

**Structures, stabilities and spectral properties of  
metalloborospherenes  $MB_{40}^{0/-}$  (M=Cu, Ag, and Au)**

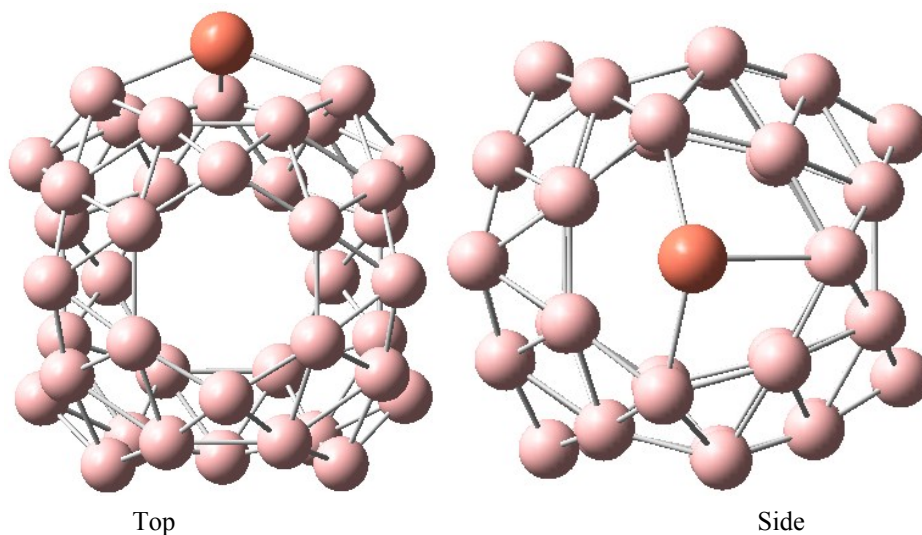
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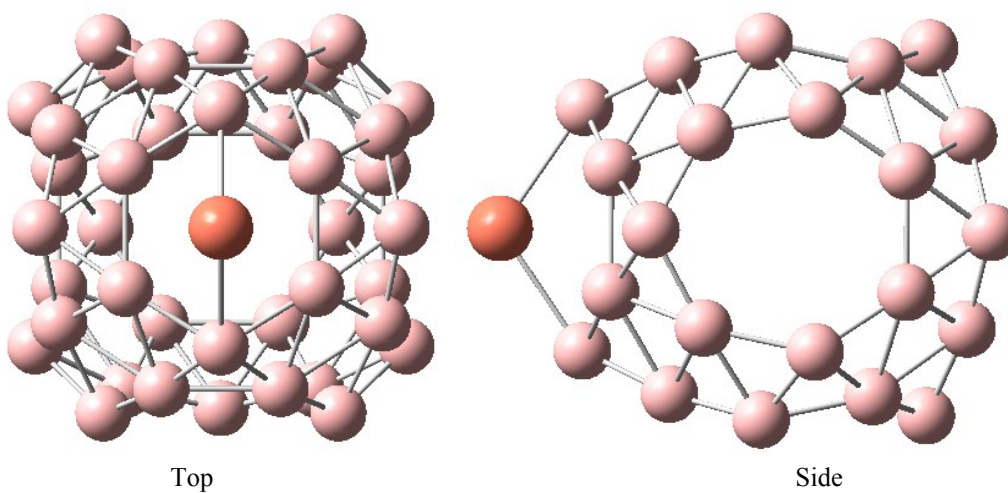
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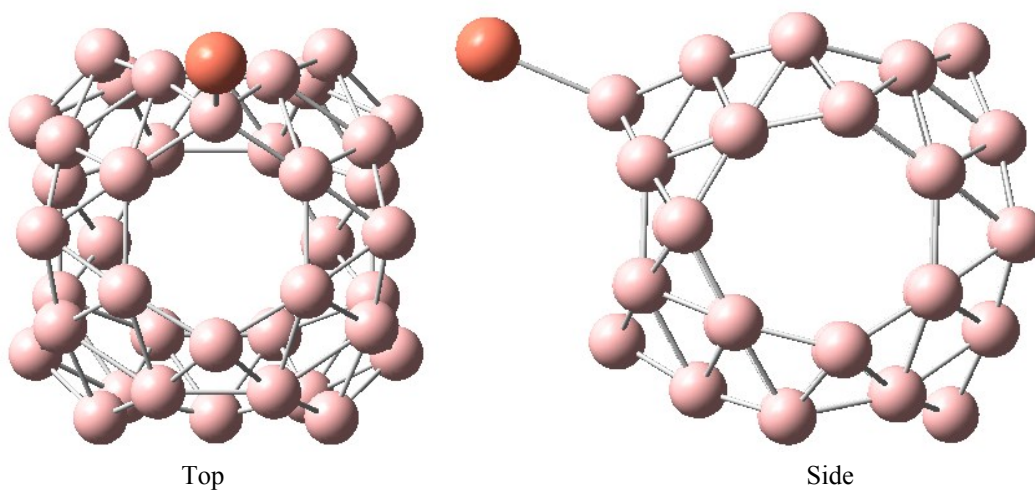
<sup>d</sup>*Key Lab of Photoelectron Technology and Application, Guizhou University, Guiyang 550025, China*



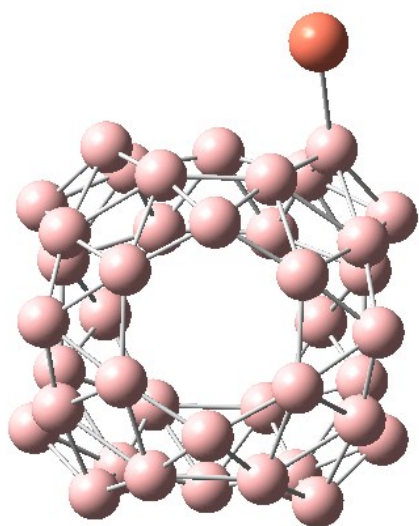
(a) Cu&B<sub>40</sub><sup>0/-</sup> path: Ly (0.00) [0.00]



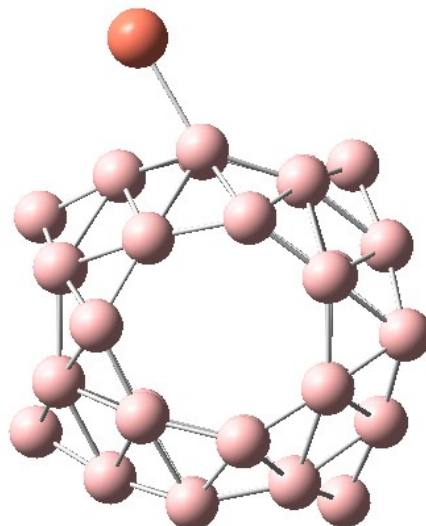
(b) Cu&B<sub>40</sub><sup>0/-</sup> path: Lz (0.33) [0.08]



(c) Cu&B<sub>40</sub><sup>0/-</sup> path: Lyz (0.70) [0.23]

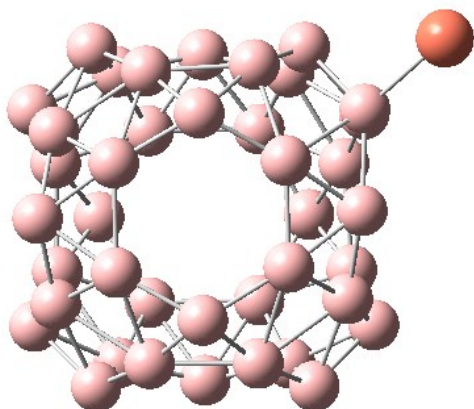


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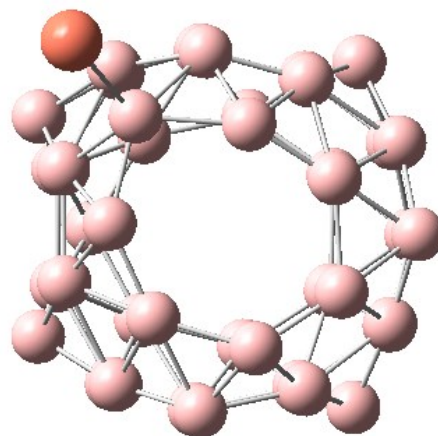


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(d) Cu&B<sub>40</sub> path: Lxyz (0.70)

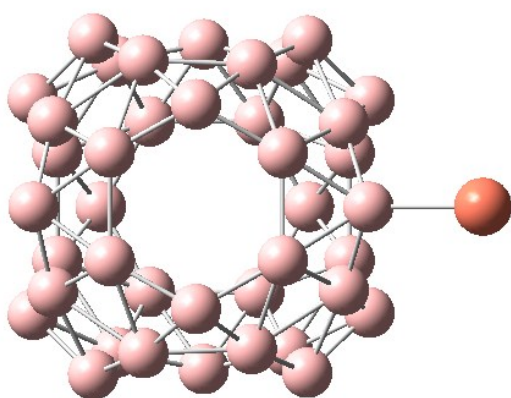


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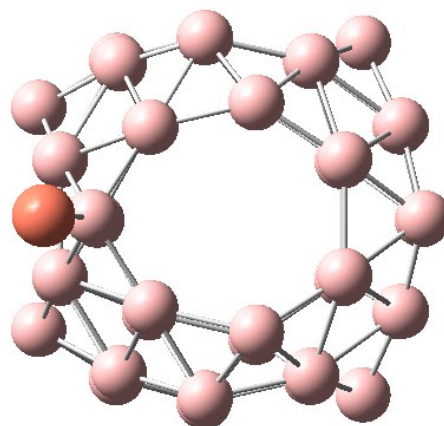


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(e) Cu&B<sub>40</sub><sup>-</sup> path: Lxyz [0.60]

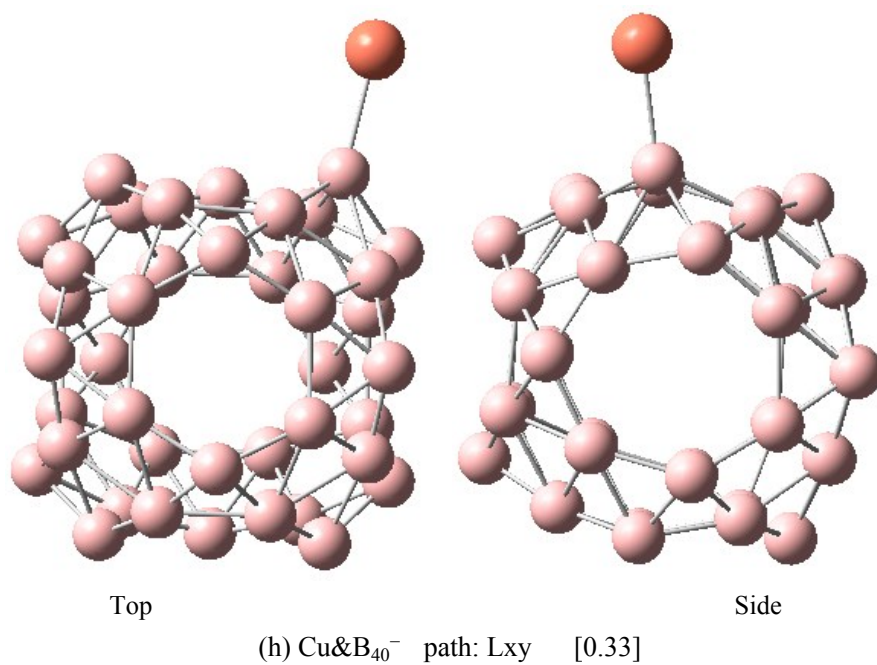
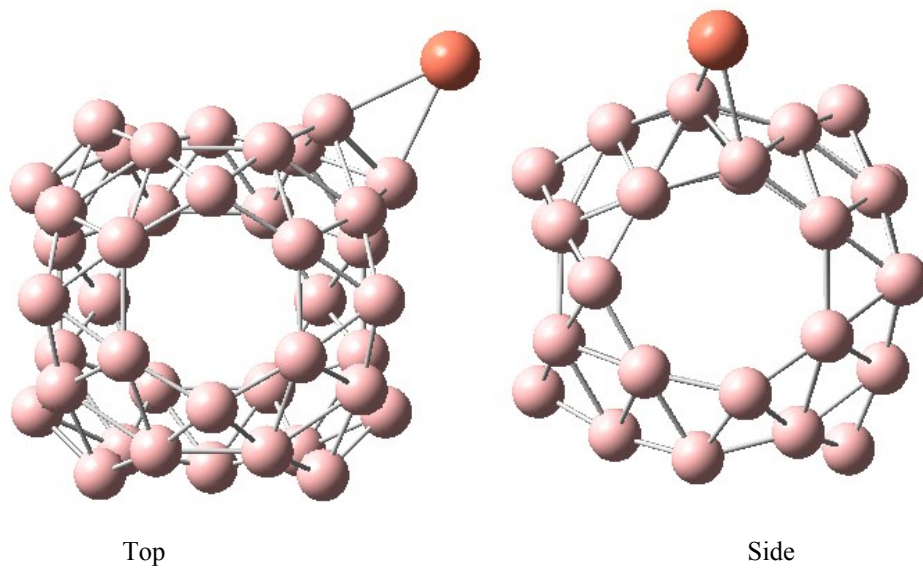


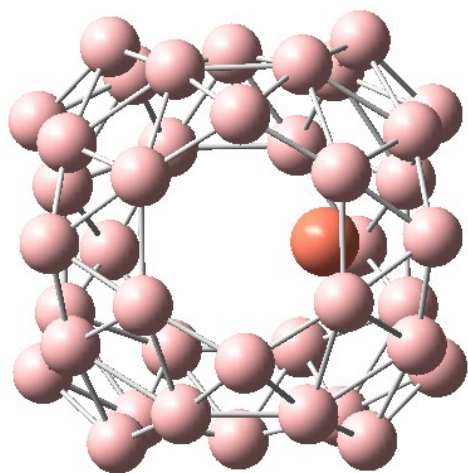
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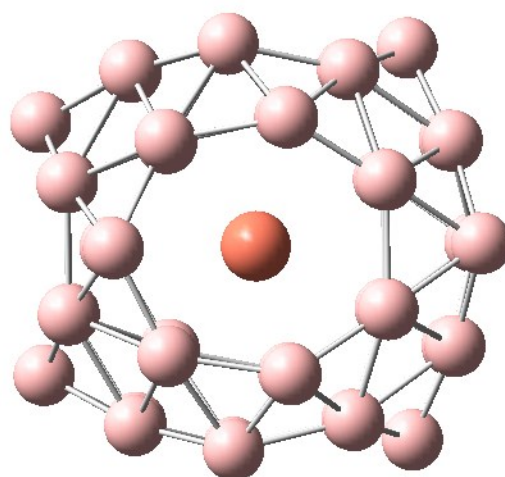
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(f) Cu&B<sub>40</sub><sup>0/-</sup> path: Lxz (0.81) [0.54]



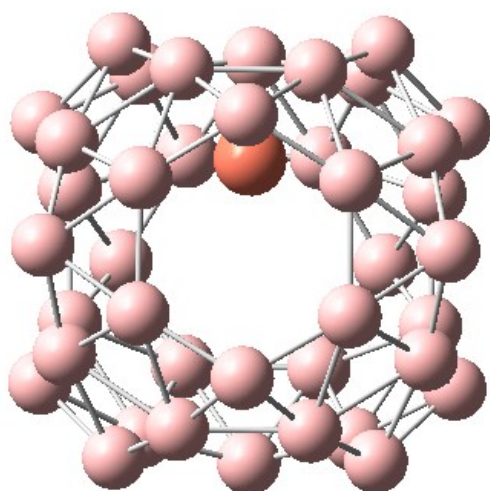


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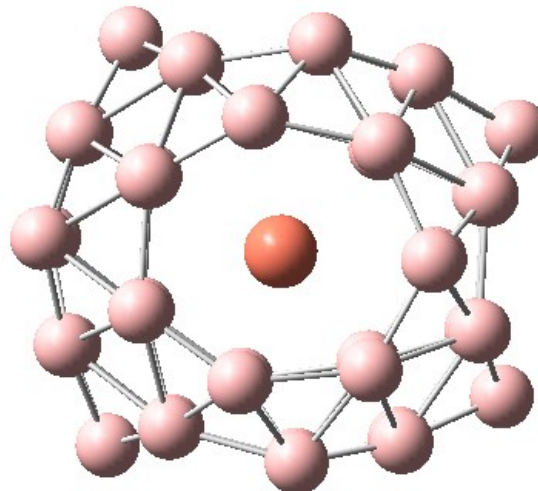


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(i) Cu@B<sub>40</sub><sup>0/-</sup> path: Lxz (1.04) [0.89]

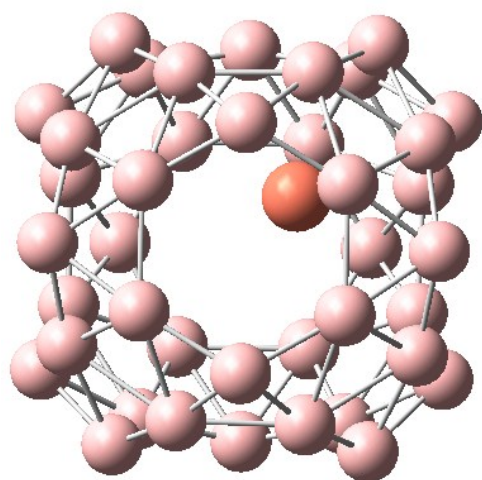


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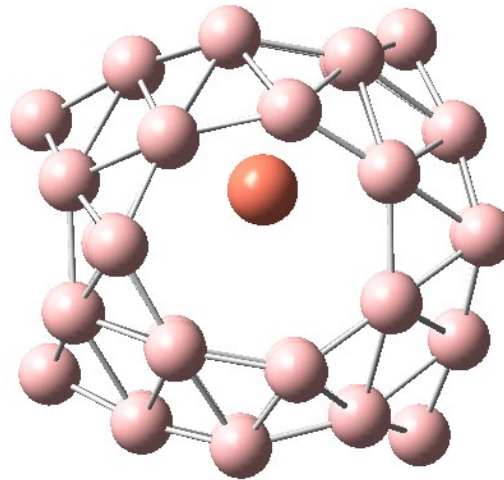


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(j) Cu@B<sub>40</sub><sup>0/-</sup> paths: Ly, Lyz, and Lxyz (1.04) [0.89]

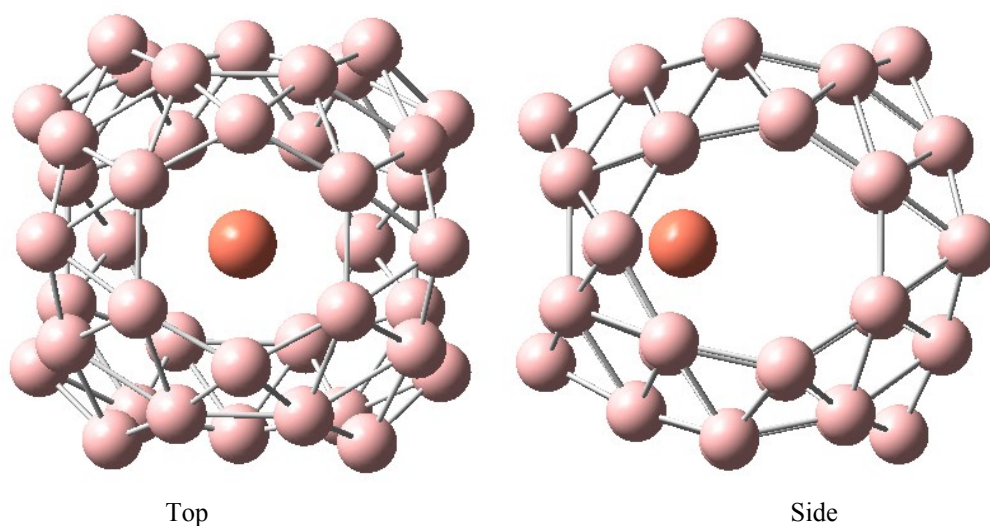


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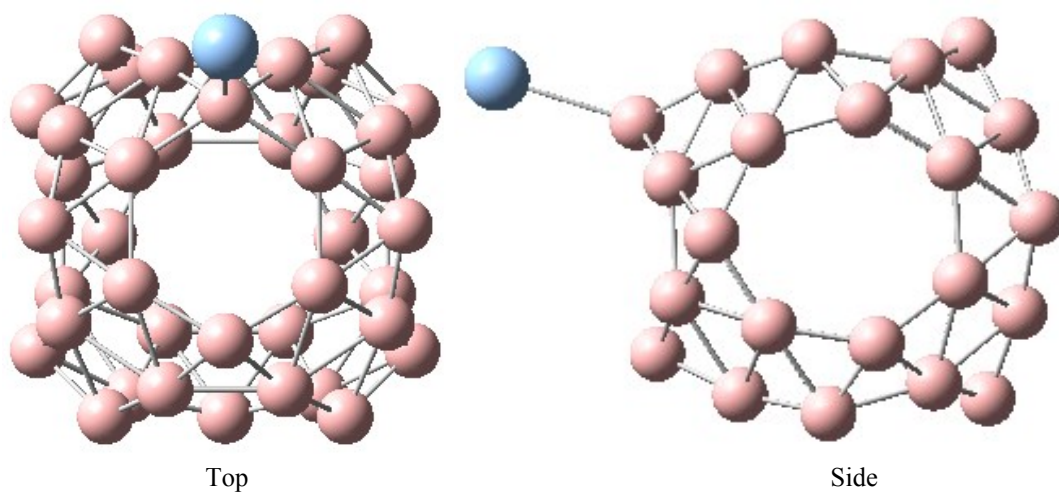
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(k) Cu@B<sub>40</sub><sup>0/-</sup> path: Lxy (1.15) [1.04]

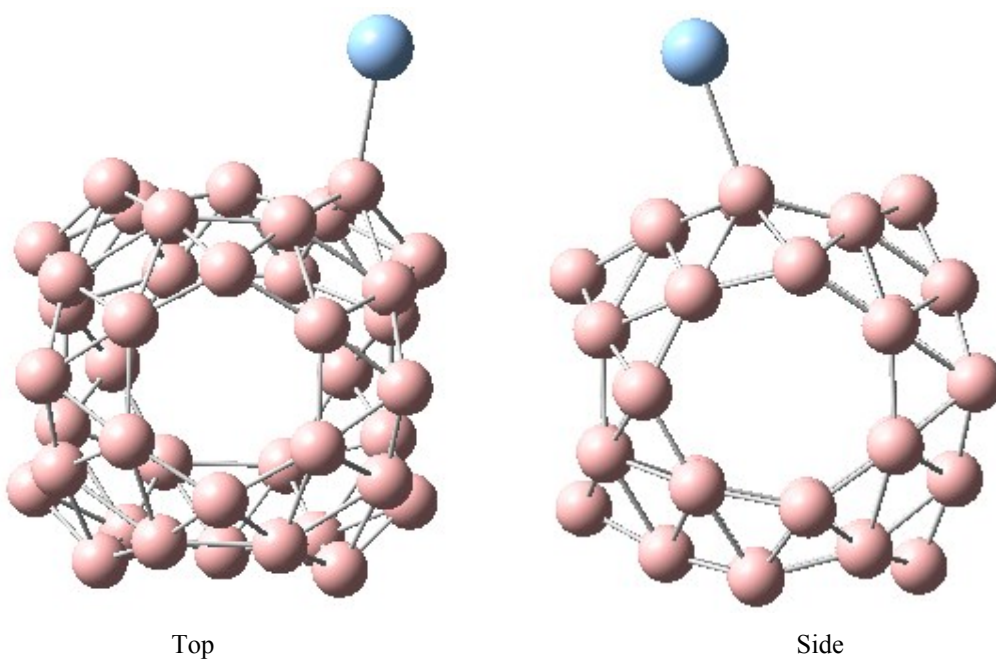


(1)  $\text{Cu@B}_{40}^{0/-}$  path: Lz (1.27) [1.15]

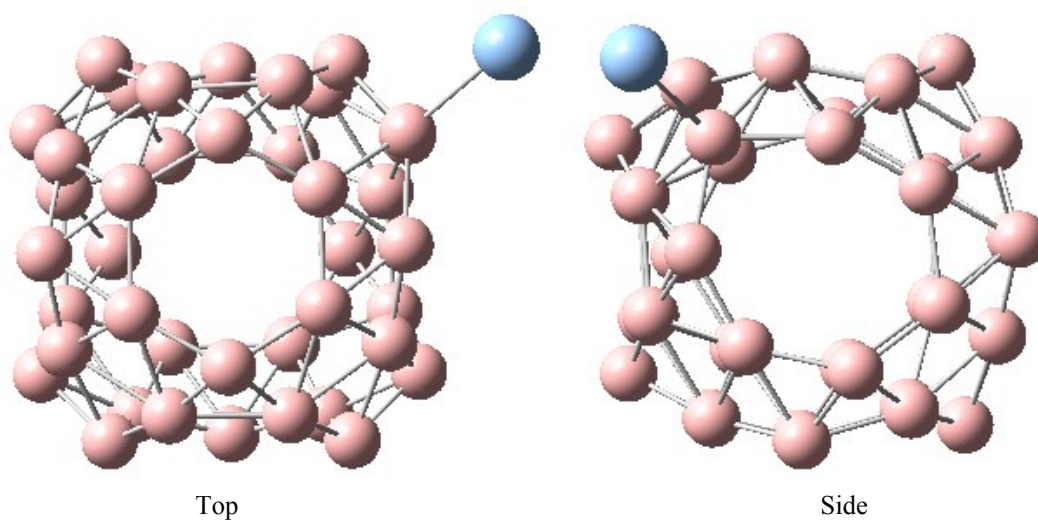
Fig. S1 Optimized structures of metalloborospherenes  $\text{CuB}_{40}^{0/-}$  for the two local minima (one corresponds to the endohedral  $\text{Cu@B}_{40}^{0/-}$ , another corresponds to the exohedral  $\text{Cu@B}_{40}^{0/-}$ ) in the six paths. The round brackets denote the relative energies (eV) of neutral metalloborospherenes  $\text{CuB}_{40}$ , the square brackets denote the relative energies (eV) of anionic metalloborospherenes  $\text{CuB}_{40}^-$ .



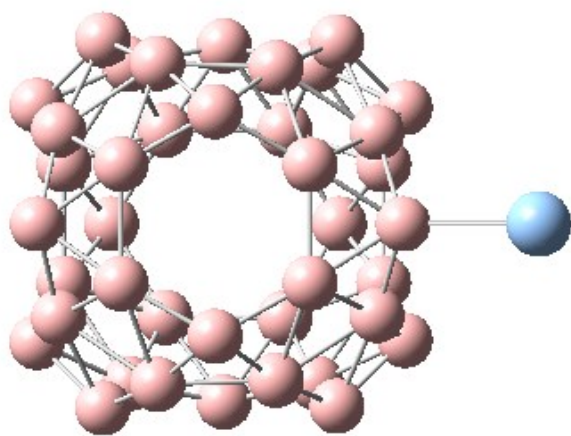
(a) Ag&B<sub>40</sub><sup>0/-</sup> path: Lyz (0.00) [0.00]



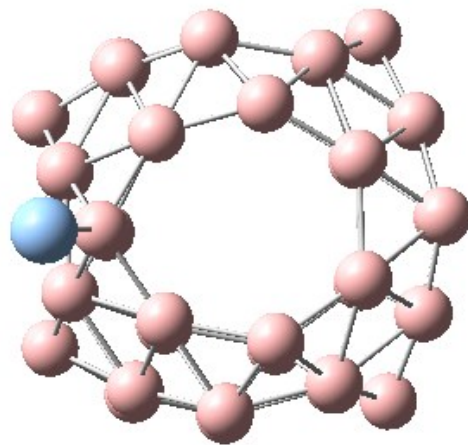
(b) Ag&B<sub>40</sub> path: Lxyz (0.07)



(c) Ag&B<sub>40</sub><sup>-</sup> path: Lxyz [0.39]

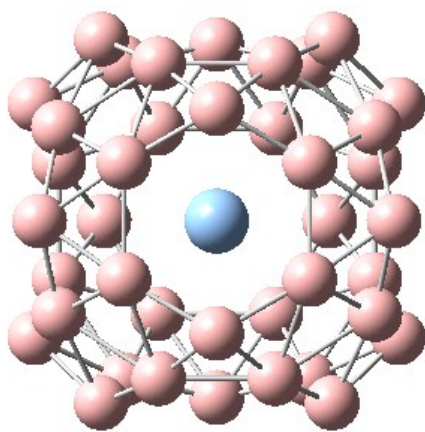


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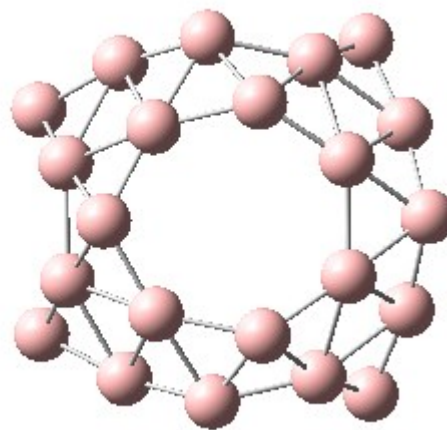


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(d) Ag&B<sub>40</sub><sup>0/-</sup> path: Lxz (0.10) [0.31]

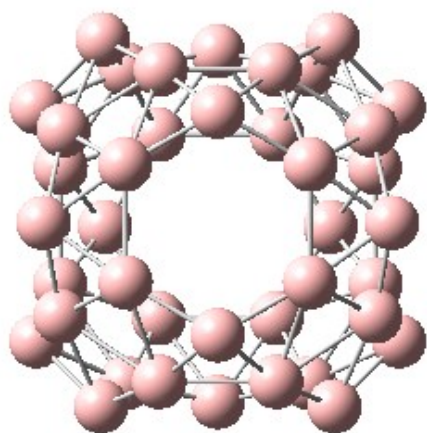


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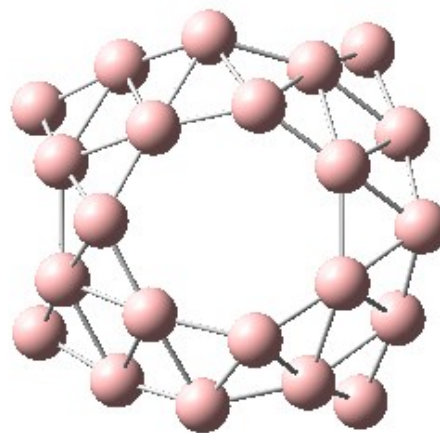


Side

(e) Ag&B<sub>40</sub><sup>0/-</sup> path: Lz (0.22) [0.31]



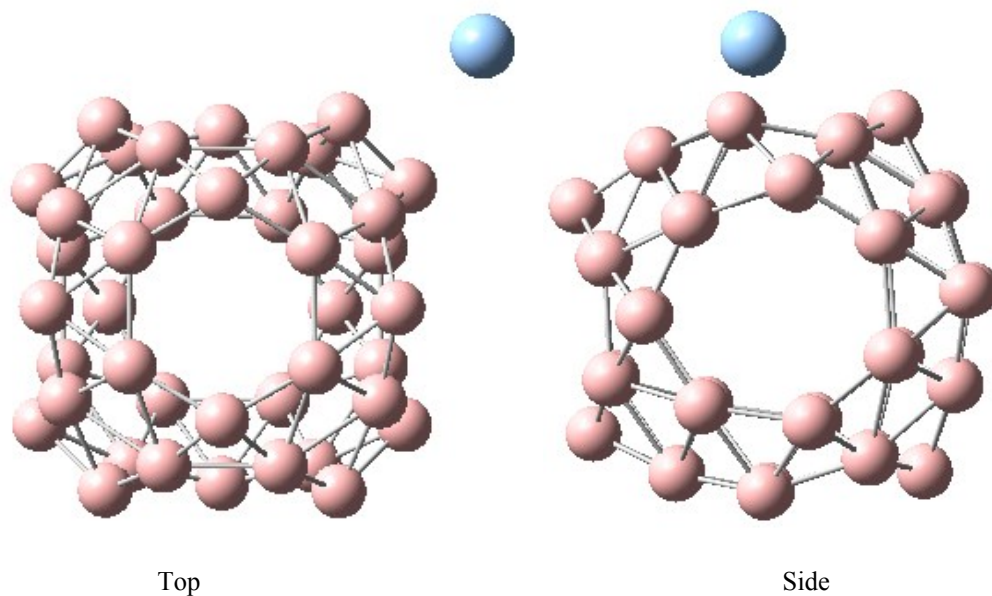
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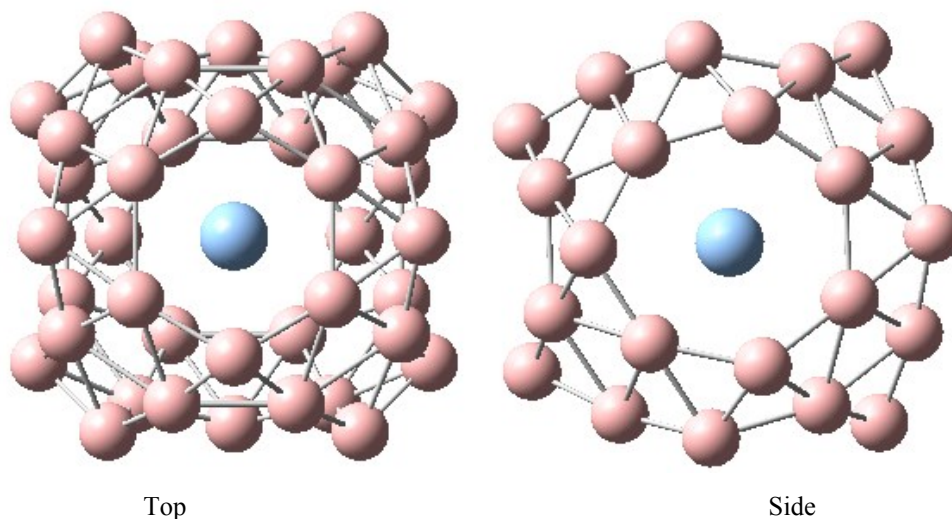
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(f) Ag&B<sub>40</sub><sup>0/-</sup> path: Ly (0.22) [0.50]



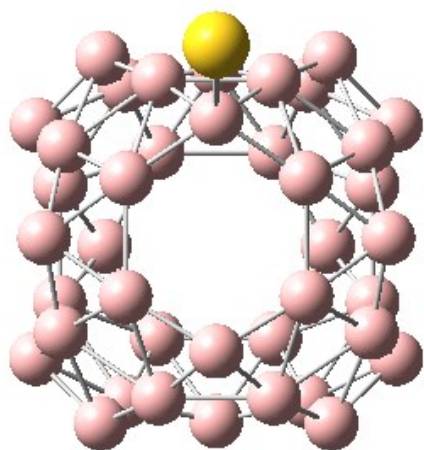


(g)  $\text{Ag}\&\text{B}_{40}^{0-}$  path: Lxy (0.39) [0.84]

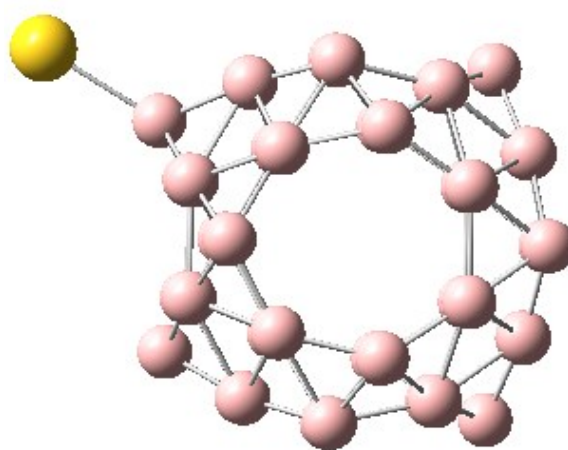


(h)  $\text{Ag}\@\text{B}_{40}^{0-}$  paths: Ly, Lz, Lxy, Lxz, Lyz, and Lxyz (1.19) [1.53]

Fig. S2 Optimized structures of metalloborospherenes  $\text{AgB}_{40}^{0-}$  for the two local minima (one corresponds to the endohedral  $\text{Ag}\&\text{B}_{40}^{0-}$ , another corresponds to the exohedral  $\text{Ag}\@\text{B}_{40}^{0-}$ ) in the six paths. The round brackets denote the relative energies (eV) of neutral metalloborospherenes  $\text{AgB}_{40}$ , the square brackets denote the relative energies (eV) of anionic metalloborospherenes  $\text{AgB}_{40}^-$ .

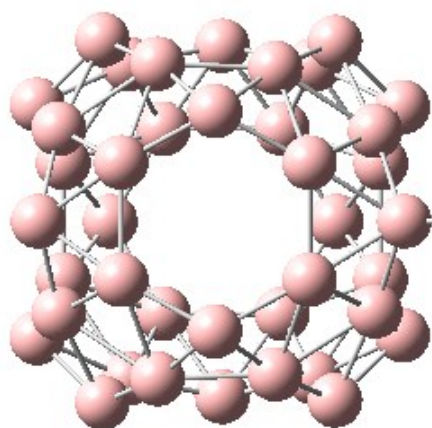


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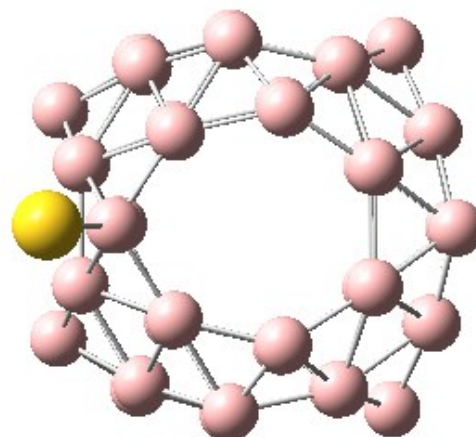


Side

(a) Au&B<sub>40</sub><sup>0/-</sup> path: Lyz (0.00) [0.00]

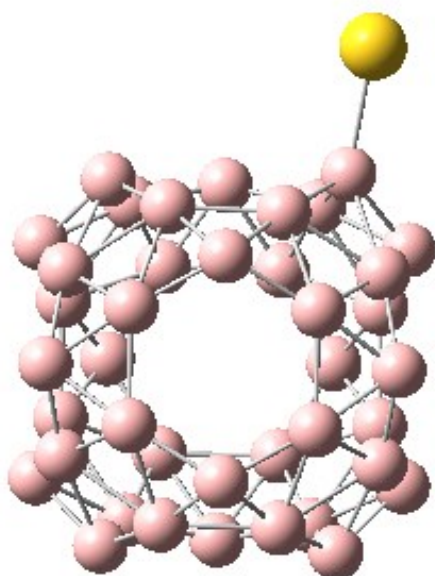


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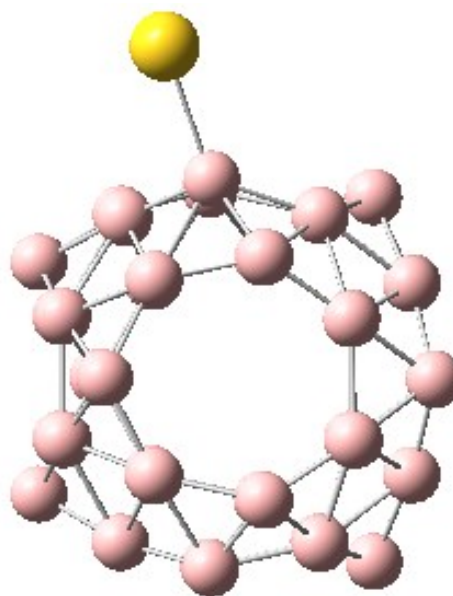


Side

(b) Au&B<sub>40</sub><sup>0/-</sup> path: Lxz (0.04) [0.22]

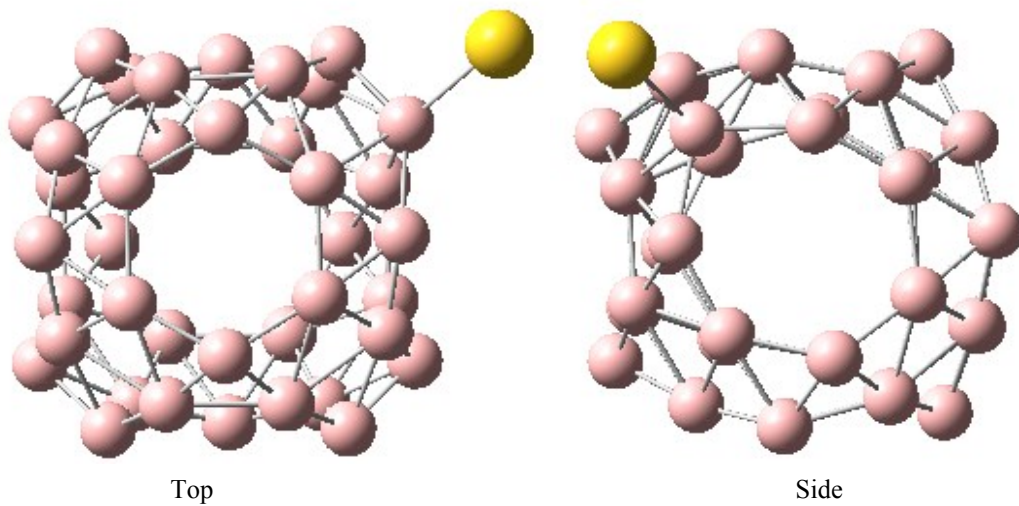


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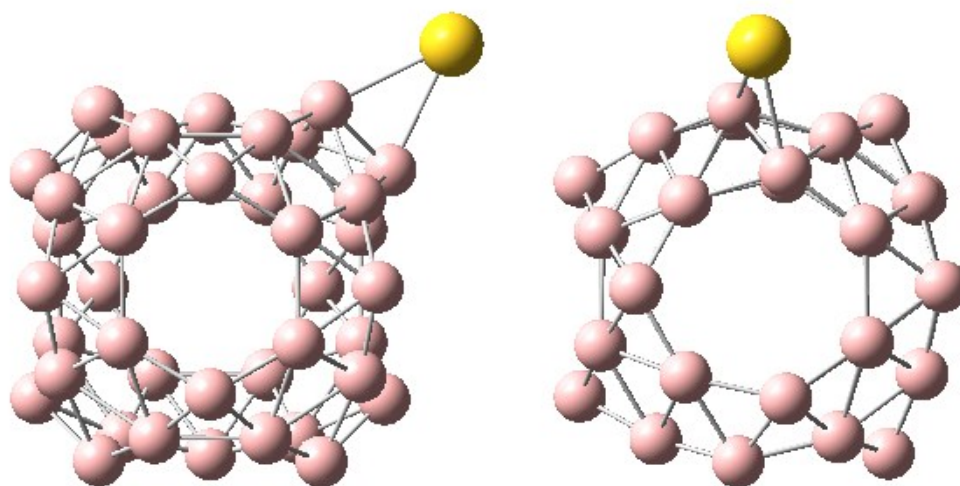


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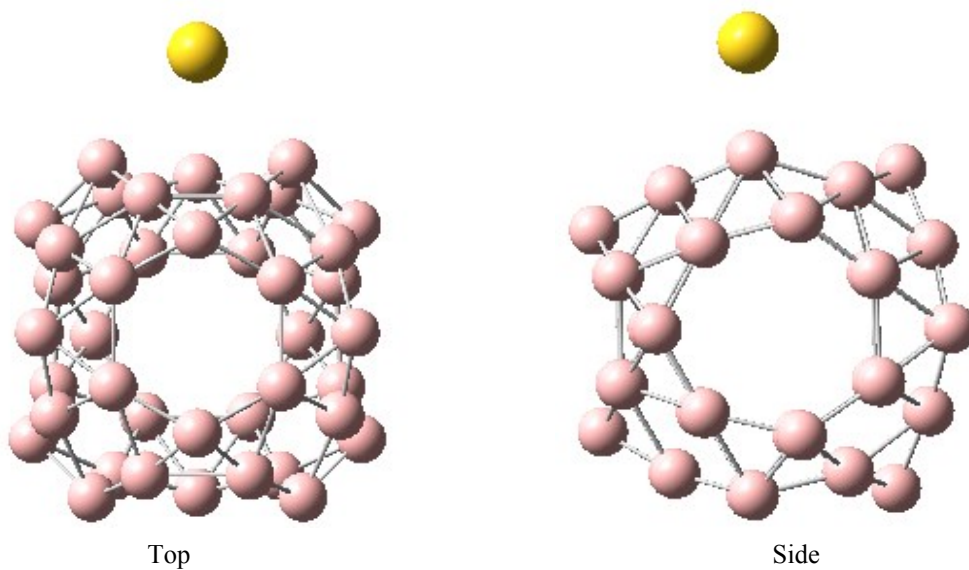
(c) Au&B<sub>40</sub> path: Lxyz (0.06)



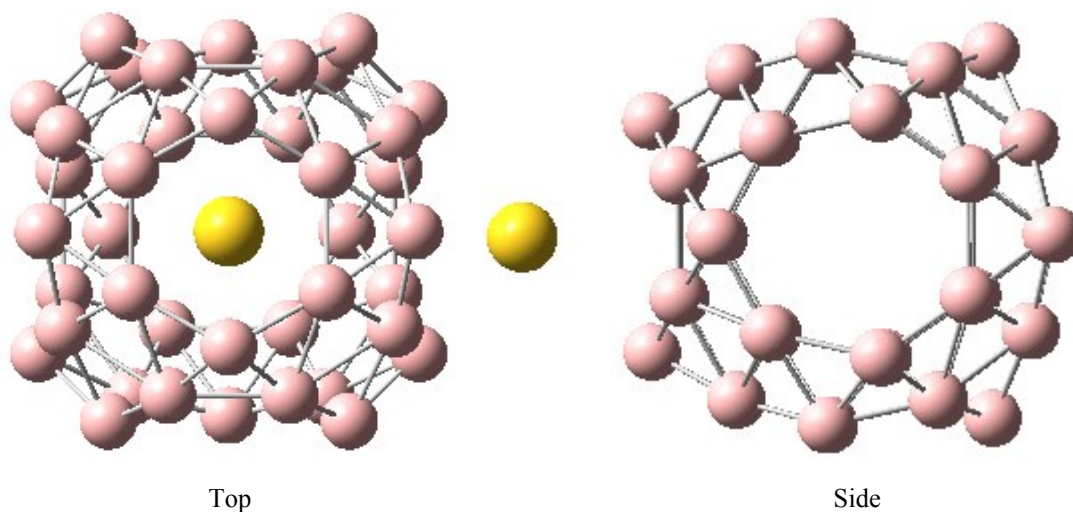
(d) Au&B<sub>40</sub><sup>-</sup> path: Lxyz [0.28]



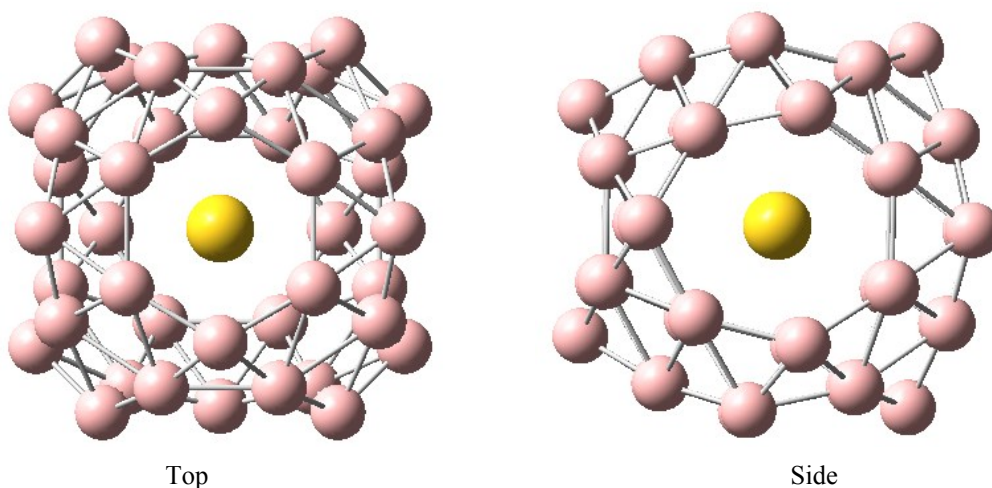
(e) Au&B<sub>40</sub><sup>0/-</sup> path: Lxy (0.24) [0.76]



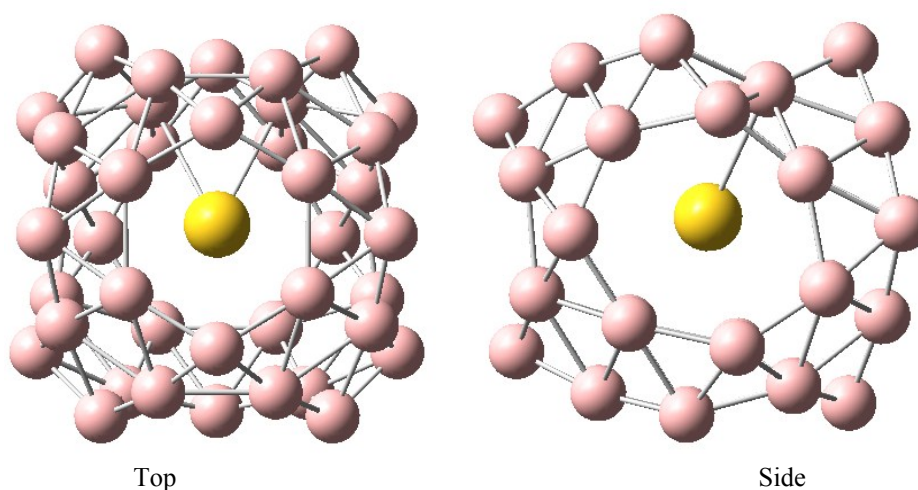
(f) Au&B<sub>40</sub><sup>0/-</sup> path: Ly (0.73) [1.05]



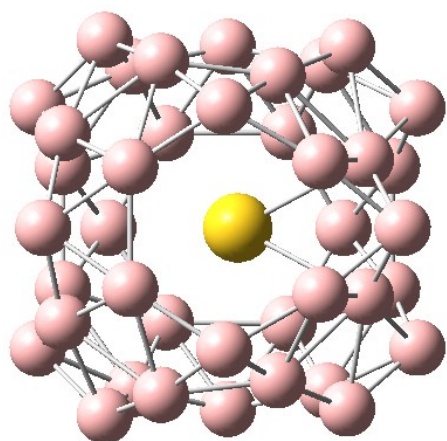
(g) Au&B<sub>40</sub><sup>0-</sup> path: Lz (0.87) [1.03]



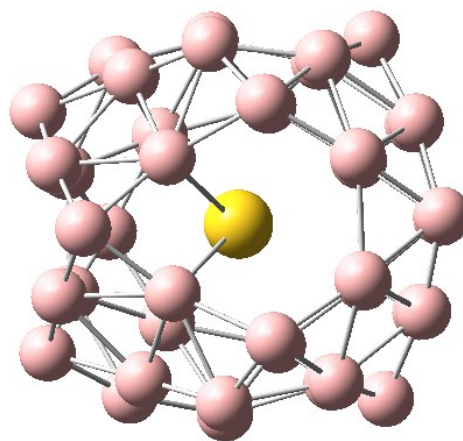
(h) Au@B<sub>40</sub> paths: Ly, Lz, Lxy, Lxz, Lyz, and Lxyz (2.50)



(i) Au@B<sub>40</sub><sup>-</sup> paths: Lyz and Lxyz [2.90]

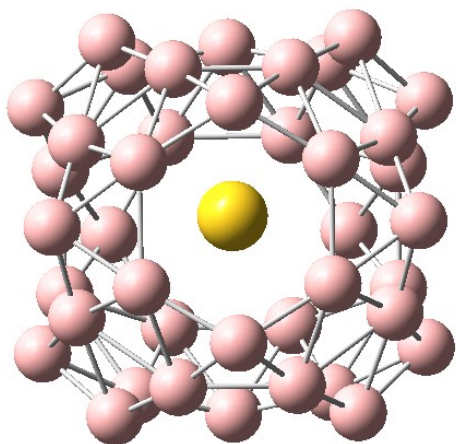


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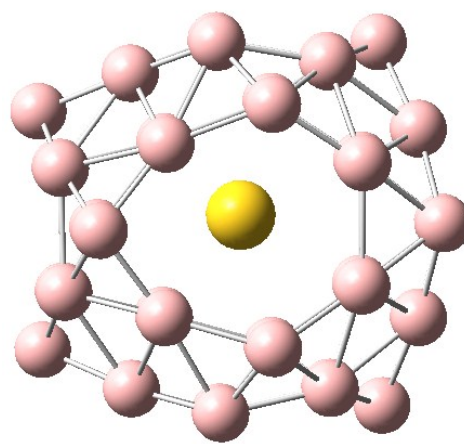


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(j) Au@B<sub>40</sub><sup>-</sup> path: Lxz [2.90]

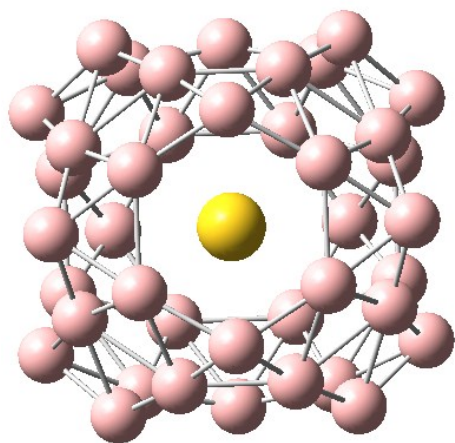


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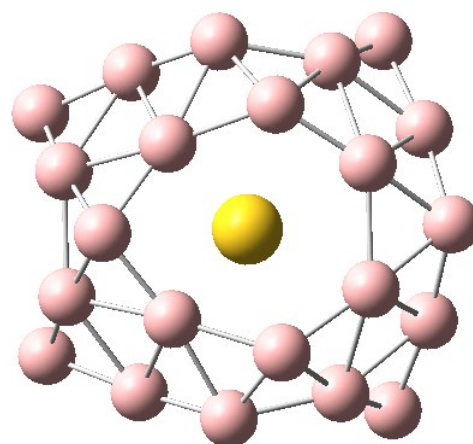


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(k) Au@B<sub>40</sub><sup>-</sup> path: Ly [3.18]

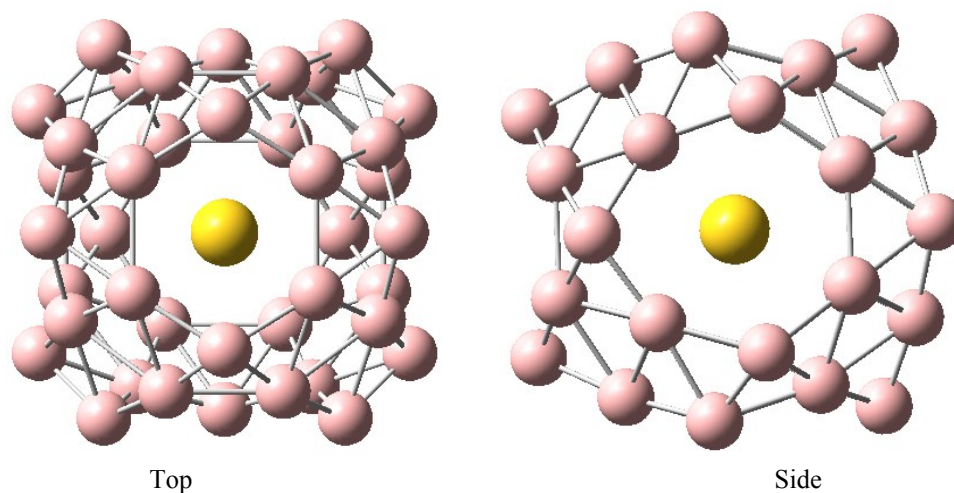


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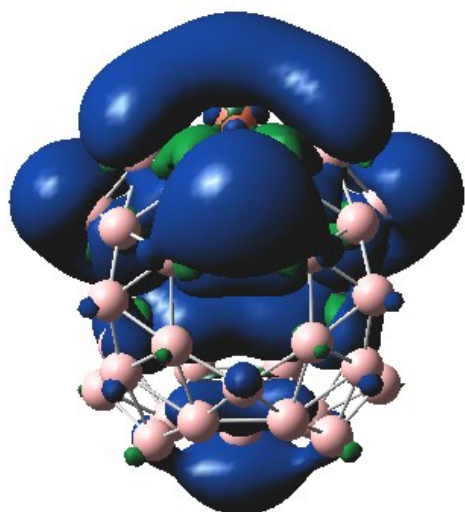
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(l) Au@B<sub>40</sub><sup>-</sup> path: Lz [3.20]

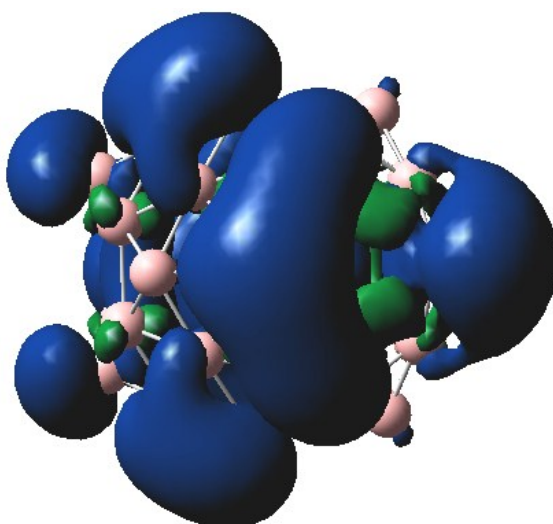


(m) Au@B<sub>40</sub><sup>-</sup> path: Lxy [3.37]

Fig. S3 Optimized structures of metalloborospherenes AuB<sub>40</sub><sup>0/-</sup> for the two local minima (one corresponds to the endohedral Au&B<sub>40</sub><sup>0/-</sup>, another corresponds to the exohedral Au@B<sub>40</sub><sup>0/-</sup>) in the six paths. The round brackets denote the relative energies (eV) of neutral metalloborospherenes AuB<sub>40</sub>, the square brackets denote the relative energies (eV) of anionic metalloborospherenes AuB<sub>40</sub><sup>-</sup>.

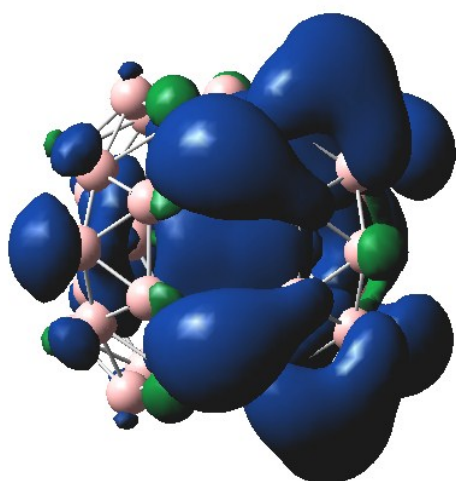


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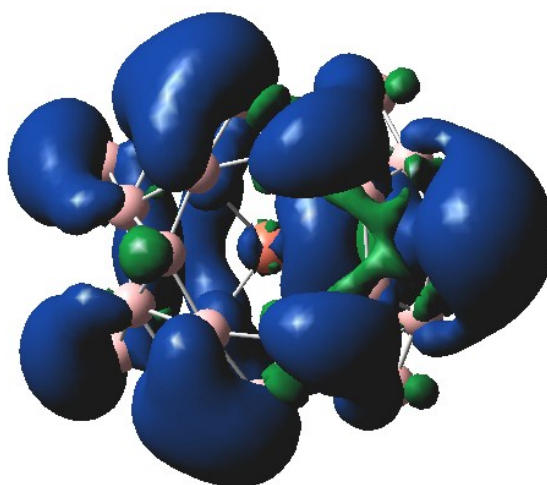


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(a)

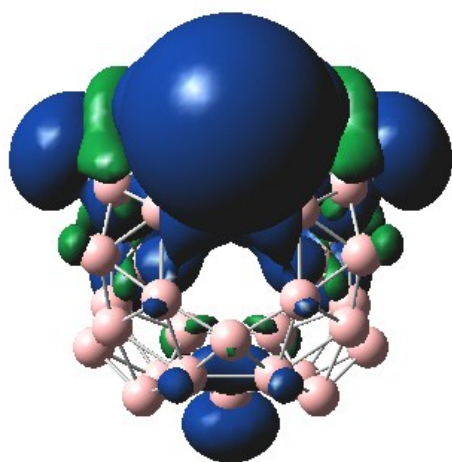


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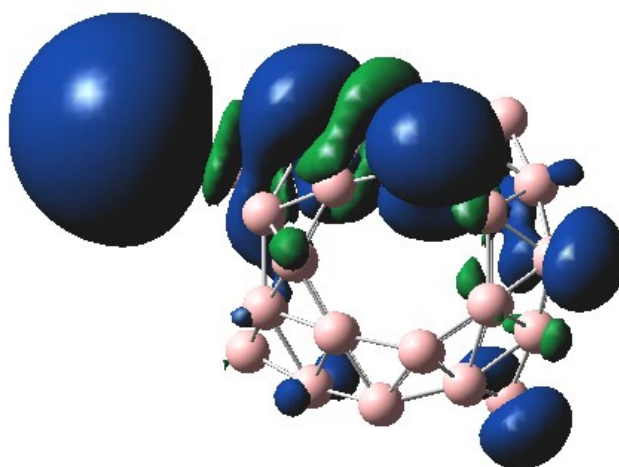


Side

(b)



Top



Side

(c)

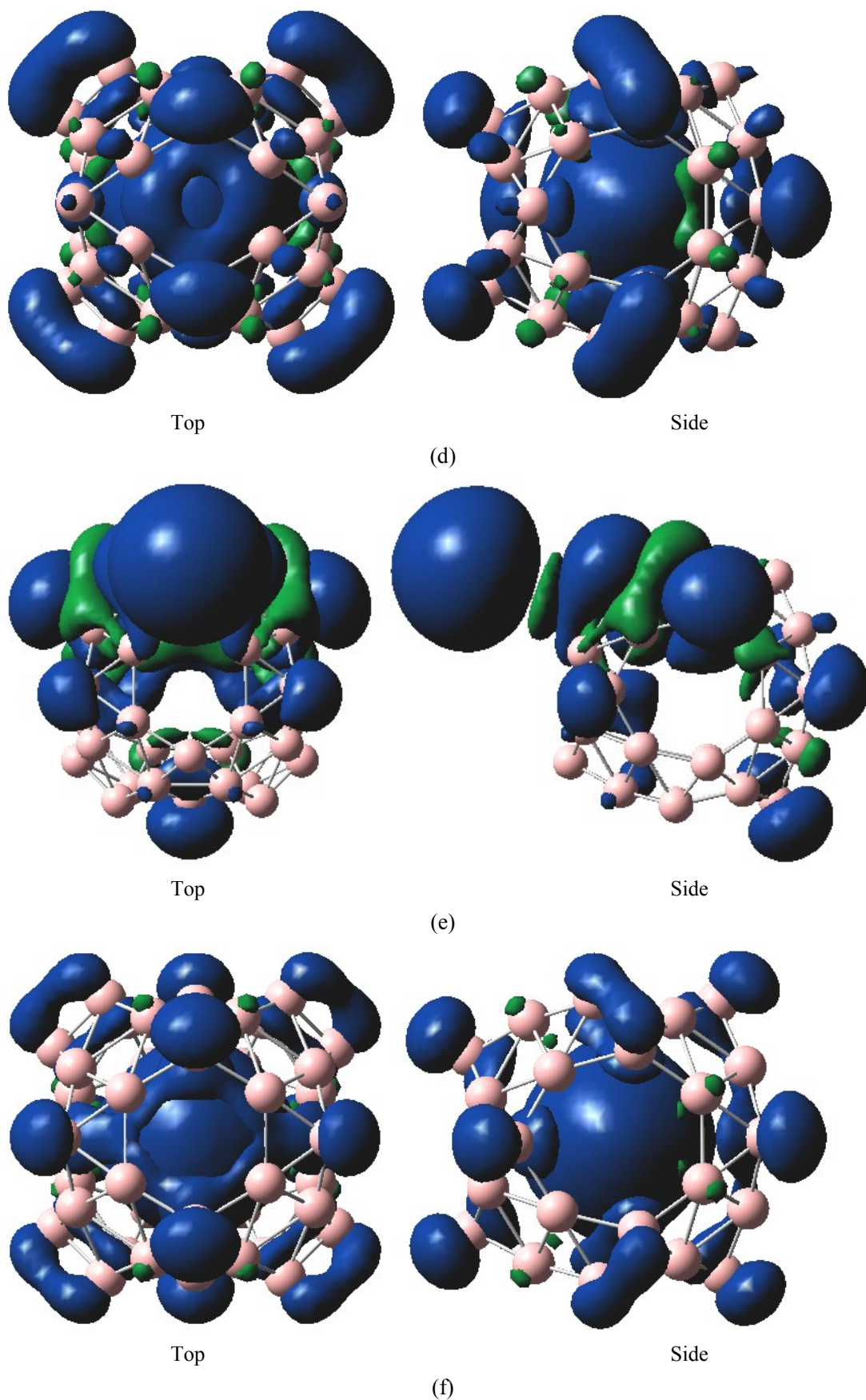


Fig. S4 Spin densities (isosurface value = 0.0004, blue denotes the positive value (up-spin component) and green denotes the negative value (down-spin component)) of



metalloborospherenes MB<sub>40</sub> (M=Cu, Ag, and Au). (a): C<sub>s</sub> Cu&B<sub>40</sub>, (b): C<sub>s</sub> Cu@B<sub>40</sub>, (c): C<sub>s</sub> Ag&B<sub>40</sub>, (d): D<sub>2d</sub> Ag@B<sub>40</sub>, (e): C<sub>s</sub> Au&B<sub>40</sub>, (f): D<sub>2d</sub> Au@B<sub>40</sub>.

Table S1. Calculated VDEs for metalloborospherenes MB<sub>40</sub><sup>-</sup> (M=Cu, Ag, and Au).

Calculated VDEs(eV)						
	Cu&B <sub>40</sub> <sup>-</sup>	Cu@B <sub>40</sub> <sup>-</sup>	Ag&B <sub>40</sub> <sup>-</sup>	Ag@B <sub>40</sub> <sup>-</sup>	Au&B <sub>40</sub> <sup>-</sup>	Au@B <sub>40</sub> <sup>-</sup>
1	2.46	2.64	2.98	2.63	3.46	3.60
2	3.22	3.49	4.34	3.34	4.45	4.17
3	3.25	3.50	4.37	3.34	4.52	4.38
4	3.38	3.80	4.39	3.64	4.54	4.52
5	3.70	4.00	4.50	3.75	4.63	4.53
6	4.03	4.19	4.57	4.15	4.76	4.60
7	4.10	4.21	4.60	4.17	4.84	4.64
8	4.27	4.32	4.64	4.17	4.99	4.87
9	4.37	4.33	4.7	4.21	5.17	4.91
10	4.39	4.36	4.75	4.40	5.35	5.23
11	4.48	4.48	4.84	4.40	5.44	5.40
12	4.51	4.50	4.90	4.40	5.62	5.53
13	4.58	4.55	5.50	4.50	5.66	5.56
14	4.77	4.56	5.51	4.53	5.75	5.62
15	4.82	4.60		4.6		5.87
16	4.95	4.62		4.62		5.88
17	4.96	4.69		4.65		5.88
18	4.98	4.70		4.71		
19	4.99	4.85		4.71		
20		5.05		4.91		
21		5.06		5.15		
22				5.22		
23				5.22		

Table S2. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Cu&B<sub>40</sub>.

Mode # ▲	Freq	Infrared	Raman Activity
1	115.83	0.1512	24.6995
2	165.82	1.0189	39.6286
3	171.16	0.1836	9.9920
4	191.08	1.0584	2.6853
5	191.97	0.0237	38.4866
6	210.52	0.0456	19.9808
7	217.43	0.0119	27.0265
8	230.29	0.0011	27.9995
9	236.77	1.5944	23.4927
10	242.51	0.1483	2.1024
11	246.85	0.3780	9.5792
12	262.04	0.0043	8.1472
13	270.91	1.4582	0.2520
14	292.55	1.6631	23.1288
15	300.53	4.6843	4.4389
16	305.99	8.8625	46.9226
17	324.74	5.4717	1.8315
18	325.39	5.0637	10.7723
19	332.90	0.3162	28.8012
20	334.84	11.3221	9.9175
21	347.49	0.4201	15.2012
22	352.75	0.6668	0.2192
23	360.39	0.8231	39.0297
24	367.63	5.7865	15.3074
25	370.94	6.0529	0.4856
26	374.51	10.5582	5.1010
27	382.75	0.2023	6.7621
28	387.82	2.4559	22.4520
29	394.20	1.2327	7.2461
30	399.67	0.6479	6.1340
31	404.89	0.8202	7.6044
32	407.19	3.6839	18.3357
33	415.49	0.6463	1.0634
34	426.66	2.6794	54.3479
35	426.98	11.8919	5.9365
36	430.63	0.1730	36.1713
37	434.76	0.4609	83.0984
38	444.03	9.1486	6.7334
39	447.67	1.8844	5.2038
40	456.02	0.7657	48.9624
41	465.85	2.7600	31.7178
42	467.66	1.1672	2.6003
43	470.88	3.0229	0.8791
44	476.18	0.6827	2.3013
45	476.88	1.3629	5.1463
46	480.22	3.1663	26.4101
47	488.50	0.0660	23.0488
48	491.84	1.2917	4.7560
49	504.77	1.9367	26.8927
50	505.87	1.3510	11.4217
51	515.98	1.4391	17.4645
52	524.80	2.0496	0.2423

53	562.87	4.1705	48.8438
54	576.47	4.6702	23.1293
55	578.15	1.9989	2.4559
56	583.21	0.0444	3.5213
57	603.04	1.8045	3.0543
58	609.42	17.1477	8.0684
59	613.15	3.0324	5.4679
60	619.95	2.8859	11.3263
61	626.99	0.0112	4.0138
62	644.86	0.6981	22.3171
63	648.39	0.0603	0.1913
64	649.90	0.4968	28.9570
65	658.57	4.9490	33.5554
66	658.96	3.8986	4.7196
67	679.45	2.4321	34.0683
68	683.49	0.1146	11.7472
69	684.82	1.2813	57.3869
70	695.27	2.9780	6.6248
71	698.93	3.9765	62.5126
72	707.20	0.7956	27.1014
73	722.77	1.7963	46.4262
74	748.37	10.9543	19.1270
75	753.11	0.3507	14.0658
76	760.01	24.6739	17.5479
77	761.90	1.4256	5.1579
78	772.86	16.7889	33.6706
79	779.81	6.4007	5.3675
80	802.15	0.3768	59.9769
81	805.00	0.0184	35.8318
82	818.00	1.9029	5.7969
83	825.21	10.8376	19.1046
84	840.02	16.0753	7.0993
85	849.64	0.0033	11.6573
86	853.80	2.5534	13.3892
87	861.00	1.1607	4.8640
88	882.11	0.3202	10.3383
89	892.62	2.4008	1.6981
90	908.46	2.0187	24.2793
91	963.92	8.9560	14.0171
92	989.44	9.0937	3.1791
93	1006.02	2.9714	19.8767
94	1015.98	0.0796	8.4262
95	1031.52	10.6079	47.6044
96	1043.66	11.7889	22.8586
97	1064.13	3.7219	26.1718
98	1093.49	18.9301	75.2000
99	1110.10	44.6790	22.0300
100	1141.17	11.3657	26.5922
101	1143.70	23.4744	89.2198
102	1154.93	17.5910	22.8470
103	1162.06	11.2456	2.3534
104	1180.44	17.3032	8.4698
105	1186.73	2.5850	35.9426
106	1197.66	5.9251	16.2046
107	1212.30	9.8652	36.8489
108	1221.14	13.6244	10.5316

109	1236.17	59.2620	54.7092
110	1245.96	106.0125	13.3200
111	1258.17	57.8787	30.4521
112	1259.21	5.4342	37.4258
113	1274.88	179.1668	133.0119
114	1278.22	81.6575	8.4668
115	1288.77	63.1945	5.4131
116	1307.84	2.2069	47.0460
117	1322.55	6.3636	75.4149

Table S3. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Cu&B<sub>40</sub><sup>-</sup>.

Mode # ▲	Freq	Infrared	Raman Activity
1	106.88	2.8633	23.2417
2	144.50	9.1581	162.5346
3	158.44	7.1790	12.1447
4	168.76	1.3529	17.1003
5	184.70	0.4509	44.9824
6	201.06	0.0133	5.1357
7	206.54	0.1141	21.3709
8	220.43	0.2901	37.5763
9	230.52	2.9731	25.0310
10	237.85	3.1704	1.4628
11	243.22	0.0170	10.5476
12	249.95	1.5881	10.7331
13	261.72	2.7330	10.7953
14	282.78	2.9793	22.1983
15	292.80	6.9862	58.6084
16	299.79	12.4779	11.3385
17	313.32	7.7655	81.7442
18	318.32	22.9496	0.6929
19	323.49	10.7313	147.2726
20	323.52	1.2797	33.8754
21	329.57	11.6478	35.0739
22	342.49	0.0167	22.3363
23	344.44	1.0457	4.5343
24	348.70	5.5393	49.5967
25	360.74	15.8300	21.5517
26	367.63	2.7882	5.5932
27	377.12	0.0274	8.7971
28	378.32	6.4892	42.0730
29	384.46	1.7606	10.3154
30	389.22	0.0660	29.3674
31	400.19	3.2458	21.6732
32	406.41	0.4058	6.5719
33	406.95	0.0058	13.9049
34	425.13	12.3839	15.3463
35	427.54	0.2486	23.5221
36	428.64	8.7964	10.0903
37	433.37	0.6899	176.0588
38	440.54	21.8469	2.0877
39	448.92	3.0076	14.4966
40	456.38	0.5956	70.5120
41	464.65	5.2090	0.0995
42	466.01	1.5420	86.9025
43	470.45	0.1961	4.3809
44	477.37	0.8500	9.8360
45	477.40	16.0807	28.5708
46	477.55	1.3636	3.1692
47	486.24	0.8257	25.3721
48	488.88	3.6061	93.4083
49	498.47	6.4222	56.5839
50	504.05	2.4529	2.9449
51	515.82	1.4606	6.3133
52	529.49	4.1256	2.9325

53	560.75	6.1617	64.8661
54	573.07	2.2164	10.7746
55	577.54	0.0979	2.6753
56	577.80	7.3763	39.3764
57	594.41	3.4829	2.2171
58	601.37	29.8709	6.4401
59	610.83	4.2089	1.9786
60	613.99	17.1370	41.4439
61	628.95	1.8493	6.4402
62	632.38	3.9509	95.2378
63	648.51	3.2250	4.4930
64	650.79	0.3365	6.7017
65	654.64	17.5531	38.1700
66	659.18	1.3054	5.2709
67	674.03	4.4560	135.2448
68	679.47	3.6997	119.2749
69	681.71	4.6942	29.9357
70	690.44	3.2974	11.2915
71	695.36	0.0083	44.7760
72	702.62	1.0730	31.3948
73	730.45	24.4355	80.2050
74	744.29	1.6505	12.2383
75	744.34	24.5427	56.1110
76	746.53	70.6709	29.3312
77	756.98	0.2283	7.2583
78	771.53	9.7797	2.5055
79	777.80	0.4566	145.2352
80	796.84	1.1616	56.5153
81	798.71	6.6277	60.3621
82	810.52	0.7045	12.8941
83	818.10	15.6382	30.0509
84	832.60	13.7820	32.1217
85	837.20	0.1439	31.5710
86	844.13	6.5395	10.7156
87	857.13	1.8749	6.6547
88	872.78	3.4242	11.8969
89	875.76	0.1518	38.2626
90	900.81	3.9841	24.3708
91	944.46	17.9603	57.5370
92	979.67	3.1468	6.3989
93	990.83	29.7618	53.5422
94	1010.33	0.0474	35.7303
95	1018.02	14.4288	30.9585
96	1039.25	13.7766	89.4487
97	1058.68	1.6734	19.2697
98	1078.25	18.7777	59.0800
99	1104.79	66.9908	73.3937
100	1126.96	25.9215	105.1861
101	1127.49	15.5946	61.1432
102	1144.80	1.4687	153.5350
103	1154.93	3.6079	1.0040
104	1172.68	30.4052	5.6542
105	1177.60	10.2786	72.0225
106	1187.68	3.8313	152.7389
107	1204.78	18.9119	155.1752
108	1210.07	38.8676	19.4404

109	1227.38	44.4147	7.5853
110	1236.14	132.2307	26.3791
111	1248.13	0.1262	40.8837
112	1255.68	72.9524	181.2961
113	1264.64	118.0428	851.6674
114	1270.86	79.3587	21.1177
115	1280.64	75.6365	107.5232
116	1304.57	3.1776	82.5482
117	1318.92	10.7727	71.2787

Table S4. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Cu@B<sub>40</sub>.

Mode # ▲	Freq	Infrared	Raman Activity
1	88.52	1.5897	0.7142
2	96.92	0.0449	0.8334
3	107.88	2.5499	3.1287
4	165.75	2.0806	28.4817
5	175.95	0.1603	76.1536
6	198.30	2.4834	4.7782
7	207.12	0.0634	0.6167
8	219.60	1.0953	32.3059
9	221.26	0.1731	16.6653
10	234.56	0.8391	17.4995
11	237.24	0.3662	18.0605
12	252.42	0.5118	25.1413
13	270.68	2.0508	17.0056
14	271.46	12.7923	18.6244
15	279.75	3.1952	9.5504
16	302.42	8.8227	26.2676
17	320.20	2.8714	16.3101
18	329.81	0.0746	40.7032
19	335.29	3.8037	0.7126
20	342.56	0.8274	10.0114
21	347.72	0.7126	2.6626
22	347.83	0.0002	1.4932
23	354.47	4.8167	30.3767
24	367.47	4.3714	3.7318
25	377.23	4.3543	14.7888
26	377.55	1.8120	2.1521
27	391.40	7.8164	2.4935
28	393.56	6.2518	28.1879
29	398.22	2.1652	32.4073
30	399.71	2.6940	2.7415
31	406.02	0.2124	23.6707
32	408.53	0.5430	10.3736
33	416.09	15.4148	21.3380
34	422.54	5.3479	22.2713
35	425.89	0.7439	8.9147
36	433.29	0.1878	40.2088
37	440.17	0.3404	10.1880
38	444.32	2.6246	11.6952
39	445.50	0.4928	66.4840
40	451.19	0.9866	3.9932
41	457.79	0.3279	60.0537
42	465.63	5.4201	80.4987
43	466.63	1.8724	13.2965
44	466.84	3.8699	6.5846
45	469.54	0.0618	2.2246
46	477.17	0.3731	23.0297
47	479.32	0.9552	14.7479
48	479.68	2.0569	7.4660
49	500.16	1.8452	1.0234
50	505.08	2.1967	1.7200
51	507.08	0.9131	35.3566
52	522.19	1.0525	7.5932



53	560.87	6.4232	36.6271
54	569.46	0.0054	0.2234
55	575.51	0.2322	1.9392
56	575.86	2.8189	4.8242
57	596.42	0.0199	4.0429
58	609.88	3.9957	17.8688
59	612.35	0.0054	4.5638
60	617.80	7.8118	6.5134
61	619.63	0.1959	7.9434
62	624.01	0.3969	9.9983
63	638.18	3.4947	42.9789
64	643.52	2.1319	31.7349
65	653.10	1.2807	4.3139
66	657.79	0.0207	4.8855
67	658.43	2.9500	200.0603
68	674.54	5.4362	56.5874
69	683.68	1.3203	86.9187
70	696.04	2.6485	4.4955
71	696.65	0.0806	43.8118
72	705.07	0.4690	20.8732
73	708.23	1.6371	20.4839
74	725.43	0.0625	3.0780
75	730.30	2.3908	1.3941
76	748.36	1.7587	7.6204
77	753.77	3.3605	52.6486
78	757.23	2.1087	0.6033
79	766.67	18.6251	34.1835
80	793.48	24.7239	8.6643
81	798.41	6.1036	14.7679
82	804.40	0.1172	27.2477
83	813.27	1.9409	19.8382
84	817.07	0.9246	93.9244
85	821.63	0.4341	24.8167
86	825.00	4.6049	27.4063
87	854.09	0.1986	5.8220
88	867.10	0.0873	4.4855
89	886.53	0.1139	0.6290
90	901.30	0.0146	10.5572
91	961.91	8.3114	5.5964
92	982.12	7.1459	2.4967
93	1009.70	1.1194	21.6814
94	1021.22	0.1441	6.6729
95	1021.90	3.5278	69.5279
96	1047.72	0.1320	0.0693
97	1064.36	3.6035	113.0394
98	1101.76	19.1486	118.1120
99	1105.04	3.9251	39.7693
100	1135.49	0.8261	71.6760
101	1154.68	36.5829	5.3232
102	1160.04	10.7762	5.6905
103	1168.30	0.1218	65.7432
104	1176.50	2.8830	37.6497
105	1188.94	17.1913	119.7527
106	1197.81	2.9271	7.1550
107	1201.40	24.1107	13.2323
108	1210.24	13.7486	130.4741

109	1237.80	72.8074	283.8518
110	1239.15	12.8695	2.5743
111	1240.53	21.9966	58.2304
112	1243.73	11.1108	33.2080
113	1248.62	43.4920	18.3362
114	1264.94	87.3148	26.0929
115	1271.99	82.3639	12.7965
116	1299.35	19.7949	106.0157
117	1314.30	14.5360	149.4519

Table S5. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Cu@B<sub>40</sub><sup>-</sup>.

Mode #	Freq	Infrared	Raman Activity
1	92.43	0.2143	2.5255
2	104.38	1.2274	2.3120
3	121.96	2.9714	13.1572
4	170.84	0.8772	72.3803
5	180.52	1.5809	55.7836
6	206.17	5.4174	9.1721
7	208.19	0.0007	6.5882
8	213.60	0.3252	2.1228
9	217.71	2.4201	19.2253
10	223.06	0.1107	16.6499
11	237.44	1.2134	19.7899
12	237.60	0.0297	12.9367
13	257.60	23.5810	4.9768
14	261.46	1.6479	68.7034
15	273.42	5.9880	27.1491
16	287.25	3.4335	5.9580
17	317.33	3.4190	1.1698
18	319.49	6.4950	0.6897
19	321.38	3.8610	44.8815
20	331.44	1.9596	7.2742
21	332.07	0.2151	7.8969
22	338.92	4.4410	3.4712
23	344.04	4.0759	12.5411
24	363.73	0.0222	8.0628
25	371.80	0.0296	0.6731
26	377.99	0.4782	32.0347
27	391.36	11.7617	29.2031
28	393.69	6.3193	12.0313
29	397.31	3.7805	10.7330
30	401.14	19.3243	6.0063
31	406.53	0.0099	2.9471
32	410.70	11.4985	17.0062
33	413.24	0.9322	30.5291
34	416.73	12.6510	13.3179
35	422.31	2.6920	34.3510
36	435.16	0.1055	1.6156
37	439.63	0.0828	82.3635
38	440.40	0.0192	13.0375
39	444.46	5.3509	59.2196
40	453.49	5.7225	27.8893
41	455.49	0.0955	47.2425
42	455.74	10.5826	20.1827
43	461.38	6.9479	81.1026
44	474.91	3.1999	18.1588
45	475.03	4.9187	5.5503
46	476.48	4.4966	16.6505
47	479.22	0.7764	8.3996
48	481.70	1.9705	5.7225
49	504.07	2.0683	2.8179
50	504.85	2.2664	0.7319
51	508.40	1.6989	2.4372
52	524.36	3.4142	11.8185

53	563.97	0.1341	0.7006
54	567.94	10.2571	17.7387
55	573.09	0.2565	1.6453
56	581.35	4.7791	3.4133
57	588.71	0.0494	1.0567
58	603.98	0.1482	39.6950
59	606.58	0.2992	3.4321
60	614.65	1.1343	0.1447
61	620.73	33.9249	30.2650
62	627.93	1.2618	23.1121
63	627.94	1.1954	25.1420
64	643.75	1.3500	101.2893
65	652.51	16.4657	26.2905
66	653.59	16.3096	114.4552
67	657.94	8.2296	15.7472
68	663.17	0.3627	14.7659
69	681.66	1.2870	19.2330
70	688.40	0.0454	63.8777
71	697.45	0.8458	6.3783
72	708.04	26.7384	9.9416
73	712.50	2.4968	30.7667
74	720.65	3.9697	27.8872
75	723.81	2.4479	21.4483
76	729.88	8.1418	12.1662
77	740.73	0.5112	5.4635
78	758.50	8.0059	44.9367
79	765.21	10.6788	46.3598
80	785.89	5.9969	29.0347
81	787.93	33.3307	3.9590
82	796.46	0.0149	6.6166
83	802.58	1.9710	93.3696
84	803.83	2.9862	14.9362
85	811.81	0.0426	49.1990
86	814.69	4.8942	62.6692
87	848.35	0.0016	7.5516
88	856.71	0.6071	0.4010
89	870.44	0.6004	3.2306
90	887.37	0.0195	14.3241
91	950.28	12.1848	10.1531
92	970.22	7.3378	1.0410
93	1002.75	0.4675	32.3008
94	1012.65	1.0800	127.4812
95	1017.81	0.8537	3.4431
96	1046.89	1.8001	0.0491
97	1056.36	7.3346	59.7012
98	1092.58	33.8054	60.9631
99	1100.51	5.0784	49.8961
100	1124.24	9.5620	141.3763
101	1145.43	39.3831	7.5543
102	1153.77	4.0167	25.2335
103	1157.94	3.0311	53.2251
104	1167.80	8.1154	99.4099
105	1180.52	34.5066	108.7864
106	1190.90	0.6193	7.2447
107	1191.72	8.9059	89.1384
108	1194.32	51.6773	15.6348

109	1214.31	37.3282	82.2693
110	1225.30	5.0030	129.2525
111	1229.08	3.2495	13.0426
112	1231.76	1.7056	3.9855
113	1240.33	54.8637	31.9596
114	1258.07	83.9149	17.4940
115	1266.43	88.5501	56.1362
116	1291.14	40.1258	82.1875
117	1304.76	31.0172	45.2234

Table S6. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Ag&B<sub>40</sub>.

Mode # ▲	Freq	Infrared	Raman Activity
1	25.49	0.5761	6.0462
2	25.82	0.4338	7.2445
3	106.46	0.2963	27.0363
4	174.54	0.1064	38.4699
5	187.12	0.8127	54.0757
6	199.22	0.0690	3.1325
7	213.90	0.5713	13.4581
8	216.49	0.1002	16.1250
9	221.18	0.1218	24.4093
10	239.05	0.1081	21.7356
11	244.10	0.0133	0.3048
12	247.39	1.9045	30.9157
13	274.04	0.0043	9.9137
14	275.88	1.3889	8.4379
15	303.47	0.0072	0.0349
16	322.52	1.0110	3.3667
17	325.90	3.1337	19.4133
18	342.53	1.6101	53.3604
19	342.97	0.2087	0.6385
20	350.45	0.0924	58.6206
21	356.62	0.7421	0.1266
22	357.64	0.8522	19.4352
23	363.07	2.0726	13.8655
24	371.44	4.7001	9.6445
25	382.48	31.4198	16.5042
26	385.20	8.9742	2.0598
27	389.79	10.5653	1.9378
28	393.90	6.2337	42.9203
29	395.08	6.7601	1.1971
30	400.44	3.5038	33.0828
31	409.54	0.3771	6.0272
32	410.97	0.0793	7.6648
33	415.73	0.9587	60.3019
34	423.36	0.5143	6.7349
35	426.64	2.4425	41.8723
36	431.32	0.5538	91.6020
37	435.18	4.7745	31.8394
38	437.30	0.7972	4.6610
39	451.57	0.2553	4.3639
40	460.24	0.2187	47.4842
41	464.12	0.0021	1.4819
42	472.03	0.7177	1.3148
43	474.59	4.6855	1.0185
44	476.63	0.4241	16.1456
45	477.49	0.7250	8.4153
46	484.51	0.3969	3.1436
47	491.25	0.1009	21.4941
48	500.26	1.3404	6.6123
49	502.59	3.6410	0.8522
50	503.67	0.9787	57.6485
51	510.03	0.4182	6.3246
52	536.94	21.8288	161.2094

53	585.74	4.8978	7.2888
54	576.38	0.1212	0.5734
55	583.91	4.3700	6.4442
56	585.82	1.2569	6.1665
57	608.66	0.2694	0.1760
58	618.90	13.0076	9.5950
59	619.06	0.0652	1.6671
60	625.98	0.0007	5.2097
61	626.81	1.8636	134.0938
62	629.58	0.1667	1.6494
63	643.45	5.2073	86.9810
64	659.72	0.0867	0.0970
65	660.40	0.2773	64.2737
66	663.33	0.6128	9.1040
67	685.42	19.8417	764.6392
68	690.38	0.0874	10.4160
69	691.14	1.4288	159.1700
70	704.04	6.9301	122.4695
71	707.79	0.9236	0.5482
72	708.13	1.9413	31.7960
73	720.47	26.1507	475.2668
74	754.22	5.5159	35.0612
75	759.49	3.0831	0.3113
76	764.60	2.4234	37.2374
77	765.44	1.8955	13.2768
78	779.67	0.0119	12.7615
79	790.28	21.7028	48.0719
80	804.58	2.8429	16.4014
81	804.72	2.4187	6.1709
82	818.97	20.7353	26.6475
83	838.27	0.5660	2.8775
84	840.34	7.6326	61.9296
85	850.17	2.8434	3.7766
86	852.97	1.2478	26.3593
87	857.93	0.0423	7.1416
88	876.91	0.1426	15.7396
89	907.25	0.1116	3.6828
90	916.67	0.0010	7.2557
91	982.53	6.1869	0.7950
92	992.73	9.6635	0.0633
93	1021.03	0.0923	14.0836
94	1037.64	7.1484	0.2772
95	1038.55	9.6132	30.8047
96	1051.62	1.2171	1.0730
97	1100.85	21.2154	18.2598
98	1130.64	24.9267	127.4159
99	1140.29	20.4333	10.8389
100	1147.83	7.2292	30.4686
101	1162.32	0.1496	2.1793
102	1186.08	2.7658	77.5957
103	1192.91	7.6500	87.8419
104	1199.80	10.7897	34.2806
105	1205.32	9.7499	6.4128
106	1223.60	7.3895	57.9643
107	1235.38	4.0840	54.4405
108	1244.10	15.6083	53.1063

109	1250.28	1.5877	51.5111
110	1256.77	79.3883	7.9356
111	1256.90	76.1452	36.2504
112	1270.38	191.5377	37.5988
113	1275.54	5.4380	9.9259
114	1289.27	35.4262	36.2274
115	1289.81	101.5530	12.9205
116	1308.51	26.0078	76.9440
117	1319.64	15.3725	157.0902



Table S7. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Ag&B<sub>40</sub><sup>-</sup>.

Mode # ▲	Freq	Infrared	Raman Activity
1	35.84	0.5487	9.1844
2	40.88	0.8931	10.3240
3	111.36	0.0403	24.2316
4	170.96	1.6686	82.2249
5	183.58	1.0597	65.6118
6	202.79	0.0715	5.6053
7	213.17	2.3703	20.0822
8	217.21	0.1844	14.4371
9	222.91	0.1500	31.5640
10	231.86	0.1686	22.3086
11	237.79	1.9874	29.6757
12	244.27	0.0197	3.4612
13	267.43	0.0474	13.8474
14	270.98	2.7348	11.9444
15	293.80	0.5979	0.5477
16	311.01	0.4966	11.5914
17	325.12	9.6146	85.4031
18	339.26	0.1397	0.6064
19	343.30	6.2926	23.2000
20	345.89	1.2036	6.5226
21	346.15	0.5466	127.9704
22	354.77	0.0193	2.7316
23	360.95	2.7174	6.9817
24	366.65	6.6904	10.4766
25	379.27	37.7560	117.9502
26	382.46	4.7962	0.7152
27	390.38	3.5211	5.9180
28	393.37	26.4813	0.6759
29	395.02	2.6255	125.5025
30	399.28	1.2323	8.0371
31	404.56	0.6264	8.4817
32	411.55	1.5539	11.7534
33	413.62	0.4697	63.1448
34	417.21	2.8184	16.9797
35	425.63	0.3552	10.8537
36	429.66	0.5403	78.2839
37	441.07	3.4033	60.9688
38	442.09	3.9306	36.3371
39	452.37	1.6632	9.7256
40	456.42	0.0077	61.4850
41	463.09	0.0399	0.7266
42	473.25	1.3977	2.2143
43	473.99	0.1441	23.3231
44	476.13	7.7725	3.7351
45	478.84	0.5700	13.2366
46	485.78	0.1041	0.5259
47	489.65	7.8165	34.4823
48	499.60	1.8286	31.9675
49	503.50	5.6504	71.6403
50	506.75	1.6247	6.3269
51	508.19	2.1785	9.7622
52	537.68	19.6131	93.5881

53	568.34	9.5311	15.0190
54	571.38	0.0234	1.3155
55	585.65	10.2827	14.2651
56	589.04	1.2974	4.9613
57	599.66	0.0155	3.8757
58	607.24	24.4291	222.4198
59	609.21	0.2570	4.7042
60	627.34	4.9243	181.3523
61	631.23	0.6501	7.6905
62	632.32	0.2807	3.5913
63	640.61	8.9784	278.5630
64	658.32	1.1716	219.2229
65	658.65	0.8295	2.5810
66	668.56	3.7204	154.1197
67	671.77	10.1792	1128.3498
68	687.25	0.2210	21.3430
69	689.35	0.1534	336.3476
70	698.42	1.1021	55.4548
71	700.44	1.7118	227.7578
72	709.25	0.1691	2.8908
73	729.10	3.8749	382.0158
74	746.77	0.4259	12.6817
75	753.66	14.7953	23.0098
76	756.65	6.3373	233.4673
77	763.57	2.7628	8.9079
78	770.55	0.3396	13.3293
79	787.03	37.8487	43.8638
80	795.97	0.5184	16.1678
81	806.23	19.2039	54.0294
82	817.85	15.1458	17.4702
83	831.20	0.4197	6.6546
84	835.33	6.8094	97.5698
85	840.71	1.4746	6.6558
86	842.28	6.2135	14.6195
87	854.85	0.2120	20.7139
88	871.16	1.7007	30.3280
89	894.39	0.3250	9.6783
90	905.62	0.1067	5.3304
91	976.26	9.6489	77.4840
92	983.26	12.7063	0.5872
93	1016.16	0.1442	0.5271
94	1030.86	3.8888	0.8442
95	1034.53	9.1919	38.9794
96	1043.93	3.0652	1.0843
97	1095.97	21.5883	73.4265
98	1122.19	19.5373	53.2109
99	1124.71	58.2564	267.5584
100	1143.29	4.3159	20.9503
101	1155.57	0.5666	26.4369
102	1178.00	10.8342	196.4400
103	1182.58	31.0003	119.9316
104	1187.69	13.3977	86.6082
105	1203.89	16.8842	26.4963
106	1210.42	7.1487	72.3729
107	1229.66	20.2762	104.2854
108	1235.72	1.8384	136.1446

109	1239.37	16.6669	2.8958
110	1250.33	62.0952	9.6759
111	1256.93	90.5385	67.4823
112	1262.38	260.7747	175.5685
113	1269.84	6.7662	54.7259
114	1282.11	42.6934	27.5311
115	1284.50	205.5345	88.5566
116	1303.46	44.7074	104.2990
117	1314.10	44.5808	120.8735

Table S8. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Ag@B<sub>40</sub>.

Mode # ▲	Freq	Infrared	Raman Activity
1	46.70	0.0038	0.4735
2	46.70	0.0038	0.4735
3	87.94	0.5418	0.1419
4	142.36	0.4541	62.2466
5	152.90	0.0000	111.8722
6	196.01	0.1418	3.7491
7	196.01	0.1418	3.7491
8	208.33	3.0531	7.4401
9	208.33	3.0531	7.4402
10	215.02	0.0000	0.0000
11	223.79	0.0000	3.3175
12	226.45	0.0000	31.3325
13	243.25	17.7366	117.5678
14	264.32	0.0000	98.3227
15	281.89	0.0000	0.0000
16	283.32	0.0066	6.9646
17	309.95	17.5974	29.9397
18	309.95	17.5974	29.9397
19	330.41	0.0000	1.8986
20	350.97	0.0000	43.4663
21	350.97	2.1939	2.1952
22	350.97	2.1939	2.1952
23	355.06	0.0000	0.0000
24	355.34	0.2655	18.5983
25	355.34	0.2655	18.5984
26	361.96	0.0000	132.5600
27	381.75	14.3367	26.9138
28	381.75	14.3366	26.9137
29	392.13	1.2159	16.6941
30	392.13	1.2159	16.6941
31	406.88	0.4131	8.3904
32	406.88	0.4131	8.3904
33	410.62	0.0000	0.0000
34	412.11	29.7597	31.9178
35	412.11	29.7597	31.9179
36	420.02	3.0571	26.3694
37	427.21	0.0000	133.2823
38	430.51	0.0000	52.6967
39	441.36	0.0000	0.0000
40	441.98	0.0000	98.6214
41	455.49	3.5711	0.0873
42	455.49	3.5711	0.0873
43	456.28	0.0000	162.6449
44	463.29	0.0000	0.0000
45	466.17	5.6307	6.4373
46	470.94	3.8407	35.1796
47	470.94	3.8407	35.1795
48	475.77	0.0000	42.3868
49	501.42	2.3881	0.8515
50	501.42	2.3881	0.8515
51	504.38	2.5657	0.0020
52	505.61	0.0000	21.7254

53	563.15	7.6560	69.2125
54	568.72	0.0000	4.2527
55	570.93	0.5377	0.0601
56	570.93	0.5377	0.0601
57	590.40	0.0000	0.0000
58	608.92	0.0000	40.9829
59	614.51	1.7334	8.4584
60	614.51	1.7334	8.4585
61	615.08	5.6398	3.7020
62	617.21	0.0000	0.0000
63	645.20	0.0000	92.4775
64	646.33	0.0000	158.0052
65	653.86	3.3396	0.1339
66	653.86	3.3396	0.1339
67	666.05	21.0851	102.6091
68	666.05	21.0851	102.6089
69	684.97	0.0000	23.0815
70	691.70	0.0597	109.8158
71	699.99	7.4799	17.4194
72	699.99	7.4799	17.4194
73	705.03	1.0710	187.5778
74	727.57	0.0000	0.0000
75	737.92	0.0002	3.4241
76	737.92	0.0002	3.4241
77	759.43	0.0000	425.8012
78	762.48	0.0000	53.8969
79	765.53	11.7315	42.0100
80	795.00	42.5031	3.6630
81	799.73	3.0035	10.0502
82	799.73	3.0035	10.0502
83	815.03	3.7631	22.8653
84	815.03	3.7631	22.8653
85	833.09	5.0642	49.7525
86	833.09	5.0642	49.7526
87	847.07	0.0000	2.1766
88	862.19	0.0000	5.2335
89	884.81	0.0000	0.0000
90	905.31	0.0000	1.5849
91	978.60	5.9270	4.5043
92	978.60	5.9270	4.5043
93	1011.00	0.0000	96.3508
94	1018.47	3.4789	27.1587
95	1018.47	3.4789	27.1587
96	1049.82	0.0000	0.0000
97	1081.31	2.5917	60.5613
98	1095.21	51.3969	73.3960
99	1095.21	51.3969	73.3958
100	1126.94	0.0000	35.0896
101	1163.85	0.0000	4.3946
102	1168.39	0.0000	9.2729
103	1175.57	46.7724	2.6757
104	1175.57	46.7724	2.6757
105	1176.84	1.6171	1.3276
106	1207.49	15.0228	16.5575
107	1207.49	15.0228	16.5575
108	1228.36	0.0000	0.0000

109	1228.90	0.0000	761.7176
110	1232.76	0.9994	8.6270
111	1232.76	0.9994	8.6270
112	1233.09	0.0000	0.0000
113	1245.01	81.9716	67.0924
114	1277.62	0.0000	652.3777
115	1278.05	159.3235	36.2202
116	1278.05	159.3235	36.2202
117	1306.72	0.0000	92.7047

Table S9. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Ag@B<sub>40</sub><sup>-</sup>.

Mode # ▲	Freq	Infrared	Raman Activity
1	52.07	0.2853	0.0946
2	52.07	0.2853	0.0946
3	96.14	5.4023	47.2005
4	103.39	1.0492	1.6396
5	157.77	0.0000	79.1706
6	197.81	0.1503	11.7279
7	197.81	0.1503	11.7279
8	200.22	0.0000	0.0000
9	203.61	26.4499	46.5886
10	207.90	2.6572	7.7134
11	207.90	2.6572	7.7134
12	211.62	0.0000	23.5966
13	219.33	0.0000	3.9906
14	252.76	0.0000	103.0987
15	258.56	0.0000	0.0000
16	275.06	0.1898	0.3632
17	308.29	0.0000	2.2108
18	310.16	11.5278	0.5004
19	310.16	11.5278	0.5004
20	333.65	0.1213	4.5189
21	333.65	0.1213	4.5189
22	343.04	0.0000	14.9109
23	352.49	0.0000	0.0000
24	352.85	0.0000	24.7064
25	355.23	7.2838	26.1778
26	355.23	7.2838	26.1778
27	377.76	0.7479	18.5702
28	377.76	0.7479	18.5703
29	397.63	2.5338	0.1329
30	397.63	2.5338	0.1329
31	404.80	37.3623	0.6035
32	404.80	37.3623	0.6035
33	405.38	0.0000	0.0000
34	409.16	0.0000	65.5872
35	409.35	7.5229	46.0189
36	409.35	7.5229	46.0189
37	419.21	0.0000	0.0000
38	424.09	0.1472	11.8879
39	439.05	0.0000	85.0490
40	444.35	0.0000	25.5724
41	444.41	10.0856	0.1137
42	444.41	10.0856	0.1137
43	451.04	0.0000	173.6595
44	462.72	7.9378	0.0028
45	471.92	8.2472	22.0646
46	471.92	8.2472	22.0647
47	475.09	0.0000	14.9010
48	476.34	0.0000	0.0000
49	503.66	3.2105	0.3453
50	505.29	3.8064	0.4423
51	505.29	3.8064	0.4423
52	507.82	0.0000	3.5779

53	563.28	0.0000	1.1092
54	569.89	14.3254	27.2888
55	573.81	1.0006	0.1672
56	573.81	1.0006	0.1672
57	583.27	0.0000	0.0000
58	602.54	1.3355	1.1724
59	602.54	1.3355	1.1725
60	613.09	0.0000	0.0000
61	617.49	0.0000	25.9585
62	622.30	15.1001	2.1510
63	638.74	0.0000	159.2667
64	645.07	0.0000	114.1109
65	648.94	27.2224	28.2211
66	648.94	27.2224	28.2214
67	664.21	0.0348	35.2196
68	664.21	0.0348	35.2194
69	686.25	0.3625	78.1426
70	686.27	0.0000	31.3609
71	704.57	45.9708	13.7177
72	704.85	0.0000	0.0000
73	722.07	15.0503	35.5155
74	722.07	15.0504	35.5154
75	724.24	0.4361	5.0969
76	724.24	0.4361	5.0969
77	742.40	0.0000	16.4324
78	755.08	3.7856	24.4421
79	774.56	0.0000	212.9177
80	793.95	2.7044	0.2274
81	793.95	2.7044	0.2273
82	794.16	48.4162	6.9740
83	808.63	2.0964	17.4609
84	808.63	2.0964	17.4609
85	817.65	1.5838	60.6149
86	817.65	1.5838	60.6147
87	845.56	0.0000	4.1509
88	851.20	0.0000	0.5662
89	870.72	0.0000	0.0000
90	893.60	0.0000	11.3982
91	967.78	7.1119	0.6955
92	967.78	7.1119	0.6955
93	1002.93	0.0000	46.8688
94	1015.02	6.1238	6.9655
95	1015.02	6.1238	6.9655
96	1050.49	0.0000	0.0000
97	1080.77	0.1406	24.7499
98	1090.80	44.7172	55.8050
99	1090.80	44.7172	55.8052
100	1122.13	0.0000	34.8996
101	1155.55	0.0000	41.1132
102	1158.98	0.0000	30.1421
103	1168.61	49.4592	0.2018
104	1168.61	49.4592	0.2018
105	1172.05	0.4279	0.0161
106	1200.85	32.6128	13.6276
107	1200.85	32.6128	13.6276
108	1214.64	0.0000	197.7755



109	1217.05	0.0000	0.0000
110	1225.02	0.0000	0.0000
111	1225.97	1.2543	22.8839
112	1225.97	1.2543	22.8839
113	1239.01	64.4304	60.1108
114	1270.70	151.9197	38.2953
115	1270.70	151.9197	38.2953
116	1273.97	0.0000	101.8820
117	1298.65	0.0000	80.9276

Table S10. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Au&B<sub>40</sub>.

Mode # ▲	Freq	Infrared	Raman Activity
1	33.96	0.1088	1.6288
2	35.04	0.1472	1.3700
3	99.05	0.0191	13.7793
4	175.00	0.0636	37.3408
5	187.89	0.4781	38.6674
6	199.18	0.0564	1.0849
7	214.38	0.3242	9.9203
8	214.66	0.0355	18.8850
9	221.52	0.6355	15.5322
10	238.38	0.0531	22.3854
11	244.53	0.0494	0.4211
12	255.46	2.7029	10.9972
13	272.99	0.0026	9.2564
14	279.34	1.1218	3.8451
15	305.01	0.0077	0.1061
16	322.14	1.4150	2.5631
17	324.61	4.5038	4.3416
18	342.20	0.1480	0.2435
19	343.38	1.0100	11.1332
20	350.25	0.0180	23.4417
21	357.41	0.8605	0.1508
22	359.79	0.7236	10.0747
23	365.35	2.2568	2.9306
24	372.99	8.5179	8.1051
25	384.36	23.3629	9.2172
26	386.55	0.2270	0.4270
27	393.30	0.0323	0.4386
28	394.14	5.7727	8.8792
29	397.48	19.2872	9.0292
30	401.44	5.5323	4.8326
31	406.95	0.8310	3.0215
32	411.13	0.0607	4.7512
33	417.34	0.5530	29.7600
34	419.04	0.8691	1.4534
35	425.76	3.5088	14.1750
36	429.50	0.2362	74.7737
37	435.81	2.1002	4.4855
38	438.38	0.2861	15.2999
39	454.16	0.0907	0.2357
40	456.92	0.0630	54.7839
41	464.99	0.0442	0.5276
42	471.45	0.9895	0.9900
43	473.92	2.8030	0.5969
44	476.26	0.6563	2.5520
45	478.99	0.7295	8.4942
46	485.29	0.5613	3.5606
47	495.00	0.5703	8.7705
48	498.35	1.4932	2.1746
49	505.23	3.4869	2.4636
50	505.70	0.0503	10.2074
51	509.41	0.3283	17.4575
52	559.43	12.9570	7.4360

53	565.33	8.3709	4.2680
54	573.24	0.1147	0.4909
55	583.37	4.0354	7.7060
56	586.13	1.1087	4.0893
57	605.21	10.6389	10.7620
58	605.22	1.2725	1.3869
59	617.64	0.0549	1.4501
60	626.20	0.0358	4.0924
61	628.66	0.1613	1.3584
62	631.85	2.1601	27.1126
63	639.31	0.5681	33.2972
64	657.43	0.0079	0.4031
65	658.34	0.5021	104.6621
66	663.14	0.4576	1.9810
67	688.27	0.3015	2.7582
68	688.95	0.5457	11.9375
69	697.74	3.1836	37.1912
70	705.36	8.8688	33.9672
71	707.31	3.9229	32.1866
72	707.59	0.9922	0.3674
73	731.01	38.7302	175.8170
74	752.58	1.8083	25.0857
75	753.31	2.9457	0.0757
76	762.95	2.0257	9.5423
77	767.18	0.5714	60.0514
78	776.88	0.5022	3.3764
79	789.58	31.8580	11.6464
80	800.79	2.3872	6.2224
81	801.93	1.8440	4.7682
82	818.71	22.0704	13.2826
83	837.20	0.1306	5.4519
84	841.66	3.7137	28.6821
85	848.61	4.0650	1.5536
86	852.61	1.9560	5.5373
87	857.26	0.0681	7.4889
88	875.67	0.1299	14.0260
89	905.41	0.1110	3.7257
90	916.51	0.0001	6.2076
91	979.03	3.2475	1.2256
92	991.41	10.4144	0.2173
93	1020.24	0.3257	6.4209
94	1036.44	7.6829	0.1077
95	1040.82	6.4067	34.6278
96	1046.73	0.8995	1.1517
97	1099.57	16.2454	1.7662
98	1123.98	4.4057	27.1435
99	1131.68	19.2000	2.3102
100	1147.53	3.7250	24.3928
101	1157.77	0.9018	1.0483
102	1185.03	2.5723	103.0027
103	1189.54	3.5206	26.0034
104	1199.67	6.7967	6.5817
105	1205.46	10.7303	8.4635
106	1216.98	4.9324	28.4218
107	1230.32	25.4054	44.3590
108	1243.16	20.0511	7.4209

109	1252.24	0.3805	37.4971
110	1257.84	70.3966	53.9763
111	1258.19	83.1406	3.5865
112	1271.43	155.3538	104.6838
113	1274.98	3.2343	7.3331
114	1290.48	46.3094	50.2907
115	1290.89	27.4580	24.7532
116	1308.27	22.5966	47.7318
117	1319.66	5.4984	188.2054

Table S11. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Au&B<sub>40</sub><sup>-</sup>.

Mode # ▲	Freq	Infrared	Raman Activity
1	43.81	0.4557	2.1046
2	46.40	0.5745	2.5556
3	102.64	0.0226	10.4149
4	172.96	0.2663	57.4945
5	183.56	0.9872	43.1120
6	200.80	0.1635	2.0612
7	212.74	2.6319	12.9902
8	217.40	0.1015	18.2586
9	224.29	0.1051	29.3542
10	235.36	0.1180	23.0094
11	243.25	3.3736	13.2508
12	245.38	0.1459	2.8629
13	270.37	0.0039	10.8481
14	272.96	1.8604	5.8055
15	298.46	0.2415	1.0329
16	315.87	1.6527	4.4249
17	327.15	5.4011	41.8352
18	342.05	0.0501	0.3917
19	345.62	4.9523	20.1919
20	347.48	1.3901	7.5290
21	349.59	0.3378	57.0814
22	357.85	0.0798	3.4644
23	361.27	3.8358	2.9953
24	368.96	7.2581	11.2096
25	381.14	35.5250	43.0582
26	382.71	2.5055	1.3918
27	392.52	1.7433	2.3835
28	395.31	27.7063	1.6113
29	396.32	3.8646	21.9609
30	400.65	0.0608	29.2768
31	404.61	2.4677	14.6676
32	411.54	1.8164	6.1511
33	416.91	0.2726	39.6648
34	418.61	3.0459	6.4585
35	426.31	0.1037	16.6898
36	429.94	0.6334	60.2489
37	441.02	4.4051	39.0544
38	443.16	0.3770	7.8974
39	454.83	0.2108	52.8426
40	456.29	0.5490	5.9635
41	465.53	0.0361	0.2718
42	471.85	2.5751	1.5696
43	474.63	0.9061	5.5315
44	477.60	4.4494	1.1767
45	480.76	0.8726	10.9494
46	487.24	0.1071	1.3474
47	494.29	6.1338	11.5670
48	500.18	2.8046	10.3008
49	505.88	1.0722	8.3704
50	506.05	2.1560	21.4384
51	506.47	2.2308	17.0221
52	548.83	16.1119	7.2996

53	568.04	0.5181	1.7339
54	570.06	13.1113	16.0920
55	587.19	8.5085	5.9230
56	589.28	2.3951	5.4196
57	599.88	0.3456	1.3772
58	601.79	27.2985	25.0237
59	610.68	0.5023	3.3710
60	630.70	0.8940	10.0679
61	631.16	1.5437	16.4297
62	634.04	0.0849	2.9822
63	639.34	5.8394	41.5188
64	655.50	1.1181	113.9974
65	655.97	0.7717	38.5556
66	665.89	1.8344	2.6294
67	686.89	4.3336	12.4112
68	686.95	2.1112	9.6950
69	694.72	3.4027	57.6751
70	697.49	5.8784	22.3995
71	708.30	0.1132	3.0963
72	718.02	50.0992	301.2864
73	736.91	48.8200	427.4050
74	739.73	2.5643	19.3620
75	755.13	13.5874	19.4023
76	758.84	4.7151	49.1793
77	767.35	3.5397	20.4856
78	776.03	2.8183	2.9714
79	789.28	29.9506	46.1283
80	796.60	0.6740	7.4226
81	807.55	21.1409	35.2517
82	819.66	26.3049	7.0245
83	832.80	0.4653	4.6595
84	839.13	8.4676	84.2820
85	843.72	2.3215	3.5731
86	845.63	4.7152	9.3581
87	855.10	0.1996	19.8738
88	872.39	2.0341	28.9535
89	894.97	0.1377	9.7608
90	907.17	0.0097	4.4941
91	975.37	11.4667	38.9978
92	984.34	11.4058	0.7089
93	1017.33	0.6248	0.2055
94	1031.09	6.5859	0.1395
95	1035.25	12.8367	22.6597
96	1036.72	3.9776	2.3181
97	1095.37	22.4393	14.8507
98	1116.31	27.3770	15.7662
99	1126.10	74.3025	36.3669
100	1143.52	5.2738	21.5522
101	1156.56	0.9085	3.9910
102	1179.99	0.8912	136.1901
103	1185.01	18.6481	31.6976
104	1189.16	29.5421	40.4914
105	1204.42	16.6971	5.7240
106	1211.00	5.7617	36.6827
107	1228.63	7.8998	79.1701
108	1240.03	0.7429	48.6030

109	1241.68	30.1510	40.5008
110	1252.88	71.3542	3.7579
111	1259.57	52.5037	30.0826
112	1268.14	272.4232	26.4921
113	1275.27	2.8733	44.7575
114	1285.22	32.7243	21.8988
115	1287.14	171.1163	61.8538
116	1304.77	37.2177	75.0559
117	1316.04	21.9351	145.3281

Table S12. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Au@B<sub>40</sub>.

Mode #	Freq	Infrared	Raman Activity
1	24.92	0.0047	0.0455
2	24.92	0.0047	0.0455
3	41.57	0.2423	0.0080
4	155.67	2.6118	40.8301
5	157.48	0.0000	32.8989
6	162.15	1.1506	0.8292
7	162.15	1.1506	0.8292
8	194.59	0.2165	2.6371
9	194.59	0.2165	2.6371
10	197.61	0.0000	0.0000
11	204.23	0.0000	2.6319
12	222.81	0.0000	2.8103
13	224.29	13.9792	0.1130
14	251.41	0.0000	5.3989
15	275.52	0.0000	0.0000
16	276.18	1.0342	1.3995
17	286.09	2.1869	7.9167
18	286.09	2.1869	7.9167
19	310.21	0.0000	5.0316
20	321.55	0.0000	26.3378
21	331.78	0.1892	0.1675
22	331.78	0.1892	0.1675
23	338.42	39.8924	14.0560
24	338.42	39.8924	14.0560
25	341.07	0.0000	0.0000
26	341.40	0.0000	16.0891
27	349.05	7.4518	0.0815
28	349.05	7.4518	0.0815
29	371.11	0.0000	0.0000
30	371.50	0.1458	14.5612
31	371.50	0.1458	14.5612
32	386.86	2.4336	4.1242
33	386.86	2.4336	4.1242
34	407.94	0.0000	5.2775
35	408.05	7.5887	26.5158
36	415.44	0.0103	1.3906
37	415.44	0.0103	1.3906
38	427.90	0.0000	51.8623
39	431.91	0.0000	0.3103
40	446.15	0.0000	86.6676
41	454.30	0.0000	0.0000
42	455.12	2.2643	0.1968
43	461.52	0.0000	18.2280
44	470.15	1.5831	0.3454
45	470.15	1.5831	0.3454
46	472.09	0.0000	0.0000
47	478.14	0.7558	7.6863
48	478.14	0.7558	7.6864
49	494.78	0.7404	1.7883
50	496.09	1.9332	1.9741
51	496.09	1.9332	1.9741
52	506.57	0.0000	60.5591



53	552.47	7.4371	3.4640
54	566.61	0.0000	0.0494
55	575.78	3.5603	11.2048
56	575.78	3.5603	11.2048
57	601.46	0.0000	0.0000
58	608.99	22.3417	0.0946
59	611.34	0.0000	0.0000
60	616.20	0.6594	0.5640
61	616.20	0.6594	0.5640
62	616.44	0.0000	3.8205
63	632.84	0.0000	73.1762
64	643.81	0.4398	0.3622
65	643.81	0.4398	0.3622
66	650.38	0.0000	76.8910
67	671.44	0.0033	0.0137
68	671.44	0.0033	0.0137
69	679.10	0.0000	46.1332
70	689.51	7.5565	11.5895
71	696.82	9.2340	21.8976
72	698.86	0.4424	0.0322
73	698.86	0.4424	0.0321
74	737.58	0.0000	11.1885
75	747.46	4.9869	2.2272
76	747.46	4.9869	2.2272
77	757.72	0.0000	0.0000
78	770.56	0.0000	1.0911
79	774.28	22.7953	10.1355
80	793.73	6.6161	5.1493
81	800.43	8.9462	17.6604
82	800.43	8.9462	17.6604
83	820.66	5.5799	2.2852
84	820.66	5.5799	2.2852
85	838.12	0.0000	9.5237
86	839.67	0.3606	3.3565
87	839.67	0.3606	3.3565
88	860.31	0.0000	21.0047
89	887.41	0.0000	0.0000
90	907.02	0.0000	10.5943
91	976.82	4.5169	0.1262
92	976.82	4.5169	0.1262
93	1007.62	0.0000	1.8333
94	1021.10	8.8935	0.3089
95	1021.10	8.8935	0.3089
96	1033.91	0.0000	0.0000
97	1077.45	16.4693	0.3554
98	1125.36	0.0000	55.8473
99	1130.44	11.6217	0.5946
100	1130.44	11.6217	0.5946
101	1158.75	0.0000	0.0047
102	1169.16	0.0000	38.8915
103	1174.00	13.5837	16.0843
104	1179.39	11.4936	0.7578
105	1179.39	11.4936	0.7578
106	1212.66	0.0000	0.0000
107	1220.54	30.5068	0.1886
108	1220.54	30.5068	0.1886

109	1225.25	0.0000	17.2550
110	1233.27	97.6870	31.0998
111	1246.69	0.0000	0.0000
112	1246.75	175.8987	6.5879
113	1246.75	175.8987	6.5879
114	1275.70	0.0000	30.5867
115	1290.86	5.7017	15.7698
116	1290.86	5.7017	15.7698
117	1303.72	0.0000	217.8701

Table S13. Predicted normal mode frequencies (cm<sup>-1</sup>) and the infrared and Raman activities for the Au@B<sub>40</sub><sup>-</sup>.

Mode #	Freq	Infrared	Raman Activity
1	66.58	0.0018	0.0289
2	77.31	1.2489	2.0152
3	87.66	2.7487	2.5637
4	147.06	15.5233	2.1010
5	151.19	3.8262	10.2311
6	177.46	0.0067	22.6894
7	183.95	5.9695	11.6164
8	189.96	1.9927	29.6314
9	192.42	0.0373	2.2156
10	216.05	0.1955	5.2674
11	226.87	1.1268	19.0406
12	235.32	0.2020	4.7024
13	255.27	4.3274	2.1783
14	259.22	4.1312	5.8647
15	280.62	18.0036	0.4541
16	288.65	0.1806	2.5161
17	289.93	25.4529	15.3627
18	304.48	0.1390	4.6732
19	309.58	1.8413	10.1302
20	319.00	0.8134	16.1632
21	323.62	7.2458	9.6736
22	332.82	6.6468	8.1557
23	344.11	8.1546	11.1158
24	350.33	0.0963	9.8097
25	357.55	3.8633	3.3731
26	366.41	1.6600	10.2532
27	367.47	35.8582	0.7630
28	372.32	0.1889	0.3994
29	386.79	11.4971	6.1171
30	391.43	0.3965	2.4414
31	397.41	0.2727	3.8066
32	398.08	0.5944	2.3688
33	401.29	2.7411	60.3822
34	409.27	16.7991	10.5773
35	421.43	1.5517	55.2214
36	428.49	0.2765	0.5991
37	429.99	0.5029	10.1778
38	438.51	0.0802	0.5922
39	443.90	0.8247	8.2353
40	445.60	1.7409	15.2973
41	450.51	2.4076	29.5073
42	455.26	0.9255	52.1424
43	460.32	0.0073	0.6612
44	467.51	0.3353	5.9114
45	467.71	0.5338	1.4587
46	475.14	15.2585	19.1240
47	479.94	6.3171	0.8274
48	489.12	0.0304	5.0116
49	496.85	5.7718	8.3182
50	502.18	0.3376	5.7941
51	504.23	4.1579	3.3384
52	509.92	1.8715	13.7316

53	538.02	0.9326	5.6515
54	542.94	12.1880	5.7957
55	568.71	0.1461	3.8599
56	577.29	1.8004	7.6725
57	577.75	9.9408	14.5556
58	581.44	2.0825	7.1227
59	594.85	0.2709	1.1461
60	615.17	0.9410	1.7078
61	616.77	10.4705	3.3057
62	618.25	18.1725	6.8860
63	631.32	0.2750	2.0001
64	640.19	5.0054	7.1233
65	645.52	0.3895	73.2691
66	648.81	1.8647	0.2132
67	654.75	0.0291	0.7866
68	656.29	0.6150	5.5329
69	667.56	7.9990	36.7354
70	676.99	7.6659	3.6802
71	690.59	0.5884	0.5199
72	691.78	1.2732	26.2364
73	706.22	0.1225	0.9590
74	707.51	3.2981	16.9160
75	711.64	4.5240	11.7234
76	731.13	1.6516	12.3848
77	738.57	7.6053	17.1303
78	749.91	10.6459	12.0409
79	765.27	0.1096	1.3495
80	777.81	22.9312	4.1256
81	782.45	8.7928	3.6175
82	794.33	7.0337	16.6455
83	794.74	11.3882	16.9177
84	821.93	10.2878	19.3184
85	830.98	1.9992	4.1408
86	831.34	1.4457	11.7468
87	841.40	1.1810	13.8894
88	844.60	1.7061	22.4799
89	872.48	0.0292	2.9412
90	888.92	0.8977	8.1747
91	937.53	1.5023	1.6342
92	951.17	9.7813	3.8946
93	987.02	1.0720	3.9733
94	987.26	9.2504	1.7912
95	1012.68	20.6128	1.3175
96	1017.28	10.2902	3.4658
97	1028.53	15.8235	2.6299
98	1087.52	7.3810	24.1442
99	1114.05	9.0258	1.7483
100	1124.19	0.1619	0.0130
101	1125.97	2.1217	39.8079
102	1148.46	16.8617	17.6822
103	1160.62	10.5318	31.6818
104	1165.44	3.2328	5.0541
105	1179.96	50.0991	30.6854
106	1197.47	9.0671	6.5351
107	1205.80	5.5172	44.4709
108	1216.76	144.4773	13.4209

109	1218.74	5.7330	4.7198
110	1220.07	0.1979	7.7783
111	1226.69	113.5062	5.9668
112	1253.64	54.5267	42.1588
113	1259.30	73.9136	5.5909
114	1281.71	0.2263	41.1887
115	1294.19	28.3925	23.6992
116	1298.61	0.1721	17.5009
117	1305.77	7.5714	280.9995