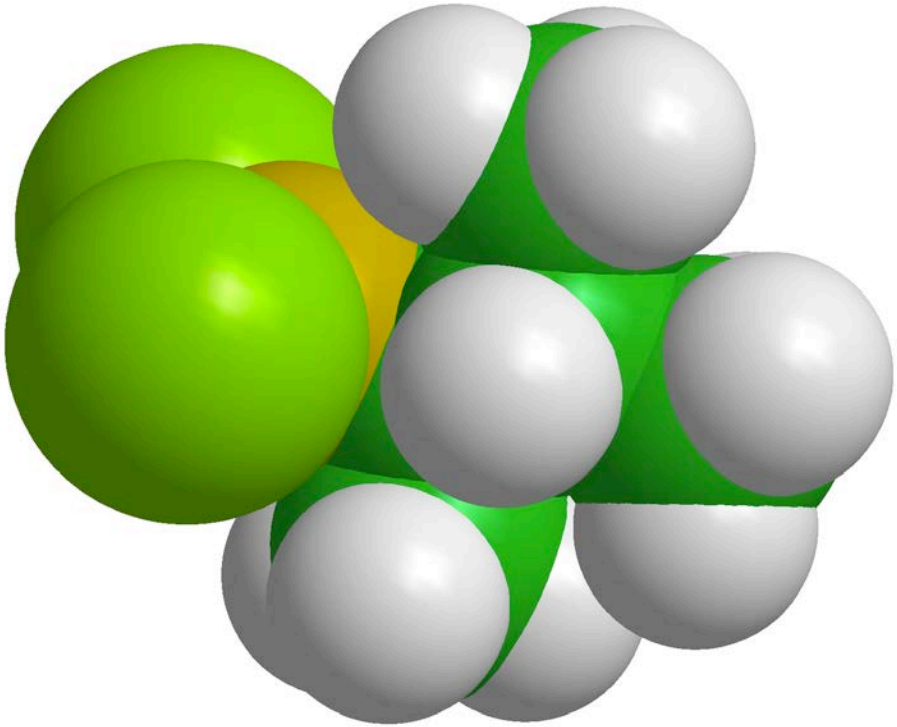
$HBCl_2$ TME sec-product B3LYP

- Zero-point correction= 0.156197 (Hartree/Particle)
- Thermal correction to Energy= 0.166743
- Thermal correction to Enthalpy= 0.167687
- Thermal correction to Gibbs Free Energy= 0.119052
- Sum of electronic and zero-point Energies= -1142.462169
- Sum of electronic and thermal Energies= -1142.451623
- Sum of electronic and thermal Enthalpies= -1142.450679
- Sum of electronic and thermal Free Energies= -1142.499315

- HBCl2T1P

- 0 1

C	-1.68245200	-0.33841100	-0.18215000
H	-1.59043500	-1.22814000	0.45263600
C	-3.08346800	0.25248800	0.03205300
H	-3.84879700	-0.45314700	-0.30337800
H	-3.21097600	1.17671000	-0.54227000
H	-3.28523900	0.47657800	1.08137600
C	-0.55535400	0.65245100	0.22664000
B	0.88950800	0.07316600	0.03312200
Cl	1.35959400	-1.49054600	0.71867500
Cl	2.15075100	0.99122700	-0.79965200
C	-0.66616100	1.13014300	1.70061900
H	-0.67272500	0.28227100	2.39087700
H	0.16934800	1.77979000	1.97683900
H	-1.58266900	1.70272900	1.85504200
H	-0.64628500	1.53875500	-0.41396400
C	-1.51618200	-0.77728300	-1.64544600
H	-1.58559900	0.08229500	-2.32054400
H	-0.55216600	-1.26381300	-1.82377300
H	-2.29614800	-1.48776900	-1.93215400

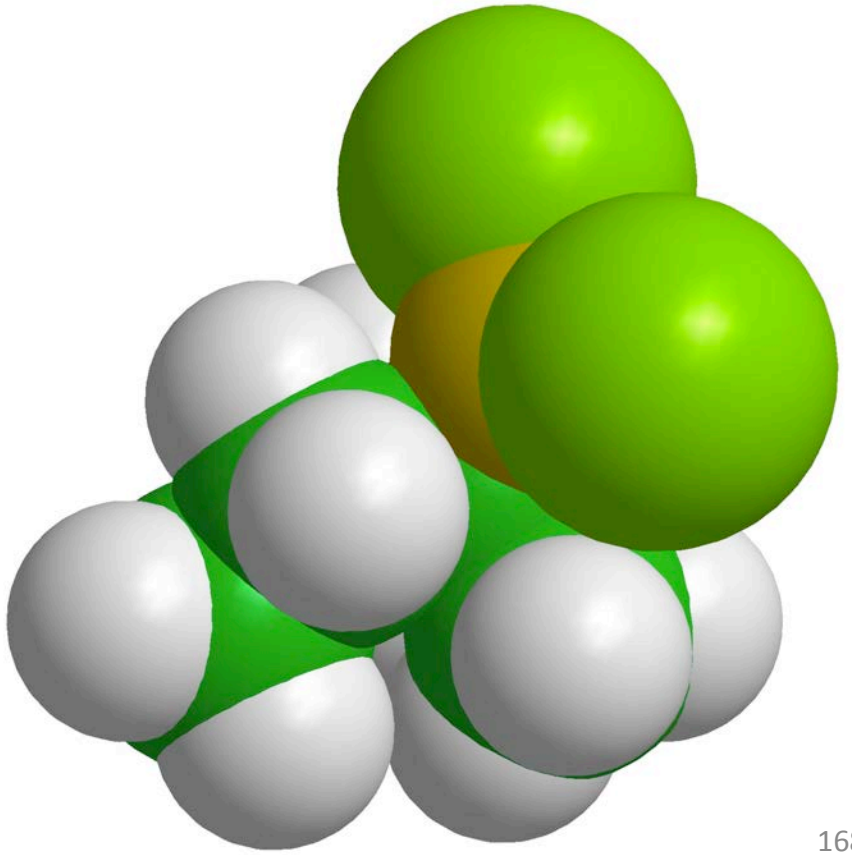


$HBCl_2$ TME tert-product B3LYP

- Zero-point correction= 0.156253 (Hartree/Particle)
- Thermal correction to Energy= 0.166758
- Thermal correction to Enthalpy= 0.167702
- Thermal correction to Gibbs Free Energy= 0.118608
- Sum of electronic and zero-point Energies= -1142.457820
- Sum of electronic and thermal Energies= -1142.447316
- Sum of electronic and thermal Enthalpies= -1142.446371
- Sum of electronic and thermal Free Energies= -1142.495466

- HBCl2T2P

- 0 1
- C 1.41250000 0.00008900 -1.01599600
- H 1.07238400 0.87725200 -1.57788800
- C 1.11079400 -1.25919700 1.19418200
- H 0.93859700 -2.17738200 0.62904300
- H 0.54077000 -1.33131800 2.12477400
- H 2.16901100 -1.22170000 1.46468800
- C 2.94712800 0.00010200 -0.99366800
- H 3.32907900 0.00019800 -2.01804500
- H 3.35015500 -0.88411200 -0.49497300
- H 3.35011900 0.88424400 -0.49481600
- C 0.71023100 -0.00008400 0.39118400
- B -0.83061100 0.00000500 0.04367100
- Cl -1.73718500 1.50008800 -0.20919100
- Cl -1.73734500 -1.49994900 -0.20929400
- H 1.07238600 -0.87695200 -1.57808100
- C 1.11084700 1.25881300 1.19453100
- H 0.93871700 2.17714700 0.62961900
- H 0.54079600 1.33071600 2.12512000
- H 2.16905300 1.22116600 1.46504300

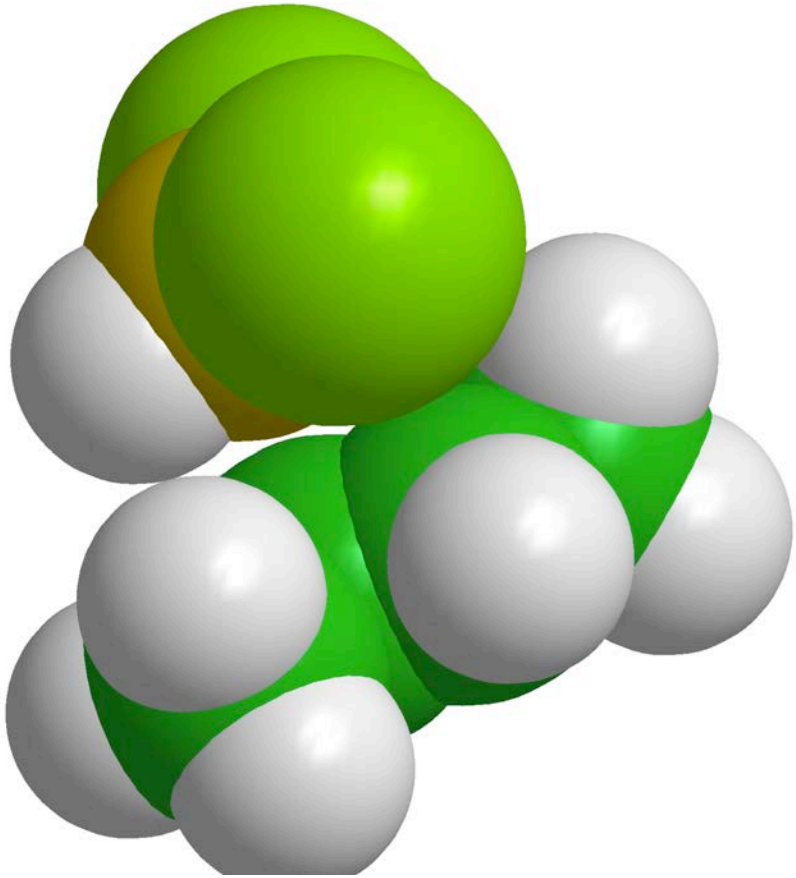


E-Butene $HBCl_2$ vdW ωB97X-D

- Zero-point correction= 0.124901 (Hartree/Particle)
- Thermal correction to Energy= 0.134640
- Thermal correction to Enthalpy= 0.135584
- Thermal correction to Gibbs Free Energy= 0.087353
- Sum of electronic and zero-point Energies= -1103.030974
- Sum of electronic and thermal Energies= -1103.021235
- Sum of electronic and thermal Enthalpies= -1103.020290
- Sum of electronic and thermal Free Energies= -1103.068522

- HBCl2EVW

- 0 1
- C 1.93119600 0.11350400 -0.52394100
- C 1.65397000 0.44584100 0.73545900
- H 1.78377900 -0.30780100 1.51228700
- C 1.17471400 1.78757400 1.19266900
- H 1.06656100 2.48169700 0.35620200
- H 0.20620400 1.70601000 1.69767700
- H 1.87437900 2.22285100 1.91313900
- B -1.04281000 -0.50893200 -0.61098400
- H -0.49869100 -1.03658600 -1.51812400
- Cl -1.70673300 1.09869700 -0.81102500
- Cl -1.34472100 -1.40625200 0.86434000
- C 2.43348400 -1.24070700 -0.95581600
- H 3.33834300 -1.52014600 -0.40952200
- H 1.68797800 -2.02136100 -0.77342900
- H 2.67000700 -1.25592200 -2.02095800
- H 1.80002000 0.86708300 -1.29894200

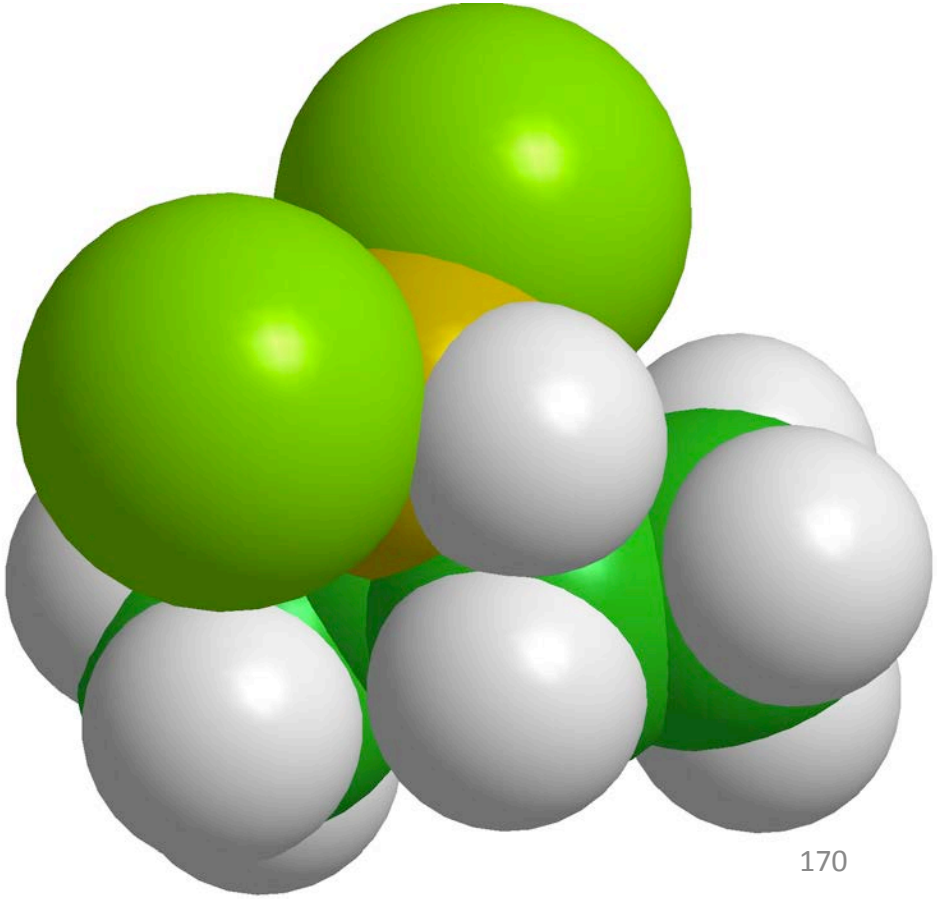


E-Butene $HBCl_2$ TS ωB97X-D

- Zero-point correction= 0.126759 (Hartree/Particle)
- Thermal correction to Energy= 0.135267
- Thermal correction to Enthalpy= 0.136211
- Thermal correction to Gibbs Free Energy= 0.093131
- Sum of electronic and zero-point Energies= -1103.016124
- Sum of electronic and thermal Energies= -1103.007616
- Sum of electronic and thermal Enthalpies= -1103.006672
- Sum of electronic and thermal Free Energies= -1103.049752

- HBETSW

- 0 1
- C -1.31358600 -0.68578300 -0.55492400
- H -1.09540200 -1.39799800 -1.34849400
- C -0.64960500 -0.86590600 0.66791000
- B 0.26225500 0.31530300 -0.26116400
- C -2.56178600 0.12680600 -0.70950500
- H -2.67486700 0.51824400 -1.72082300
- H -2.58587300 0.95085600 0.00418900
- H -3.40513600 -0.53754100 -0.49584200
- Cl 0.17284800 1.94135300 0.59091700
- Cl 1.93128400 -0.31960100 -0.66095900
- H -0.28961200 0.47349200 -1.35118300
- C 0.07196900 -2.14429700 1.02065600
- H 0.39325300 -2.68851100 0.13137700
- H 0.95808100 -1.93881400 1.62299500
- H -0.59563000 -2.78848500 1.59970100
- H -1.06829000 -0.32245100 1.50980700

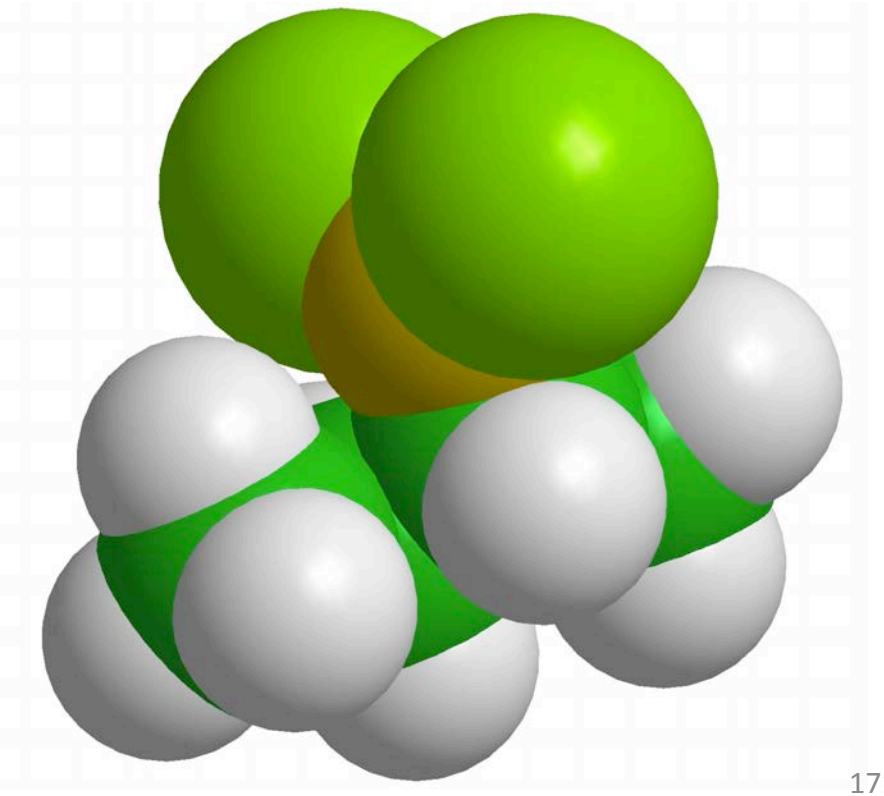


E-Butene $HBCl_2$ product ωB97X-D

- Zero-point correction= 0.129668 (Hartree/Particle)
- Thermal correction to Energy= 0.138735
- Thermal correction to Enthalpy= 0.139679
- Thermal correction to Gibbs Free Energy= 0.094378
- Sum of electronic and zero-point Energies= -1103.074425
- Sum of electronic and thermal Energies= -1103.065358
- Sum of electronic and thermal Enthalpies= -1103.064414
- Sum of electronic and thermal Free Energies= -1103.109715

- HBCl2EPW

- 0 1
- C 2.04785900 -0.01094200 -0.04155900
- H 2.08495300 0.70821700 0.78363700
- C 0.76341000 -0.84680900 0.06183100
- B -0.56299300 -0.01384000 -0.00543900
- Cl -0.73970600 1.51462600 0.85798400
- Cl -1.97606100 -0.61651900 -0.86825700
- C 0.73440900 -1.66092700 1.37598900
- H 0.75330800 -1.00043400 2.24776400
- H -0.15381500 -2.29434100 1.44729800
- H 1.61262800 -2.31028200 1.42807100
- H 0.75104800 -1.56250200 -0.76883600
- C 2.18340900 0.72074200 -1.37452600
- H 2.14221600 0.01770700 -2.21190500
- H 1.38232100 1.45399000 -1.51384200
- H 3.13226800 1.25840000 -1.43589200
- H 2.90354300 -0.68175600 0.09511600

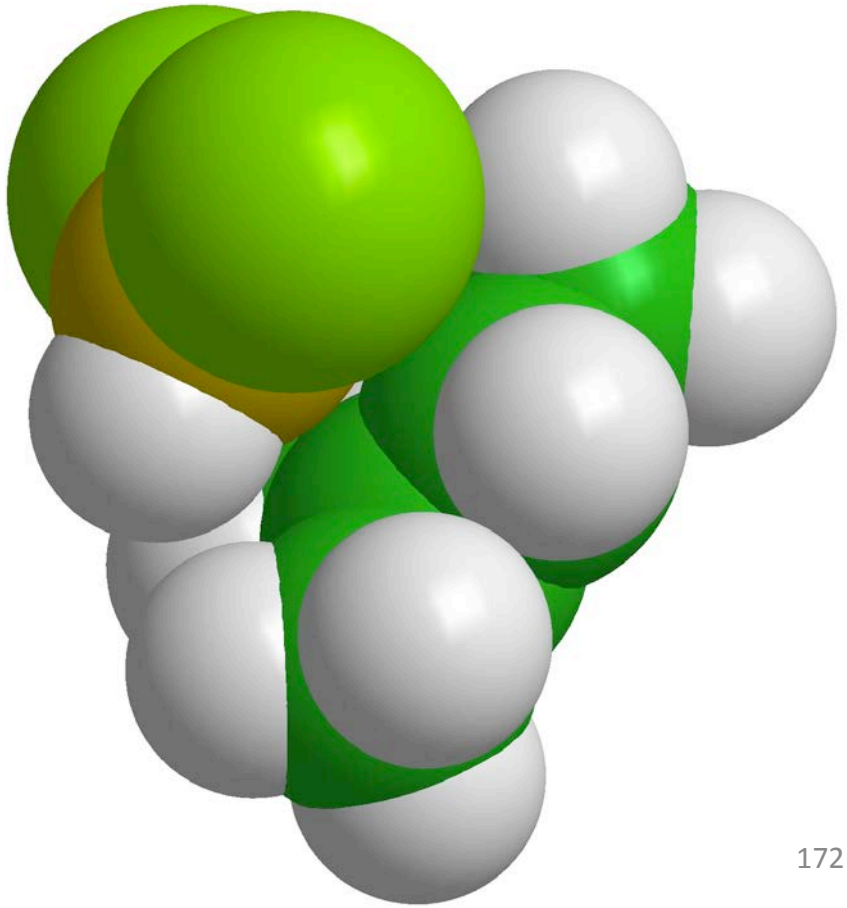


TME $HBCl_2$ VdW ωB97X-D

- Zero-point correction= 0.154015 (Hartree/Particle)
- Thermal correction to Energy= 0.165483
- Thermal correction to Enthalpy= 0.166428
- Thermal correction to Gibbs Free Energy= 0.115214
- Sum of electronic and zero-point Energies= -1142.321889
- Sum of electronic and thermal Energies= -1142.310420
- Sum of electronic and thermal Enthalpies= -1142.309476
- Sum of electronic and thermal Free Energies= -1142.360690

- HBCl2TVW

- 0 1
- C 2.18438700 1.08119900 -0.64495000
- H 1.90901300 1.90883300 0.00731400
- H 1.71292400 1.24985000 -1.61970500
- H 3.26702000 1.11780900 -0.80594100
- C 1.78722900 -0.26365700 -0.10363500
- C 1.18545300 -0.46757900 1.07456500
- H 0.96267200 -1.49994100 1.33912700
- C 0.79268300 0.54012400 2.11040200
- H 0.99161600 1.56901900 1.81002100
- H -0.27594600 0.45792300 2.33631600
- H 1.32952700 0.35095900 3.04542900
- B -1.16251700 -0.12363100 -0.78351800
- H -0.52498200 -0.45092600 -1.72363600
- Cl -1.41658800 1.58028000 -0.45430200
- Cl -2.04551300 -1.32897800 0.13565400
- C 2.14417300 -1.42369600 -0.99440600
- H 3.22981900 -1.48766600 -1.12536800
- H 1.79058600 -2.37280700 -0.58742800
- H 1.71250400 -1.29537600 -1.99338500

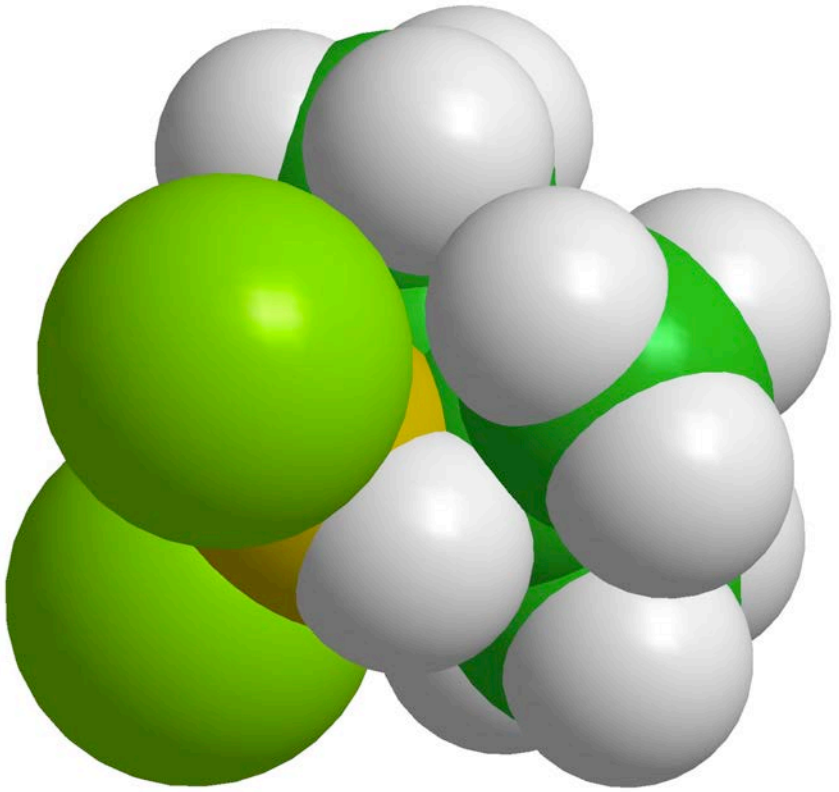


TME $HBCl_2$ sec-TS ωB97X-D

- Zero-point correction= 0.155009 (Hartree/Particle)
- Thermal correction to Energy= 0.164814
- Thermal correction to Enthalpy= 0.165759
- Thermal correction to Gibbs Free Energy= 0.120232
- Sum of electronic and zero-point Energies= -1142.308789
- Sum of electronic and thermal Energies= -1142.298984
- Sum of electronic and thermal Enthalpies= -1142.298039
- Sum of electronic and thermal Free Energies= -1142.343566

- HBT2TSFW

- 0 1
- C 1.34096600 0.37477000 -0.14419100
- C 0.62504700 -0.05310200 1.00427700
- B -0.57228800 0.10104500 -0.22519200
- C 0.80331900 -1.41042600 1.64729000
- H 1.02229700 -2.19900300 0.92857100
- H -0.10836200 -1.69615900 2.17430800
- H 1.61937000 -1.36949300 2.37466900
- C 2.11970300 -0.59350700 -0.98890600
- H 2.31824700 -0.18122000 -1.97863100
- H 1.61164400 -1.55083300 -1.09527000
- H 3.07630800 -0.76867500 -0.48519800
- Cl -1.31125900 -1.52285600 -0.65971900
- Cl -1.75656300 1.44261900 0.20587800
- H -0.00109600 0.47899800 -1.25374900
- C 1.70782400 1.82512300 -0.28779000
- H 2.67499900 1.95726400 0.20920000
- H 1.81505300 2.11516900 -1.33396900
- H 0.98089500 2.47493400 0.19864800
- H 0.42389700 0.74066200 1.71860300



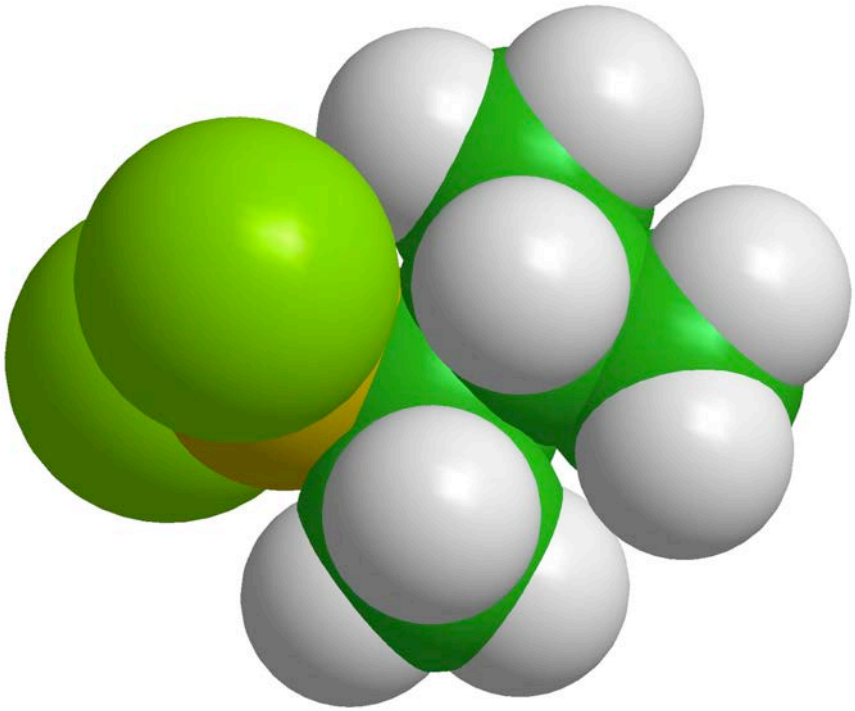
TME $HBCl_2$ sec-product WB97xD

- Zero-point correction= 0.158167 (Hartree/Particle)
- Thermal correction to Energy= 0.168473
- Thermal correction to Enthalpy= 0.169417
- Thermal correction to Gibbs Free Energy= 0.121473
- Sum of electronic and zero-point Energies= -1142.359297
- Sum of electronic and thermal Energies= -1142.348991
- Sum of electronic and thermal Enthalpies= -1142.348047
- Sum of electronic and thermal Free Energies= -1142.395991

- HBCl2T1PW

- 0 1

C	1.66808600	0.30985600	-0.23346500
H	1.57737200	1.28096200	0.26871600
C	3.06802400	-0.23939400	0.04437900
H	3.82772400	0.41362500	-0.39362600
H	3.18831500	-1.23483000	-0.39747100
H	3.27798700	-0.31525200	1.11322800
C	0.56115000	-0.61662000	0.32213300
B	-0.88418300	-0.07231900	0.04949200
Cl	-1.34798400	1.56875900	0.50774300
Cl	-2.13996500	-1.09165600	-0.64898400
C	0.68294700	-0.86133700	1.84308400
H	0.71214400	0.08648400	2.38824100
H	-0.15831700	-1.44522900	2.22765500
H	1.59370200	-1.41664800	2.07532000
H	0.65498200	-1.58652000	-0.18259900
C	1.47753500	0.52785400	-1.73698400
H	1.53241200	-0.42534800	-2.27364900
H	0.51046500	0.98693500	-1.96716200
H	2.25280500	1.18451100	-2.13988900

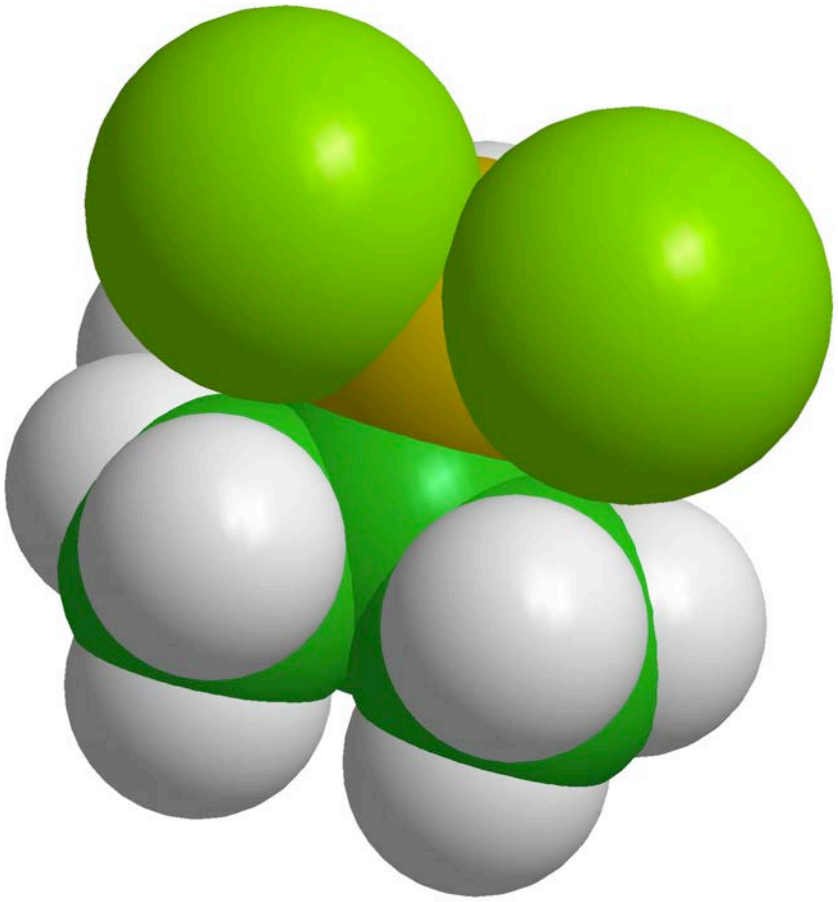


TME $HBCl_2$ tert-TS ωB97X-D

- Zero-point correction= 0.155296 (Hartree/Particle)
- Thermal correction to Energy= 0.165017
- Thermal correction to Enthalpy= 0.165961
- Thermal correction to Gibbs Free Energy= 0.120495
- Sum of electronic and zero-point Energies= -1142.299996
- Sum of electronic and thermal Energies= -1142.290275
- Sum of electronic and thermal Enthalpies= -1142.289331
- Sum of electronic and thermal Free Energies= -1142.334797

- HBT1TSFW

- 0 1
- C 1.07272200 -0.44136100 1.00605800
- H 0.77501200 -1.15791100 1.76827100
- C 0.74754700 -0.78006400 -0.32594700
- B -0.51532300 0.29111000 0.32385600
- C 1.52129300 -0.19300200 -1.49133900
- H 1.94271400 0.78945000 -1.29012100
- H 0.87000200 -0.09656100 -2.36242000
- H 2.33817900 -0.87269800 -1.75419300
- C 2.12992900 0.53882800 1.41958700
- H 2.01106100 0.83075100 2.46317300
- H 2.12297200 1.43435800 0.79904800
- H 3.10078000 0.04798900 1.29910100
- Cl -0.51631900 1.91267200 -0.53458100
- Cl -2.13532800 -0.55709400 0.41772400
- H -0.22676800 0.55015200 1.49524400
- C 0.24963800 -2.18787500 -0.60600500
- H -0.22632700 -2.64509700 0.26144400
- H -0.47700400 -2.18755700 -1.42070200
- H 1.09722800 -2.81240400 -0.90568100

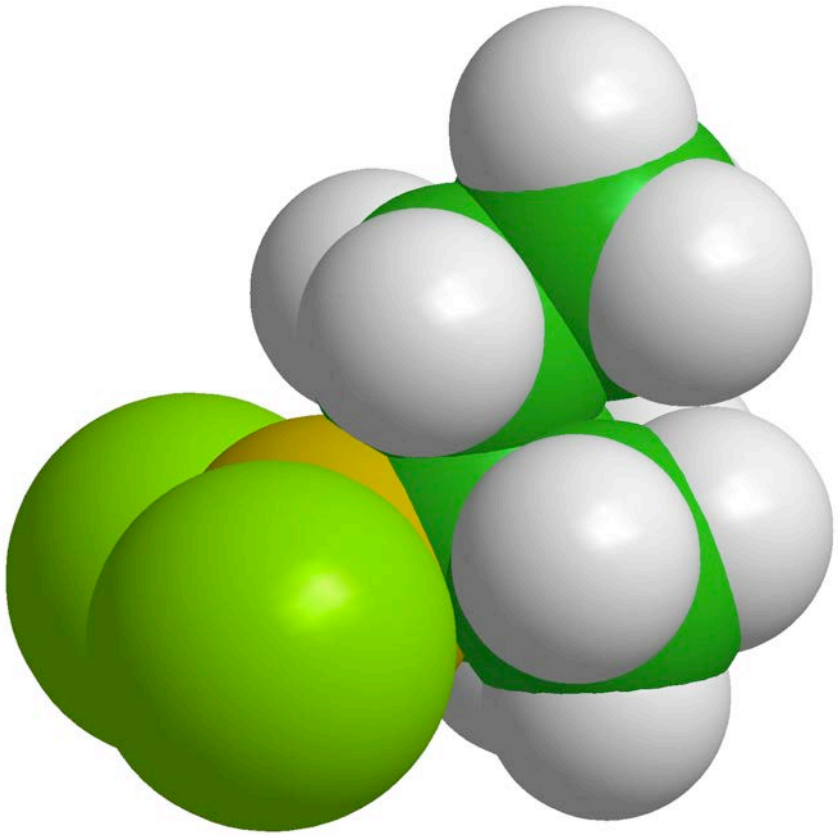


TME $HBCl_2$ tert-product ωB97X-D

- Zero-point correction= 0.157924 (Hartree/Particle)
- Thermal correction to Energy= 0.168221
- Thermal correction to Enthalpy= 0.169166
- Thermal correction to Gibbs Free Energy= 0.120820
- Sum of electronic and zero-point Energies= -1142.356083
- Sum of electronic and thermal Energies= -1142.345785
- Sum of electronic and thermal Enthalpies= -1142.344841
- Sum of electronic and thermal Free Energies= -1142.393187

- HBCl2T2PW

- 0 1
- C -1.40256500 -0.00004700 -1.01638800
- H -1.06386600 -0.87850200 -1.57802600
- C -1.11285400 1.25356400 1.18310900
- H -0.94782400 2.17169100 0.61477000
- H -0.54232800 1.32967000 2.11322700
- H -2.17094500 1.20921400 1.45430900
- C -2.93091400 -0.00003200 -0.98479200
- H -3.32310400 -0.00009400 -2.00455400
- H -3.32698800 0.88472500 -0.48129200
- H -3.32700200 -0.88471800 -0.48118000
- C -0.71058000 0.00003000 0.38498400
- B 0.83061800 -0.00000200 0.04400900
- Cl 1.73210400 -1.49670300 -0.20477400
- Cl 1.73216800 1.49665300 -0.20481200
- H -1.06385000 0.87833400 -1.57813300
- C -1.11286500 -1.25341500 1.18324700
- H -0.94784100 -2.17160600 0.61501000
- H -0.54234300 -1.32942300 2.11337500
- H -2.17095700 -1.20902500 1.45443800



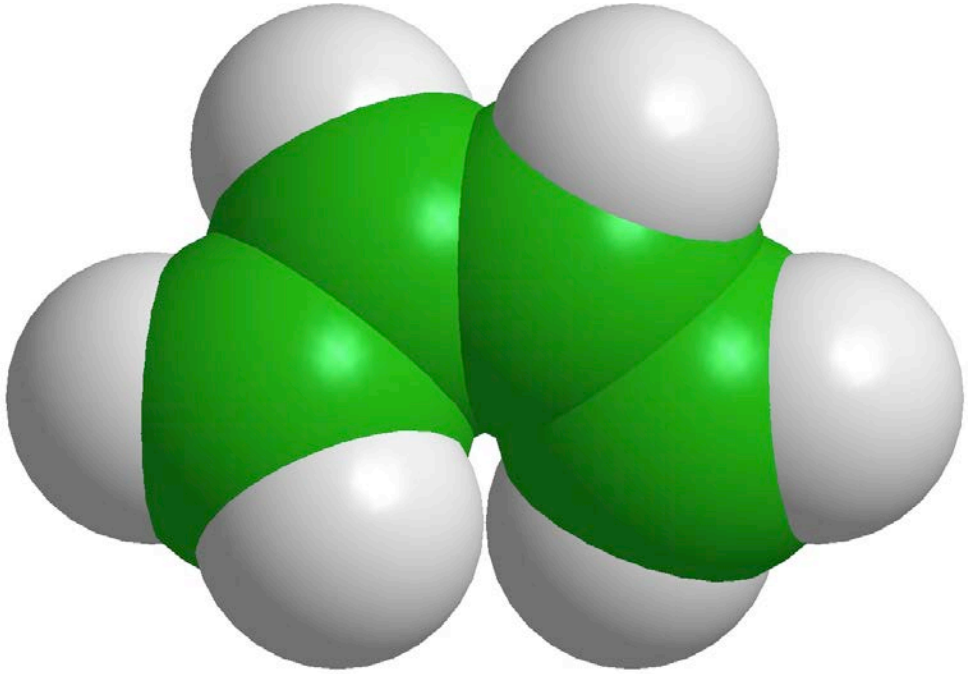
S-cis-butadiene B3LYP

Zero-point correction= 0.084688 (Hartree/Particle)
Thermal correction to Energy= 0.089385
Thermal correction to Enthalpy= 0.090330
Thermal correction to Gibbs Free Energy= 0.058014
Sum of electronic and zero-point Energies= -155.948221
Sum of electronic and thermal Energies= -155.943524
Sum of electronic and thermal Enthalpies= -155.942580
Sum of electronic and thermal Free Energies= -155.974895

Bdgauche

0 1

C 0	-1.544710	-0.489119	0.080378
C 0	-0.726326	0.548580	-0.109392
C 0	0.726328	0.548581	0.109394
C 0	1.544710	-0.489120	-0.080378
H 0	-1.182239	-1.440798	0.454441
H 0	-2.607232	-0.412422	-0.118486
H 0	-1.154111	1.496455	-0.430269
H 0	1.154111	1.496457	0.430264
H 0	1.182220	-1.440793	-0.454438
H 0	2.607236	-0.412434	0.118474



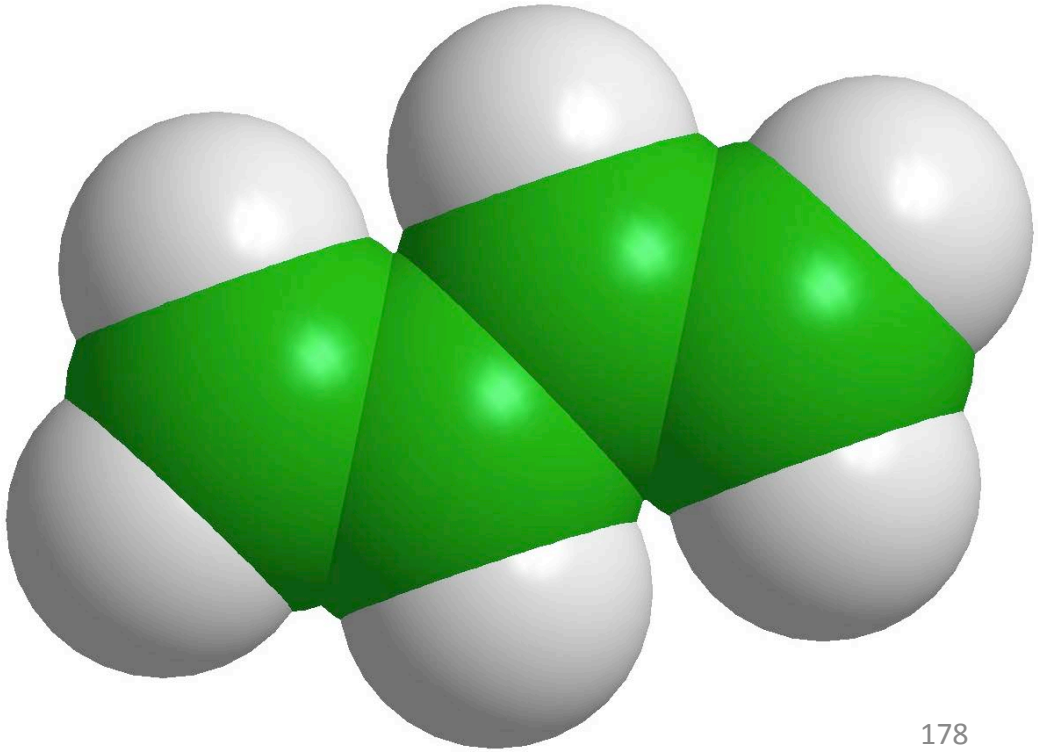
S-trans butadiene B3LYP

Zero-point correction= 0.084798 (Hartree/Particle)
Thermal correction to Energy= 0.089445
Thermal correction to Enthalpy= 0.090389
Thermal correction to Gibbs Free Energy= 0.058357
Sum of electronic and zero-point Energies= -155.953705
Sum of electronic and thermal Energies= -155.949058
Sum of electronic and thermal Enthalpies= -155.948114
Sum of electronic and thermal Free Energies= -155.980146

BDtrans

0 1

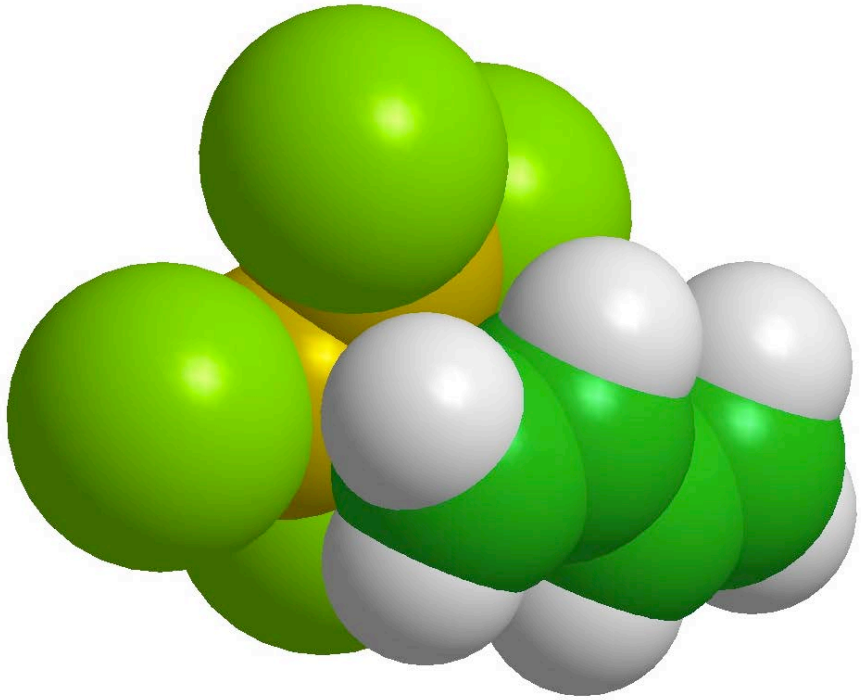
C	1.10864200	-1.47056100	0.00000000
H	2.09078300	-1.00888500	0.00000000
H	1.06994500	-2.55249400	0.00000000
C	-0.00000800	-0.73045300	0.00000000
H	-0.97399400	-1.21452100	0.00000000
C	0.00000000	0.73044300	0.00000000
H	0.97399300	1.21449600	0.00000000
C	-1.10863800	1.47056800	0.00000000
H	-2.09079100	1.00892200	0.00000000
H	-1.06991100	2.55250100	0.00000000



B_2Cl_4 s-trans-butadiene vdW B3LYP

- Zero-point correction= 0.098628 (Hartree/Particle)
- Thermal correction to Energy= 0.111620
- Thermal correction to Enthalpy= 0.112564
- Thermal correction to Gibbs Free Energy= 0.054829
- Sum of electronic and zero-point Energies= -2046.708722
- Sum of electronic and thermal Energies= -2046.695730
- Sum of electronic and thermal Enthalpies= -2046.694785
- Sum of electronic and thermal Free Energies= -2046.752520
- B2Cl4CBV1

- 0 1
- C 1.97269200 -0.20844100 1.44234800
- H 2.14313200 0.85059700 1.62529000
- B -0.59433900 0.98930800 -0.39590100
- Cl 0.52484800 1.45451600 -1.66891700
- Cl -1.10679500 2.22909400 0.74652300
- C 0.92170700 -0.81085700 2.02057100
- H 0.25119500 -0.27317900 2.67931700
- B -1.23217800 -0.59523600 -0.32835500
- Cl -0.59385700 -1.87643200 -1.35260600
- Cl -2.61250700 -0.97264200 0.69801300
- H 0.73060700 -1.87005400 1.88082700
- C 2.92970000 -0.87515900 0.57485200
- H 2.76199700 -1.93302000 0.38654500
- C 3.97691900 -0.26117500 0.01324600
- H 4.17096600 0.79345500 0.18044600
- H 4.66985800 -0.79148900 -0.62847700



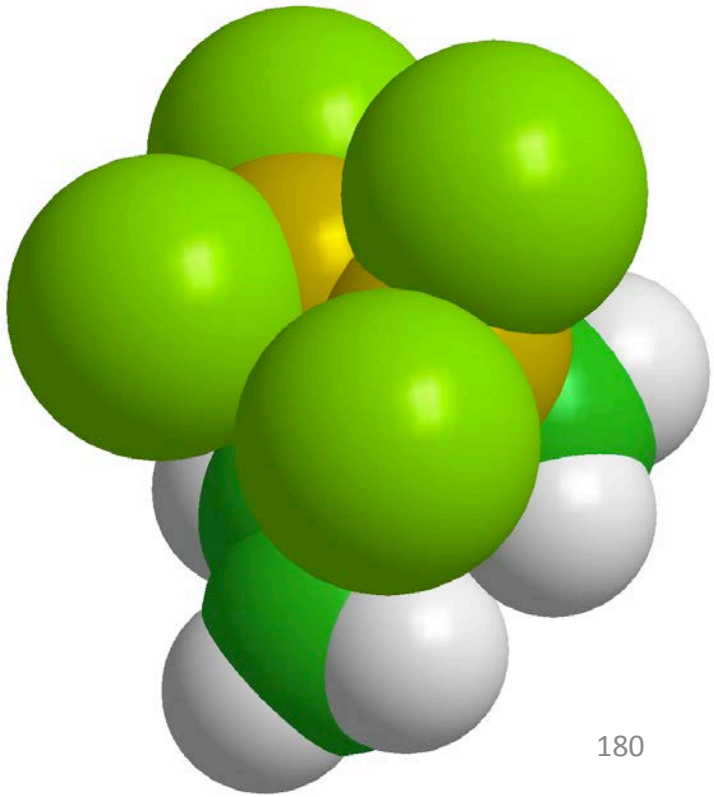
B_2Cl_4 s-cis-butadiene 1,2-addition TS B3LYP

Zero-point correction= 0.100152 (Hartree/Particle)
Thermal correction to Energy= 0.111770
Thermal correction to Enthalpy= 0.112714
Thermal correction to Gibbs Free Energy= 0.060896
Sum of electronic and zero-point Energies= -2046.668176
Sum of electronic and thermal Energies= -2046.656558
Sum of electronic and thermal Enthalpies= -2046.655614
Sum of electronic and thermal Free Energies= -2046.707432

B2Cl4DTSF1

0 1

C	0.73961600	-0.51540900	-1.39715700
H	-0.08700800	-0.85280300	-2.00861300
B	-0.80947900	-0.54550200	0.17441000
Cl	-0.63049400	-1.21785700	1.78216200
Cl	-2.24253100	-1.08632400	-0.72633700
C	1.12842800	0.87153300	-1.59686800
H	0.65290600	1.35905700	-2.44135500
B	0.28517400	0.96853500	-0.22060300
Cl	1.38348200	1.28022500	1.22114800
Cl	-1.22444300	2.05734200	-0.27887700
C	1.60079200	-1.58751800	-0.88356800
C	2.87256700	-1.43329600	-0.50466200
H	3.45118300	-2.28051400	-0.15678300
H	1.14453600	-2.57131000	-0.83362900
H	3.37404400	-0.47385800	-0.52210900
H	2.17522500	1.12485500	-1.48065700



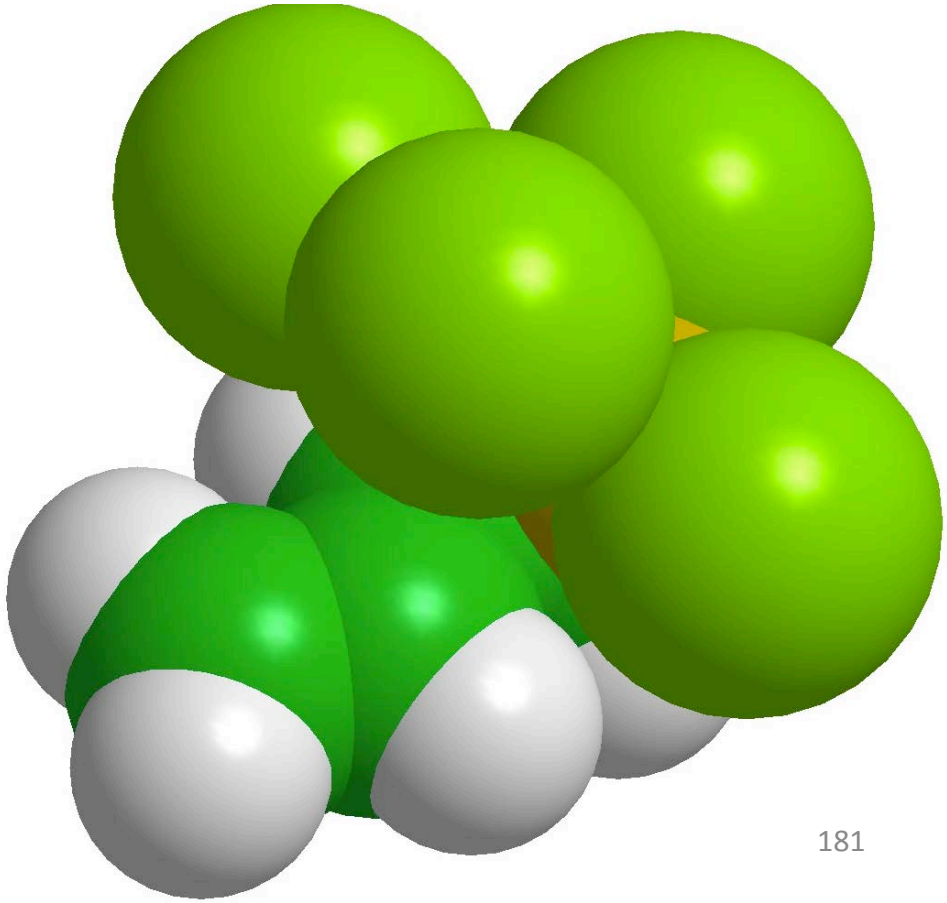
B_2Cl_4 s-Trans-butadiene TS B3LYP

Zero-point correction= 0.100017 (Hartree/Particle)
Thermal correction to Energy= 0.111666
Thermal correction to Enthalpy= 0.112610
Thermal correction to Gibbs Free Energy= 0.060780
Sum of electronic and zero-point Energies= -2046.670944
Sum of electronic and thermal Energies= -2046.659295
Sum of electronic and thermal Enthalpies= -2046.658351
Sum of electronic and thermal Free Energies= -2046.710182

B2Cl4DTSF2

0 1

C	-0.84957800	-0.77755500	-1.16361700
H	-1.27410100	0.06022000	-1.70114800
B	-0.24476600	0.80523600	0.25452200
Cl	-0.46104200	0.81770200	1.99247500
Cl	-0.80433200	2.26003800	-0.60528900
C	0.37973100	-1.34072600	-1.71237500
H	0.70469400	-0.90529300	-2.65108500
B	0.89376200	-0.56323800	-0.39850300
Cl	1.32273400	-1.72201700	0.96468800
Cl	2.16000100	0.78027800	-0.68108100
C	-1.79667200	-1.56079100	-0.36443100
C	-3.09445700	-1.25026600	-0.30302500
H	-3.79544800	-1.87534100	0.23667400
H	-1.40906900	-2.43610900	0.14455500
H	-3.49784100	-0.37270100	-0.79765900
H	0.49751200	-2.41674800	-1.65421000

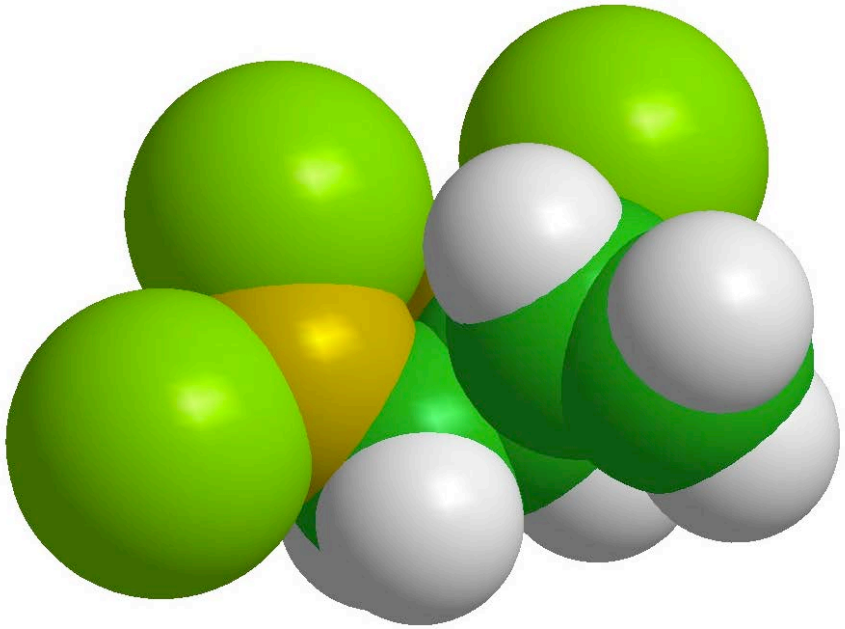


B_2Cl_4 Butadiene 1,2 addition gauche product B3LYP

- Zero-point correction= 0.101393 (Hartree/Particle)
- Thermal correction to Energy= 0.113424
- Thermal correction to Enthalpy= 0.114369
- Thermal correction to Gibbs Free Energy= 0.059853
- Sum of electronic and zero-point Energies= -2046.748624
- Sum of electronic and thermal Energies= -2046.736592
- Sum of electronic and thermal Enthalpies= -2046.735648
- Sum of electronic and thermal Free Energies= -2046.790164

- B2Cl4PPG1

- 0 1
- C 0.85715000 0.47698900 -1.12946000
- H 0.87222300 -0.31909700 -1.88931500
- B 1.79717000 -0.03866000 0.00748100
- Cl 1.17383000 -0.72060900 1.51399000
- Cl 3.54671400 -0.01661400 -0.21464800
- C -0.61685900 0.83845300 -0.78090300
- H -1.09920800 1.09652000 -1.73966000
- B -1.49961100 -0.37744300 -0.29685400
- Cl -1.38038300 -1.94206200 -1.12047900
- Cl -2.73629900 -0.21559700 0.94365500
- H 1.33240400 1.33456200 -1.61710400
- C -0.69200500 2.06526000 0.09633700
- H -0.30518000 1.95648800 1.10716700
- C -1.17745000 3.24184100 -0.28613400
- H -1.58094300 3.39815200 -1.28240700
- H -1.19777800 4.09164700 0.38632900

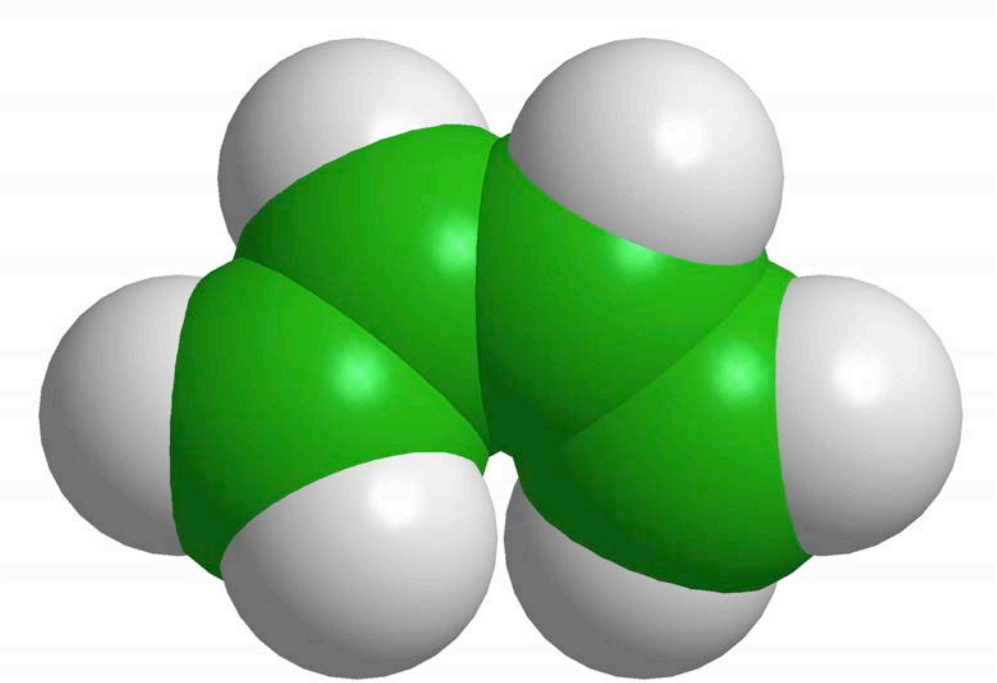


Cis-Butadiene WB97-xD

- Zero-point correction= 0.085610 (Hartree/Particle)
- Thermal correction to Energy= 0.090227
- Thermal correction to Enthalpy= 0.091172
- Thermal correction to Gibbs Free Energy= 0.059046
- Sum of electronic and zero-point Energies= -155.883626
- Sum of electronic and thermal Energies= -155.879008
- Sum of electronic and thermal Enthalpies= -155.878064
- Sum of electronic and thermal Free Energies= -155.910190

- BDgauche

- 0 1
- C 1.53239700 -0.48814100 -0.08881600
- C 0.72533500 0.54912100 0.11981600
- C -0.72533400 0.54912000 -0.11981600
- C -1.53239700 -0.48814000 0.08881600
- H 1.15806700 -1.42260400 -0.49511100
- H 2.59354200 -0.42799100 0.12369400
- H 1.15135500 1.48471500 0.47572900
- H -1.15135500 1.48471500 -0.47572900
- H -1.15806800 -1.42260500 0.49511100
- H -2.59354200 -0.42799000 -0.12369400

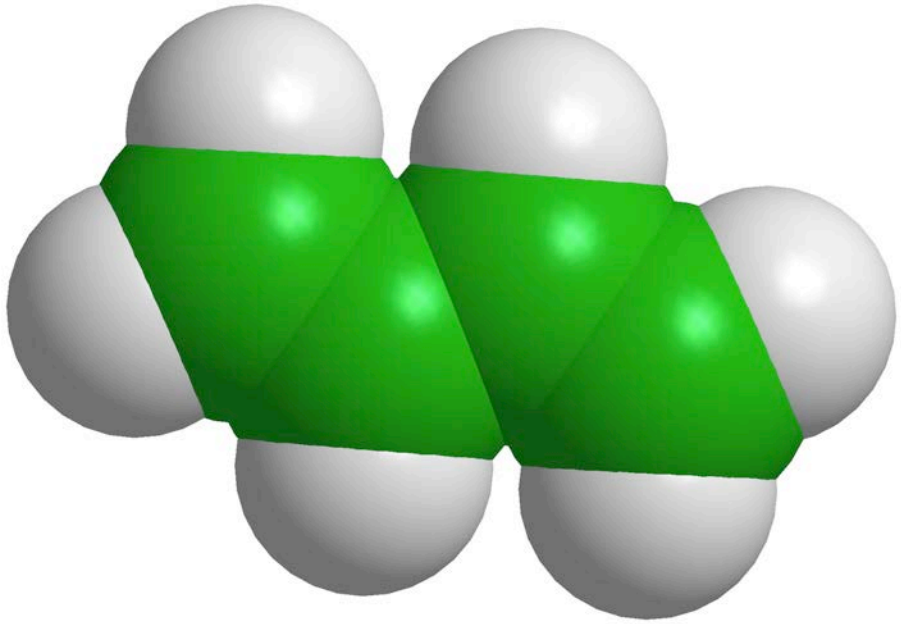


Trans-Butadiene WB97xD

- Zero-point correction= 0.085515 (Hartree/Particle)
- Thermal correction to Energy= 0.090188
- Thermal correction to Enthalpy= 0.091132
- Thermal correction to Gibbs Free Energy= 0.059014
- Sum of electronic and zero-point Energies= -155.887968
- Sum of electronic and thermal Energies= -155.883296
- Sum of electronic and thermal Enthalpies= -155.882351
- Sum of electronic and thermal Free Energies= -155.914470

- BDtransW

- 0 1
- C 1.10388800 -1.47472500 0.00000000
- H 2.09047800 -1.02090200 0.00000000
- H 1.05800000 -2.55740700 0.00000000
- C 0.00000000 -0.72984500 0.00000000
- H -0.97440100 -1.21427400 0.00000000
- C 0.00000000 0.72984500 0.00000000
- H 0.97440100 1.21427300 0.00000000
- C -1.10388800 1.47472500 0.00000000
- H -2.09047800 1.02090300 0.00000000
- H -1.05800000 2.55740700 0.00000000

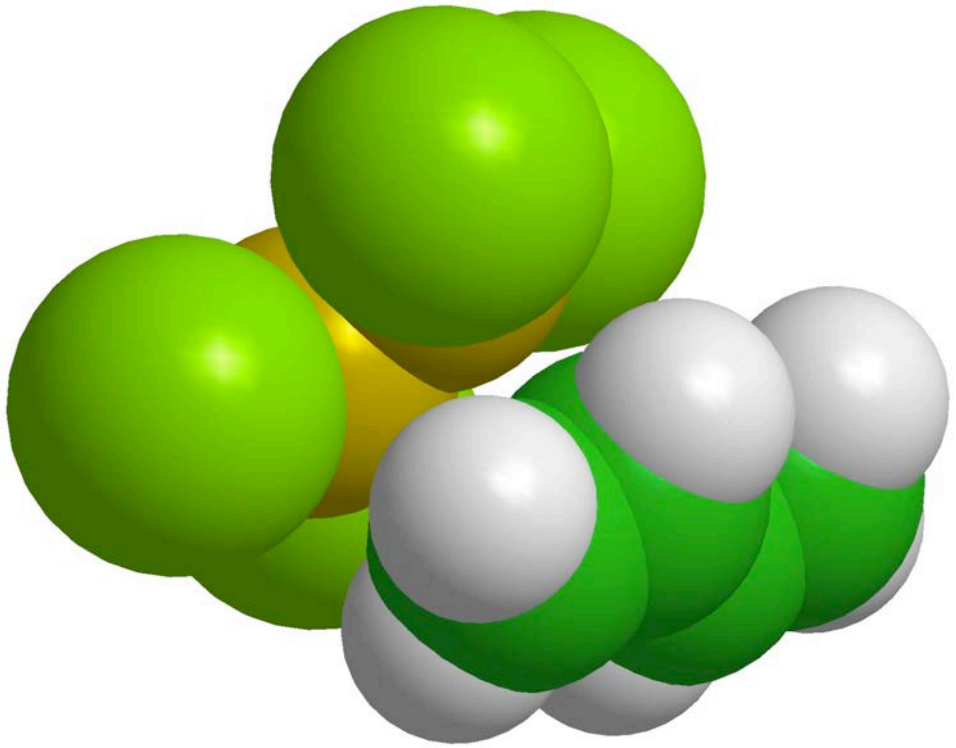


BD B_2Cl_4 trans VdW WB97xD

- Zero-point correction= 0.100664 (Hartree/Particle)
- Thermal correction to Energy= 0.113943
- Thermal correction to Enthalpy= 0.114888
- Thermal correction to Gibbs Free Energy= 0.057863
- Sum of electronic and zero-point Energies= -2046.564880
- Sum of electronic and thermal Energies= -2046.551601
- Sum of electronic and thermal Enthalpies= -2046.550657
- Sum of electronic and thermal Free Energies= -2046.607681

- B2Cl4CBV1W

- 0 1
- C -1.65175700 -0.21802000 -1.54948300
- H -1.83658100 0.84491400 -1.69514600
- B 0.45713200 0.99815500 0.42442500
- Cl -0.77418800 1.41933000 1.59848600
- Cl 1.03676600 2.26149200 -0.65154000
- C -0.57770800 -0.77861300 -2.11552300
- H 0.10843400 -0.20095200 -2.72346400
- B 1.12966400 -0.57815700 0.38704400
- Cl 0.38963300 -1.89772700 1.27848200
- Cl 2.63494300 -0.89861500 -0.45904100
- H -0.37307700 -1.83962200 -2.00553200
- C -2.61729800 -0.93891900 -0.72984800
- H -2.44423000 -2.00337100 -0.59150400
- C -3.66315400 -0.35324700 -0.14924400
- H -3.85167900 0.70935600 -0.26903700
- H -4.35896700 -0.91367800 0.46337000

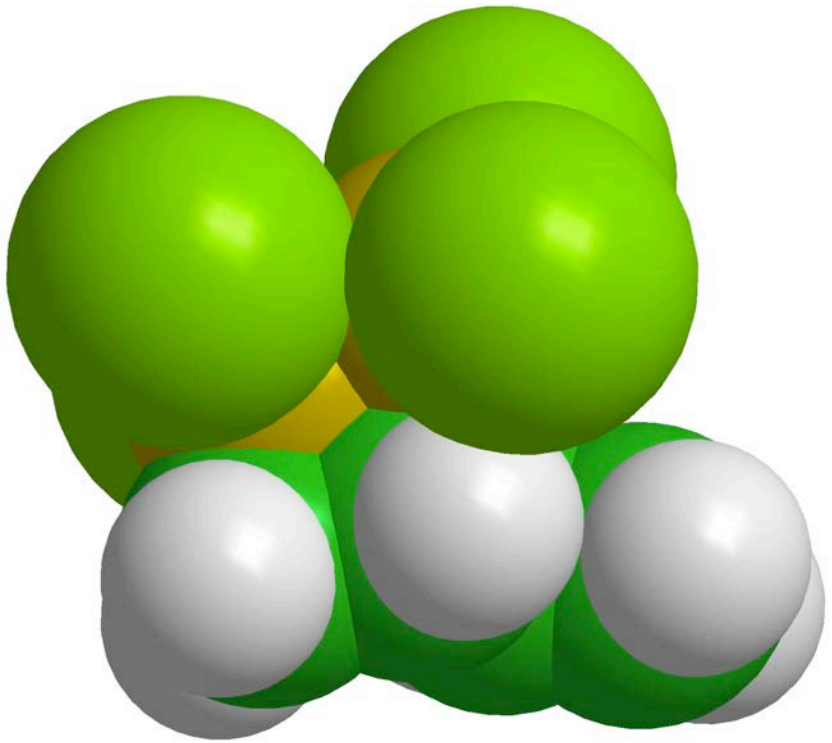


BD B_2Cl_4 trans TS WB97xD

- Zero-point correction= 0.101385 (Hartree/Particle)
- Thermal correction to Energy= 0.112857
- Thermal correction to Enthalpy= 0.113802
- Thermal correction to Gibbs Free Energy= 0.062191
- Sum of electronic and zero-point Energies= -2046.536818
- Sum of electronic and thermal Energies= -2046.525346
- Sum of electronic and thermal Enthalpies= -2046.524401
- Sum of electronic and thermal Free Energies= -2046.576012

- B2Cl4DTSF2W

- 0 1
- C -0.63678700 -0.93518900 -1.19972800
- H -1.17428000 -0.17426600 -1.75195000
- B -0.37754700 0.73800600 0.25279600
- Cl -0.62261300 0.73140800 1.98349200
- Cl -1.20969100 2.03377900 -0.63152600
- C 0.66689700 -1.29020200 -1.69661900
- H 0.96758500 -0.81223200 -2.62142400
- B 0.96358600 -0.38775700 -0.36659200
- Cl 1.57954800 -1.43895100 1.00378500
- Cl 1.97460900 1.13889200 -0.67696900
- C -1.46700000 -1.83967300 -0.39290200
- C -2.78498300 -1.67963500 -0.30795900
- H -3.39968200 -2.37608100 0.24913400
- H -0.96456600 -2.66013600 0.10767700
- H -3.28990900 -0.85044100 -0.79424500
- H 0.99039200 -2.31707900 -1.57625700



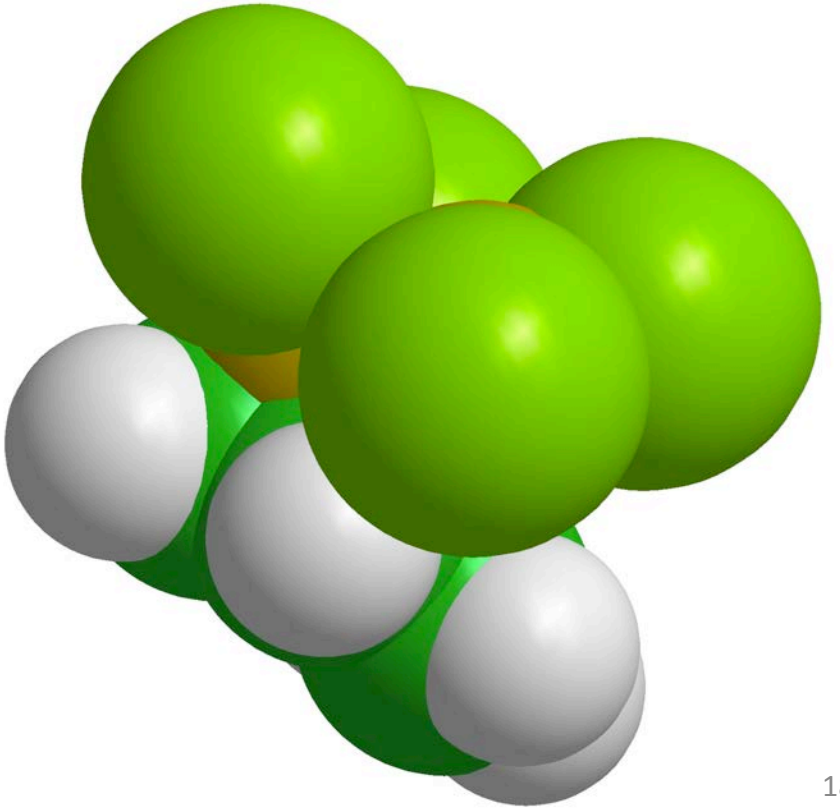
BD B_2Cl_4 cis TS WB97xD

- Zero-point correction= 0.101783 (Hartree/Particle)
- Thermal correction to Energy= 0.113096
- Thermal correction to Enthalpy= 0.114040
- Thermal correction to Gibbs Free Energy= 0.063020
- Sum of electronic and zero-point Energies= -2046.534135
- Sum of electronic and thermal Energies= -2046.522822
- Sum of electronic and thermal Enthalpies= -2046.521878
- Sum of electronic and thermal Free Energies= -2046.572899

- B2Cl4DTSF1

- 0 1

C	0.69377300	-0.40407600	-1.44967600
H	-0.15820500	-0.66228900	-2.06693500
B	-0.80443100	-0.53582400	0.17100100
Cl	-0.59005100	-1.32640600	1.71448100
Cl	-2.25693900	-1.00434000	-0.72725200
C	1.14044100	0.95770800	-1.56158900
H	0.67090800	1.54060600	-2.34522000
B	0.28295100	0.95376800	-0.16616500
Cl	1.40893200	1.17027500	1.26569600
Cl	-1.17337600	2.09587700	-0.17806900
C	1.50949300	-1.54667200	-1.00651800
C	2.76882900	-1.45400000	-0.58796000
H	3.31464800	-2.33875500	-0.28346300
H	1.01774200	-2.51387000	-1.03673100
H	3.29160900	-0.50702700	-0.52574500
H	2.18985900	1.17193400	-1.40419400



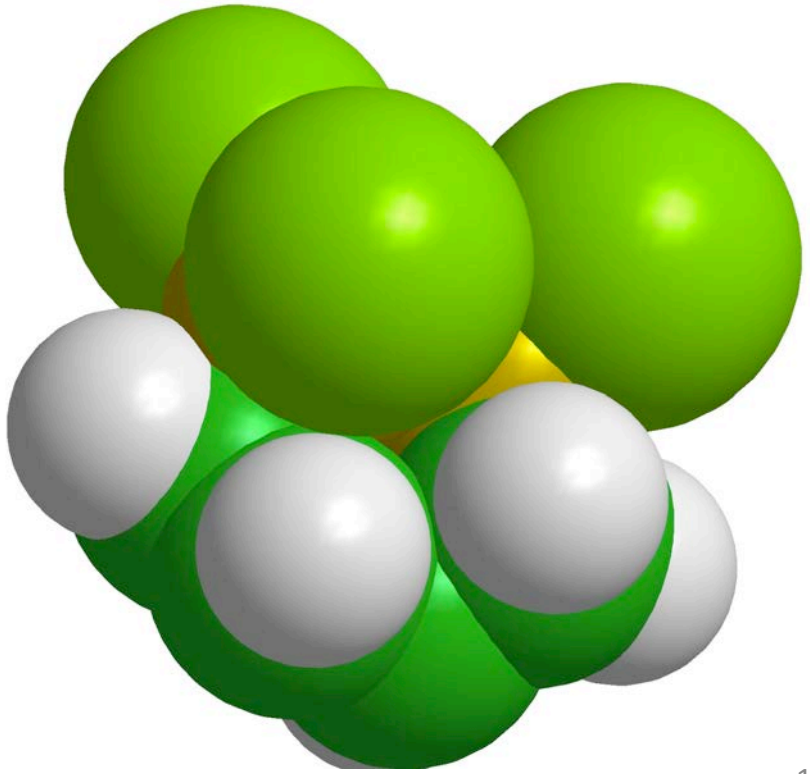
BD B_2Cl_4 alt TS WB97xD

- Zero-point correction= 0.100083 (Hartree/Particle)
- Thermal correction to Energy= 0.111179
- Thermal correction to Enthalpy= 0.112123
- Thermal correction to Gibbs Free Energy= 0.062649
- Sum of electronic and zero-point Energies= -2046.485722
- Sum of electronic and thermal Energies= -2046.474626
- Sum of electronic and thermal Enthalpies= -2046.473682
- Sum of electronic and thermal Free Energies= -2046.523156

- B2Cl4TSaltW

- 0 1

C	1.07277300	1.48417800	-1.10891500
C	0.68758300	2.39373200	-0.09889500
C	-0.68758300	2.39373200	0.09889400
C	-1.07277300	1.48417900	1.10891500
H	0.42726700	1.38858600	-1.97952000
H	1.34756300	2.51333400	0.75626600
H	-1.34756200	2.51333400	-0.75626700
H	-0.42726500	1.38858600	1.97952000
H	2.13853500	1.40152500	-1.34172900
B	1.03018700	-0.11281600	-0.26673400
H	-2.13853400	1.40152500	1.34173000
B	-1.03018700	-0.11281600	0.26673400
Cl	-2.03307900	-0.17798200	-1.22429400
Cl	-1.29370100	-1.46947900	1.39585400
Cl	2.03307900	-0.17798200	1.22429500
Cl	1.29370000	-1.46947900	-1.39585400

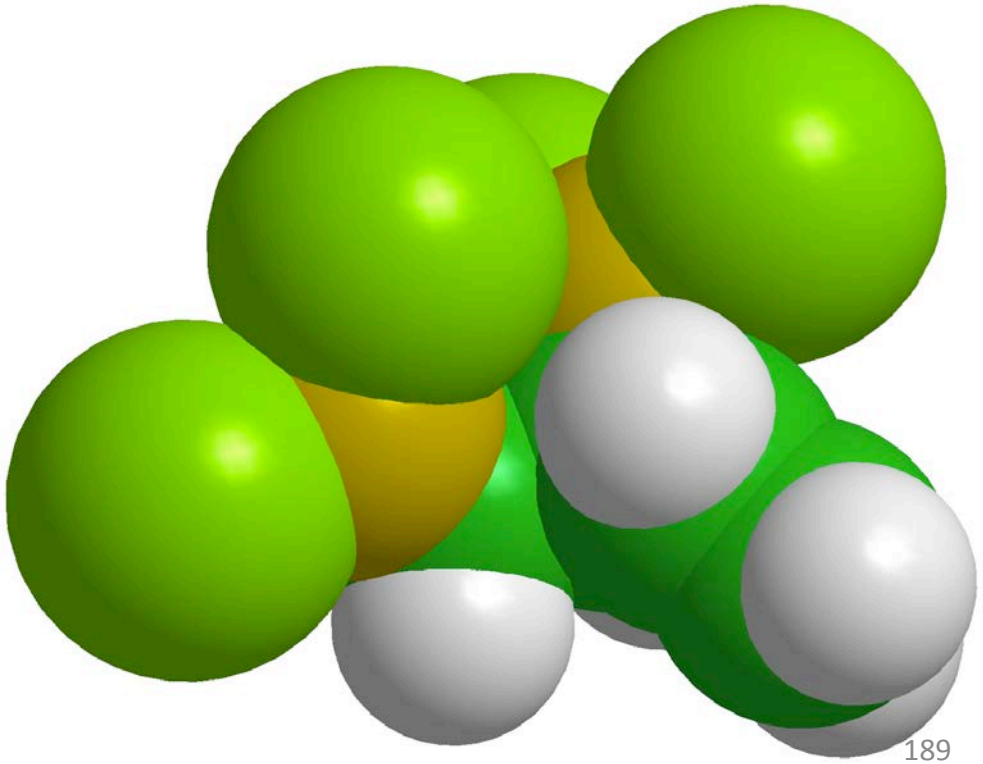


BD B_2Cl_4 gauchePWB97xD

- Zero-point correction= 0.102899 (Hartree/Particle)
- Thermal correction to Energy= 0.114726
- Thermal correction to Enthalpy= 0.115670
- Thermal correction to Gibbs Free Energy= 0.061981
- Sum of electronic and zero-point Energies= -2046.614418
- Sum of electronic and thermal Energies= -2046.602591
- Sum of electronic and thermal Enthalpies= -2046.601647
- Sum of electronic and thermal Free Energies= -2046.655337

- B2Cl4PPGW

- 0 1
- C 0.85343700 0.49699100 -1.14228100
- H 0.89448300 -0.29360700 -1.90604500
- B 1.78249400 -0.00964200 0.00857300
- Cl 1.14213500 -0.66407500 1.51560800
- Cl 3.52770100 0.00121100 -0.19598500
- C -0.61809800 0.82942600 -0.80048500
- H -1.11365200 1.07327900 -1.75571700
- B -1.47238700 -0.39976600 -0.30247800
- Cl -1.29278600 -1.97399700 -1.08371000
- Cl -2.72825300 -0.24017600 0.91107200
- H 1.32259100 1.36672600 -1.61421000
- C -0.71155600 2.05047900 0.07647400
- H -0.28533600 1.95854900 1.07379700
- C -1.25807400 3.20115100 -0.29001800
- H -1.70129200 3.33396100 -1.27295800
- H -1.29113800 4.04946400 0.38375900

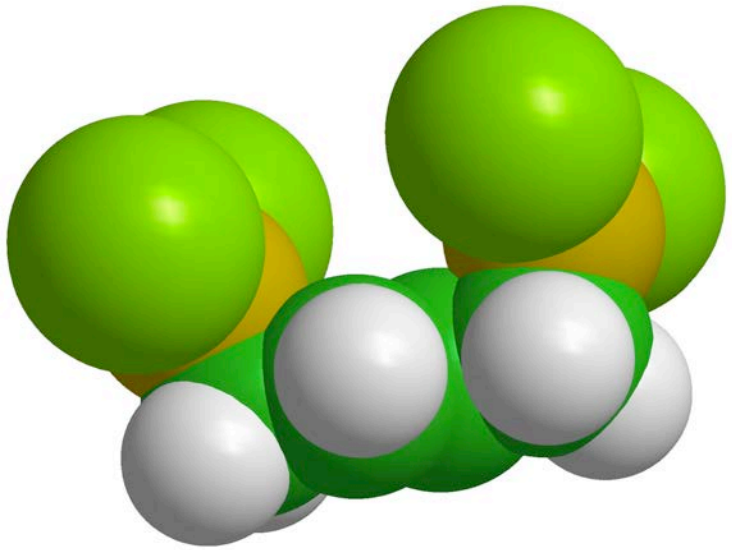


BD B_2Cl_4 alt14P WB97xD

- Zero-point correction= 0.103280 (Hartree/Particle)
- Thermal correction to Energy= 0.115290
- Thermal correction to Enthalpy= 0.116234
- Thermal correction to Gibbs Free Energy= 0.059278
- Sum of electronic and zero-point Energies= -2046.619353
- Sum of electronic and thermal Energies= -2046.607343
- Sum of electronic and thermal Enthalpies= -2046.606399
- Sum of electronic and thermal Free Energies= -2046.663355

- B2Cl4BD14PW

- 0 1
- C -1.92381200 -0.38519600 1.61709900
- H -2.65031700 0.11942000 2.25912000
- H -1.82324500 -1.42405500 1.93895100
- C -0.58653700 0.31601400 1.68550300
- H -0.61054000 1.40406300 1.67043000
- C 0.58725700 -0.31015700 1.68701500
- H 0.61131300 -1.39825800 1.67680000
- C 1.92450600 0.39087000 1.61580900
- H 2.65122600 -0.11134000 2.25946000
- H 1.82393100 1.43088600 1.93386400
- B 2.34397300 0.30273900 0.10775300
- B -2.34389500 -0.30238400 0.10890000
- Cl 3.15128400 -1.12825400 -0.52224700
- Cl 1.92915300 1.58486500 -1.02152900
- Cl -1.92904900 -1.58815700 -1.01620000
- Cl -3.15205000 1.12615500 -0.52557900

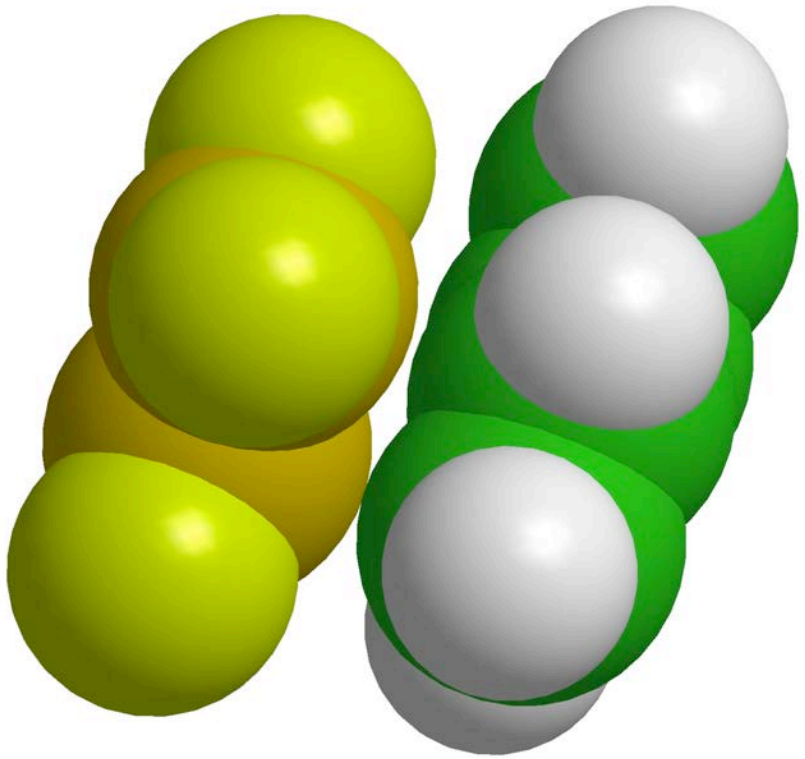


B_2F_4 butadiene VdW ωB97X-D

- Zero-point correction= 0.106001 (Hartree/Particle)
- Thermal correction to Energy= 0.118330
- Thermal correction to Enthalpy= 0.119275
- Thermal correction to Gibbs Free Energy= 0.064774
- Sum of electronic and zero-point Energies= -605.175268
- Sum of electronic and thermal Energies= -605.162938
- Sum of electronic and thermal Enthalpies= -605.161994
- Sum of electronic and thermal Free Energies= -605.216494

- B2F4BDVW

- 0 1
- C 1.43099600 -0.31078200 1.10841200
- H 1.54795400 0.65640200 1.59424800
- B -1.01821900 1.06931900 -0.08019500
- C 0.57110300 -1.19822900 1.61676600
- H -0.01311200 -0.97918000 2.50242600
- B -1.34710200 -0.52942200 -0.58239500
- H 0.44139800 -2.17842900 1.16701900
- C 2.23639700 -0.53811100 -0.08634900
- H 2.13375000 -1.50725300 -0.56781800
- C 3.04877500 0.38088900 -0.60334000
- H 3.15560100 1.35972500 -0.14620200
- H 3.62472000 0.18833500 -1.50043000
- F -1.56753900 1.57662400 1.01469800
- F -2.28039300 -1.26530400 0.00550500
- F -0.69695400 -1.09602800 -1.58917100
- F -0.20926200 1.86896600 -0.75872400

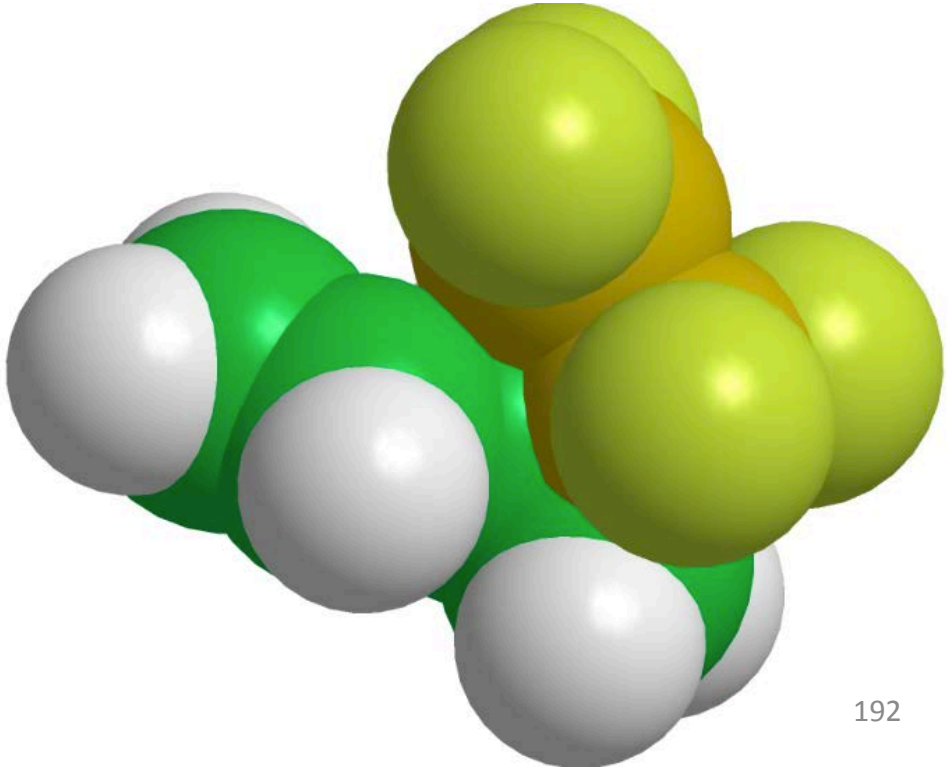


B_2F_4 butadiene trans-12 TS ωB97X-D

- Zero-point correction= 0.106546 (Hartree/Particle)
- Thermal correction to Energy= 0.116857
- Thermal correction to Enthalpy= 0.117801
- Thermal correction to Gibbs Free Energy= 0.070229
- Sum of electronic and zero-point Energies= -605.128091
- Sum of electronic and thermal Energies= -605.117780
- Sum of electronic and thermal Enthalpies= -605.116836
- Sum of electronic and thermal Free Energies= -605.164408

- B2F4DTSFW

- 0 1
- C -0.54006000 -0.91713200 -0.60889700
- H -0.69562700 -0.46609400 -1.58532800
- B 0.08295600 1.11859000 -0.01433600
- C 0.50422400 -1.85712900 -0.47865400
- H 1.04516600 -2.14924300 -1.36884600
- B 1.13378500 -0.37219200 0.08610900
- C -1.68839000 -0.87274300 0.31395700
- C -2.87004400 -0.39360400 -0.06064300
- H -3.72217200 -0.41805700 0.60746800
- H -1.53180500 -1.28818100 1.30395700
- H -3.02354300 0.03512100 -1.04615000
- H 0.46134200 -2.56898000 0.33628400
- F -0.25209800 1.70052000 1.12184000
- F -0.12185300 1.81403600 -1.12675300
- F 1.39365600 -0.49420100 1.44542800
- F 2.19680200 0.02043300 -0.72949600

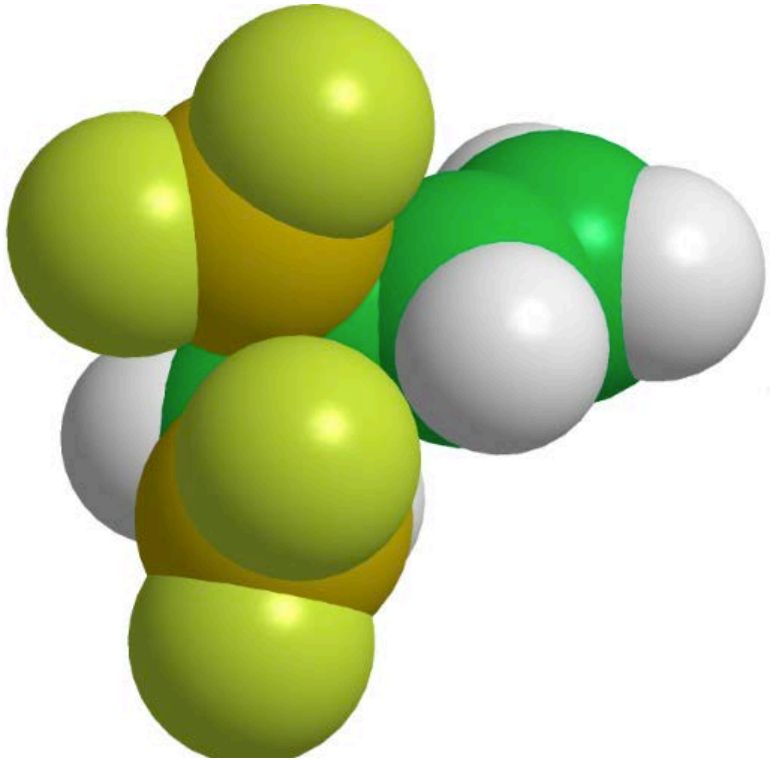


B_2F_4 Butadiene 1,2-gauche product ωB97X-D

- Zero-point correction= 0.108840 (Hartree/Particle)
- Thermal correction to Energy= 0.119570
- Thermal correction to Enthalpy= 0.120514
- Thermal correction to Gibbs Free Energy= 0.070298
- Sum of electronic and zero-point Energies= -605.230511
- Sum of electronic and thermal Energies= -605.219781
- Sum of electronic and thermal Enthalpies= -605.218837
- Sum of electronic and thermal Free Energies= -605.269053

- B2F4BDPW

- 0 1
- C 0.77556200 0.50789500 -1.04545900
- H 1.03695800 -0.18363600 -1.85742700
- B 1.79750500 0.23623800 0.10112700
- C -0.70771700 0.31914200 -0.65059600
- H -1.31172700 0.43235200 -1.56360700
- B -0.99947700 -1.14641200 -0.16227900
- H 0.93812800 1.50991100 -1.45456500
- C -1.16655200 1.36233000 0.33335900
- H -0.69508300 1.33317200 1.31433600
- C -2.07820100 2.29206200 0.08411700
- H -2.57695600 2.35535300 -0.87898100
- H -2.36510600 3.01877800 0.83532300
- F -1.92415200 -1.43372500 0.73813000
- F -0.34914200 -2.17911100 -0.69034600
- F 1.42848800 -0.39193100 1.21810400
- F 3.07203800 0.58214200 0.02101800



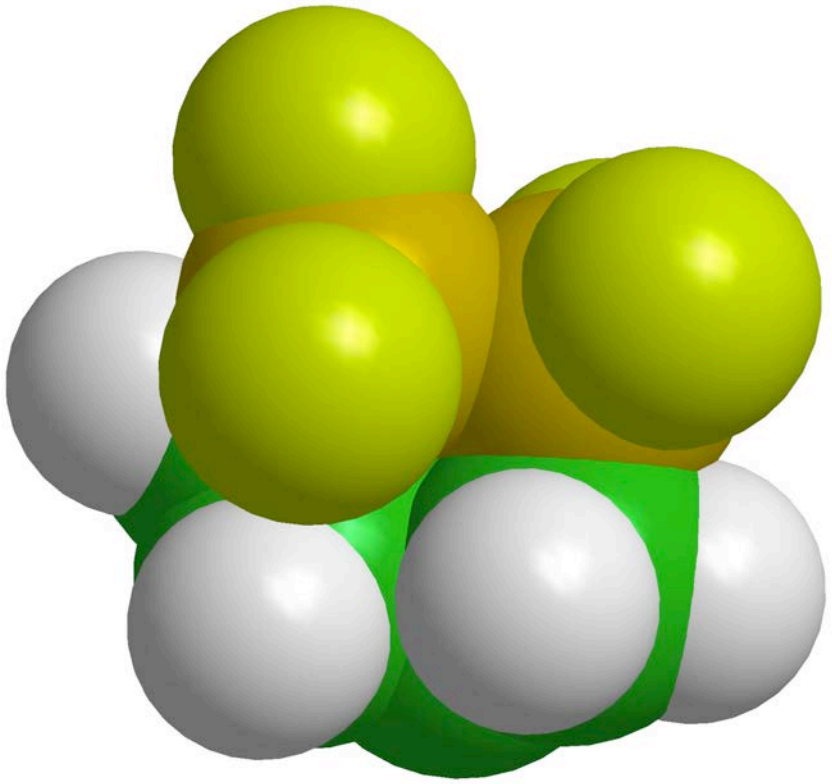
B_2F_4 Butadiene altTS for14 addition ωB97X-D

- Zero-point correction= 0.105954 (Hartree/Particle)
- Thermal correction to Energy= 0.115843
- Thermal correction to Enthalpy= 0.116787
- Thermal correction to Gibbs Free Energy= 0.071174
- Sum of electronic and zero-point Energies= -605.094535
- Sum of electronic and thermal Energies= -605.084646
- Sum of electronic and thermal Enthalpies= -605.083702
- Sum of electronic and thermal Free Energies= -605.129315

B2F4TSaltW

0 1

C	1.28712500	1.03038400	-0.85460900
C	0.69331700	1.93637900	0.04640300
C	-0.69325000	1.93640200	-0.04640200
C	-1.28708400	1.03042500	0.85461000
H	0.82992600	0.90746600	-1.83384600
H	1.15054900	2.03434700	1.02776800
H	-1.15048300	2.03438800	-1.02776500
H	-0.82987800	0.90748800	1.83384300
H	2.37427200	0.92002600	-0.86079000
B	1.03259700	-0.54944800	0.04346300
H	-2.37423500	0.92010100	0.86080000
B	-1.03261700	-0.54941400	-0.04346600
F	1.47140500	-1.60288700	-0.66036600
F	1.45703800	-0.49888700	1.32007100
F	-1.45706800	-0.49883700	-1.32007100
F	-1.47145300	-1.60283900	0.66036500

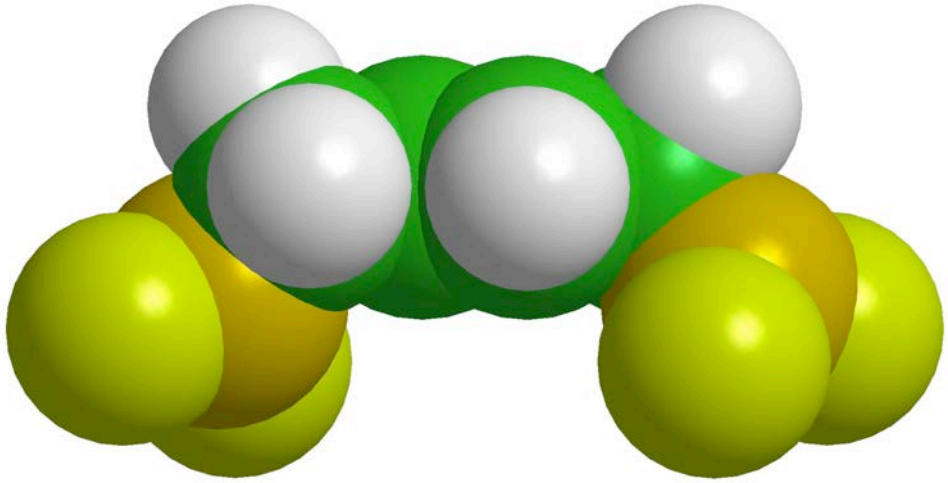


B_2F_4 Butadiene alt-product from 1,4-addition ωB97X-D

- Zero-point correction= 0.108426 (Hartree/Particle)
- Thermal correction to Energy= 0.119412
- Thermal correction to Enthalpy= 0.120356
- Thermal correction to Gibbs Free Energy= 0.067387
- Sum of electronic and zero-point Energies= -605.235223
- Sum of electronic and thermal Energies= -605.224237
- Sum of electronic and thermal Enthalpies= -605.223293
- Sum of electronic and thermal Free Energies= -605.276262

- B2F4BD14PW

- 0 1
- C -1.92582000 0.94595300 0.34689700
- H -2.48753300 1.85437500 0.07757400
- H -1.83091100 0.98078100 1.43666000
- C -0.58085000 0.96339300 -0.31959600
- H -0.58235500 0.96137800 -1.40842700
- C 0.58050100 0.96132000 0.32312900
- H 0.58194900 0.95329400 1.41193200
- C 1.92549600 0.94683000 -0.34336400
- H 2.48695000 1.85440900 -0.07067100
- H 1.83061700 0.98577400 -1.43299900
- B 2.84474100 -0.25207100 0.05766300
- B -2.84465200 -0.25176400 -0.05860400
- F 3.89451100 -0.59479800 -0.67710100
- F 2.64770700 -0.96025800 1.16164000
- F -2.64836700 -0.95467400 -1.16607100
- F -3.89331000 -0.59869300 0.67578100

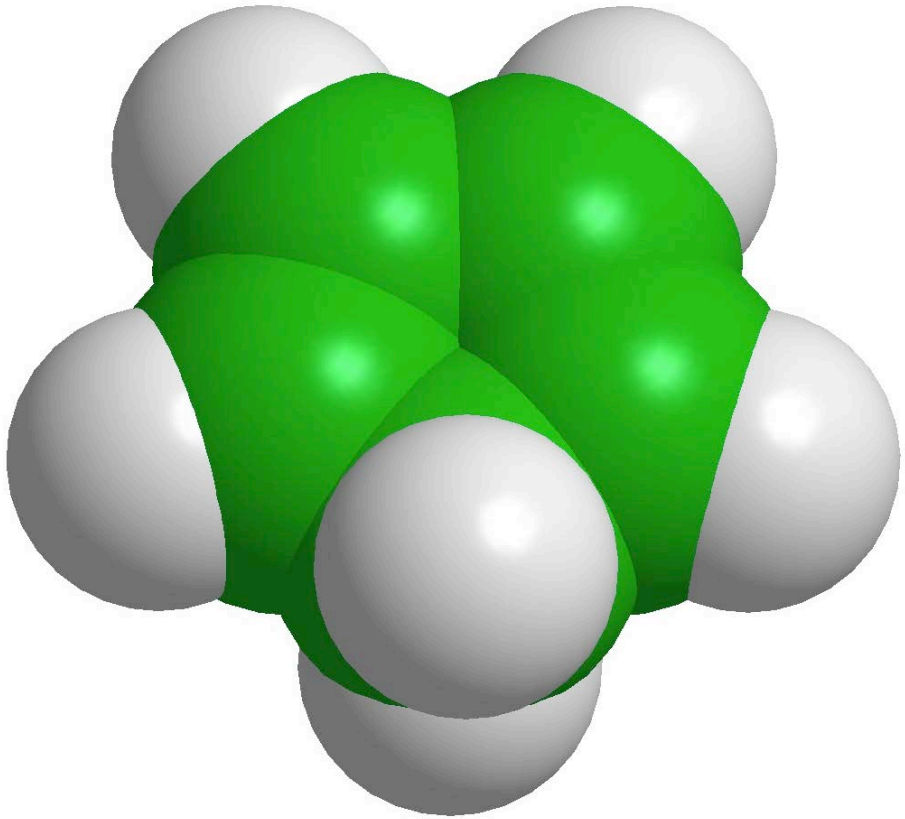


Cyclopentadiene B3LYP

- Zero-point correction= 0.092150 (Hartree/Particle)
- Thermal correction to Energy= 0.096303
- Thermal correction to Enthalpy= 0.097248
- Thermal correction to Gibbs Free Energy= 0.065554
- Sum of electronic and zero-point Energies= -194.061570
- Sum of electronic and thermal Energies= -194.057417
- Sum of electronic and thermal Enthalpies= -194.056472
- Sum of electronic and thermal Free Energies= -194.088166

- CycloP1

- 0 1
- C 1.17937400 -0.28245700 0.00006100
- C 0.73554100 0.98855800 0.00005000
- C -0.73338700 0.99017100 -0.00004600
- C -1.17999000 -0.27990000 -0.00007200
- H 2.21009200 -0.60990500 0.00011800
- H 1.34979100 1.88000100 0.00009200
- H -1.34565400 1.88298100 -0.00008600
- H -2.21141800 -0.60511700 -0.00013700
- C -0.00131500 -1.21520600 0.00000200
- H -0.00202800 -1.87749600 -0.87657700
- H -0.00212400 -1.87745700 0.87661300

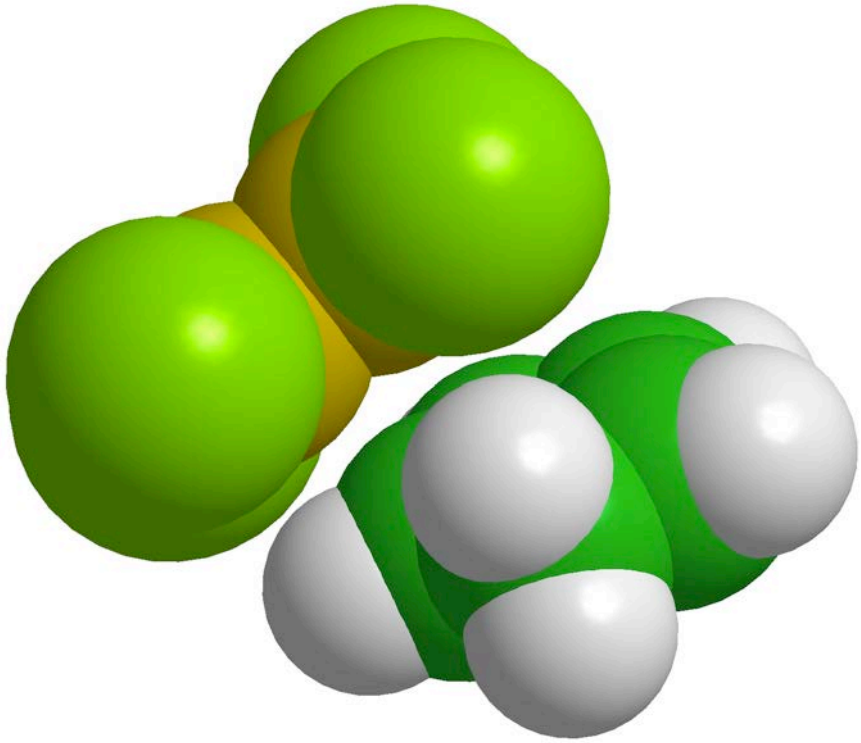


B_2Cl_4 cyclopentadiene vdW B3LYP

- Zero-point correction= 0.106200 (Hartree/Particle)
- Thermal correction to Energy= 0.119503
- Thermal correction to Enthalpy= 0.120448
- Thermal correction to Gibbs Free Energy= 0.061406
- Sum of electronic and zero-point Energies= -2084.817835
- Sum of electronic and thermal Energies= -2084.804531
- Sum of electronic and thermal Enthalpies= -2084.803587
- Sum of electronic and thermal Free Energies= -2084.862629

- B2Cl4

- 0 1
- C 1.35300200 -1.44539400 -0.88282100
- H 0.56569200 -2.15288700 -1.10177400
- B -1.49907500 -0.34661500 0.03167300
- Cl -1.87436900 -1.63484000 1.17626100
- Cl -2.24376700 -0.42957100 -1.56404100
- C 1.62678700 -0.30388500 -1.55666900
- H 1.06762200 0.08903100 -2.39578500
- B -0.54037800 0.98475200 0.49641000
- C 2.39535100 -1.64690700 0.18127500
- H 1.96086300 -1.70798500 1.18734300
- H 2.94326800 -2.58710800 0.03113000
- Cl 0.41680500 0.94871000 1.97211100
- Cl -0.57391000 2.48795500 -0.42353300
- C 2.82732500 0.31666500 -0.99252900
- H 3.25783900 1.24580800 -1.34134800
- C 3.28595900 -0.44660800 0.01892400
- H 4.15054000 -0.24909900 0.63738100



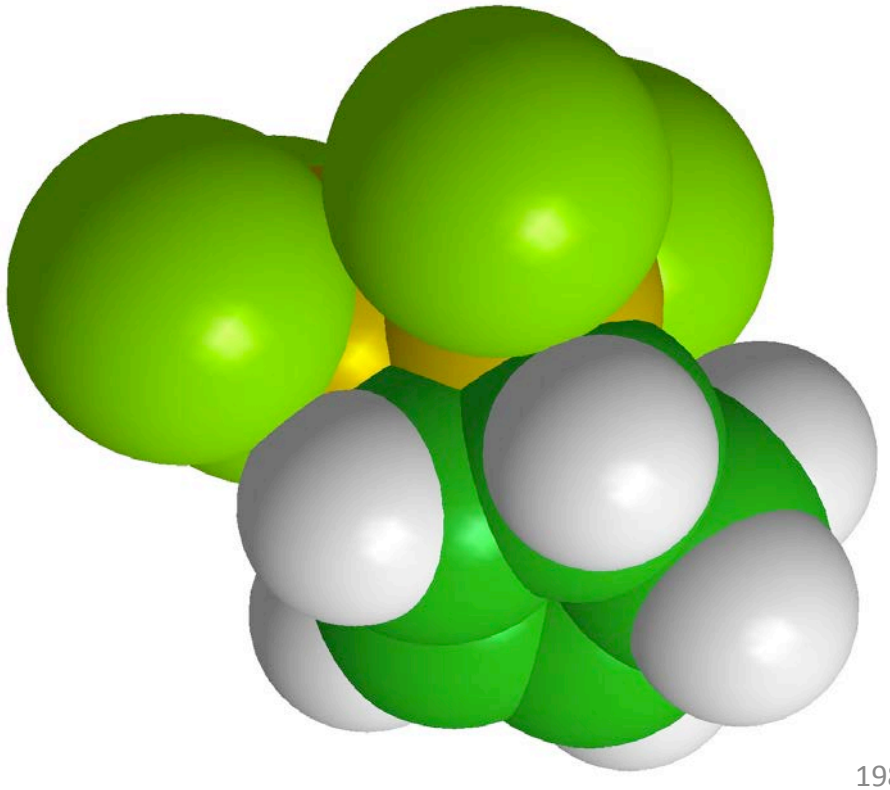
B2Cl4 cyclopentadiene TS for 1,2-addition B3LYP

- Zero-point correction= 0.107541 (Hartree/Particle)
- Thermal correction to Energy= 0.118714
- Thermal correction to Enthalpy= 0.119658
- Thermal correction to Gibbs Free Energy= 0.069117
- Sum of electronic and zero-point Energies= -2084.782392
- Sum of electronic and thermal Energies= -2084.771219
- Sum of electronic and thermal Enthalpies= -2084.770275
- Sum of electronic and thermal Free Energies= -2084.820816

- B2Cl4Cp12TSF

- 0 1

C	0.57547100	-0.38582300	-1.31265900
H	-0.18471900	-0.33657500	-2.08405200
B	-1.10127500	-0.49574400	-0.03169700
Cl	-1.16103800	-1.89758500	1.03172500
Cl	-2.58681300	-0.16657200	-0.93403400
C	1.42478400	0.76420900	-0.99910600
H	1.37830600	1.62904900	-1.64993600
B	0.26618300	0.83541300	0.16606500
C	2.80186200	0.20669400	-0.64543000
Cl	0.91971700	0.51474000	1.85816800
Cl	-0.72346300	2.39204700	0.00355100
C	1.33828300	-1.60556200	-1.02052700
C	2.58430500	-1.27607100	-0.63880800
H	3.35073900	-1.98798500	-0.35719200
H	0.93231800	-2.60363500	-1.09893200
H	3.18561200	0.57022000	0.31376600
H	3.54210700	0.48519000	-1.40626200

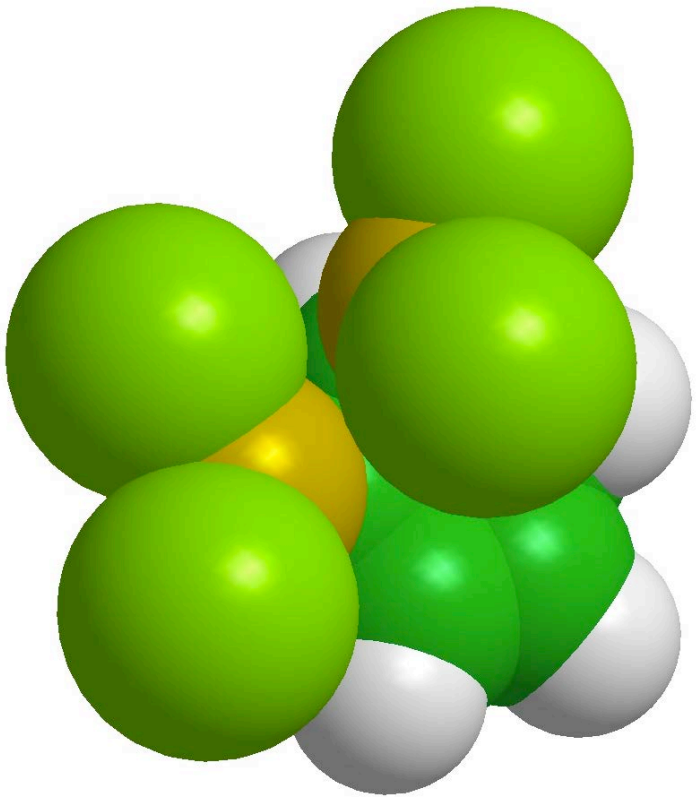


B_2Cl_4 Cyclopentadiene 1,2-addition product B3LYP

- Zero-point correction= 0.109196 (Hartree/Particle)
- Thermal correction to Energy= 0.120941
- Thermal correction to Enthalpy= 0.121885
- Thermal correction to Gibbs Free Energy= 0.068259
- Sum of electronic and zero-point Energies= -2084.852643
- Sum of electronic and thermal Energies= -2084.840898
- Sum of electronic and thermal Enthalpies= -2084.839954
- Sum of electronic and thermal Free Energies= -2084.893580

- B2Cl4Cp12P

- 0 1
- C 0.70051800 0.89848000 -0.79758600
- C -0.84821100 0.65905600 -0.89999200
- C -1.47597100 2.08704100 -0.64444700
- C -0.35476600 2.85092300 0.01317100
- C 0.81117400 2.21762700 -0.06159800
- H 1.07348800 1.06657400 -1.82976400
- H -1.12274000 0.30792800 -1.89567700
- H -1.77473900 2.55227600 -1.59169700
- H -2.38075000 2.05679300 -0.02700800
- H -0.50500200 3.82472600 0.46403700
- H 1.75317300 2.59589300 0.31429000
- B -1.48809600 -0.30086300 0.15915700
- B 1.61470900 -0.29818100 -0.36731500
- Cl 3.09244900 -0.06946700 0.56495400
- Cl 1.27453500 -1.92882800 -0.97183500
- Cl -0.81939400 -0.49025300 1.78394500
- Cl -2.99894000 -1.14014200 -0.20357500

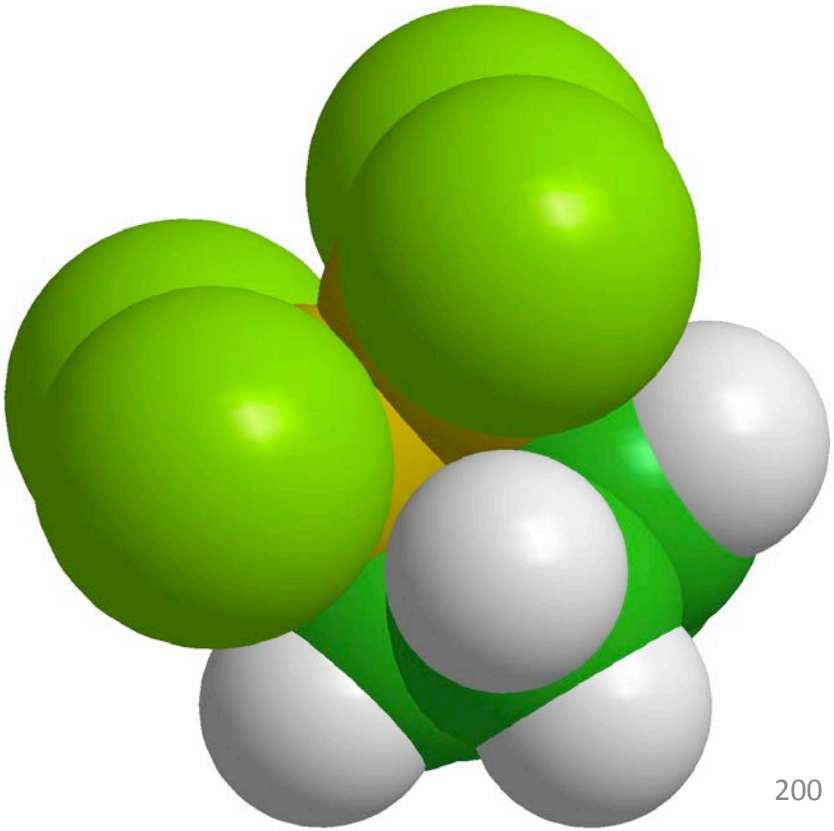


B_2Cl_4 cyclopentadiene TS for 1,4-addition B3LYP

- Zero-point correction= 0.106796 (Hartree/Particle)
- Thermal correction to Energy= 0.118123
- Thermal correction to Enthalpy= 0.119067
- Thermal correction to Gibbs Free Energy= 0.068397
- Sum of electronic and zero-point Energies= -2084.767822
- Sum of electronic and thermal Energies= -2084.756494
- Sum of electronic and thermal Enthalpies= -2084.755550
- Sum of electronic and thermal Free Energies= -2084.806221

- B2Cl4CpTSF1

- 0 1
- C -1.07053300 2.18160500 -0.38691800
- C 0.28626000 2.42859900 -0.48403800
- C 0.85815500 1.38913200 -1.25628600
- C -0.24153000 0.76675500 -2.06817500
- C -1.36777900 0.92938800 -1.04952900
- H -1.77077700 2.74518200 0.21464500
- H 0.83473800 3.19168400 0.04986400
- H -0.05517400 -0.25242100 -2.39782200
- H -0.43660500 1.39211800 -2.95171300
- B -1.00706500 -0.33407000 0.09361800
- B 1.04074000 -0.18412800 0.15128100
- H -2.40090200 0.75309600 -1.34940800
- H 1.90255200 1.37875300 -1.55014400
- Cl -1.64656700 -0.05528500 1.77178800
- Cl -1.44429800 -1.97928900 -0.53778600
- Cl 1.75898700 0.39791800 1.67237100
- Cl 1.97719300 -1.46865500 -0.65756400

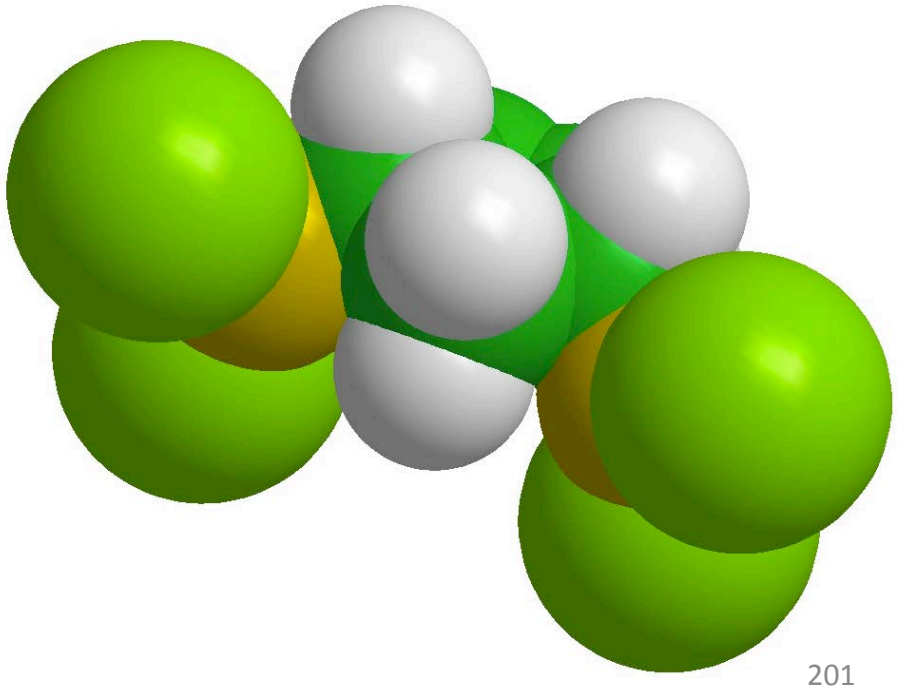


B_2Cl_4 cyclopentadiene 1,4 addition product B3LYP

- Zero-point correction= 0.109718 (Hartree/Particle)
- Thermal correction to Energy= 0.121511
- Thermal correction to Enthalpy= 0.122455
- Thermal correction to Gibbs Free Energy= 0.066820
- Sum of electronic and zero-point Energies= -2084.854845
- Sum of electronic and thermal Energies= -2084.843053
- Sum of electronic and thermal Enthalpies= -2084.842108
- Sum of electronic and thermal Free Energies= -2084.897743

- B2Cl4Cp14P

- 0 1
- C 0.66526200 0.92463800 1.65801800
- C -0.66522600 0.92461300 1.65804200
- C -1.24292300 -0.29653200 0.97073300
- C 0.00003800 -0.84705200 0.18387400
- C 1.24298900 -0.29650200 0.97070600
- H 1.28432300 1.67523200 2.13436900
- H -1.28429300 1.67519900 2.13439900
- H -1.53338500 -1.03873900 1.72903000
- H 0.00004700 -1.93376800 0.10335800
- H 0.00002300 -0.43700100 -0.83130200
- H 1.53352500 -1.03869600 1.72898300
- B -2.45892600 -0.09647000 0.00482100
- B 2.45894000 -0.09629200 0.00475200
- Cl 2.79759700 1.45198600 -0.76524800
- Cl 3.50241500 -1.46327300 -0.40236400
- Cl -2.79835100 1.45195400 -0.76452800
- Cl -3.50172800 -1.46380800 -0.40285600

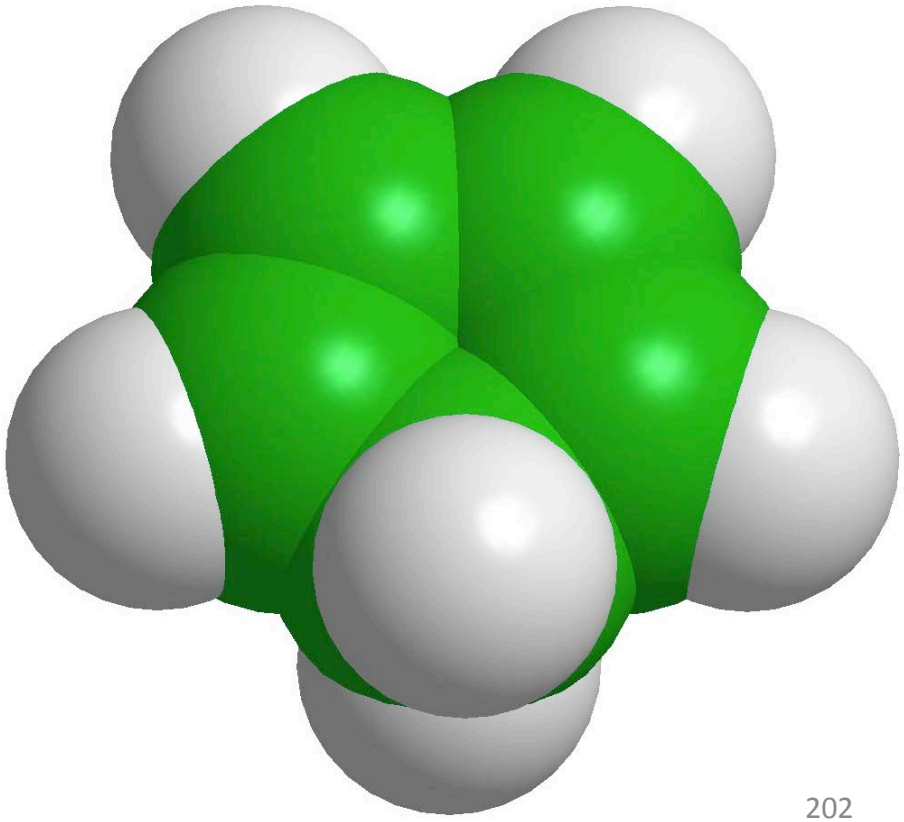


Cyclopentadiene ωB97X-D

- Zero-point correction= 0.092945 (Hartree/Particle)
- Thermal correction to Energy= 0.097091
- Thermal correction to Enthalpy= 0.098035
- Thermal correction to Gibbs Free Energy= 0.066350
- Sum of electronic and zero-point Energies= -193.988282
- Sum of electronic and thermal Energies= -193.984136
- Sum of electronic and thermal Enthalpies= -193.983192
- Sum of electronic and thermal Free Energies= -194.014877

- CycloP2

- 0 1
- C 1.17543900 -0.28033000 0.00005600
- C 0.73353500 0.98646400 0.00006000
- C -0.73374000 0.98631200 -0.00005700
- C -1.17538200 -0.28057400 -0.00006300
- H 2.20674600 -0.60589100 0.00011300
- H 1.34833500 1.87741400 0.00010800
- H -1.34872400 1.87713600 -0.00010100
- H -2.20662000 -0.60635000 -0.00012800
- C 0.00012700 -1.21187200 0.00000000
- H 0.00023700 -1.87117200 -0.87754300
- H 0.00015500 -1.87112900 0.87757700

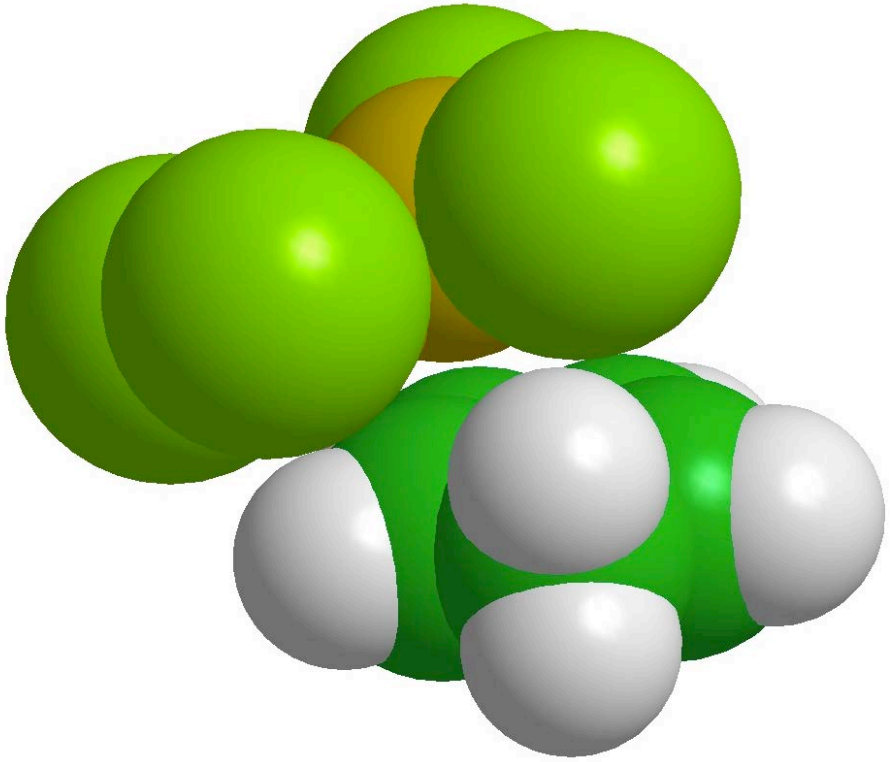


B_2Cl_4 Cyclopentadiene vdW ωB97X-D

- Zero-point correction= 0.108010 (Hartree/Particle)
- Thermal correction to Energy= 0.120872
- Thermal correction to Enthalpy= 0.121817
- Thermal correction to Gibbs Free Energy= 0.065428
- Sum of electronic and zero-point Energies= -2084.668056
- Sum of electronic and thermal Energies= -2084.655194
- Sum of electronic and thermal Enthalpies= -2084.654250
- Sum of electronic and thermal Free Energies= -2084.710638

- B2Cl4CpVW

- 0 1
- C 1.08480900 -1.49260300 -1.01168700
- H 0.26478200 -2.15758500 -1.24684700
- B -1.45154100 -0.25630200 0.07339800
- Cl -1.82073800 -1.59510100 1.15345000
- Cl -2.32313000 -0.17303200 -1.45079900
- C 1.39303800 -0.34116300 -1.64235500
- H 0.83415900 0.10874500 -2.45306100
- B -0.37173400 0.98317800 0.55145400
- C 2.12714400 -1.77775200 0.02511900
- H 1.70022200 -1.86131000 1.03220000
- H 2.63554900 -2.72961100 -0.17334600
- Cl 0.60206900 0.82070300 2.00071900
- Cl -0.28685300 2.50293800 -0.32610400
- C 2.62520100 0.20715100 -1.07274300
- H 3.08811900 1.13217000 -1.38877900
- C 3.06013000 -0.61189400 -0.10179700
- H 3.93867600 -0.47285400 0.51281900

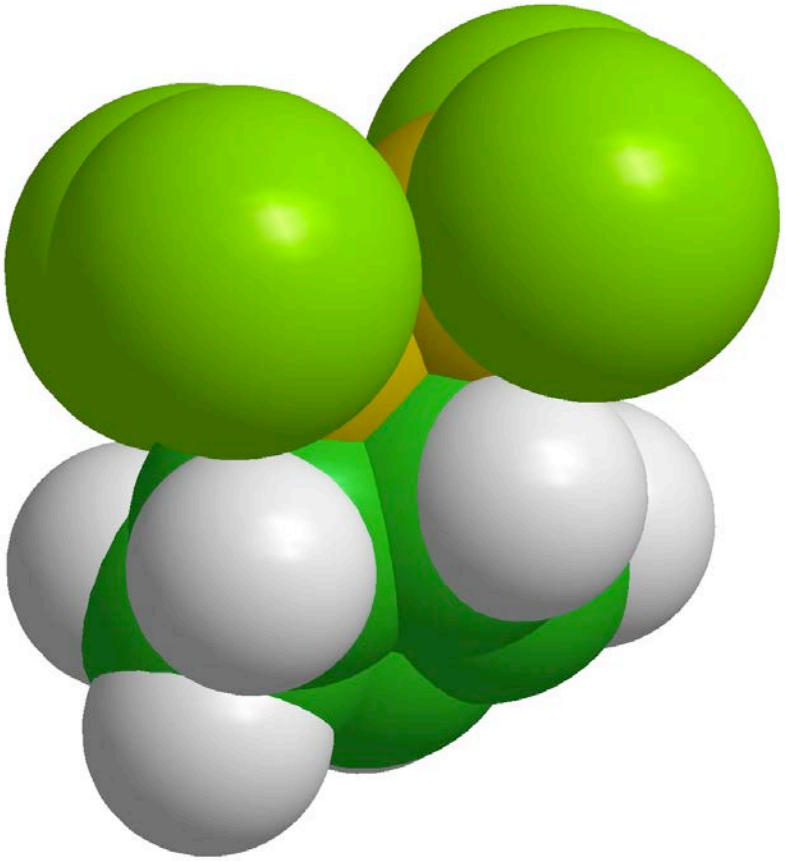


B_2Cl_4 Cyclopentadiene 1,2-TS ωB97X-D

- Zero-point correction= 0.109162 (Hartree/Particle)
- Thermal correction to Energy= 0.120138
- Thermal correction to Enthalpy= 0.121082
- Thermal correction to Gibbs Free Energy= 0.071073
- Sum of electronic and zero-point Energies= -2084.640361
- Sum of electronic and thermal Energies= -2084.629385
- Sum of electronic and thermal Enthalpies= -2084.628441
- Sum of electronic and thermal Free Energies= -2084.678450

- BCP12WTS

- 0 1
- C 0.56907700 -0.32966700 -1.32007900
- H -0.19974400 -0.24964800 -2.08143400
- B -1.10037200 -0.48361900 -0.02682400
- Cl -1.14422200 -1.91768000 0.98504400
- Cl -2.58694200 -0.13557000 -0.90851700
- C 1.43412800 0.78490500 -0.98888400
- H 1.39093000 1.68085400 -1.59471900
- B 0.25550800 0.81659000 0.17836000
- C 2.79175500 0.20338000 -0.63510800
- Cl 0.92088400 0.46790800 1.85113000
- Cl -0.70447000 2.38234200 0.03509800
- C 1.30648400 -1.57186900 -1.04985400
- C 2.54790400 -1.27200400 -0.64982300
- H 3.29708700 -2.00076400 -0.36695100
- H 0.87962300 -2.55861200 -1.15300600
- H 3.17755600 0.54969600 0.32856700
- H 3.53352200 0.47616900 -1.39448000



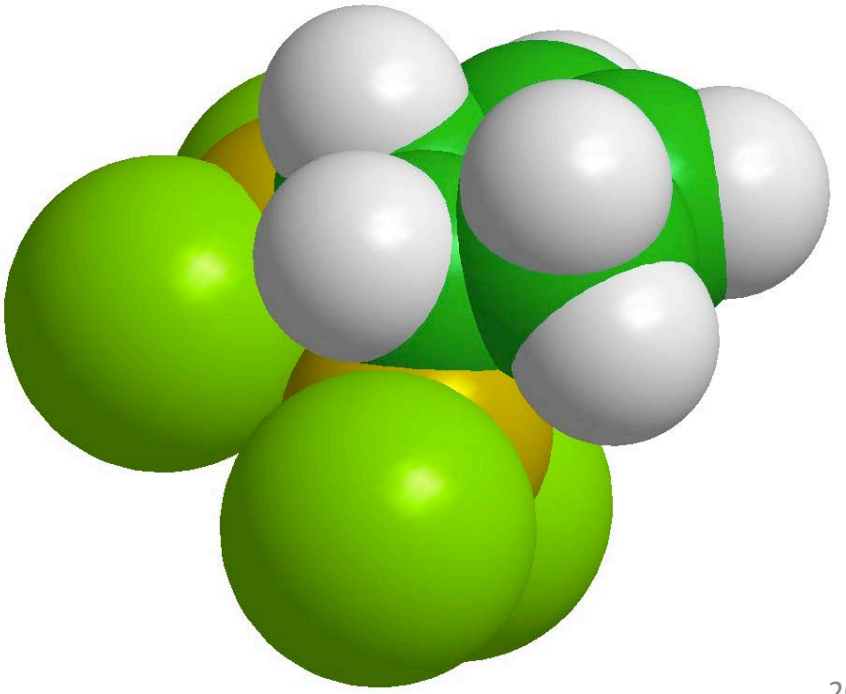
B_2Cl_4 Cyclopentadiene 1,2-addition product ωB97X-D

Zero-point correction= 0.110747 (Hartree/Particle)
Thermal correction to Energy= 0.122324
Thermal correction to Enthalpy= 0.123268
Thermal correction to Gibbs Free Energy= 0.070315
Sum of electronic and zero-point Energies= -2084.710726
Sum of electronic and thermal Energies= -2084.699149
Sum of electronic and thermal Enthalpies= -2084.698205
Sum of electronic and thermal Free Energies= -2084.751159

B2Cl4Cp12W

0 1

C	0.68720400	0.91042600	-0.80731400
C	-0.84521000	0.64732300	-0.91861300
C	-1.49436100	2.05594100	-0.68089600
C	-0.40591000	2.82181100	0.02329600
C	0.76819700	2.20967300	-0.04030400
H	1.07064700	1.10484100	-1.82923900
H	-1.11192500	0.26929500	-1.90694600
H	-1.75318400	2.52938700	-1.63484700
H	-2.42276500	2.01399200	-0.10070600
H	-0.58025700	3.78229400	0.49245700
H	1.69609600	2.59268900	0.36533000
B	-1.46027200	-0.30639200	0.16323000
B	1.60095100	-0.28588900	-0.37702600
Cl	3.07277700	-0.05997200	0.55336900
Cl	1.24844800	-1.91098100	-0.97504100
Cl	-0.76316000	-0.46572700	1.77478100
Cl	-2.96168400	-1.16344600	-0.16335000

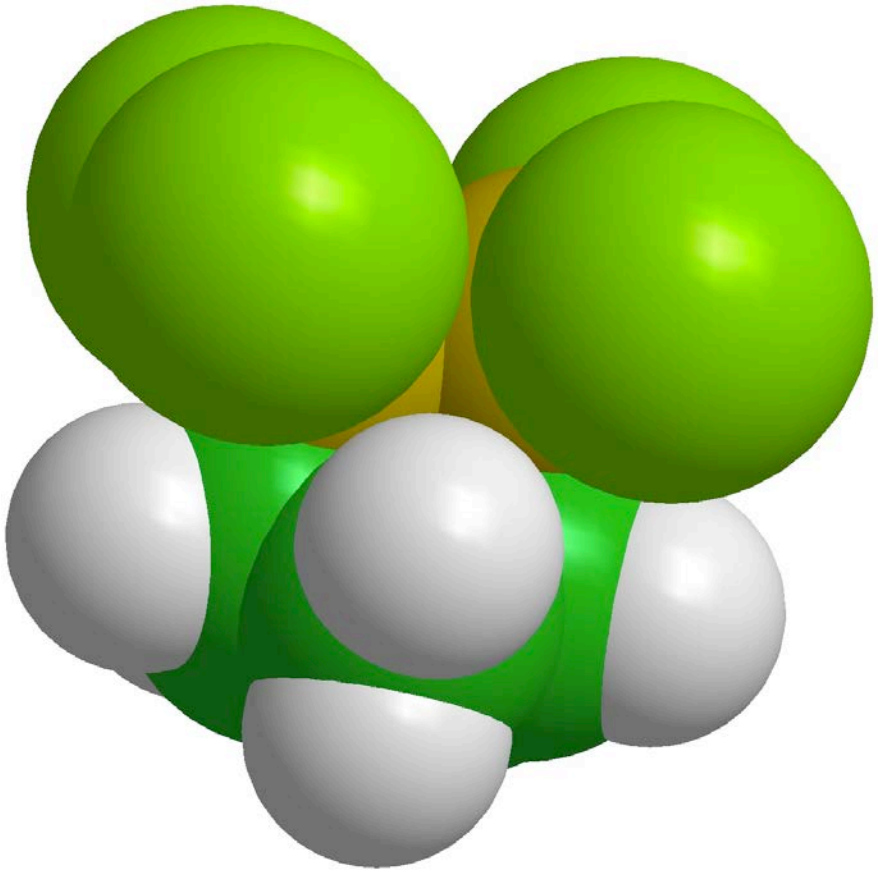


B_2Cl_4 Cyclopentadiene 1,4-addition TS ωB97X-D

- Zero-point correction= 0.108044 (Hartree/Particle)
- Thermal correction to Energy= 0.119257
- Thermal correction to Enthalpy= 0.120201
- Thermal correction to Gibbs Free Energy= 0.069713
- Sum of electronic and zero-point Energies= -2084.621070
- Sum of electronic and thermal Energies= -2084.609856
- Sum of electronic and thermal Enthalpies= -2084.608912
- Sum of electronic and thermal Free Energies= -2084.659401

- BCP14WTS

- 0 1
- C -1.09913600 2.13807300 -0.42467700
- C 0.25190200 2.39730300 -0.53231300
- C 0.82216900 1.35618600 -1.29078000
- C -0.26852700 0.70634100 -2.08145100
- C -1.38674400 0.88397200 -1.06819500
- H -1.80117700 2.70094100 0.17563600
- H 0.79812100 3.16688700 -0.00621800
- H -0.07221300 -0.31941100 -2.38570600
- H -0.46961500 1.30999500 -2.97705700
- B -0.99364000 -0.33796200 0.10679900
- B 1.03573400 -0.17140500 0.14693400
- H -2.42039800 0.68147400 -1.34728800
- H 1.86852900 1.34002100 -1.58007400
- Cl -1.61548400 -0.01711500 1.77707500
- Cl -1.42210700 -1.99838200 -0.47099300
- Cl 1.76428600 0.46441900 1.63476700



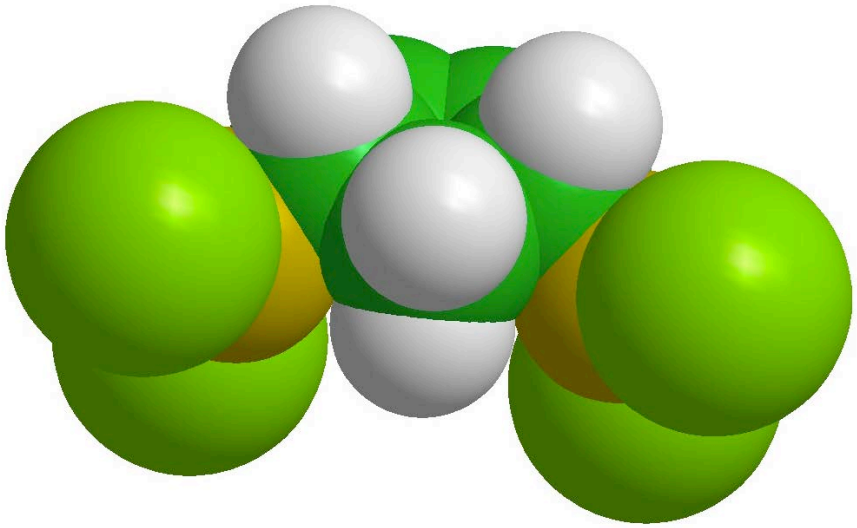
B_2Cl_4 Cyclopentadiene 1,4-addition product ωB97X-D

- Zero-point correction= 0.111009 (Hartree/Particle)
- Thermal correction to Energy= 0.122752
- Thermal correction to Enthalpy= 0.123696
- Thermal correction to Gibbs Free Energy= 0.067859
- Sum of electronic and zero-point Energies= -2084.709879
- Sum of electronic and thermal Energies= -2084.698136
- Sum of electronic and thermal Enthalpies= -2084.697192
- Sum of electronic and thermal Free Energies= -2084.753029

- B2Cl4Cp14W

- 0 1

C	0.66334700	0.95926200	1.67134800
C	-0.66334500	0.95926800	1.67133900
C	-1.23810900	-0.27997000	1.02638200
C	0.00000000	-0.86501800	0.27414500
C	1.23811000	-0.27997200	1.02638100
H	1.28288300	1.72768700	2.11782800
H	-1.28288000	1.72769700	2.11781300
H	-1.55375500	-0.99007700	1.80313800
H	-0.00000100	-1.95448600	0.24451000
H	0.00000100	-0.50758100	-0.76280000
H	1.55375500	-0.99008300	1.80313400
B	-2.41473800	-0.09510100	0.01139700
B	2.41473800	-0.09509800	0.01139600
Cl	2.70671300	1.43592200	-0.79853700
Cl	3.43202300	-1.46602200	-0.42073500
Cl	-2.70672600	1.43592100	-0.79852900
Cl	-3.43201200	-1.46603100	-0.42073800



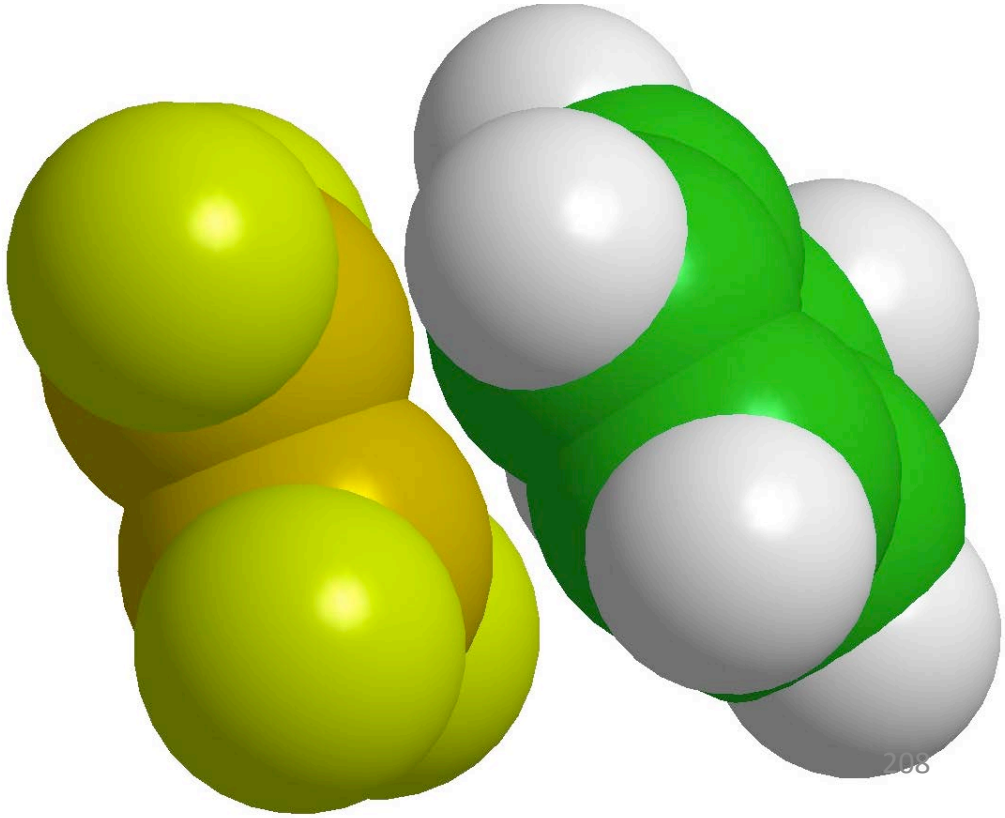
B_2F_4 Cyclopentadiene vdW B3LYP

Zero-point correction= 0.112230 (Hartree/Particle)
Thermal correction to Energy= 0.124271
Thermal correction to Enthalpy= 0.125215
Thermal correction to Gibbs Free Energy= 0.070439
Sum of electronic and zero-point Energies= -643.479290
Sum of electronic and thermal Energies= -643.467249
Sum of electronic and thermal Enthalpies= -643.466305
Sum of electronic and thermal Free Energies= -643.521081

CpF

0 1

C	1.19966900	0.79269800	1.17576900
C	2.11231800	-0.35097600	1.05815900
C	2.59432100	-0.40365700	-0.19834100
C	2.01579600	0.72784400	-1.00200300
C	1.12550000	1.42996700	-0.01404700
H	0.68381900	1.07646500	2.08417900
H	2.34048700	-1.03679500	1.86305900
H	1.46196200	0.36628100	-1.87787700
H	2.79498100	1.39795900	-1.38922300
B	-1.80549500	0.40059700	-0.01893800
B	-1.01678900	-1.09533700	-0.23236500
H	0.56315800	2.32647600	-0.23552500
H	3.28019400	-1.13765100	-0.59787600
F	-2.25290400	0.79149000	1.16829600
F	-2.04537500	1.21884000	-1.03749500
F	-0.93630500	-1.99175800	0.74000300



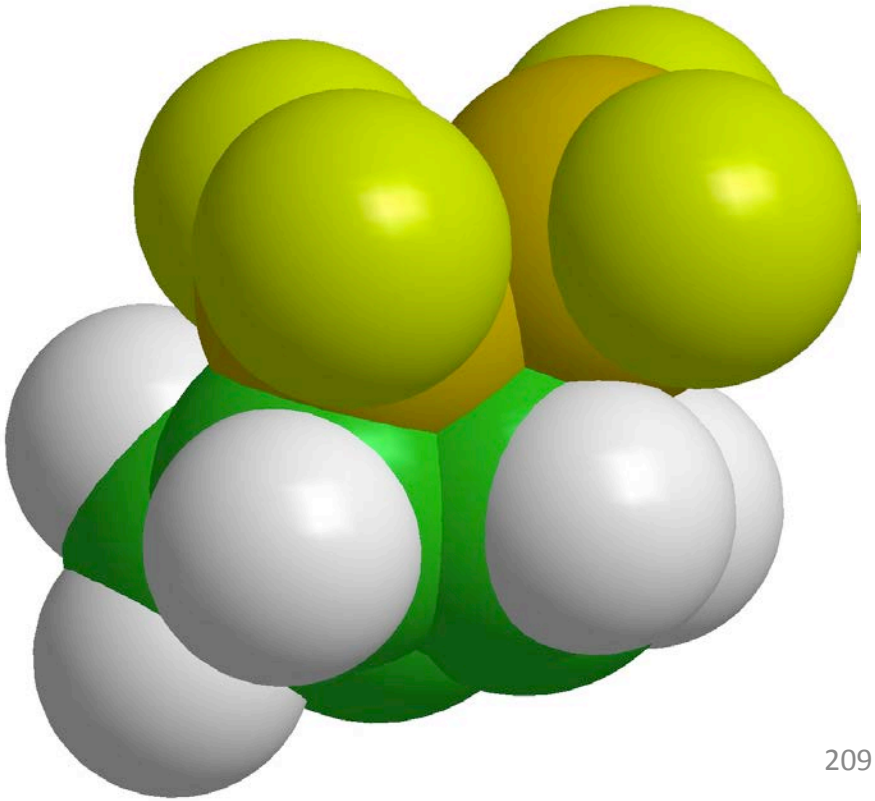
B_2F_4 Cyclopentadiene 1,2-addition TS B3LYP

Zero-point correction= 0.112854 (Hartree/Particle)
Thermal correction to Energy= 0.122844
Thermal correction to Enthalpy= 0.123788
Thermal correction to Gibbs Free Energy= 0.077105
Sum of electronic and zero-point Energies= -643.428437
Sum of electronic and thermal Energies= -643.418447
Sum of electronic and thermal Enthalpies= -643.417503
Sum of electronic and thermal Free Energies= -643.464186

BCP12B3FTS

0 1

C	0.42100000	-0.38831500	-1.04683000
H	-0.24166500	-0.50758800	-1.89719000
B	-1.46938200	-0.49273800	0.06073600
C	1.11044000	0.83729200	-0.74908700
H	1.10962900	1.65417300	-1.46030500
B	-0.29425100	0.91982000	0.19172800
C	2.36786800	0.46731600	0.02384400
C	1.15229400	-1.50106500	-0.42794200
C	2.25234600	-1.01999500	0.17611000
H	2.96447700	-1.61835600	0.73120500
H	0.82220600	-2.53011900	-0.44592300
H	2.42029400	0.95909200	1.00353800
H	3.28007300	0.74350500	-0.51943200
F	0.03504500	0.89813000	1.54659800
F	-1.08709200	1.98063000	-0.24611300
F	-2.48135700	-0.47018100	-0.79825800
F	-1.50665600	-1.43163700	0.99435300

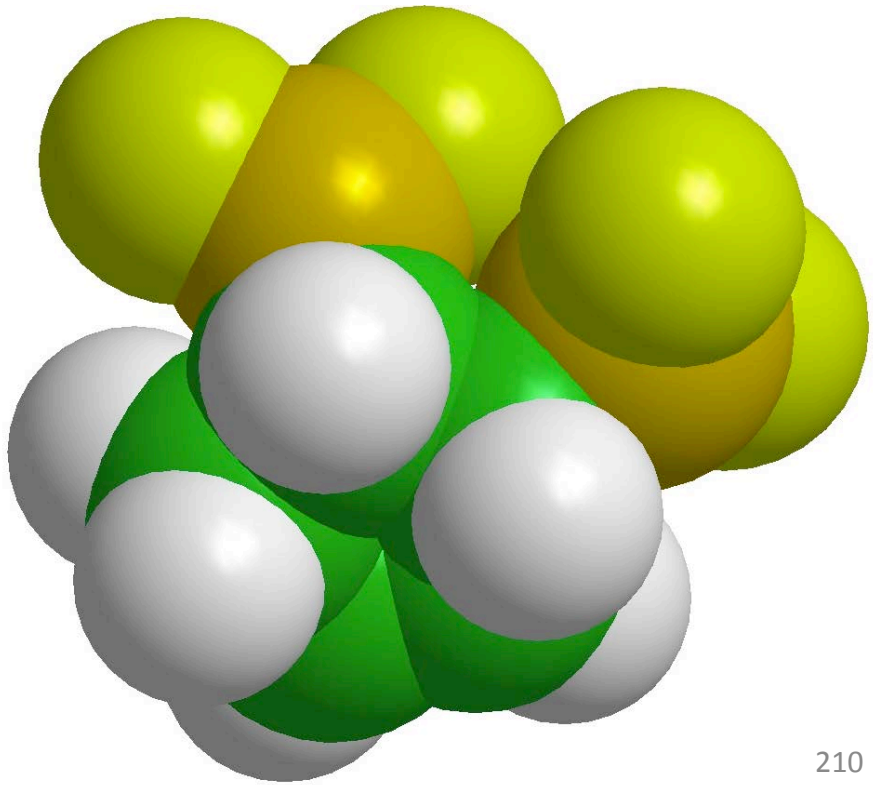


B_2F_4 Cyclopentadiene 1,2-addition product B3LYP

- Zero-point correction= 0.115186 (Hartree/Particle)
- Thermal correction to Energy= 0.125586
- Thermal correction to Enthalpy= 0.126530
- Thermal correction to Gibbs Free Energy= 0.077078
- Sum of electronic and zero-point Energies= -643.524598
- Sum of electronic and thermal Energies= -643.514197
- Sum of electronic and thermal Enthalpies= -643.513253
- Sum of electronic and thermal Free Energies= -643.562706

- B2F4Cp12P1

- 0 1
- C 0.42189700 0.88561700 -0.57190200
- C -0.85671900 -0.00180300 -0.77901300
- C -2.04692800 0.95055400 -0.42089000
- C -1.39579100 1.97247200 0.48162600
- C -0.06654600 1.93907500 0.40416900
- H 0.65055900 1.38324400 -1.53087600
- H -0.94206100 -0.34190600 -1.81664000
- H -2.45115300 1.43332700 -1.31935300
- H -2.88238000 0.42656200 0.05140900
- H -1.96850700 2.67584700 1.07472300
- H 0.60702200 2.60952500 0.92447900
- B -0.88715600 -1.27322400 0.12459200
- B 1.73908500 0.12780200 -0.20940900
- F 0.15878200 -1.64141800 0.87591700
- F -1.94758500 -2.06875600 0.20806100
- F 2.22125500 -0.83881000 -0.99258600
- F 2.49992500 0.44509700 0.83709600



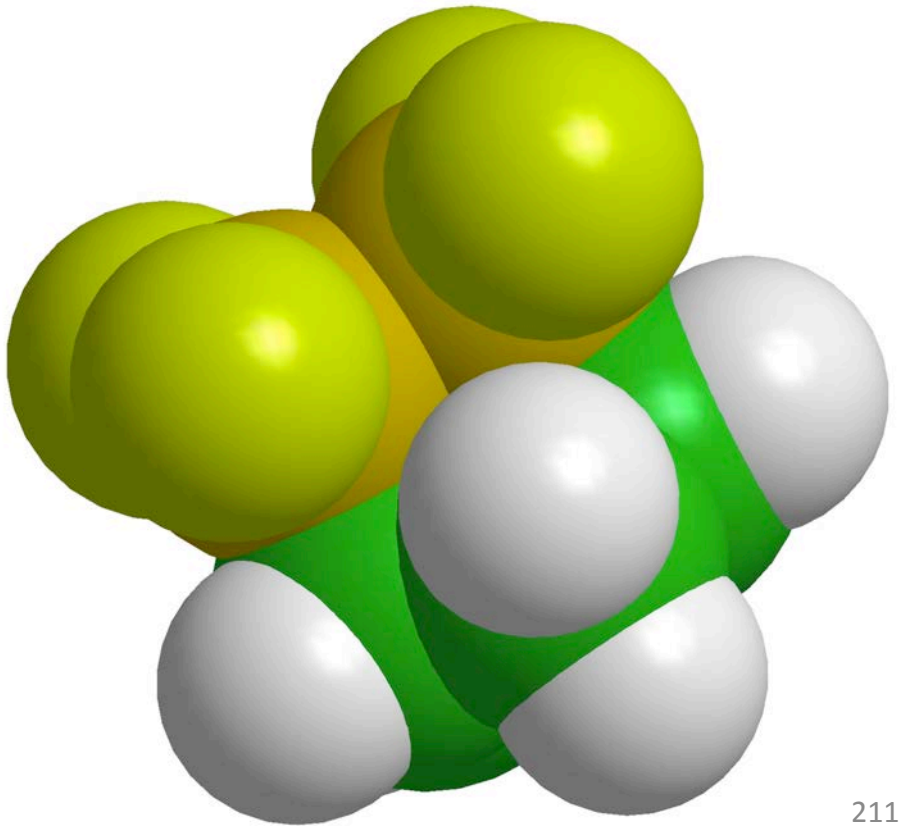
B_2F_4 Cyclopentadiene 1,4-addition TS B3LYP

Zero-point correction= 0.112100 (Hartree/Particle)
Thermal correction to Energy= 0.122470
Thermal correction to Enthalpy= 0.123414
Thermal correction to Gibbs Free Energy= 0.075667
Sum of electronic and zero-point Energies= -643.432222
Sum of electronic and thermal Energies= -643.421852
Sum of electronic and thermal Enthalpies= -643.420908
Sum of electronic and thermal Free Energies= -643.468654

BCP14B3FTS

0 1

C	1.83329400	0.69683900	0.70230400
C	1.83336300	-0.69661500	0.70229700
C	1.13249600	-1.14369700	-0.44171200
C	1.14645900	0.00008100	-1.43108300
C	1.13241900	1.14384700	-0.44171300
H	2.17173700	1.32539300	1.51487200
H	2.17189100	-1.32513900	1.51485300
H	0.33369700	0.00006200	-2.15395300
H	2.10471500	0.00011800	-1.97201600
B	-0.73724200	0.97626500	0.08190000
B	-0.73702100	-0.97639500	0.08187200
H	1.14176500	2.18515500	-0.75165100
H	1.14206700	-2.18499600	-0.75168200
F	-0.97786300	-1.47767800	1.30527900
F	-1.47539100	-1.52145500	-0.90303500
F	-1.47558500	1.52125900	-0.90305200
F	-0.97813300	1.47757700	1.30526900



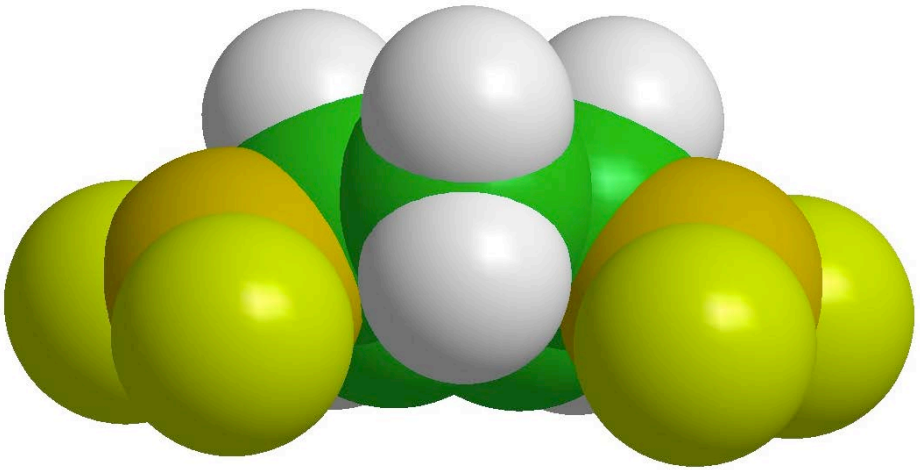
Cyclopentadiene B_2F_4 1, 4 addition product B3LYP

- Zero-point correction= 0.115716 (Hartree/Particle)
- Thermal correction to Energy= 0.126242
- Thermal correction to Enthalpy= 0.127186
- Thermal correction to Gibbs Free Energy= 0.075W 92
- Sum of electronic and zero-point Energies= -643.519749
- Sum of electronic and thermal Energies= -643.509223
- Sum of electronic and thermal Enthalpies= -643.508279
- Sum of electronic and thermal Free Energies= -643.559473

- B2F4Cp14B

- 0 1

C	-0.66508700	1.54020700	0.25079600
C	0.66502800	1.54023300	0.25080400
C	1.24255900	0.42894100	-0.61681800
C	0.00001700	-0.44982200	-0.93545300
C	-1.24254900	0.42889800	-0.61684700
H	-1.28769500	2.26159900	0.76661500
H	1.28760200	2.26164000	0.76664200
H	1.64017900	0.89751900	-1.53299300
H	0.00004500	-0.80334000	-1.96786400
H	0.00003700	-1.33701900	-0.29865900
H	-1.64019700	0.89746600	-1.53301700
B	2.45083400	-0.29942400	0.05842000
B	-2.45082700	-0.29944300	0.05841400
F	-3.54244200	0.37188000	0.41270400
F	-2.45761400	-1.60045100	0.32175500
F	2.45760500	-1.60043700	0.32174800
F	3.54247100	0.37186600	0.41270600



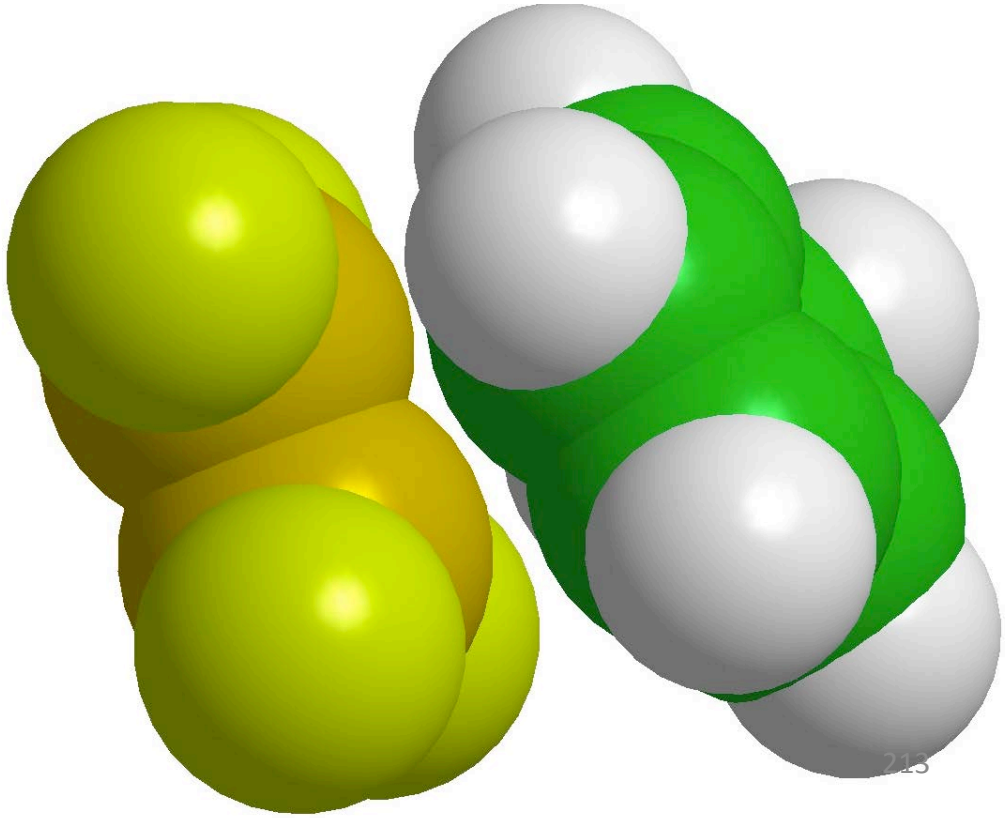
B_2F_4 Cyclopentadiene vdW B3LYP

Zero-point correction= 0.112230 (Hartree/Particle)
Thermal correction to Energy= 0.124271
Thermal correction to Enthalpy= 0.125215
Thermal correction to Gibbs Free Energy= 0.070439
Sum of electronic and zero-point Energies= -643.479290
Sum of electronic and thermal Energies= -643.467249
Sum of electronic and thermal Enthalpies= -643.466305
Sum of electronic and thermal Free Energies= -643.521081

CpF

0 1

C	1.19966900	0.79269800	1.17576900
C	2.11231800	-0.35097600	1.05815900
C	2.59432100	-0.40365700	-0.19834100
C	2.01579600	0.72784400	-1.00200300
C	1.12550000	1.42996700	-0.01404700
H	0.68381900	1.07646500	2.08417900
H	2.34048700	-1.03679500	1.86305900
H	1.46196200	0.36628100	-1.87787700
H	2.79498100	1.39795900	-1.38922300
B	-1.80549500	0.40059700	-0.01893800
B	-1.01678900	-1.09533700	-0.23236500
H	0.56315800	2.32647600	-0.23552500
H	3.28019400	-1.13765100	-0.59787600
F	-2.25290400	0.79149000	1.16829600
F	-2.04537500	1.21884000	-1.03749500
F	-0.93630500	-1.99175800	0.74000300
F	-0.46528300	-1.42904900	-1.29285300



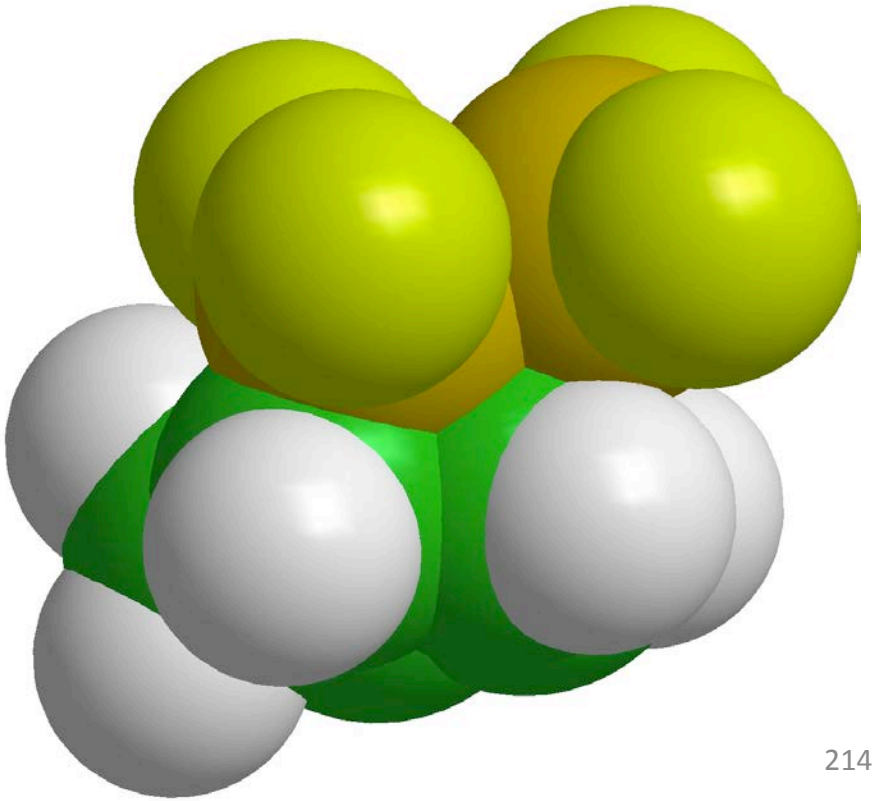
B_2F_4 Cyclopentadiene 1,2-addition TS B3LYP

Zero-point correction= 0.112854 (Hartree/Particle)
Thermal correction to Energy= 0.122844
Thermal correction to Enthalpy= 0.123788
Thermal correction to Gibbs Free Energy= 0.077105
Sum of electronic and zero-point Energies= -643.428437
Sum of electronic and thermal Energies= -643.418447
Sum of electronic and thermal Enthalpies= -643.417503
Sum of electronic and thermal Free Energies= -643.464186

BCP12B3FTS

0 1

C	0.42100000	-0.38831500	-1.04683000
H	-0.24166500	-0.50758800	-1.89719000
B	-1.46938200	-0.49273800	0.06073600
C	1.11044000	0.83729200	-0.74908700
H	1.10962900	1.65417300	-1.46030500
B	-0.29425100	0.91982000	0.19172800
C	2.36786800	0.46731600	0.02384400
C	1.15229400	-1.50106500	-0.42794200
C	2.25234600	-1.01999500	0.17611000
H	2.96447700	-1.61835600	0.73120500
H	0.82220600	-2.53011900	-0.44592300
H	2.42029400	0.95909200	1.00353800
H	3.28007300	0.74350500	-0.51943200
F	0.03504500	0.89813000	1.54659800
F	-1.08709200	1.98063000	-0.24611300
F	-2.48135700	-0.47018100	-0.79825800
F	-1.50665600	-1.43163700	0.99435300

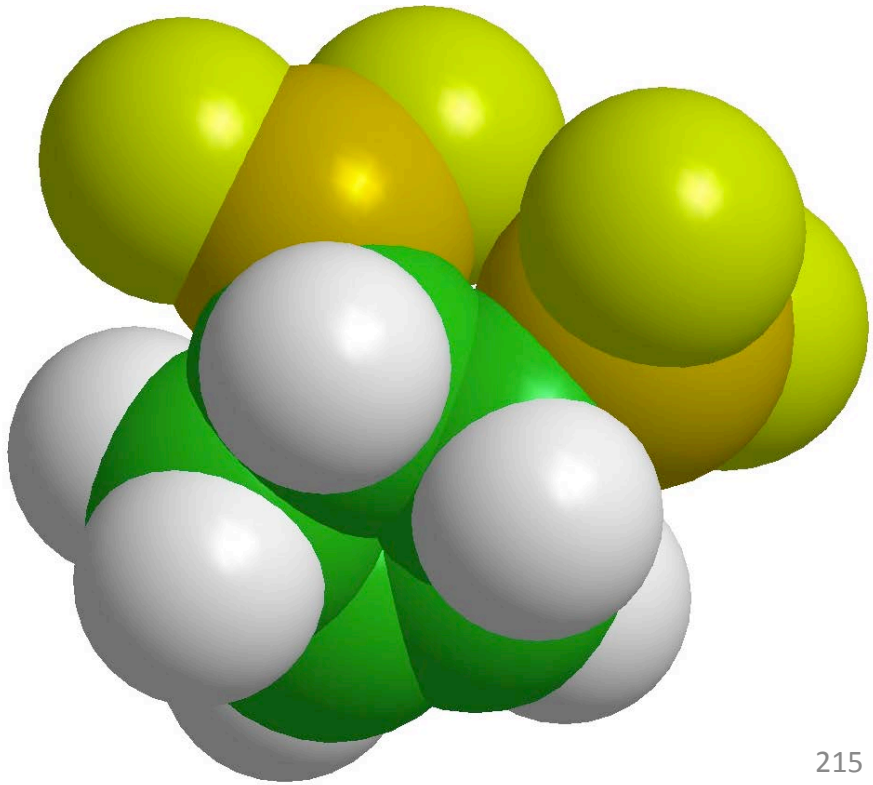


B_2F_4 Cyclopentadiene 1,2-addition product B3LYP

- Zero-point correction= 0.115186 (Hartree/Particle)
- Thermal correction to Energy= 0.125586
- Thermal correction to Enthalpy= 0.126530
- Thermal correction to Gibbs Free Energy= 0.077078
- Sum of electronic and zero-point Energies= -643.524598
- Sum of electronic and thermal Energies= -643.514197
- Sum of electronic and thermal Enthalpies= -643.513253
- Sum of electronic and thermal Free Energies= -643.562706

- B2F4Cp12P1

- 0 1
- C 0.42189700 0.88561700 -0.57190200
- C -0.85671900 -0.00180300 -0.77901300
- C -2.04692800 0.95055400 -0.42089000
- C -1.39579100 1.97247200 0.48162600
- C -0.06654600 1.93907500 0.40416900
- H 0.65055900 1.38324400 -1.53087600
- H -0.94206100 -0.34190600 -1.81664000
- H -2.45115300 1.43332700 -1.31935300
- H -2.88238000 0.42656200 0.05140900
- H -1.96850700 2.67584700 1.07472300
- H 0.60702200 2.60952500 0.92447900
- B -0.88715600 -1.27322400 0.12459200
- B 1.73908500 0.12780200 -0.20940900
- F 0.15878200 -1.64141800 0.87591700
- F -1.94758500 -2.06875600 0.20806100
- F 2.22125500 -0.83881000 -0.99258600
- F 2.49992500 0.44509700 0.83709600



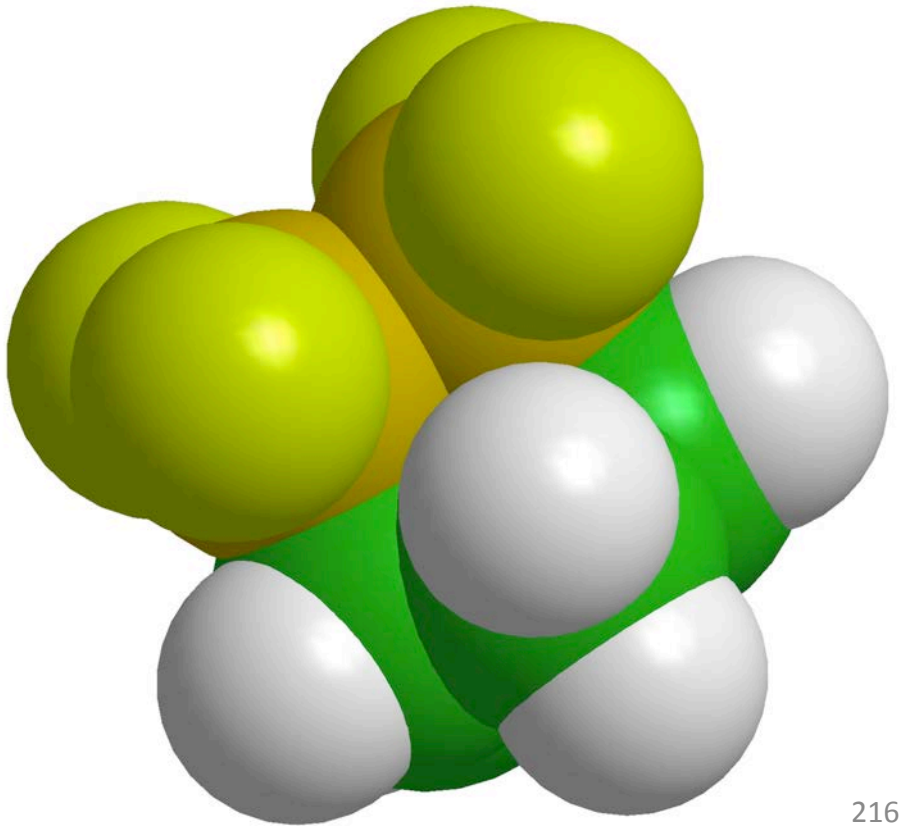
B_2F_4 Cyclopentadiene 1,4-addition TS B3LYP

Zero-point correction= 0.112100 (Hartree/Particle)
Thermal correction to Energy= 0.122470
Thermal correction to Enthalpy= 0.123414
Thermal correction to Gibbs Free Energy= 0.075667
Sum of electronic and zero-point Energies= -643.432222
Sum of electronic and thermal Energies= -643.421852
Sum of electronic and thermal Enthalpies= -643.420908
Sum of electronic and thermal Free Energies= -643.468654

BCP14B3FTS

0 1

C	1.83329400	0.69683900	0.70230400
C	1.83336300	-0.69661500	0.70229700
C	1.13249600	-1.14369700	-0.44171200
C	1.14645900	0.00008100	-1.43108300
C	1.13241900	1.14384700	-0.44171300
H	2.17173700	1.32539300	1.51487200
H	2.17189100	-1.32513900	1.51485300
H	0.33369700	0.00006200	-2.15395300
H	2.10471500	0.00011800	-1.97201600
B	-0.73724200	0.97626500	0.08190000
B	-0.73702100	-0.97639500	0.08187200
H	1.14176500	2.18515500	-0.75165100
H	1.14206700	-2.18499600	-0.75168200
F	-0.97786300	-1.47767800	1.30527900
F	-1.47539100	-1.52145500	-0.90303500
F	-1.47558500	1.52125900	-0.90305200
F	-0.97813300	1.47757700	1.30526900

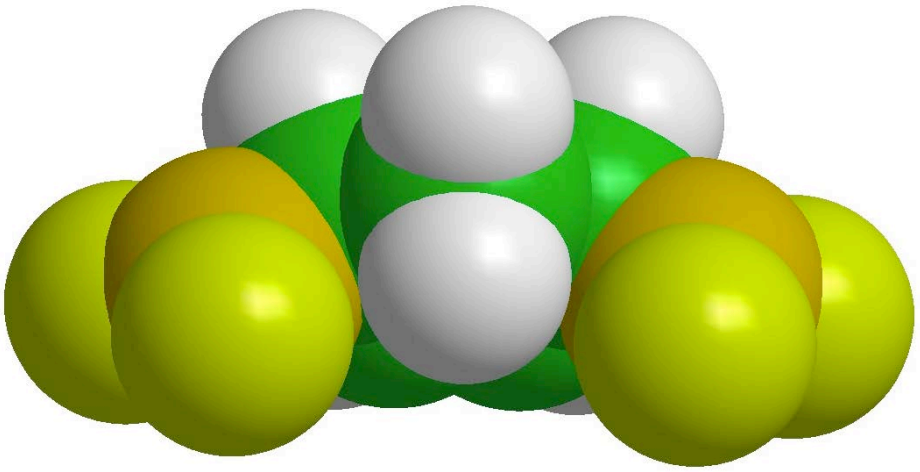


Cyclopentadiene B_2F_4 1, 4 addition product B3LYP

- Zero-point correction= 0.115716 (Hartree/Particle)
- Thermal correction to Energy= 0.126242
- Thermal correction to Enthalpy= 0.127186
- Thermal correction to Gibbs Free Energy= 0.075W 92
- Sum of electronic and zero-point Energies= -643.519749
- Sum of electronic and thermal Energies= -643.509223
- Sum of electronic and thermal Enthalpies= -643.508279
- Sum of electronic and thermal Free Energies= -643.559473

- B2F4Cp14B

- 0 1
- C -0.66508700 1.54020700 0.25079600
- C 0.66502800 1.54023300 0.25080400
- C 1.24255900 0.42894100 -0.61681800
- C 0.00001700 -0.44982200 -0.93545300
- C -1.24254900 0.42889800 -0.61684700
- H -1.28769500 2.26159900 0.76661500
- H 1.28760200 2.26164000 0.76664200
- H 1.64017900 0.89751900 -1.53299300
- H 0.00004500 -0.80334000 -1.96786400
- H 0.00003700 -1.33701900 -0.29865900
- H -1.64019700 0.89746600 -1.53301700
- B 2.45083400 -0.29942400 0.05842000
- B -2.45082700 -0.29944300 0.05841400
- F -3.54244200 0.37188000 0.41270400
- F -2.45761400 -1.60045100 0.32175500
- F 2.45760500 -1.60043700 0.32174800
- F 3.54247100 0.37186600 0.41270600

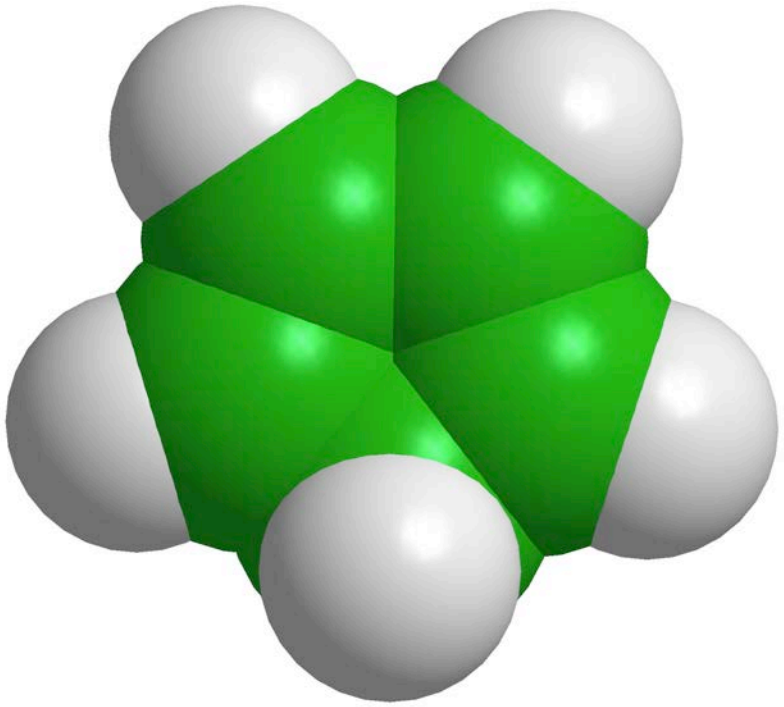


Cyclopentadiene ωB97xD

- Zero-point correction= 0.092945 (Hartree/Particle)
- Thermal correction to Energy= 0.097092
- Thermal correction to Enthalpy= 0.098036
- Thermal correction to Gibbs Free Energy= 0.066349
- Sum of electronic and zero-point Energies= -193.988285
- Sum of electronic and thermal Energies= -193.984138
- Sum of electronic and thermal Enthalpies= -193.983194
- Sum of electronic and thermal Free Energies= -194.014880

- CpW

- 0 1
- C 1.17150700 -0.29672800 -0.00000500
- C 0.74732700 0.97605200 -0.00000200
- C -0.71951900 0.99654500 0.00001000
- C -1.17929300 -0.26371800 -0.00001100
- H 2.19777400 -0.63770300 -0.00000600
- H 1.37390900 1.85881700 -0.00000100
- H -1.32120300 1.89646000 0.00001700
- H -2.21481100 -0.57553100 -0.00001700
- C -0.01709400 -1.21221200 0.00000500
- H -0.02661600 -1.87085300 -0.87789700
- H -0.02661900 -1.87083000 0.87792500

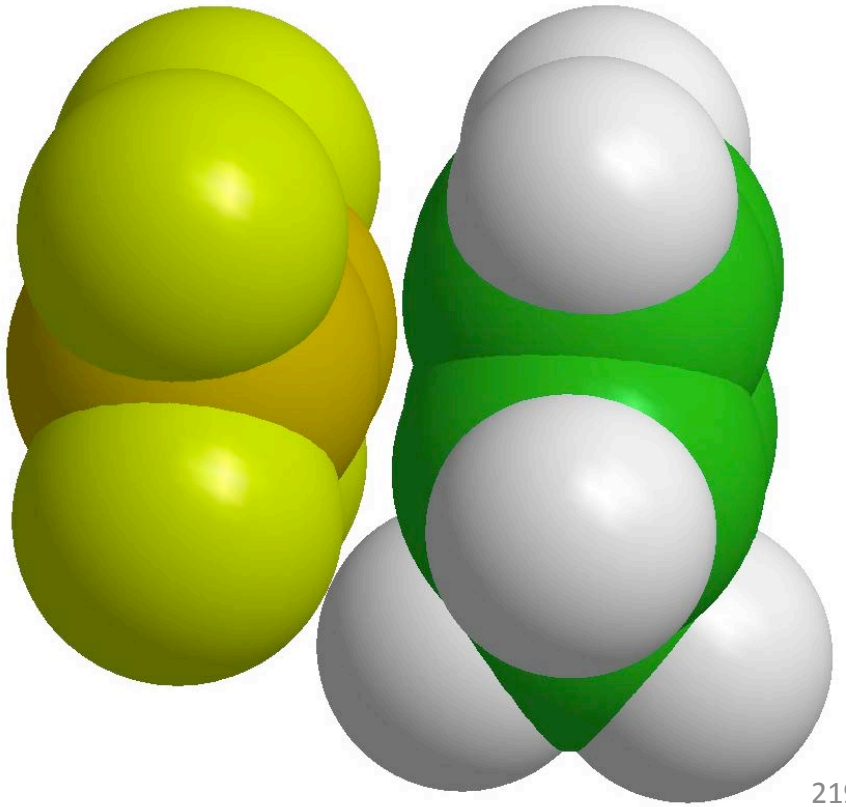


B_2F_4 Cyclopentadiene vdW ωB97X-D

- Zero-point correction= 0.113410 (Hartree/Particle)
- Thermal correction to Energy= 0.124326
- Thermal correction to Enthalpy= 0.125270
- Thermal correction to Gibbs Free Energy= 0.074810
- Sum of electronic and zero-point Energies= -643.279525
- Sum of electronic and thermal Energies= -643.268610
- Sum of electronic and thermal Enthalpies= -643.267666
- Sum of electronic and thermal Free Energies= -643.318126

- B2F4CpVW

- 0 1
- C 1.60577200 -1.30837100 0.13917400
- H 1.51302900 -2.33595800 0.46156400
- B -1.40656300 -0.74871200 0.08324100
- C 1.43831200 -0.84012500 -1.10969700
- H 1.18172800 -1.42572100 -1.98261100
- B -1.21144100 0.95741900 0.10959700
- C 1.95452000 -0.17067800 1.05093400
- H 1.22860700 -0.05880000 1.86608300
- H 2.93193200 -0.31653500 1.52678200
- C 1.65442900 0.61214300 -1.11278700
- H 1.57517400 1.24346400 -1.98772000
- C 1.95305600 1.01479600 0.13340800
- H 2.15619000 2.02718300 0.45310000
- F -1.42642600 1.70233400 -0.96324300
- F -0.93884800 1.59973800 1.23807800
- F -1.33269200 -1.46613100 1.19762000
- F -1.76127500 -1.39413600 -1.01774000

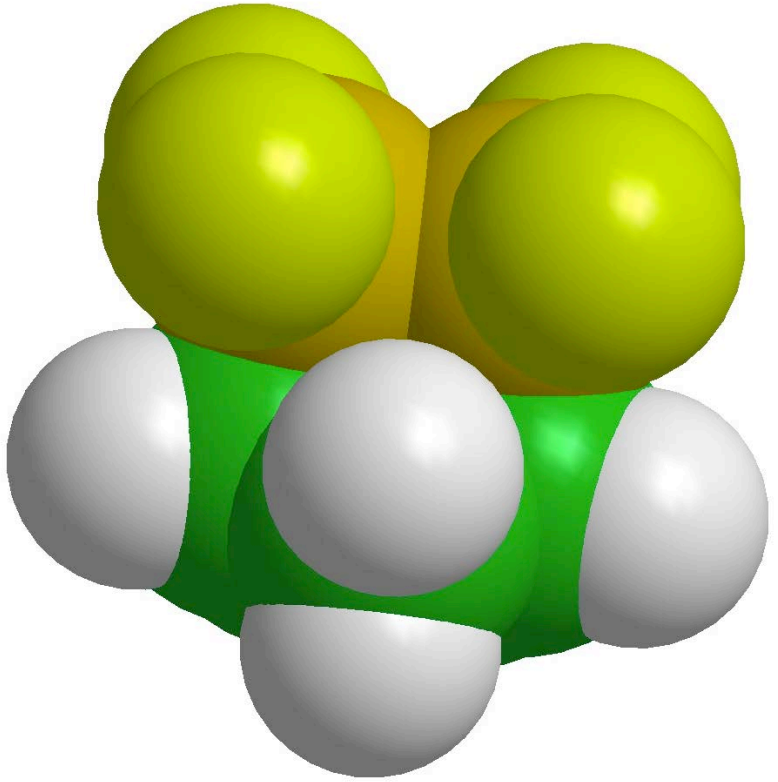


B_2F_4 Cyclopentadiene TS for 1,4 addition ωB97X-D

- Zero-point correction= 0.113237 (Hartree/Particle)
- Thermal correction to Energy= 0.123464
- Thermal correction to Enthalpy= 0.124408
- Thermal correction to Gibbs Free Energy= 0.077214
- Sum of electronic and zero-point Energies= -643.233727
- Sum of electronic and thermal Energies= -643.223500
- Sum of electronic and thermal Enthalpies= -643.222556
- Sum of electronic and thermal Free Energies= -643.269750

- B2F4W14TS

- 0 1
- C -1.80900500 -0.69544200 0.70501300
- C -1.80899900 0.69545800 0.70500300
- C -1.12946000 1.13849100 -0.44429000
- C -1.14456600 -0.00000800 -1.42866900
- C -1.12947300 -1.13849500 -0.44427500
- H -2.13249900 -1.32538500 1.52208000
- H -2.13248900 1.32541400 1.52206200
- H -0.33473400 -0.00001900 -2.15466500
- H -2.10558800 -0.00000600 -1.96217000
- B 0.73102700 -0.97118100 0.07991600
- B 0.73102300 0.97118300 0.07990800
- H -1.13131600 -2.18061400 -0.75104800
- H -1.13130900 2.18060600 -0.75107900
- F 0.96536400 1.47632200 1.30239300
- F 1.46723300 1.52409500 -0.90134100
- F 1.46722200 -1.52410400 -0.90133800
- F 0.96537000 -1.47631600 1.30240000

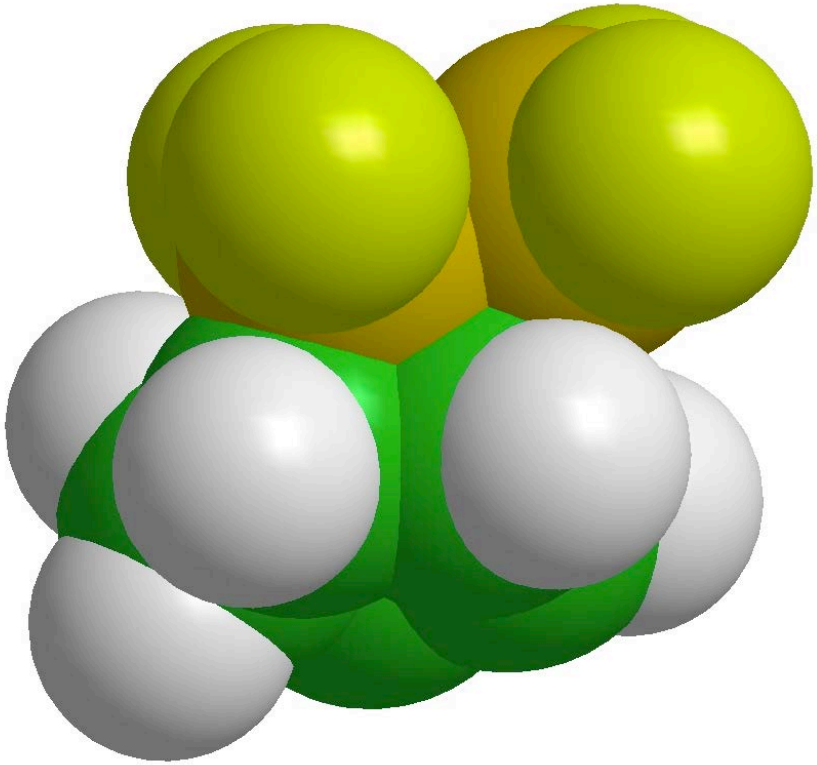


B_2F_4 Cyclopentadiene TS for 1,2 addition ωB97X-D

- Zero-point correction= 0.114140 (Hartree/Particle)
- Thermal correction to Energy= 0.124013
- Thermal correction to Enthalpy= 0.124957
- Thermal correction to Gibbs Free Energy= 0.078562
- Sum of electronic and zero-point Energies= -643.232977
- Sum of electronic and thermal Energies= -643.223104
- Sum of electronic and thermal Enthalpies= -643.222160
- Sum of electronic and thermal Free Energies= -643.268555

- BC2F4W12TS

- 0 1
- C 0.40410900 -0.36209500 -1.04984700
- H -0.26510400 -0.46018100 -1.89862400
- B -1.46600900 -0.47990800 0.06093000
- C 1.11918400 0.83639700 -0.75068900
- H 1.11327800 1.67217600 -1.43792200
- B -0.28665600 0.90964900 0.20234000
- C 2.36456500 0.44270600 0.01599900
- C 1.11418600 -1.49517700 -0.43844500
- C 2.21676700 -1.03839900 0.16682600
- H 2.91352000 -1.65135300 0.72476400
- H 0.75963000 -2.51558300 -0.45954700
- H 2.43132600 0.93204000 0.99447100
- H 3.27669400 0.69494400 -0.53626000
- F 0.06218600 0.87317700 1.55035400
- F -1.05682300 1.99202100 -0.21889800
- F -2.48326000 -0.44034200 -0.78956200
- F -1.49753400 -1.43833800 0.97296100

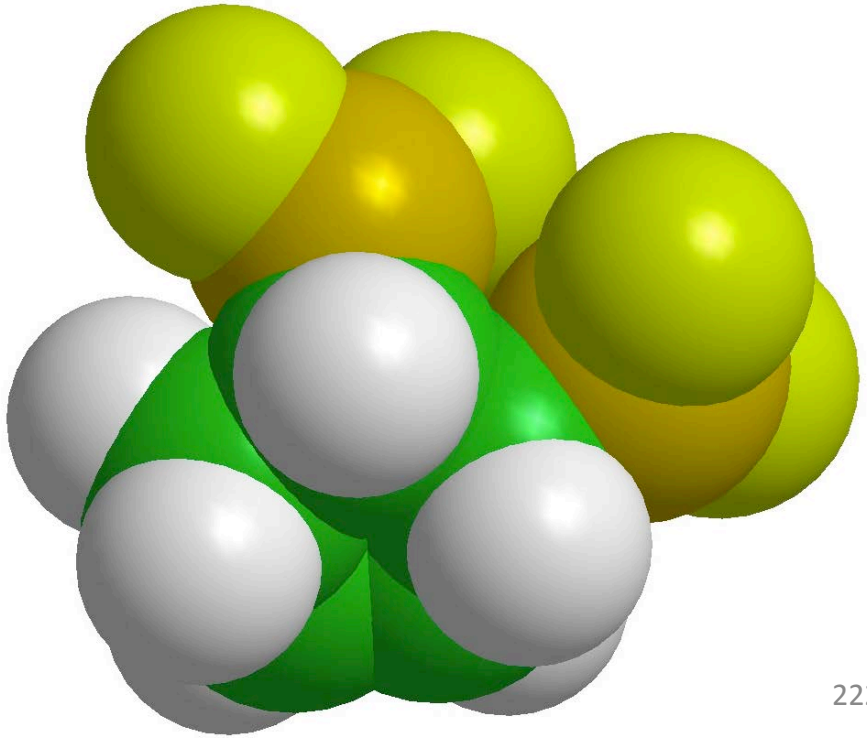


B_2F_4 Cyclopentadiene 1,2 addition product ωB97X-D

- Zero-point correction= 0.116915 (Hartree/Particle)
- Thermal correction to Energy= 0.127195
- Thermal correction to Enthalpy= 0.128139
- Thermal correction to Gibbs Free Energy= 0.079165
- Sum of electronic and zero-point Energies= -643.325817
- Sum of electronic and thermal Energies= -643.315537
- Sum of electronic and thermal Enthalpies= -643.314593
- Sum of electronic and thermal Free Energies= -643.363567

- B2F4Cp12WP

- 0 1
- C 0.45238100 0.86010400 -0.57094100
- C -0.83693800 0.01859500 -0.79802500
- C -1.99440400 1.00728100 -0.46857800
- C -1.33390500 1.97244900 0.48508800
- C -0.00926000 1.89516700 0.43100000
- H 0.69657600 1.38423900 -1.51232400
- H -0.91783500 -0.34392200 -1.82731500
- H -2.33412400 1.53367300 -1.36919200
- H -2.87342200 0.51238600 -0.04684400
- H -1.89342300 2.67011800 1.09624900
- H 0.67805100 2.51485900 0.99348100
- B -0.92652500 -1.21589900 0.16010300
- B 1.74925400 0.05265700 -0.23130400
- F 0.03622200 -1.50102900 1.03634500
- F -1.97224500 -2.02866900 0.16351900
- F 2.08563700 -1.01673100 -0.94665600
- F 2.61297400 0.43790600 0.69686800

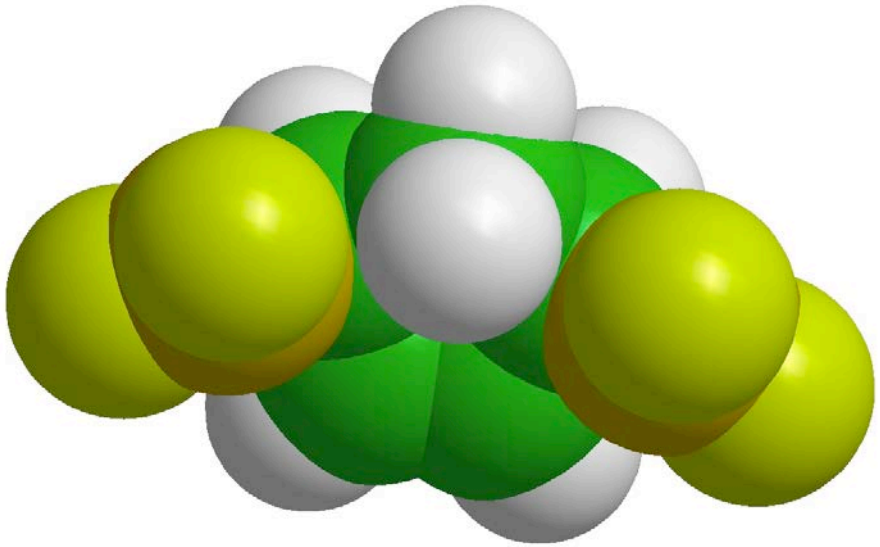


B_2F_4 Cyclopentadiene 1,4 addition product ωB97X-D

- Zero-point correction= 0.116805 (Hartree/Particle)
- Thermal correction to Energy= 0.127324
- Thermal correction to Enthalpy= 0.128268
- Thermal correction to Gibbs Free Energy= 0.076666
- Sum of electronic and zero-point Energies= -643.325533
- Sum of electronic and thermal Energies= -643.315014
- Sum of electronic and thermal Enthalpies= -643.314070
- Sum of electronic and thermal Free Energies= -643.365672

- B2F4Cp14WP

- 0 1
- C -0.66319300 1.54061100 0.21015200
- C 0.66334800 1.54058300 0.21009800
- C 1.23459100 0.40339100 -0.61793800
- C -0.00001500 -0.49060300 -0.88365800
- C -1.23455200 0.40345700 -0.61783600
- H -1.28619700 2.27829100 0.70154900
- H 1.28642300 2.27824400 0.70143400
- H 1.61604500 0.83827300 -1.55636700
- H -0.00007100 -0.91033200 -1.89047200
- H -0.00001300 -1.33500500 -0.19030400
- H -1.61601600 0.83837600 -1.55625400
- B 2.45663400 -0.29431400 0.06314600
- B -2.45665900 -0.29423600 0.06314100
- F -3.52463900 0.40514900 0.42881700
- F -2.49795100 -1.59561900 0.31299000
- F 2.49770100 -1.59561400 0.31346700
- F 3.52476500 0.40500400 0.42851300

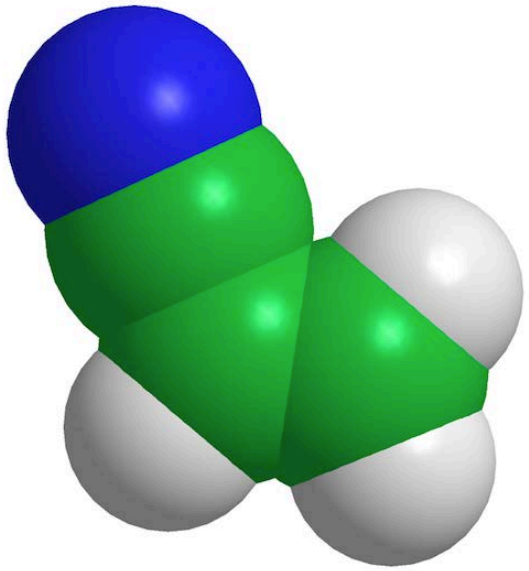


Acrylonitrile wB97x-D

- Zero-point correction= 0.051183 (Hartree/Particle)
- Thermal correction to Energy= 0.055309
- Thermal correction to Enthalpy= 0.056253
- Thermal correction to Gibbs Free Energy= 0.025326
- Sum of electronic and zero-point Energies= -170.757475
- Sum of electronic and thermal Energies= -170.753350
- Sum of electronic and thermal Enthalpies= -170.752405
- Sum of electronic and thermal Free Energies= -170.783333

- ANW

- 0 1
- C 1.31458000 -0.97474000 0.00000000
- H 2.01496400 -0.14793600 0.00000000
- H 1.71990600 -1.97911300 0.00000000
- C 0.00000000 -0.77589900 0.00000000
- H -0.70086000 -1.60331400 0.00000000
- C -0.58060100 0.53188800 0.00000000
- N -1.06255500 1.57755300 0.00000000

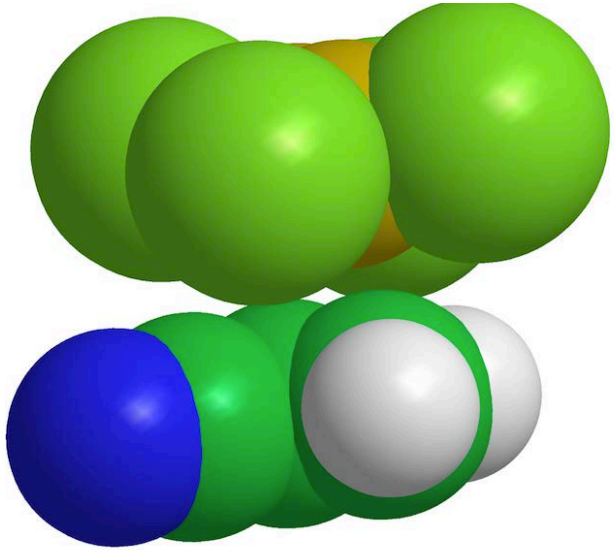


B2Cl4 AN vdW

- Zero-point correction= 0.065646 (Hartree/Particle)
- Thermal correction to Energy= 0.078772
- Thermal correction to Enthalpy= 0.079717
- Thermal correction to Gibbs Free Energy= 0.021079
- Sum of electronic and zero-point Energies= -2061.429863
- Sum of electronic and thermal Energies= -2061.416737
- Sum of electronic and thermal Enthalpies= -2061.415793
- Sum of electronic and thermal Free Energies= -2061.474430

- B2Cl4ANVW

- 0 1
- C -1.81817200 -0.32850400 1.57760200
- H -1.69599900 -1.39508000 1.73474000
- B 0.72426000 -0.91321800 -0.41757100
- Cl -0.27367800 -1.72410000 -1.60066700
- Cl 1.56548800 -1.89177300 0.77313500
- C -1.04057700 0.55925900 2.19597400
- H -0.26053500 0.23019300 2.87182100
- B 0.88707100 0.79799100 -0.42625500
- Cl -0.21597700 1.79897700 -1.33824300
- Cl 2.17422700 1.57709000 0.47571500
- H -1.16740000 1.62554200 2.04742200
- C -2.85951500 0.05639500 0.67578900
- N -3.69630900 0.35275600 -0.05715000



B2Cl4 AN TS1 wB97x-D

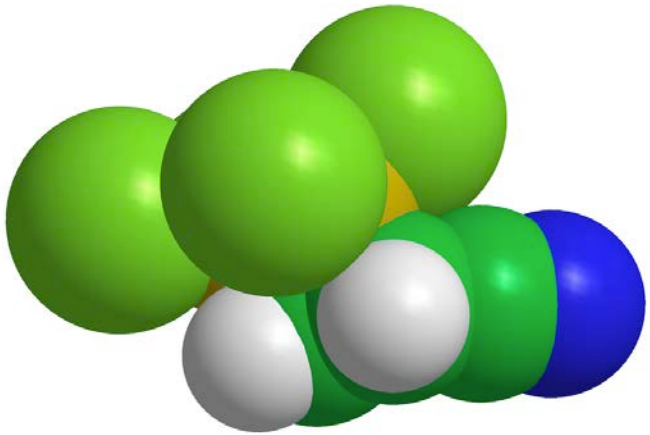
- **Zero-point correction= 0.066695 (Hartree/Particle)**
- **Thermal correction to Energy= 0.077710**
- **Thermal correction to Enthalpy= 0.078654**
- **Thermal correction to Gibbs Free Energy= 0.027724**
- **Sum of electronic and zero-point Energies= -2061.395566**
- **Sum of electronic and thermal Energies= -2061.384550**
- **Sum of electronic and thermal Enthalpies= -2061.383606**
- **Sum of electronic and thermal Free Energies= -2061.434536**

- **v=-306.5**

- **B2Cl4ANTSW1**

- **0 1**

C	**1.62908800**	**0.52458000**	**1.07650200**
H	**1.84836500**	**1.56902800**	**1.25400700**
C	**0.43202200**	**-0.02377100**	**1.56090500**
B	**-1.19395900**	**-0.43685100**	**0.11290300**
Cl	**-1.27179900**	**-2.16579300**	**-0.15574000**
Cl	**-2.68742700**	**0.39529700**	**0.46486700**
H	**0.38053500**	**-1.09098500**	**1.74450700**
H	**-0.24041300**	**0.61483700**	**2.12335200**
B	**0.31719800**	**0.52752100**	**-0.19295800**
Cl	**-0.11961300**	**2.29580300**	**-0.38484300**
Cl	**1.00062200**	**-0.28514100**	**-1.67616700**
C	**2.75930700**	**-0.31115700**	**0.80984700**
N	**3.68607500**	**-0.96670700**	**0.62527200**



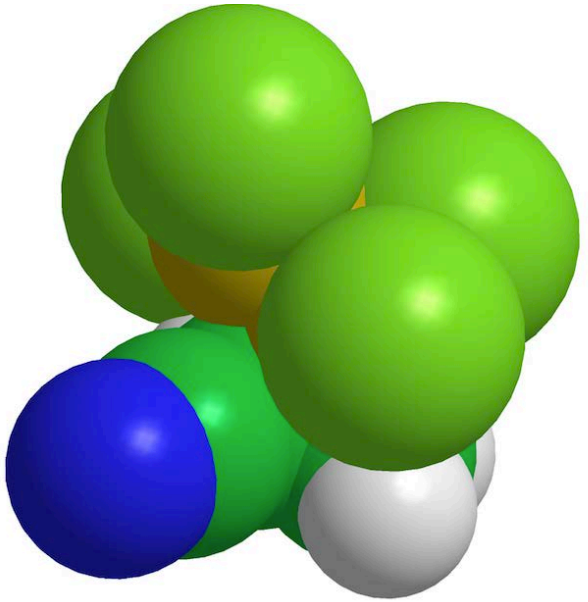
B2Cl4 AN TS2 wB97x-D

- Zero-point correction= 0.066468 (Hartree/Particle)
- Thermal correction to Energy= 0.077445
- Thermal correction to Enthalpy= 0.078389
- Thermal correction to Gibbs Free Energy= 0.027840
- Sum of electronic and zero-point Energies= -2061.389325
- Sum of electronic and thermal Energies= -2061.378348
- Sum of electronic and thermal Enthalpies= -2061.377404
- Sum of electronic and thermal Free Energies= -2061.427953

- v= –220 cm-1

- B2Cl4ANTSW2

- 0 1
- C 1.61016100 -0.29064000 1.62290600
- H 2.62108200 -0.54991600 1.34199800
- C 1.02361400 0.89324900 1.12662400
- B -0.90787600 0.27184600 -0.20667900
- Cl -2.01919300 1.24807900 0.76721200
- Cl -1.27065600 0.12774000 -1.90461700
- H 0.23904200 1.37182700 1.69867300
- B 0.53518200 -0.68099000 0.34823400
- Cl 1.52330500 -1.30900200 -1.04308800
- Cl -0.81035200 -1.81699000 0.97778700
- H 1.24605600 -0.65824700 2.57301500
- C 1.69544600 1.76190500 0.20013100
- N 2.22702800 2.49256100 -0.51049200

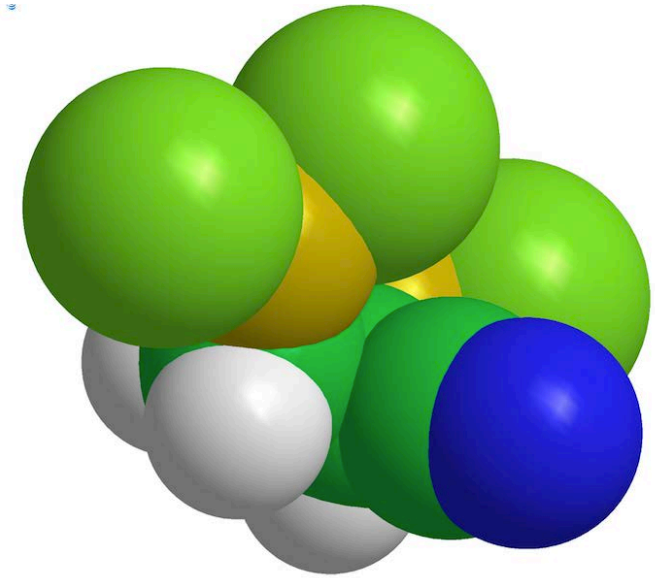


B2Cl4 AN product wB97x-D

- Zero-point correction= 0.068335 (Hartree/Particle)
- Thermal correction to Energy= 0.079635
- Thermal correction to Enthalpy= 0.080579
- Thermal correction to Gibbs Free Energy= 0.027957
- Sum of electronic and zero-point Energies= -2061.486376
- Sum of electronic and thermal Energies= -2061.475077
- Sum of electronic and thermal Enthalpies= -2061.474132
- Sum of electronic and thermal Free Energies= -2061.526754

- B2Cl4ANPW

- 0 1
- C -0.58615700 0.60628600 -1.13583000
- H -1.05190400 0.59454000 -2.13418700
- B -1.53601000 -0.35349800 -0.29514300
- Cl -2.81779300 0.25309700 0.71522700
- Cl -1.38961600 -2.08934300 -0.53009600
- C 0.87640400 0.12743200 -1.30005200
- H 1.40840700 0.79737300 -1.98285600
- B 1.72746800 -0.03643800 0.00829900
- Cl 0.98901200 -0.03374800 1.60151500
- Cl 3.45803200 -0.28367500 -0.11183000
- C -0.62307900 1.99588000 -0.68733900
- N -0.61051300 3.09182400 -0.34045300
- H 0.88299700 -0.85021400 -1.79813100

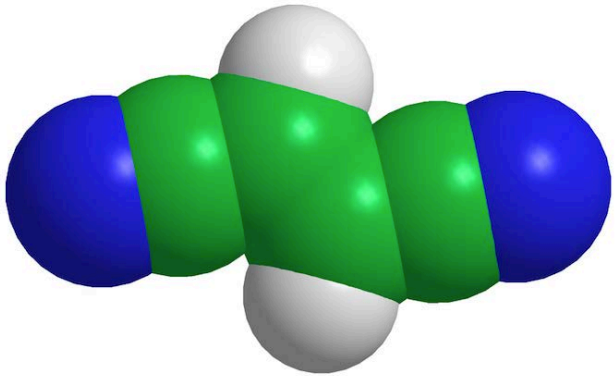


(E)-dicyanoethene

- Zero-point correction= 0.050205 (Hartree/Particle)
- Thermal correction to Energy= 0.055930
- Thermal correction to Enthalpy= 0.056875
- Thermal correction to Gibbs Free Energy= 0.021833
- Sum of electronic and zero-point Energies= -262.981042
- Sum of electronic and thermal Energies= -262.975317
- Sum of electronic and thermal Enthalpies= -262.974373
- Sum of electronic and thermal Free Energies= -263.009415

- DCW

- 0 1
- C -0.33543700 0.57765600 0.00000000
- H -1.41925800 0.60205700 0.00000000
- C 0.33543700 -0.57765600 0.00000000
- H 1.41925800 -0.60205700 0.00000000
- C -0.33543700 -1.83641800 0.00000000
- N -0.86238500 -2.85978800 0.00000000
- C 0.33543700 1.83641800 0.00000000
- N 0.86238500 2.85978800 0.00000000

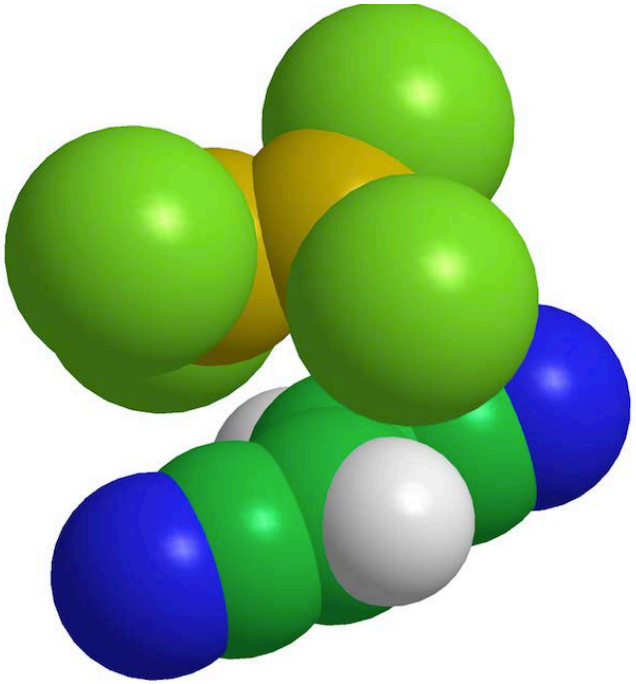


B2Cl4 DCE vdW wB97x-D

- Zero-point correction= 0.064173 (Hartree/Particle)
- Thermal correction to Energy= 0.077512
- Thermal correction to Enthalpy= 0.078457
- Thermal correction to Gibbs Free Energy= 0.018849
- Sum of electronic and zero-point Energies= -2153.653677
- Sum of electronic and thermal Energies= -2153.640337
- Sum of electronic and thermal Enthalpies= -2153.639393
- Sum of electronic and thermal Free Energies= -2153.699001

- B2Cl4DCVW

- 0 1
- C -2.48003000 -0.36436900 -0.56396500
- B 1.24061700 -0.78224200 0.32653500
- Cl 2.02877700 -2.08255600 -0.53101500
- Cl 0.49656900 -1.11570400 1.88009400
- C -2.48136200 0.35221300 0.56416900
- H -2.47913200 -0.12384000 1.53767800
- B 1.23572000 0.78835100 -0.32658200
- Cl 0.49033100 1.11706000 -1.88050000
- Cl 2.01549500 2.09349800 0.53129000
- H -2.48127400 0.11171200 -1.53746600
- C -2.45737800 1.77802900 0.54547600
- N -2.41795900 2.92853900 0.54739300
- C -2.44850500 -1.79003600 -0.54533500
- N -2.40312200 -2.94032500 -0.54736600



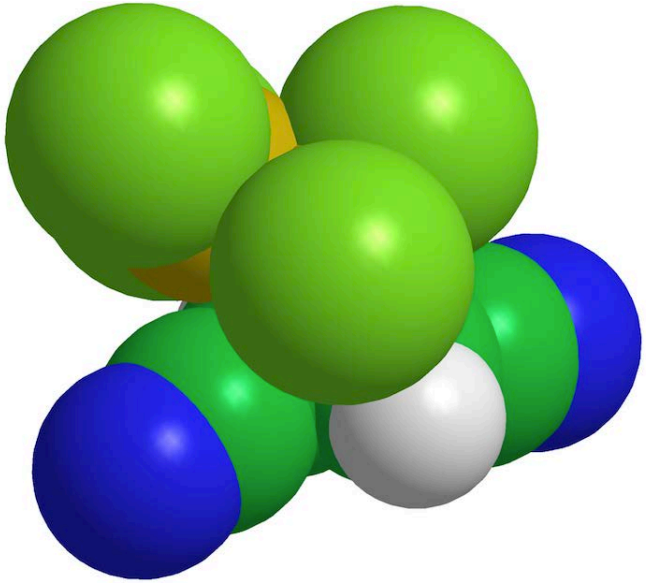
B2Cl4 DCE TS wB97x-D

- Zero-point correction= 0.064934 (Hartree/Particle)
- Thermal correction to Energy= 0.077827
- Thermal correction to Enthalpy= 0.078771
- Thermal correction to Gibbs Free Energy= 0.023548
- Sum of electronic and zero-point Energies= -2153.604812
- Sum of electronic and thermal Energies= -2153.591919
- Sum of electronic and thermal Enthalpies= -2153.590975
- Sum of electronic and thermal Free Energies= -2153.646198

- v = -231 cm-1

- B2Cl4ANTSW1

- 0 1
- C 1.83612200 -0.77971200 -0.31111500
- H 2.08280900 -1.73035500 0.14282700
- C 0.72386000 -0.68041100 -1.16493600
- B -1.14532300 0.55341100 -0.17369100
- Cl -1.20395800 1.74261100 -1.46666000
- Cl -2.63276200 0.11663700 0.60434400
- H 0.68750500 0.14418100 -1.86731800
- B 0.34305800 -0.16502500 0.56533900
- Cl -0.02697100 -1.50004000 1.74078900
- Cl 0.74070000 1.47953600 1.28816400
- C 2.90053300 0.16798100 -0.40843100
- N 3.77705600 0.90857700 -0.48522000
- C -0.04476000 -1.83441800 -1.53662100
- N -0.65743700 -2.74501100 -1.87763100

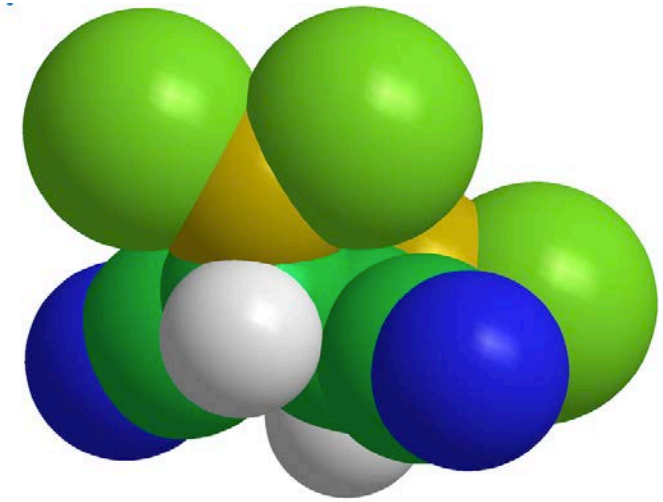


B2Cl4 DCE product wB97x-D

- Zero-point correction= 0.067097 (Hartree/Particle)
- Thermal correction to Energy= 0.080138
- Thermal correction to Enthalpy= 0.081082
- Thermal correction to Gibbs Free Energy= 0.024125
- Sum of electronic and zero-point Energies= -2153.700359
- Sum of electronic and thermal Energies= -2153.687318
- Sum of electronic and thermal Enthalpies= -2153.686374
- Sum of electronic and thermal Free Energies= -2153.743331

- B2Cl4DCPW

- 0 1
- C -0.78141800 -0.00184500 1.11743700
- H -1.10844300 0.66855000 1.92750000
- B -1.48886600 0.61652500 -0.17389000
- Cl -3.15715200 0.26338300 -0.51521200
- Cl -0.61948500 1.74587900 -1.18639500
- C 0.78139500 0.00183500 1.11745800
- H 1.10839500 -0.66856900 1.92752700
- B 1.48887600 -0.61654300 -0.17384700
- Cl 0.61954000 -1.74594800 -1.18633100
- Cl 3.15713200 -0.26329100 -0.51522400
- C -1.29132000 -1.32350300 1.46932100
- N -1.66271700 -2.37042500 1.76395200
- C 1.29128500 1.32349800 1.46934900
- N 1.66268400 2.37039900 1.76405100



B2Cl4 in solvent 1=heptane, 2=THF, 3=MeCN

- Zero-point correction= 0.013200 (Hartree/Particle)
- Thermal correction to Energy= 0.020424
- Thermal correction to Enthalpy= 0.021369
- Thermal correction to Gibbs Free Energy= -0.021499
- Sum of electronic and zero-point Energies= -1890.669315
- Sum of electronic and thermal Energies= -1890.662091
- Sum of electronic and thermal Enthalpies= -1890.661146
- Sum of electronic and thermal Free Energies= -1890.704014

- B2Cl41

- 0 1
- B 0.00000000 0.00000000 0.84578800
- B 0.00000000 0.00000000 -0.84578800
- Cl -1.51174200 -0.00018100 -1.72960200
- Cl 1.51174200 0.00018100 -1.72960200
- Cl 0.00000000 -1.51174200 1.72960200
- Cl 0.00000000 1.51174200 1.72960200

- Zero-point correction= 0.013083 (Hartree/Particle)
- Thermal correction to Energy= 0.020330
- Thermal correction to Enthalpy= 0.021274
- Thermal correction to Gibbs Free Energy= -0.021737
- Sum of electronic and zero-point Energies= -1890.670316
- Sum of electronic and thermal Energies= -1890.663069
- Sum of electronic and thermal Enthalpies= -1890.662125
- Sum of electronic and thermal Free Energies= -1890.705136

- B2Cl42

- 0 1
- B 0.00000000 0.00000000 0.84586100
- B 0.00000000 0.00000000 -0.84586100
- Cl 0.00000000 -1.51148900 -1.73145700
- Cl 0.00000000 1.51148900 -1.73145700
- Cl 1.51148900 -0.00024300 1.73145700
- Cl -1.51148900 0.00024300 1.73145700

- Zero-point correction= 0.013045 (Hartree/Particle)
- Thermal correction to Energy= 0.020296
- Thermal correction to Enthalpy= 0.021240
- Thermal correction to Gibbs Free Energy= -0.021759
- Sum of electronic and zero-point Energies= -1890.670706
- Sum of electronic and thermal Energies= -1890.663454
- Sum of electronic and thermal Enthalpies= -1890.662510
- Sum of electronic and thermal Free Energies= -1890.705509

- B2Cl43

- 0 1
- B 0.00000000 0.00000000 0.84586900
- B 0.00000000 0.00000000 -0.84586900
- Cl 0.00000000 -1.51132800 -1.73225800
- Cl 0.00000000 1.51132800 -1.73225800
- Cl 1.51132700 -0.00022800 1.73225800
- Cl -1.51132700 0.00022800 1.73225800

(E)-butene in solvent 1=heptane, 2=THF, 3=MeCN

1

- Zero-point correction= 0.108144 (Hartree/Particle)
- Thermal correction to Energy= 0.113674
- Thermal correction to Enthalpy= 0.114618
- Thermal correction to Gibbs Free Energy= 0.080651
- Sum of electronic and zero-point Energies= -157.105271
- Sum of electronic and thermal Energies= -157.099742
- Sum of electronic and thermal Enthalpies= -157.098797
- Sum of electronic and thermal Free Energies= -157.132764

EBW1

0 1

C	1.95639200	-0.07902400	0.00002500
H	2.01406500	-1.17032400	-0.00003100
H	2.49365600	0.29075200	0.87942300
H	2.49370500	0.29084500	-0.87930400
C	0.53435300	0.39455200	0.00001100
H	0.38618500	1.47447200	0.00002400
C	-0.53435300	-0.39455200	-0.00001400
H	-0.38618500	-1.47447200	-0.00003000
C	-1.95639300	0.07902400	-0.00002200
H	-2.49367900	-0.29080800	-0.87938300
H	-2.49368200	-0.29078900	0.87934400
H	-2.01406500	1.17032400	-0.00003400

2

- Zero-point correction= 0.108030 (Hartree/Particle)
- Thermal correction to Energy= 0.113559
- Thermal correction to Enthalpy= 0.114503
- Thermal correction to Gibbs Free Energy= 0.080542
- Sum of electronic and zero-point Energies= -157.105997
- Sum of electronic and thermal Energies= -157.100468
- Sum of electronic and thermal Enthalpies= -157.099524
- Sum of electronic and thermal Free Energies= -157.133485

EBW2

0 1

C	1.95702900	-0.07928500	0.00002500
H	2.01492700	-1.17068700	-0.00003100
H	2.49438900	0.29117400	0.87905400
H	2.49443700	0.29126700	-0.87893500
C	0.53473600	0.39464100	0.00001100
H	0.38704900	1.47476000	0.00002400
C	-0.53473600	-0.39464100	-0.00001500
H	-0.38704900	-1.47476000	-0.00003000
C	-1.95702900	0.07928500	-0.00002200
H	-2.49441100	-0.29123000	-0.87901400
H	-2.49441400	-0.29121100	0.87897500
H	-2.01492700	1.17068700	-0.00003400

3

- Zero-point correction= 0.107986 (Hartree/Particle)
- Thermal correction to Energy= 0.113514
- Thermal correction to Enthalpy= 0.114458
- Thermal correction to Gibbs Free Energy= 0.080498
- Sum of electronic and zero-point Energies= -157.106280
- Sum of electronic and thermal Energies= -157.100751
- Sum of electronic and thermal Enthalpies= -157.099807
- Sum of electronic and thermal Free Energies= -157.133768

EBW3

0 1

C	1.95727600	-0.07939400	0.00002500
H	2.01527500	-1.17083900	-0.00003100
H	2.49469000	0.29134700	0.87889000
H	2.49473900	0.29144000	-0.87877200
C	0.53488900	0.39468000	0.00001100
H	0.38741400	1.47487900	0.00002400
C	-0.53488900	-0.39468000	-0.00001500
H	-0.38741400	-1.47487900	-0.00003000
C	-1.95727600	0.07939400	-0.00002300
H	-2.49471300	-0.29140300	-0.87885000
H	-2.49471600	-0.29138400	0.87881200
H	-2.01527500	1.17083900	-0.00003300

E-butene B2Cl4 vdW / solvent 1-3

- Zero-point correction= 0.123920 (Hartree/Particle)
- Thermal correction to Energy= 0.137703
- Thermal correction to Enthalpy= 0.138647
- Thermal correction to Gibbs Free Energy= 0.080799
- Sum of electronic and zero-point Energies= -2047.782812
- Sum of electronic and thermal Energies= -2047.769029
- Sum of electronic and thermal Enthalpies= -2047.768084
- Sum of electronic and thermal Free Energies= -2047.825933

- EBNVW1

- 0 1
- C 0.52036600 2.26292600 -0.42140300
- C -0.51630900 2.26364200 0.41954300
- H -0.31645000 2.26539900 1.49092200
- C -1.95441200 2.36274200 0.01078200
- H -2.07093200 2.29049100 -1.07252300
- H -2.56843300 1.58785100 0.47908300
- H -2.36630500 3.32431600 0.33396200
- B -0.85572800 -0.90471200 -0.03590600
- Cl -1.70082400 -0.81995700 -1.57038200
- Cl -1.81418600 -1.10005600 1.42226300
- C 1.95857700 2.36018200 -0.01258100
- H 2.37175500 3.32115700 -0.33590600
- H 2.07491700 2.28793500 1.07074500
- H 2.57166400 1.58442900 -0.48067600
- H 0.32052400 2.26483400 -1.49278400
- B 0.85410100 -0.90600900 0.03663700
- Cl 1.81216200 -1.10466400 -1.42133800
- Cl 1.69944000 -0.82060300 1.57095500

- Zero-point correction= 0.123708 (Hartree/Particle)
- Thermal correction to Energy= 0.137504
- Thermal correction to Enthalpy= 0.138448
- Thermal correction to Gibbs Free Energy= 0.080620
- Sum of electronic and zero-point Energies= -2047.784155
- Sum of electronic and thermal Energies= -2047.770359
- Sum of electronic and thermal Enthalpies= -2047.769415
- Sum of electronic and thermal Free Energies= -2047.827243

- EBNVW2

- 0 1
- C 0.52265500 2.25762000 -0.41996200
- C -0.51695300 2.25850600 0.41812500
- H -0.32078500 2.26044400 1.49016800
- C -1.95350400 2.36062500 0.00435200
- H -2.06661200 2.28804400 -1.07933800
- H -2.57069400 1.58804700 0.47236000
- H -2.36411500 3.32318600 0.32613400
- B -0.85583300 -0.90267200 -0.03333000
- Cl -1.70611400 -0.82449000 -1.56617200
- Cl -1.81171200 -1.09160400 1.42815700
- C 1.95937500 2.35701100 -0.00615000
- H 2.37184700 3.31863300 -0.32838200
- H 2.07224900 2.28479600 1.07759800
- H 2.57525200 1.58308100 -0.47364600
- H 0.32652100 2.26021700 -1.49201200
- B 0.85357200 -0.90428600 0.03400800
- Cl 1.80897200 -1.09735300 -1.42723100
- Cl 1.70404200 -0.82621400 1.56674800

- Zero-point correction= 0.123574 (Hartree/Particle)
- Thermal correction to Energy= 0.137396
- Thermal correction to Enthalpy= 0.138340
- Thermal correction to Gibbs Free Energy= 0.080448
- Sum of electronic and zero-point Energies= -2047.784722
- Sum of electronic and thermal Energies= -2047.770900
- Sum of electronic and thermal Enthalpies= -2047.769956
- Sum of electronic and thermal Free Energies= -2047.827849

- EBNVW3

- 0 1
- C 0.52311200 2.25616400 -0.42022200
- C -0.51607000 2.25731400 0.41866600
- H -0.31944200 2.25929500 1.49061100
- C -1.95279000 2.36046700 0.00552800
- H -2.06641400 2.28798000 -1.07812900
- H -2.57036000 1.58869200 0.47438600
- H -2.36241000 3.32330300 0.32778100
- B -0.85592000 -0.90182000 -0.03371200
- Cl -1.70619500 -0.82289600 -1.56689300
- Cl -1.81288500 -1.09168600 1.42725900
- C 1.96006400 2.35580200 -0.00705600
- H 2.37211800 3.31745200 -0.32975600
- H 2.07343200 2.28356300 1.07665100
- H 2.57580500 1.58230000 -0.47546700
- H 0.32650500 2.25886900 -1.49216900
- B 0.85311600 -0.90404100 0.03432800
- Cl 1.80947400 -1.09799400 -1.42649700
- Cl 1.70365800 -0.82569700 1.56739600

E-butene B2Cl4 TS /solvent 1-3

- Zero-point correction= 0.124654 (Hartree/ Particle)
- Thermal correction to Energy= 0.136723
- Thermal correction to Enthalpy= 0.137667
- Thermal correction to Gibbs Free Energy= 0.085511
- Sum of electronic and zero-point Energies= -2047.758871
- Sum of electronic and thermal Energies= -2047.746803
- Sum of electronic and thermal Enthalpies= -2047.745859
- Sum of electronic and thermal Free Energies= -2047.798014
-
- v= -356.3 cm-1
- B2Cl4EBTSW1
- 0 1

C	1.83477000	0.03954100	0.84581400
H	2.33826200	0.98134800	1.04385600
C	0.54924100	-0.09951300	1.47762000
B	-1.03373300	-0.27459900	0.03586400
C	2.75053400	-1.16071500	0.74133300
H	3.44120300	-1.04592700	-0.09594100
H	2.19145700	-2.08581200	0.58649600
H	3.33750300	-1.26397100	1.65799200
Cl	-1.57917200	-1.94968000	0.20308400
Cl	-2.30254900	0.91125200	-0.18155200
H	0.27021100	-1.12061900	1.71742600
B	0.70774900	0.28277500	-0.33585900
Cl	0.66806100	2.05366000	-0.83395800
Cl	0.84893300	-0.87900400	-1.76794700
C	-0.02258900	0.96871600	2.36964700
H	0.53858400	0.91132000	3.30767100
H	0.11935700	1.96409000	1.94862000
H	-1.07803900	0.81467000	2.59371000

- Zero-point correction= 0.124475 (Hartree/ Particle)
- Thermal correction to Energy= 0.136562
- Thermal correction to Enthalpy= 0.137506
- Thermal correction to Gibbs Free Energy= 0.085427
- Sum of electronic and zero-point Energies= -2047.762964
- Sum of electronic and thermal Energies= -2047.750876
- Sum of electronic and thermal Enthalpies= -2047.749932
- Sum of electronic and thermal Free Energies= -2047.802012
- v= –378.6 cm-1
- B2Cl4EBTSW2
- 0 1

C	1.80119200	0.11336700	0.88330700
H	2.27881700	1.07197300	1.06466400
C	0.49766900	-0.02373800	1.48883100
B	-1.03187900	-0.28738700	0.04754500
C	2.74524700	-1.07000600	0.87787400
H	3.47474300	-0.97535900	0.07148700
H	2.21321900	-2.01331100	0.74006100
H	3.28689500	-1.11832200	1.82594700
Cl	-1.55505900	-1.96817800	0.20862000
Cl	-2.31471700	0.87781500	-0.20962700
H	0.23625600	-1.03846800	1.77413800
B	0.71925800	0.27020700	-0.34015400
Cl	0.64696200	2.01485400	-0.93801000
Cl	0.93532500	-0.95079800	-1.71433100
C	-0.10447200	1.07563300	2.32099200
H	0.45748000	1.07295700	3.26017400
H	0.02090800	2.05285900	1.85476200
H	-1.15570400	0.90924300	2.55271100

- Zero-point correction= 0.124450 (Hartree/ Particle)
- Thermal correction to Energy= 0.136521
- Thermal correction to Enthalpy= 0.137465
- Thermal correction to Gibbs Free Energy= 0.085511
- Sum of electronic and zero-point Energies= -2047.764619
- Sum of electronic and thermal Energies= -2047.752549
- Sum of electronic and thermal Enthalpies= -2047.751604
- Sum of electronic and thermal Free Energies= -2047.803558
- B2Cl4EBTSW3
- 0 1

C	1.79053800	0.13579800	0.89321800
H	2.26056700	1.09909500	1.06989000
C	0.48136300	-0.00001000	1.49141800
B	-1.03139800	-0.29125800	0.05326500
C	2.74224700	-1.04138300	0.91954200
H	3.48280300	-0.95380200	0.12239300
H	2.21806300	-1.99015600	0.79011600
H	3.27002100	-1.07073400	1.87594300
Cl	-1.54869800	-1.97323800	0.21154800
Cl	-2.31761700	0.86838500	-0.21792800
H	0.22464200	-1.01181000	1.79188400
B	0.72353300	0.26578800	-0.34086500
Cl	0.64185900	2.00074400	-0.97143200
Cl	0.96066000	-0.97306400	-1.69701400
C	-0.12801600	1.10948100	2.30452400
H	0.43241800	1.11951600	3.24456800
H	-0.00258200	2.08091500	1.82639600
H	-1.17885100	0.94294500	2.53662600

E-Butene B2Cl4 product / solvent 1-3

- Zero-point correction= 0.126141 (Hartree/ Particle)
- Thermal correction to Energy= 0.138508
- Thermal correction to Enthalpy= 0.139452
- Thermal correction to Gibbs Free Energy= 0.085027
- Sum of electronic and zero-point Energies= -2047.828793
- Sum of electronic and thermal Energies= -2047.816425
- Sum of electronic and thermal Enthalpies= -2047.815481
- Sum of electronic and thermal Free Energies= -2047.869906

- B2Cl4EPW1

- 0 1
- C 0.77767200 0.06553400 1.28565700
- H 1.13609700 -0.68800900 2.01008800
- B 1.49273900 -0.42042400 -0.02578900
- Cl 3.09073400 0.15356800 -0.48998300
- Cl 0.78041800 -1.66986300 -1.05873100
- C -1.25915000 -1.41687500 1.82219700
- H -0.97415900 -2.23319200 1.15524500
- H -2.34366200 -1.44334400 1.93749300
- H -0.81383700 -1.60935500 2.80194000
- C 1.25926200 1.42536800 1.81567000
- H 2.34372700 1.45222500 1.93128400
- H 0.81355400 1.62249400 2.79430700
- H 0.97467900 2.23857700 1.14476800
- C -0.77755000 -0.05948600 1.28599600
- H -1.13594700 0.69736400 2.00699100
- B -1.49273500 0.42038300 -0.02761700
- Cl -0.78068200 1.66514800 -1.06635700
- Cl -3.09058000 -0.15613500 -0.48917700

- Zero-point correction= 0.125958 (Hartree/ Particle)
- Thermal correction to Energy= 0.138343
- Thermal correction to Enthalpy= 0.139288
- Thermal correction to Gibbs Free Energy= 0.084715
- Sum of electronic and zero-point Energies= -2047.830606
- Sum of electronic and thermal Energies= -2047.818220
- Sum of electronic and thermal Enthalpies= -2047.817276
- Sum of electronic and thermal Free Energies= -2047.871848

- B2Cl4EPW2

- 0 1
- C 0.77722600 0.05474200 1.28571400
- H 1.13744900 -0.70468300 2.00297600
- B 1.49454200 -0.41913000 -0.02607400
- Cl 3.09377100 0.16161000 -0.48660500
- Cl 0.78661200 -1.65858200 -1.07705100
- C -1.25619400 -1.43810600 1.80710800
- H -0.97071100 -2.24731700 1.13159300
- H -2.34041000 -1.46616100 1.92508400
- H -0.80820400 -1.63873700 2.78365600
- C 1.25583300 1.41029500 1.82945500
- H 2.33998400 1.43631600 1.94848300
- H 0.80732400 1.59595100 2.80871500
- H 0.97092500 2.22989700 1.16636300
- C -0.77757100 -0.07423400 1.28457400
- H -1.13798500 0.67401300 2.01338100
- B -1.49462300 0.41961900 -0.01999000
- Cl -0.78571000 1.67370400 -1.05278000
- Cl -3.09430400 -0.15308000 -0.48892000

- Zero-point correction= 0.125903 (Hartree/ Particle)
- Thermal correction to Energy= 0.138291
- Thermal correction to Enthalpy= 0.139236
- Thermal correction to Gibbs Free Energy= 0.084655
- Sum of electronic and zero-point Energies= -2047.831345
- Sum of electronic and thermal Energies= -2047.818956
- Sum of electronic and thermal Enthalpies= -2047.818012
- Sum of electronic and thermal Free Energies= -2047.872593

- B2Cl4EPW3

- 0 1
- C 0.77759600 0.06180800 1.28595300
- H 1.13719800 -0.69430000 2.00690800
- B 1.49387100 -0.42058800 -0.02211100
- Cl 3.09223000 0.15859700 -0.49090300
- Cl 0.78531300 -1.66679500 -1.06612800
- C -1.25750000 -1.42482700 1.81860500
- H -0.97231700 -2.23958300 1.14953500
- H -2.34175000 -1.45025200 1.93721500
- H -0.80942100 -1.61789300 2.79649300
- C 1.25797200 1.41951900 1.82250000
- H 2.34222000 1.44415100 1.94134200
- H 0.80982000 1.61019500 2.80083200
- H 0.97332100 2.23629600 1.15565300
- C -0.77746200 -0.06551500 1.28579800
- H -1.13706800 0.68858900 2.00886200
- B -1.49386900 0.42061500 -0.02078600
- Cl -0.78564100 1.67004900 -1.06119900
- Cl -3.09223500 -0.15733700 -0.49115200