Theoretical Probing of Deltahedral Closo-Auro-Boranes $B_xAu_x^{2-}$ ($x = 5-12$)

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Supporting Information

Complete references 16 and 17:

16. NWChem 4.7. Aprà, E.; Windus, T.L.; Straatsma, T.P.; Bylaska, E.J.; de Jong, W.; Hirata, S.; Valiev, M.; Hackler, M.; Pollack, L.; Kowalski, K.; Harrison, R.; Dupuis, M.; Smith, D.M.A.; Nieplocha, J.; Tipparaju V.; Krishnan, M.; Auer, A.A.; Brown, E.; Cisneros, G.; Fann, G.; Fruchtl, H.; Garza, J.; Hirao, K.; Kendall, R.; Nichols, J.; Tsemekhman, K.; Wolinski, K.; Anchell, J.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsel, H.; Deegan, M.; Dyall, K.; Elwood, D.; Glendening, E.; Gutowski, M.; Hess, A.; Jaffe, J.; Johnson, B.; Ju, J.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nakajima, T.; Niu, S.; Rosing, M.; Sandrone, G.; Stave, M.; Taylor, H.; Thomas, G.; van Lenthe, J.; Wong, A.; Zhang, Z.; "NWChem, A Computational Chemistry Package for Parallel Computers, Version 4.7" (2005), Pacific Northwest National Laboratory, Richland, Washington 99352-0999, USA.

(17) Gaussian 03 (revision A.1). Frisch, M. J.; Trucks, G. M.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith,

T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.;

Wong, M. W.; Gonzales, C. ; Pople, J. A., Gaussian, Inc., Pittsburgh PA, 2003.

$\text{B}_5\text{H}_5^{2-} \text{D}_{3h} {}^1\text{A}_1'$ B3LYP/aug-cc-pvTZ

B	0.000000	1.051462	0.000000
B	0.910593	-0.525731	0.000000
B	-0.910593	-0.525731	0.000000
B	0.000000	0.000000	1.306253
B	0.000000	0.000000	-1.306253
H	1.962165	-1.132857	0.000000
H	0.000000	2.265713	0.000000
H	-1.962165	-1.132857	0.000000
H	0.000000	0.000000	-2.511066
H	0.000000	0.000000	2.511066

1	2	3	4	5	6
Fr 390.6306	392.2144	455.4253	455.4701	522.2201	633.8355
7	8	9	10	11	12
Fr 633.8812	641.8058	643.7404	736.1475	737.7197	765.4103
13	14	15	16	17	18
Fr 768.2288	809.8371	810.1182	916.7051	916.9464	974.9540
19	20	21	22	23	24
Fr 1023.4690	2378.9509	2378.9642	2404.4034	2472.9566	2479.8963

Zero-point vibrational energy= 36.23097 kcal/mol

$E_{\text{tot}}(\text{B3LYP})=-127.186814$ a. u.

B₆H₆²⁻ O_h ¹A_{1g} B3LYP/aug-cc-pvTZ

B	0	0.000000	0.000000	1.225851
B	0	0.000000	1.225851	0.000000
B	0	0.000000	0.000000	-1.225851
B	0	0.000000	-1.225851	0.000000
B	0	1.225851	0.000000	0.000000
B	0	-1.225851	0.000000	0.000000
H	0	0.000000	-2.437750	0.000000
H	0	0.000000	0.000000	2.437750
H	0	0.000000	2.437750	0.000000
H	0	0.000000	0.000000	-2.437750
H	0	-2.437750	0.000000	0.000000
H	0	2.437750	0.000000	0.000000

	1	2	3	4	5	6
Fr	444.1598	444.1598	444.1598	645.1755	645.1755	645.1755
	7	8	9	10	11	12
Fr	687.4664	687.4665	687.4665	738.9378	738.9378	738.9378
	13	14	15	16	17	18
Fr	821.5844	821.5844	822.2791	822.2791	822.2791	851.8426
	19	20	21	22	23	24
Fr	851.8426	851.8427	960.8848	1025.9671	1025.9671	1025.9671
	25	26	27	28	29	30
Fr	2402.0598	2402.0598	2413.6975	2413.6975	2413.6975	2458.9925

Zero-point vibrational energy= 46.82669 kcal/mol

E_{tot}(B3LYP)=-152.7416847 a. u.

B₇H₇²⁻ D_{5h} ¹A₁' B3LYP/aug-cc-pvTZ

B	0.000000	1.406589	0.000000
B	1.337746	0.434660	0.000000
B	0.826772	-1.137955	0.000000
B	-0.826772	-1.137955	0.000000
B	-1.337746	0.434660	0.000000
B	0.000000	0.000000	1.164707
B	0.000000	0.000000	-1.164707
H	0.000000	2.619013	0.000000
H	2.490830	0.809320	0.000000
H	1.539417	-2.118826	0.000000
H	-1.539417	-2.118826	0.000000
H	-2.490830	0.809320	0.000000
H	0.000000	0.000000	2.378732
H	0.000000	0.000000	-2.378732

	1	2	3	4	5	6
Fr	450.3379	450.3385	461.2872	461.2872	528.3590	528.3590
	7	8	9	10	11	12
Fr	568.5956	568.5997	607.5922	743.4604	743.4614	765.6421
	13	14	15	16	17	18
Fr	765.6553	767.7201	767.7201	798.5367	842.8965	842.8965
	19	20	21	22	23	24
Fr	864.7979	864.7981	883.5168	883.5264	890.0287	895.9927
	25	26	27	28	29	30
Fr	916.5332	981.3579	981.3579	1071.2204	1071.2210	2384.5596
	31	32	33	34	35	36
Fr	2385.5347	2385.5347	2388.2536	2409.9103	2409.9103	2449.4724

Zero-point vibrational energy= 55.43918 kcal/mol

E_{tot}(B3LYP)=-178.2315176 a. u.

B₈H₈²⁻ D_{2d} ¹A₁ B3LYP/aug-cc-pvTZ

B	-0.57008324	0.57008324	-1.32770521
B	0.57008324	-0.57008324	-1.32770521
B	-0.90040097	0.90040097	0.31447109
B	0.90040097	-0.90040097	0.31447109
B	-0.57008324	-0.57008324	1.32770521
B	0.57008324	0.57008324	1.32770521
B	0.90040097	0.90040097	-0.31447109
B	-0.90040097	-0.90040097	-0.31447109
H	-1.11443111	-1.11443111	2.25898806
H	1.11443111	1.11443111	2.25898806
H	-1.11443111	1.11443111	-2.25898806
H	1.11443111	-1.11443111	-2.25898806
H	1.73094595	-1.73094595	0.61846999
H	-1.73094595	1.73094595	0.61846999
H	1.73094595	1.73094595	-0.61846999
H	-1.73094595	-1.73094595	-0.61846999

Fr	1	2	3	4	5	6
	20.0460	20.0460	20.1779	22.7431	23.9650	29.3331
Fr	7	8	9	10	11	12
	31.0381	31.0381	31.2990	31.6116	43.0277	43.0277
Fr	13	14	15	16	17	18
	44.8671	97.5383	107.5681	107.5681	110.4032	114.1151
Fr	19	20	21	22	23	24
	176.4993	245.7713	245.7713	264.2734	264.2734	352.3101
Fr	25	26	27	28	29	30
	369.6521	369.6521	396.4837	482.2825	519.2333	540.8089
Fr	31	32	33	34	35	36
	653.8640	683.6251	683.6251	694.4181	797.0160	797.0160
Fr	37	38	39	40	41	42
	897.2947	962.1834	962.1834	964.1719	1003.6206	1012.6449

Zero-point vibrational energy= 21.83 kcal/mol
E_{tot}(B3LYP)= -203.71105959 a. u.

B₉H₉²⁻ D_{3h} ¹A₁' B3LYP/cc-pvTZ

B	1.15807254	1.15807254	0.00000000
B	-1.58195652	0.42388397	0.00000000
B	0.42388397	-1.58195652	0.00000000
B	-0.29715241	1.10898791	0.89213839
B	-0.81183550	-0.81183550	0.89213839
B	1.10898791	-0.29715241	0.89213839
B	-0.29715241	1.10898791	-0.89213839
B	-0.81183550	-0.81183550	-0.89213839
B	1.10898791	-0.29715241	-0.89213839
H	2.00878895	2.00878895	0.00000000
H	-2.74405673	0.73526779	0.00000000
H	0.73526779	-2.74405673	0.00000000
H	-1.40879701	-1.40879701	1.75402416
H	1.92445250	-0.51565549	1.75402416
H	-0.51565549	1.92445250	1.75402416
H	1.92445250	-0.51565549	-1.75402416
H	-1.40879701	-1.40879701	-1.75402416
H	-0.51565549	1.92445250	-1.75402416

	1	2	3	4	5	6
Fr	164.12	341.80	341.80	435.30	435.30	531.08
	7	8	9	10	11	12
Fr	557.19	592.51	592.51	642.20	667.11	667.11
	13	14	15	16	17	18
Fr	712.57	721.40	721.40	754.10	754.10	761.43
	19	20	21	22	23	24
Fr	774.23	774.23	786.13	841.48	841.48	864.74
	25	26	27	28	29	30
Fr	877.29	882.38	886.03	886.03	888.02	888.02
	31	32	33	34	35	36
Fr	914.17	916.52	916.52	977.49	977.49	991.25
	37	38	39	40	41	42
Fr	998.75	1073.62	1073.62	2439.68	2439.68	2452.01
	43	44	45	46	47	48
Fr	2452.01	2455.70	2456.06	2482.85	2482.85	2513.26

Zero-point vibrational energy= 73.78309381 kcal/mol

E_{tot}(B3LYP)=-229.21223585 a. u.

B₁₀H₁₀²⁻ D_{4d} ¹A₁ B3LYP/cc-pvTZ

B	-0.91886818	0.91886818	-0.76062045
B	0.91886818	0.91886818	-0.76062045
B	0.91886818	-0.91886818	-0.76062045
B	-0.91886818	-0.91886818	-0.76062045
B	0.00000000	1.29947584	0.76062045
B	-1.29947584	0.00000000	0.76062045
B	0.00000000	-1.29947584	0.76062045
B	1.29947584	0.00000000	0.76062045
B	0.00000000	0.00000000	-1.85507414
B	0.00000000	0.00000000	1.85507414
H	-1.71948972	1.71948972	-1.16840616
H	-1.71948972	-1.71948972	-1.16840616
H	1.71948972	-1.71948972	-1.16840616
H	1.71948972	1.71948972	-1.16840616
H	0.00000000	-2.43172569	1.16840616
H	-2.43172569	0.00000000	1.16840616
H	0.00000000	2.43172569	1.16840616
H	2.43172569	0.00000000	1.16840616
H	0.00000000	0.00000000	3.05499627
H	0.00000000	0.00000000	-3.05499627

	1	2	3	4	5	6
Fr	420.50	459.05	459.05	490.51	490.51	565.73
	7	8	9	10	11	12
Fr	565.73	596.79	596.79	610.95	622.01	622.01
	13	14	15	16	17	18
Fr	645.20	645.20	716.80	716.80	732.25	742.33
	19	20	21	22	23	24
Fr	747.30	747.30	747.39	747.39	812.47	831.10
	25	26	27	28	29	30
Fr	854.06	854.06	880.90	880.90	886.17	886.17
	31	32	33	34	35	36
Fr	903.28	904.54	912.12	912.12	917.72	917.72
	37	38	39	40	41	42
Fr	932.64	932.64	936.06	936.06	1011.95	1032.07
	43	44	45	46	47	48
Fr	1032.07	1106.68	2466.48	2466.48	2470.26	2470.26
	49	50	51	52	53	54
Fr	2474.65	2488.42	2488.42	2493.44	2506.67	2536.28

Zero-point vibrational energy= 84.11609761 kcal/mol
E_{tot}(B3LYP)=-254.73842980 a. u.

B₁₁H₁₁²⁻ C_{2v} ¹A₁ B3LYP/cc-pvTZ

B	0.00000000	0.00000000	-1.43212048
B	0.00000000	1.66137809	-0.91137793
B	0.00000000	-1.66137809	-0.91137793
B	0.00000000	-1.48104522	0.83365135
B	0.00000000	1.48104522	0.83365135
B	-1.33431832	0.93489137	-0.22606999
B	1.33431832	0.93489137	-0.22606999
B	1.33431832	-0.93489137	-0.22606999
B	-1.33431832	-0.93489137	-0.22606999
B	-0.91281384	0.00000000	1.22919963
B	0.91281384	0.00000000	1.22919963
H	0.00000000	0.00000000	-2.63400577
H	0.00000000	2.63973052	-1.60669440
H	0.00000000	-2.63973052	-1.60669440
H	-2.44236202	1.37768813	-0.37775934
H	-2.44236202	-1.37768813	-0.37775934
H	2.44236202	-1.37768813	-0.37775934
H	2.44236202	1.37768813	-0.37775934
H	0.00000000	-2.42976800	1.57208710
H	0.00000000	2.42976800	1.57208710
H	1.62701281	0.00000000	2.19433702
H	-1.62701281	0.00000000	2.19433702

	1	2	3	4	5	6
Fr	172.54	291.57	378.69	443.75	476.68	500.05
	7	8	9	10	11	12
Fr	534.44	545.52	546.17	583.91	603.31	620.42
	13	14	15	16	17	18
Fr	623.58	638.85	678.16	704.55	710.66	710.72
	19	20	21	22	23	24
Fr	724.35	729.87	744.02	754.99	766.89	786.75
	25	26	27	28	29	30
Fr	788.71	812.09	830.07	834.42	835.11	864.39
	31	32	33	34	35	36
Fr	869.83	870.18	901.74	903.77	906.41	911.37
	37	38	39	40	41	42
Fr	921.83	923.25	930.07	940.90	941.14	946.41
	43	44	45	46	47	48
Fr	949.25	964.06	965.32	1021.88	1062.55	1066.32
	49	50	51	52	53	54
Fr	1095.93	2462.67	2466.56	2474.84	2479.83	2480.64
	55	56	57	58	59	60
Fr	2488.10	2490.06	2496.38	2508.53	2510.81	2544.76

Zero-point vibrational energy= 92.56481213 kcal/mol; E_{tot}(B3LYP)=-280.20796735 a. u.

B₁₂H₁₂²⁻ I_h ¹A_g B3LYP/cc-pvTZ

B	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.782616
B	1.543791	0.000000	0.891308
B	-1.150674	-1.029194	0.891308
B	-0.318038	-1.665271	-0.550859
B	1.347232	-1.029194	-0.550859
B	1.029194	-2.694465	0.000000
B	-0.514597	-2.694465	0.891308
B	-0.318038	-1.665271	2.333475
B	1.347232	-1.029194	2.333475
B	2.179868	-1.665271	0.891308
B	1.029194	-2.694465	1.782616
H	2.272286	0.953613	0.891308
H	3.358598	-1.890388	0.891308
H	1.936598	-0.804077	3.354285
H	1.393442	-3.648077	-0.630896
H	-1.243093	-3.648077	0.891308
H	-0.907404	-1.890388	3.354285
H	1.393442	-3.648077	2.413512
H	-0.364248	0.953613	-0.630896
H	-0.364248	0.953613	2.413512
H	-2.329404	-0.804076	0.891308
H	-0.907404	-1.890389	-1.571669
H	1.936598	-0.804076	-1.571669

1	2	3	4	5	6
Fr 519.2044	519.2060	519.2072	519.2074	519.2093	574.9859
7	8	9	10	11	12
Fr 574.9876	574.9880	574.9903	574.9908	656.5192	656.5207
13	14	15	16	17	18
Fr 656.5226	656.5243	705.2135	705.2163	705.2168	738.3051
19	20	21	22	23	24
Fr 738.3098	738.3129	738.3163	739.3503	757.5302	757.5327
25	26	27	28	29	30
Fr 757.5351	757.5372	757.5388	761.5028	761.5050	761.5083
31	32	33	34	35	36
Fr 870.2941	870.2951	870.2991	870.3011	946.6990	946.7012
37	38	39	40	41	42
Fr 946.7042	946.7060	950.0263	950.0267	950.0299	950.0307
43	44	45	46	47	48
Fr 950.0317	951.7348	951.7374	951.7398	951.7405	951.7425
49	50	51	52	53	54
Fr 967.3852	967.3868	967.3916	1072.0026	1072.0052	1072.0111
55	56	57	58	59	60
Fr 2494.3921	2494.3935	2494.3957	2501.1954	2501.1963	2501.1975
61	62	63	64	65	66
Fr 2501.1982	2501.1987	2521.0163	2521.0166	2521.0175	2557.1052

Zero-point vibrational energy= 104.33278 kcal/mol
E_{tot}(B3LYP)=-305.7938604 a. u.

B₅Au₅²⁻ D_{3h} B3LYP/B/aug-cc-pvTZ/Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	0.75361856	0.75361856	0.00000000
B	0.00000000	0.00000000	-1.27806031
B	0.00000000	0.00000000	1.27806031
B	0.27584354	-1.02946210	0.00000000
B	-1.02946210	0.27584354	0.00000000
Au	2.20773283	2.20773283	0.00000000
Au	0.80808630	-3.01581914	0.00000000
Au	-3.01581914	0.80808630	0.00000000
Au	0.00000000	0.00000000	-3.32350856
Au	0.00000000	0.00000000	3.32350856

Fr	12.49	12.49	26.58	26.58	35.20	41.40
	7	8	9	10	11	12
Fr	41.40	106.36	118.55	282.42	282.42	293.28
	13	14	15	16	17	18
Fr	307.80	307.80	359.67	433.14	433.14	548.57
	19	20	21	22	23	24
Fr	548.57	809.11	853.29	853.29	1103.49	1108.75

Zero-Point Energy = 12.79250536 kcal/mol

E_{tot}(B3LYP)=-804.01623645 a. u.

B₆Au₆²⁻ O_h B3LYP/B/aug-cc-pvTZ//Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	-1.21761000	0.00000000	0.00000000
B	0.00000000	-1.21761000	0.00000000
B	0.00000000	1.21761000	0.00000000
B	1.21761000	0.00000000	0.00000000
B	0.00000000	0.00000000	-1.21761000
B	0.00000000	0.00000000	1.21761000
Au	-3.27476000	0.00000000	0.00000000
Au	0.00000000	-3.27476000	0.00000000
Au	0.00000000	3.27476000	0.00000000
Au	3.27476000	0.00000000	0.00000000
Au	0.00000000	0.00000000	-3.27476000
Au	0.00000000	0.00000000	3.27476000

	1	2	3	4	5	6
Fr	26.85	26.85	26.85	27.18	27.18	27.18
	7	8	9	10	11	12
Fr	44.57	44.57	44.57	114.10	114.10	118.22
	13	14	15	16	17	18
Fr	293.65	293.65	293.65	333.69	333.69	333.69
	19	20	21	22	23	24
Fr	433.91	433.91	433.91	681.17	681.17	681.17
	25	26	27	28	29	30
Fr	862.74	862.74	994.99	994.99	994.99	1095.15

Zero-Point Energy = 16.69543049 kcal/mol

E_{tot}(B3LYP)=-964.897162713809 a. u.

B₇Au₇²⁻ D_{5h} B3LYP/B/aug-cc-pvTZ/Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	0.00000000	1.40121859	0.00000000
B	0.00000000	0.00000000	-1.15102979
B	0.00000000	0.00000000	1.15102979
B	-1.33263807	0.43300036	0.00000000
B	1.33263807	0.43300036	0.00000000
B	-0.82361562	-1.13360965	0.00000000
B	0.82361562	-1.13360965	0.00000000
Au	0.00000000	3.47053538	0.00000000
Au	-3.30067529	1.07245441	0.00000000
Au	3.30067529	1.07245441	0.00000000
Au	-2.03992951	-2.80772210	0.00000000
Au	2.03992951	-2.80772210	0.00000000
Au	0.00000000	0.00000000	-3.21727874
Au	0.00000000	0.00000000	3.21727874

	1	2	3	4	5	6
Fr	26.59	26.59	26.68	26.68	29.19	29.19

	7	8	9	10	11	12
Fr	29.53	29.53	44.18	44.18	47.82	104.92

	13	14	15	16	17	18
Fr	104.92	113.07	114.94	286.41	304.69	304.69

	19	20	21	22	23	24
Fr	307.29	329.71	329.71	474.98	474.98	487.15

	25	26	27	28	29	30
Fr	487.15	602.85	602.85	722.10	722.10	838.40

	31	32	33	34	35	36
Fr	840.14	983.10	983.10	1006.36	1006.36	1027.29

Zero-Point Energy = 19.90558620 kcal/mol

E_{tot}(B3LYP)=-1125.73587848 a. u.

B₈Au₈²⁻ D_{2d} B3LYP/B/aug-cc-pvTZ/Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	-0.57825193	0.57825193	-1.30636176
B	0.57825193	-0.57825193	-1.30636176
B	-0.90097467	0.90097467	0.31350901
B	0.90097467	-0.90097467	0.31350901
B	-0.57825193	-0.57825193	1.30636176
B	0.57825193	0.57825193	1.30636176
B	0.90097467	0.90097467	-0.31350901
B	-0.90097467	-0.90097467	-0.31350901
Au	-1.46355419	-1.46355419	2.94461166
Au	1.46355419	1.46355419	2.94461166
Au	-1.46355419	1.46355419	-2.94461166
Au	1.46355419	-1.46355419	-2.94461166
Au	2.31015066	-2.31015066	0.89428932
Au	-2.31015066	2.31015066	0.89428932
Au	2.31015066	2.31015066	-0.89428932
Au	-2.31015066	-2.31015066	-0.89428932

	1	2	3	4	5	6
Fr	23.77	23.77	25.16	27.97	28.54	28.81
	7	8	9	10	11	12
Fr	29.91	30.21	30.21	32.19	45.07	45.07
	13	14	15	16	17	18
Fr	49.18	99.69	106.87	106.87	108.06	114.13
	19	20	21	22	23	24
Fr	289.33	289.33	301.70	312.38	312.38	343.74
	25	26	27	28	29	30
Fr	396.47	396.47	413.60	504.51	567.77	576.73
	31	32	33	34	35	36
Fr	665.24	702.45	702.45	707.02	797.23	797.23
	37	38	39	40	41	42
Fr	876.64	944.64	944.64	948.72	1018.89	1024.41

Zero-Point Energy = 22.57892974 kcal/mol

E_{tot}(B3LYP)=-1286.55444249 a. u.

B₉Au₉²⁻ D_{3h} B3LYP/B/cc-pvTZ/Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	-1.15762592	-1.15762592	0.00000000
B	1.58134642	-0.42372049	0.00000000
B	-0.42372049	1.58134642	0.00000000
B	0.29859045	-1.11435475	0.88466468
B	0.81576429	0.81576429	0.88466468
B	-1.11435475	0.29859045	0.88466468
B	0.29859045	-1.11435475	-0.88466468
B	0.81576429	0.81576429	-0.88466468
B	-1.11435475	0.29859045	-0.88466468
Au	-2.61158405	-2.61158405	0.00000000
Au	3.56749016	-0.95590611	0.00000000
Au	-0.95590611	3.56749016	0.00000000
Au	1.80215999	1.80215999	2.39540134
Au	-2.46179633	0.65963634	2.39540134
Au	0.65963634	-2.46179633	2.39540134
Au	-2.46179633	0.65963634	-2.39540134
Au	1.80215999	1.80215999	-2.39540134
Au	0.65963634	-2.46179633	-2.39540134

	1	2	3	4	5	6
Fr	3.73	24.97	24.97	28.19	28.69	28.69
	7	8	9	10	11	12
Fr	28.77	28.77	30.45	30.45	30.54	31.53
	13	14	15	16	17	18
Fr	36.48	47.98	47.98	101.08	101.08	105.05
	19	20	21	22	23	24
Fr	105.05	108.70	112.46	176.79	286.84	310.11
	25	26	27	28	29	30
Fr	310.11	328.29	328.29	364.02	364.02	364.65
	31	32	33	34	35	36
Fr	488.87	488.87	526.12	540.66	667.50	667.50
	37	38	39	40	41	42
Fr	716.62	716.62	819.04	827.11	833.03	833.03
	43	44	45	46	47	48
Fr	953.35	953.35	966.87	984.55	1002.22	1002.22

Zero-Point Energy = 25.60595895 kcal/mol

E_{tot}(B3LYP)=-1447.34172714 a. u.

B₁₀Au₁₀²⁻ D_{4d} B3LYP/B/cc-pvTZ/Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	-0.91946081	0.91946081	0.75869997
B	-0.91946081	-0.91946081	0.75869997
B	0.91946081	-0.91946081	0.75869997
B	0.91946081	0.91946081	0.75869997
B	-1.30031394	0.00000000	-0.75869997
B	0.00000000	1.30031394	-0.75869997
B	1.30031394	0.00000000	-0.75869997
B	0.00000000	-1.30031394	-0.75869997
B	0.00000000	0.00000000	1.84951271
B	0.00000000	0.00000000	-1.84951271
Au	-2.28074371	2.28074371	1.49244011
Au	2.28074371	2.28074371	1.49244011
Au	2.28074371	-2.28074371	1.49244011
Au	-2.28074371	-2.28074371	1.49244011
Au	3.22545869	0.00000000	-1.49244011
Au	0.00000000	3.22545869	-1.49244011
Au	-3.22545869	0.00000000	-1.49244011
Au	0.00000000	-3.22545869	-1.49244011
Au	0.00000000	0.00000000	-3.89998813
Au	0.00000000	0.00000000	3.89998813

	1	2	3	4	5	6
Fr	27.04	27.04	29.45	29.84	29.84	30.77
	7	8	9	10	11	12
Fr	30.77	32.71	33.16	33.16	37.04	37.04
	13	14	15	16	17	18
Fr	37.78	37.78	41.90	41.90	53.72	103.14
	19	20	21	22	23	24
Fr	103.14	108.08	110.56	110.56	111.82	113.65
	25	26	27	28	29	30
Fr	291.59	291.59	325.71	325.71	326.81	332.16
	31	32	33	34	35	36
Fr	387.80	493.56	493.56	505.66	505.66	577.78
	37	38	39	40	41	42
Fr	577.78	624.04	624.04	658.26	658.26	668.69
	43	44	45	46	47	48
Fr	793.33	793.33	813.38	813.38	822.33	876.68
	49	50	51	52	53	54
Fr	885.89	885.89	896.95	896.95	1024.84	1031.39

Zero-Point Energy = 29.39349341 kcal/mol

E_{tot}(B3LYP)=-1608.18496397 a. u.

B₁₁Au₁₁²⁻ C_{2v} B3LYP/B/cc-pvTZ/Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	0.00000000	0.00000000	-1.44539099
B	0.00000000	-1.65891477	-0.92447749
B	0.00000000	1.65891477	-0.92447749
B	0.00000000	1.47683184	0.82783094
B	0.00000000	-1.47683184	0.82783094
B	1.33718319	-0.93117073	-0.23729582
B	-1.33718319	-0.93117073	-0.23729582
B	-1.33718319	0.93117073	-0.23729582
B	1.33718319	0.93117073	-0.23729582
B	0.92363794	0.00000000	1.22238642
B	-0.92363794	0.00000000	1.22238642
Au	0.00000000	0.00000000	-3.51737647
Au	0.00000000	-3.35268323	-2.09800554
Au	0.00000000	3.35268323	-2.09800554
Au	3.21162569	-1.75575531	-0.54148680
Au	3.21162569	1.75575531	-0.54148680
Au	-3.21162569	1.75575531	-0.54148680
Au	-3.21162569	-1.75575531	-0.54148680
Au	0.00000000	3.12621172	2.07280363
Au	0.00000000	-3.12621172	2.07280363
Au	-2.15840712	0.00000000	2.88271764
Au	2.15840712	0.00000000	2.88271764

Fr	1	2	3	4	5	6
	34.236	38.536	38.777	40.419	41.005	41.482
Fr	7	8	9	10	11	12
	41.645	41.932	42.154	42.210	42.321	42.416
Fr	13	14	15	16	17	18
	42.876	42.951	45.053	45.830	56.426	57.344
Fr	19	20	21	22	23	24
	59.699	94.371	102.537	108.034	109.679	110.826
Fr	25	26	27	28	29	30
	111.804	113.238	115.132	311.323	325.593	326.517
Fr	31	32	33	34	35	36
	332.789	343.839	344.224	390.429	437.055	474.130
Fr	37	38	39	40	41	42
	494.109	500.627	580.063	586.636	599.166	633.074
Fr	43	44	45	46	47	48
	637.471	680.041	681.301	738.342	745.397	749.056
Fr	49	50	51	52	53	54
	783.566	810.890	822.244	849.051	875.689	876.553
Fr	55	56	57	58	59	60
	908.632	911.443	952.916	974.640	1000.660	1017.279

E_{tot}(B3LYP)=-1769.055913 a. u.

B₁₂Au₁₂²⁻ I_h B3LYP/B/cc-pvTZ/Au/Stuttgart_rsc_1997_ecp

	x	y	z
B	0.00000000	0.00000000	1.69501238
B	1.22652248	-0.89112074	0.75803258
B	1.51606516	0.00000000	-0.75803258
B	0.46848990	1.44186365	-0.75803258
B	-1.22652248	-0.89112074	-0.75803258
B	-1.22652248	0.89112074	-0.75803258
B	-0.46848990	-1.44186365	0.75803258
B	0.00000000	0.00000000	-1.69501238
B	-0.46848990	1.44186365	0.75803258
B	1.22652248	0.89112074	0.75803258
B	-1.51606516	0.00000000	0.75803258
B	0.46848990	-1.44186365	-0.75803258
Au	0.00000000	0.00000000	3.75812991
Au	2.71940835	-1.97576581	1.68068679
Au	3.36137358	0.00000000	-1.68068679
Au	1.03872156	3.19685624	-1.68068679
Au	-2.71940835	-1.97576581	-1.68068679
Au	-2.71940835	1.97576581	-1.68068679
Au	-1.03872156	-3.19685624	1.68068679
Au	0.00000000	0.00000000	-3.75812991
Au	-1.03872156	3.19685624	1.68068679
Au	2.71940835	1.97576581	1.68068679
Au	-3.36137358	0.00000000	1.68068679
Au	1.03872156	-3.19685624	-1.68068679

Fr	1	2	3	4	5	6
	37.643	37.643	37.643	37.643	38.453	38.453
Fr	7	8	9	10	11	12
	38.453	38.453	38.453	38.965	38.965	38.965
Fr	13	14	15	16	17	18
	38.965	39.587	39.587	39.587	39.587	39.587
Fr	19	20	21	22	23	24
	63.622	63.622	63.622	109.098	109.098	109.098
Fr	25	26	27	28	29	30
	109.098	109.098	114.045	114.330	114.330	114.330
Fr	31	32	33	34	35	36
	337.863	337.863	337.863	353.932	353.932	353.932
Fr	37	38	39	40	41	42
	552.301	552.301	552.301	552.301	552.301	664.729
Fr	43	44	45	46	47	48
	664.729	664.729	664.729	664.729	717.197	717.197
Fr	49	50	51	52	53	54
	717.197	717.197	793.397	793.397	793.397	793.397
Fr	55	56	57	58	59	60
	842.121	842.121	842.121	853.584	904.949	904.949
Fr	61	62	63	64	65	66
	904.949	904.949	904.949	926.080	926.080	926.080

E_{tot}(B3LYP)=-1929.877711 a. u.