Supplementary Information (SI)

A reinvestigation of the boron cluster $B_{15}^{+/0/-}$: A benchmark of density functionals and consideration of aromaticity models

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Tables of supplementary information (SI)

Table S1. The T1 diagnostic of CCSD(T)/aug-cc-pVTZ single point of $B_{15}^{+/0/-}$.

Isomer	T1	Isomer	T1	Isomer	T1	Isomer	T1
1a	0.036	**2a**	0.023	**3a**	0.018	**4a**	0.023
5a	0.020	**6a**	0.023	**7a**	0.032	**8a**	0.024
1n	0.045	**2n**	0.029	**3n**	0.031	**4n**	0.021
1c	0.020	**2c**	0.022	**3c**	0.021	**4c**	0.020

Table S2. Relative energies (kcal/mol) of $\Delta E_{\mathbf{3a-2a}}$, $\Delta E_{\mathbf{7a-2a}}$ and $\Delta E_{\mathbf{4a-2a}}$ and their errors $\Delta\Delta E_{\mathbf{3a-2a}}$, $\Delta\Delta E_{\mathbf{7a-2a}}$ and $\Delta\Delta E_{\mathbf{4a-2a}}$ of B_{15}^{-}. The MAE is in the last column.

	$\Delta E_{\mathbf{3a-2a}}$	$\Delta E_{\mathbf{7a-2a}}$	$\Delta E_{\mathbf{4a-2a}}$	$\Delta\Delta E_{\mathbf{3a-2a}}$	$\Delta\Delta E_{\mathbf{7a-2a}}$	$\Delta\Delta E_{\mathbf{4a-2a}}$	**MAE**
CCSD(T)[c]	2.4	6.3	5.5	-	-	-	-
B3LYP[a]	-1.19	0.83	12.95	-3.59	-5.47	7.45	5.50
B3LYP[b]	-1.71	0.30	12.10	-4.11	-6.00	6.60	5.57
M06[a]	5.78	5.56	11.57	3.38	-0.74	6.07	3.40
M06[b]	5.34	5.56	10.47	2.94	-0.74	4.97	2.88
VSXC[a]	1.16	1.65	10.56	-1.24	-4.65	5.06	3.65
VSXC[b]	0.51	1.21	9.72	-1.89	-5.09	4.22	3.73
B1B95[a]	4.04	6.10	3.87	1.64	-0.20	-1.63	1.16
B1B95[b]	3.69	5.71	3.19	1.29	-0.59	-2.31	1.40
BPBE[a]	0.55	1.41	9.30	-1.85	-4.89	3.80	3.51
BPBE[b]	0.15	1.02	8.46	-2.25	-5.28	2.96	3.50
TPSSh[a]	0.25	1.44	5.16	-2.15	-4.86	-0.34	2.45
TPSSh[b]	-0.29	1.02	4.36	-2.69	-5.28	-1.14	3.04
PBE[a]	1.50	2.26	9.04	-0.90	-4.04	3.54	2.83
PBE[b]	1.02	1.83	8.24	-1.38	-4.47	2.74	2.86
PBE0[a]	4.02	2.61	7.83	1.62	-3.69	2.33	2.55
PBE0[b]	3.55	2.22	7.00	1.15	-4.08	1.50	2.24
HSE06[a]	3.40	2.18	8.41	1.00	-4.12	2.91	2.68
HSE06[b]	2.96	1.81	7.55	0.56	-4.49	2.05	2.37
B2PLYPD3[a]	2.44	4.59	2.44	0.04	-1.71	-3.06	1.60
B2PLYPD3[b]	3.07	4.52	2.52	0.67	-1.78	-2.98	1.81

[a)] The DFT functional in conjunction with the 6-311+G(d) basis set, [b)] The DFT functional in conjunction with the def2-TZVPP basis set, [c)] The singlet-point CCSD(T)/aug-cc-pVTZ references values.

Table S3. Relative energies (kcal/mol) of ΔE_{2n-1n}, ΔE_{3n-1n} and ΔE_{4n-1n} and their errors $\Delta\Delta E_{2n-1n}$, $\Delta\Delta E_{3n-1n}$ and $\Delta\Delta E_{4n-1n}$ of B_{15}. The MAE is in the last column.

	ΔE_{2n-1n}	ΔE_{3n-1n}	ΔE_{4n-1n}	$\Delta\Delta E_{2n-1n}$	$\Delta\Delta E_{3n-1n}$	$\Delta\Delta E_{4n-1n}$	**MAE**
CCSD(T)[c]	1.9	3.9	16.0	-	-	-	-
B3LYP[a]	2.40	0.65	42.02	0.50	-3.25	26.02	15.14
B3LYP[b]	2.22	0.54	41.87	0.32	-3.36	25.87	15.06
M06[a]	3.04	3.60	3.26	1.14	-0.30	-12.74	7.39
M06[b]	2.09	3.50	2.11	0.19	-0.40	-13.89	8.03
VSXC[a]	2.77	1.83	26.14	0.87	-2.07	10.14	6.00
VSXC[b]	2.38	1.39	26.07	0.48	-2.51	10.07	6.00
B1B95[a]	1.82	3.51	-6.93	-0.08	-0.39	-22.93	13.24
B1B95[b]	-0.92	3.27	-7.05	-2.82	-0.63	-23.05	13.41
BPBE[a]	2.73	2.85	22.30	0.83	-1.05	6.30	3.72
BPBE[b]	2.42	2.63	21.86	0.52	-1.27	5.86	3.47
TPSSh[a]	1.52	1.68	10.05	-0.38	-2.22	-5.95	3.68
TPSSh[b]	1.16	1.37	9.78	-0.74	-2.53	-6.22	3.90
PBE[a]	2.94	3.49	18.45	1.04	-0.41	2.45	1.56
PBE[b]	2.61	3.22	18.18	0.71	-0.68	2.18	1.38
PBE0[a]	2.15	3.74	10.43	0.25	-0.16	-5.57	3.22
PBE0[b]	1.87	3.56	10.24	-0.03	-0.34	-5.76	3.33
HSE06[a]	2.32	3.43	12.50	0.42	-0.47	-3.50	2.05
HSE06[b]	2.01	3.24	12.22	0.11	-0.66	-3.78	2.21
B2PLYPD3[a]	2.06	1.42	37.10	0.16	-2.48	21.10	12.26
B2PLYPD3[b]	1.91	1.29	36.74	0.01	-2.61	20.74	12.07

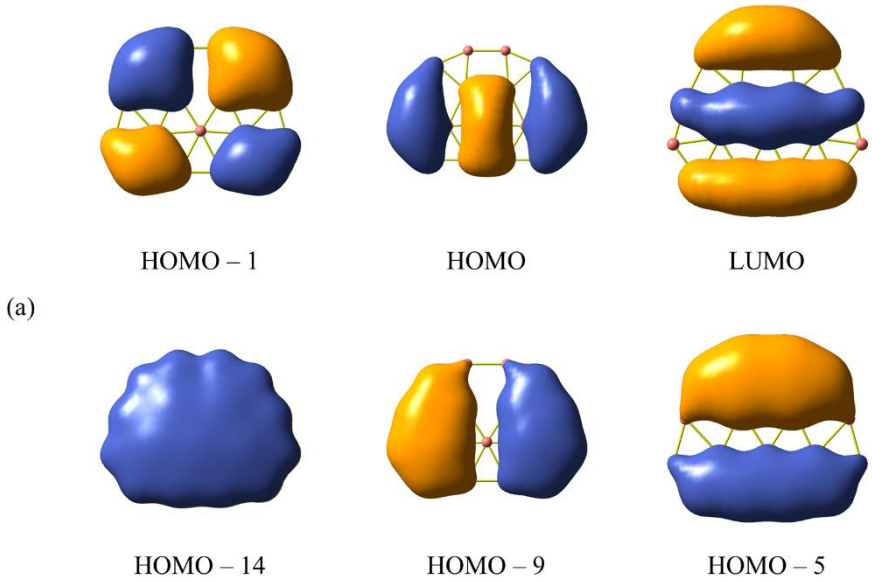
[a)] The DFT functional in conjunction with the 6-311+G(d) basis set, [b)] The DFT functional in conjunction with the def2-TZVPP basis set, [c)] The singlet-point CCSD(T)/aug-cc-pVTZ references values.

Table S4. Relative energies (kcal/mol) of ΔE_{2c-1c}, ΔE_{3c-1c} and ΔE_{4c-1c} and their errors $\Delta\Delta E_{2c-1c}$, $\Delta\Delta E_{3c-1c}$ and $\Delta\Delta E_{4c-1c}$ of B_{15}^{+}. The MAE is in the last column.

	ΔE_{2c-1c}	ΔE_{3c-1c}	ΔE_{4c-1c}	$\Delta\Delta E_{2c-1c}$	$\Delta\Delta E_{3c-1c}$	$\Delta\Delta E_{4c-1c}$	**MAE**
CCSD(T)[c]	1.9	3.9	16.0	-	-	-	-
B3LYP[a]	2.40	0.65	42.02	0.50	-3.25	26.02	15.14
B3LYP[b]	2.22	0.54	41.87	0.32	-3.36	25.87	15.06
M06[a]	3.04	3.60	3.26	1.14	-0.30	-12.74	7.39
M06[b]	2.09	3.50	2.11	0.19	-0.40	-13.89	8.03
VSXC[a]	2.77	1.83	26.14	0.87	-2.07	10.14	6.00
VSXC[b]	2.38	1.39	26.07	0.48	-2.51	10.07	6.00
B1B95[a]	1.82	3.51	-6.93	-0.08	-0.39	-22.93	13.24
B1B95[b]	-0.92	3.27	-7.05	-2.82	-0.63	-23.05	13.41
BPBE[a]	2.73	2.85	22.30	0.83	-1.05	6.30	3.72
BPBE[b]	2.42	2.63	21.86	0.52	-1.27	5.86	3.47
TPSSh[a]	1.52	1.68	10.05	-0.38	-2.22	-5.95	3.68
TPSSh[b]	1.16	1.37	9.78	-0.74	-2.53	-6.22	3.90
PBE[a]	2.94	3.49	18.45	1.04	-0.41	2.45	1.56
PBE[b]	2.61	3.22	18.18	0.71	-0.68	2.18	1.38
PBE0[a]	2.15	3.74	10.43	0.25	-0.16	-5.57	3.22
PBE0[b]	1.87	3.56	10.24	-0.03	-0.34	-5.76	3.33
HSE06[a]	2.32	3.43	12.50	0.42	-0.47	-3.50	2.05
HSE06[b]	2.01	3.24	12.22	0.11	-0.66	-3.78	2.21
B2PLYPD3[a]	2.06	1.42	37.10	0.16	-2.48	21.10	12.26
B2PLYPD3[b]	1.91	1.29	36.74	0.01	-2.61	20.74	12.07

[a)] The DFT functional in conjunction with the 6-311+G(d) basis set, [b)] The DFT functional in conjunction with the def2-TZVPP basis set, [c)] The singlet-point CCSD(T)/aug-cc-pVTZ references values.

Figures of supplementary information (SI)



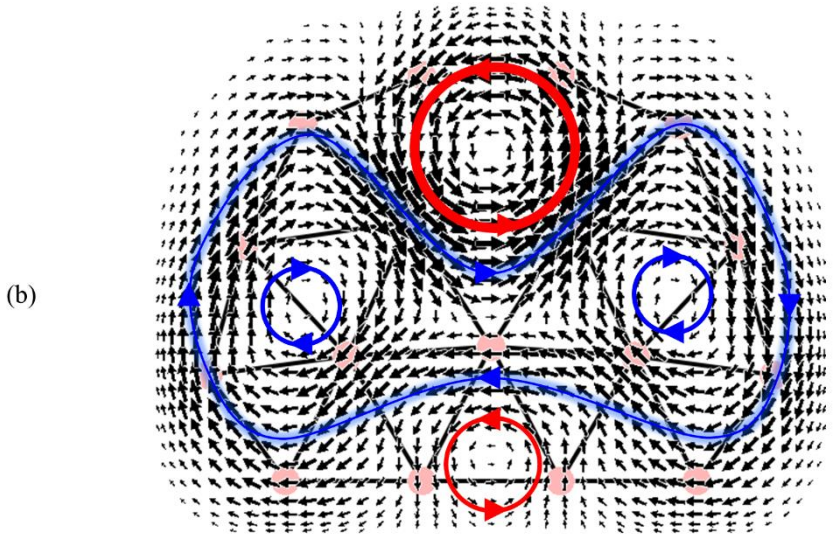


Figure S1. (a) The π-MOs and (b) the π ring current map of B_{17}^-. Local diatropic and local paramagnetic ring currents are highlighted by blue and red rings, respectively.

SI: The python code

The python code to compute the dimensions $L_a \times L_b$ of a rectangle box and the root mean square error (RMSE) (namely rectanglebox.py):

```
import matplotlib.pyplot as plt
import numpy as np
import math
from numpy import random
import scipy.special as sp
import scipy.optimize as opt

def find_La_Lb(C,abE):
    E_RM = (abE[:,0]**2)*C[0] + (abE[:,1]**2)*C[1]
    E_dft = E_RM*C[2] + C[3]
    return np.sum((E_dft - abE[:,2])**2)

plt.rcParams["figure.figsize"] = (5,5)
Edft = np.loadtxt("aC2v.txt", usecols=(0,1,2))
n_occ = 5
n_unocc = 3
xmin = math.floor(100*(np.min(Edft[:, 2]) - 0.02))/100
xmax = math.ceil(100*(np.max(Edft[:, 2]) + 0.02))/100
x = np.linspace(xmin, xmax, 11)
y = x
plt.plot(x, y,'k--')
plt.axis('equal')

c_guess = np.ones(4)
c_guess[3] = -1

Eocc = Edft[:n_occ, :]
Eunocc = Edft[-n_unocc:, :]
Cminimo = opt.minimize(find_La_Lb,c_guess,args=(Eocc))
c_out = Cminimo.x
La = 0.529177249*np.pi/np.sqrt(2*c_out[0]*c_out[2])
Lb = 0.529177249*np.pi/np.sqrt(2*c_out[1]*c_out[2])
E_1 = (Eocc[:,0]**2)*c_out[0] + (Eocc[:,1]**2)*c_out[1]
E_r_occ = E_1*c_out[2] + c_out[3]
RMSE = np.sqrt(np.sum((E_r_occ - Eocc[:,2])**2)/n_occ)
E_2 = (Eunocc[:,0]**2)*c_out[0] + (Eunocc[:,1]**2)*c_out[1]
E_r_unocc = E_2*c_out[2] + c_out[3]
plt.plot(E_r_occ, Eocc[:,2], 'ro',markersize=12,fillstyle='none')
plt.plot(E_r_unocc, Eunocc[:,2], 'bs',markersize=12,fillstyle='none')
print(f"Rectangle box:")
print(f"     La = {La:.4f} Angstrom")
print(f"     Lb = {Lb:.4f} Angstrom")
print(f"     La/Lb = {La/Lb:.4f} ")
print(f"     RMSE = {RMSE:.4f} ")
print(f"     ")
```

```
plt.savefig('rectangle.png', dpi=300)
```

will read the MO information of **1a-C_{2v}** in the file “aC2v.txt”:

1	1	-0.212942157
2	1	-0.147224498
1	2	-0.127987704
3	1	-0.076135935
2	2	-0.034904343
1	3	-0.014415061
4	1	0.045922111
3	2	0.046338683

content with three columns representing the quantum numbers *a*, *b*, and MO energy (Hartree), respectively.

Additional information on isomers

Cartesian coordinates (in angstrom), energies (E, Hartree), and zero-point energies (ZPE, Hartree) of lower-lying isomers optimized at the PBE/6-311+G(d) level.

1a

E = -372.115403224, ZPE = 0.05783

5	-0.029089000	1.145113000	2.018757000
5	-0.101002000	-0.124567000	0.844625000
5	-0.101002000	-0.124567000	-0.844625000
5	0.052006000	-0.356989000	2.481697000
5	-0.302907000	-1.639556000	0.000000000
5	0.169519000	1.501723000	0.000000000
5	-0.046903000	2.587783000	1.387771000
5	-0.029089000	1.145113000	-2.018757000
5	0.111916000	3.223220000	0.000000000
5	-0.046903000	2.587783000	-1.387771000
5	0.012482000	-1.765314000	1.748570000
5	0.052006000	-0.356989000	-2.481697000
5	0.123241000	-3.028720000	-0.777840000
5	0.123241000	-3.028720000	0.777840000
5	0.012482000	-1.765314000	-1.748570000

1a-*C*$_{2v}$

E = -372.104077266; Number of imaginary frequencies = 2

5	0.000000000	1.987156000	1.157686000
5	0.000000000	0.831981000	-0.115526000
5	0.000000000	-0.831981000	-0.115526000
5	0.000000000	2.461528000	-0.367077000
5	0.000000000	0.000000000	-1.612398000
5	0.000000000	0.000000000	1.491774000
5	0.000000000	1.398267000	2.600467000
5	0.000000000	-1.987156000	1.157686000
5	0.000000000	0.000000000	3.234548000
5	0.000000000	-1.398267000	2.600467000
5	0.000000000	1.777568000	-1.790919000
5	0.000000000	-2.461528000	-0.367077000
5	0.000000000	-0.779837000	-3.041593000
5	-0.000000000	0.779837000	-3.041593000
5	0.000000000	-1.777568000	-1.790919000

2a

E = -372.1150576, ZPE = 0.060007

5	-0.905151000	1.484710000	0.085927000
5	-2.521820000	1.337327000	0.283473000
5	0.420672000	2.374192000	-0.363829000
5	-3.414754000	0.092577000	-0.054838000
5	-0.210561000	-0.369298000	0.216782000
5	-2.788013000	-1.348954000	-0.003908000
5	1.940809000	2.059005000	-0.211776000
5	-1.212331000	-1.707871000	-0.048346000
5	-1.768234000	-0.048161000	-0.320804000
5	2.706952000	0.679755000	0.053403000
5	0.831446000	0.982935000	0.398174000
5	3.044811000	-0.894104000	0.040617000
5	2.037124000	-2.083896000	-0.097765000
5	1.434431000	-0.593688000	0.164052000
5	0.404620000	-1.964529000	-0.141162000

3a

E = -372.1112236; ZPE = 0.057794

5	0.000000000	1.496216000	0.809929000
5	0.000000000	0.775607000	3.503188000
5	0.000000000	0.000000000	1.865603000
5	0.000000000	1.496216000	-0.809929000
5	0.000000000	0.000000000	0.000000000
5	0.000000000	0.000000000	-1.865603000
5	0.000000000	-1.496216000	-0.809929000
5	0.000000000	0.775607000	-3.503188000
5	0.000000000	-1.747941000	-2.323776000
5	0.000000000	-0.775607000	-3.503188000
5	0.000000000	1.747941000	-2.323776000
5	0.000000000	1.747941000	2.323776000
5	0.000000000	-1.747941000	2.323776000
5	0.000000000	-1.496216000	0.809929000
5	0.000000000	-0.775607000	3.503188000

4a

E = -372.1003049; ZPE = 0.058385

5	0.846014000	-1.878289000	0.246587000
5	-0.765450000	-1.919832000	-0.165139000
5	2.404071000	-1.579971000	-0.197393000
5	-2.877405000	-0.117223000	-0.679180000
5	-0.006934000	-0.552544000	0.978314000
5	-2.194824000	1.147776000	0.070816000
5	-0.977225000	0.848647000	1.160449000
5	-0.683477000	1.916180000	-0.215047000
5	-1.522815000	-0.429151000	0.208715000
5	2.916554000	-0.154518000	-0.511854000
5	1.572260000	-0.317377000	0.413381000
5	2.055070000	1.254064000	-0.476570000
5	-2.200836000	-1.555384000	-0.758700000
5	0.836960000	2.237915000	-0.630622000
5	0.598037000	1.099708000	0.556244000

7a

E = -372.1094639; ZPE = 0.057329

5	1.437965000	1.818120000	0.000000000
5	0.000000000	0.856403000	0.000000000
5	-0.178027000	-0.854047000	0.000000000
5	0.010183000	2.525251000	0.000000000
5	-1.589264000	0.191612000	0.000000000
5	1.535687000	-0.031232000	0.000000000
5	2.847994000	1.072090000	0.000000000
5	0.800083000	-2.311850000	0.000000000
5	3.164948000	-0.443276000	0.000000000
5	2.263997000	-1.691376000	0.000000000
5	-1.483061000	1.959544000	0.000000000
5	-0.739165000	-2.435986000	0.000000000
5	-3.136340000	-0.347316000	0.000000000
5	-2.894275000	1.195502000	0.000000000
5	-2.040723000	-1.503439000	0.000000000

1n

E = -371.9983039; ZPE = 0.057496

5	0.087491000	-0.111842000	0.834027000
5	0.087491000	-0.111842000	-0.834027000
5	0.159348000	-1.613954000	0.000000000
5	-0.045039000	-0.360303000	2.473948000
5	-0.063580000	3.230969000	0.000000000
5	-0.019394000	-1.781906000	-1.768842000
5	0.016741000	2.604263000	1.392239000
5	-0.061622000	-3.042801000	-0.772206000
5	-0.045039000	-0.360303000	-2.473948000
5	0.006086000	1.141441000	-2.002951000
5	0.006086000	1.141441000	2.002951000
5	-0.019394000	-1.781906000	1.768842000
5	-0.061622000	-3.042801000	0.772206000
5	-0.064296000	1.485281000	0.000000000
5	0.016741000	2.604263000	-1.392239000

2n

E = -371.9944239; ZPE = 0.057778

5	1.708828000	-0.146988000	2.371212000
5	1.708828000	-0.146988000	-2.371212000
5	1.957679000	-0.079749000	0.815514000
5	1.957679000	-0.079749000	-0.815514000
5	0.140722000	0.073371000	1.524789000
5	-1.051260000	-0.071887000	2.812425000
5	-1.851812000	-0.082413000	-1.457325000
5	-1.851812000	-0.082413000	1.457325000
5	0.421464000	-0.130394000	3.228233000
5	-2.434115000	-0.173922000	0.000000000
5	0.421464000	-0.130394000	-3.228233000
5	0.140722000	0.073371000	-1.524789000
5	-0.906516000	0.438462000	0.000000000
5	0.689387000	0.611581000	0.000000000
5	-1.051260000	-0.071887000	-2.812425000

3n

E = -371.9932837; ZPE = 0.057609

5	0.000000000	1.499362000	0.800986000
5	0.000000000	0.769733000	3.512854000
5	0.000000000	0.000000000	1.852530000
5	0.000000000	1.499362000	-0.800986000
5	0.000000000	0.000000000	0.000000000
5	0.000000000	0.000000000	-1.852530000
5	0.000000000	-1.499362000	-0.800986000
5	0.000000000	0.769733000	-3.512854000
5	0.000000000	-1.746338000	-2.326075000
5	0.000000000	-0.769733000	-3.512854000
5	0.000000000	1.746338000	-2.326075000
5	0.000000000	1.746338000	2.326075000
5	0.000000000	-1.746338000	2.326075000
5	0.000000000	-1.499362000	0.800986000
5	0.000000000	-0.769733000	3.512854000

4n

E = -371.9697324; ZPE = 0.057893

5	0.000000000	2.740992000	-0.760910000
5	0.000000000	0.000000000	0.982202000
5	-1.364664000	2.114714000	-0.345955000
5	-1.540502000	-0.833879000	0.525114000
5	0.000000000	0.874746000	-0.861337000
5	1.364664000	-2.114714000	-0.345955000
5	0.000000000	-2.740992000	-0.760910000
5	0.000000000	1.681438000	0.772830000
5	1.540502000	-0.833879000	0.525114000
5	-1.540502000	0.833879000	0.525114000
5	1.364664000	2.114714000	-0.345955000
5	1.540502000	0.833879000	0.525114000
5	0.000000000	-0.874746000	-0.861337000
5	0.000000000	-1.681438000	0.772830000
5	-1.364664000	-2.114714000	-0.345955000

1c

E = -371.7264283; ZPE = 0.057656

5	0.000000000	2.011920000	1.133402000
5	0.000000000	0.828408000	-0.099590000
5	0.000000000	-0.828408000	-0.099590000
5	0.000000000	2.483099000	-0.362520000
5	0.000000000	0.000000000	-1.601634000
5	0.000000000	0.000000000	1.480677000
5	0.000000000	1.392336000	2.620698000
5	0.000000000	-2.011920000	1.133402000
5	0.000000000	0.000000000	3.245881000
5	0.000000000	-1.392336000	2.620698000
5	0.000000000	1.785204000	-1.796829000
5	0.000000000	-2.483099000	-0.362520000
5	0.000000000	-0.768621000	-3.057623000
5	0.000000000	0.768621000	-3.057623000
5	0.000000000	-1.785204000	-1.796829000

2c

E = -371.722467; ZPE = 0.057787

5	-1.701549000	-0.179149000	2.377875000
5	-0.131706000	0.145856000	1.525773000
5	0.900317000	0.436479000	0.000000000
5	2.454531000	-0.133267000	0.000000000
5	-0.697471000	0.623994000	0.000000000
5	-1.969018000	-0.090192000	-0.803562000
5	-0.421401000	-0.111590000	3.243433000
5	1.852126000	-0.107794000	1.445367000
5	-0.131706000	0.145856000	-1.525773000
5	1.042860000	-0.120733000	2.823498000
5	-1.969018000	-0.090192000	0.803562000
5	1.852126000	-0.107794000	-1.445367000
5	-0.421401000	-0.111590000	-3.243433000
5	-1.701549000	-0.179149000	-2.377875000
5	1.042860000	-0.120733000	-2.823498000

3c

E = -371.7149238; ZPE = 0.057062

5	0.000000000	1.504883000	0.794659000
5	0.000000000	0.766642000	3.534257000
5	0.000000000	0.000000000	1.842476000
5	0.000000000	1.504883000	-0.794659000
5	0.000000000	0.000000000	0.000000000
5	0.000000000	0.000000000	-1.842476000
5	0.000000000	-1.504883000	-0.794659000
5	0.000000000	0.766642000	-3.534257000
5	0.000000000	-1.747418000	-2.335721000
5	0.000000000	-0.766642000	-3.534257000
5	0.000000000	1.747418000	-2.335721000
5	0.000000000	1.747418000	2.335721000
5	0.000000000	-1.747418000	2.335721000
5	0.000000000	-1.504883000	0.794659000
5	0.000000000	-0.766642000	3.534257000

4c

E = -371.7171278; ZPE = 0.058825

5	0.000000000	2.035841000	0.000000000
5	1.601949000	1.822882000	0.000000000
5	-1.601949000	1.822882000	0.000000000
5	0.000000000	-0.993863000	0.907847000
5	0.860711000	0.496932000	-0.907847000
5	2.379636000	0.475888000	0.000000000
5	1.763090000	-1.017920000	0.000000000
5	-0.860711000	0.496932000	0.907847000
5	0.860711000	0.496932000	0.907847000
5	-2.379636000	0.475888000	0.000000000
5	-0.860711000	0.496932000	-0.907847000
5	-1.763090000	-1.017920000	0.000000000
5	-0.777687000	-2.298769000	0.000000000
5	0.000000000	-0.993863000	-0.907847000
5	0.777687000	-2.298769000	0.000000000