

Supporting Information for:

Three-fold Aromatic Boranes. Spherical Aromaticity in borane *ortho*-carboranes as a Useful Trimer Node for Cluster-Based Architectures

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Table S1. Energy Decomposition Analysis (EDA) for different adducts given by $\text{BH}_3 \cdot \text{NH}_3$, **1**- NH_3 , **1**-CO, and $\text{B}(\text{B}_8\text{C}_2\text{H}_9)_3\text{-MeCN}$. Values in kcal/mol.

	$\text{BH}_3 \cdot \text{NH}_3$		1 - NH_3		1 -CO		$\text{B}(\text{B}_8\text{C}_2\text{H}_9)_3\text{-MeCN}$	
ΔE_{Pauli}	111.9		188.7		188.5		170.8	
ΔE_{Elstat}	-80.3	50.2% ^a	-122.0	49.1%	-90.1	41.0%	-96.2	45.4%
ΔE_{Orb}	-78.5	49.1% ^a	-119.4	48.0%	-123.8	56.3%	-109.8	51.8%
ΔE_{Disp}	-1.1	0.7% ^a	-7.2	2.9%	-6.0	2.7%	-5.9	2.8%
ΔE_{Int}	-48.0		-59.8		-31.5		-41.1	
Δr_1	-68.1	86.7% ^b	-96.3	80.7%	-91.7	74.0%	-80.3	73.2%
Δr_2	-2.3	2.9% ^b	-4.3	3.6%	-10.6	8.6%	-8.2	7.4%
Δr_3	-2.2	2.9% ^b	-4.3	3.6%	-10.6	8.6%	-8.2	7.4%
Δr_4	-2.2	2.8% ^b	-4.3	3.6%	-6.6	5.3%	-8.2	7.4%

^aPercentual contribution related to stabilizing interactions. ^bPercentual contribution relative to the overall orbital interaction (ΔE_{Orb}).

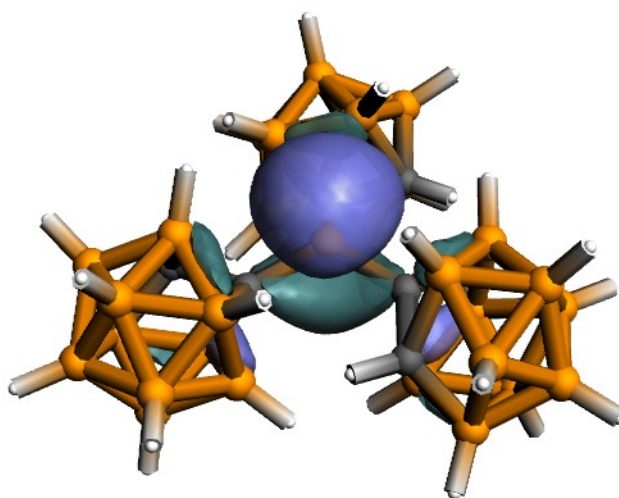


Figure S1. Lowest-unoccupied molecular orbital (LUMO) for $\text{B}(\text{B}_8\text{C}_2\text{H}_9)_3$ (**1**), responsible for its observed Lewis acid character. Isosurface set at ± 0.03 a.u.

Table S2. Optimized coordinates for the studied species in a MultipleXYZ format.
Values given in Angstrom (Å).

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BoCb3 (1)			
C	-1.606420625	0.139224903	0.000935664
C	0.923782616	1.321588619	0.000935664
C	0.682638010	-1.460813522	0.000935664
C	-0.295971213	-2.805761300	0.000597620
H	-1.356482528	-2.610648572	0.001387387
B	-2.682568360	-0.892405593	0.887429587
H	-2.230067860	-1.774349439	1.534810060
C	2.577846169	1.146562061	0.000597620
H	2.939129248	0.130575957	0.001387387
B	-3.701339418	1.779188954	0.885870344
H	-3.891737905	2.786502387	1.485604944
B	-4.209286947	-0.894170172	-0.000377627
H	-4.893409483	-1.866733817	-0.001400936
C	-2.281874956	1.659199239	0.000597620
H	-1.582646720	2.480072615	0.001387387
B	-4.007133822	0.125983951	1.443555106
H	-4.543091224	-0.097399615	2.481365462
B	-2.351211764	0.756521446	-1.444744700
H	-1.638683984	1.039967329	-2.349916336
B	-2.681820630	-0.892947110	-0.886851564
H	-2.227601164	-1.774907232	-1.533201390
B	-4.847786974	0.759346706	-0.001429870
H	-6.010781459	1.008983128	-0.001876932
B	-4.005074752	0.125416624	-1.444538556
H	-4.539344287	-0.097554241	-2.483066544
B	-3.700447398	1.779002228	-0.886587621
H	-3.889248789	2.786161461	-1.487470490
B	-2.353112536	0.756907048	1.445662521
H	-1.641972351	1.040214421	2.351403290
B	0.000000000	0.000000000	0.001671890
B	2.879017557	-3.198264342	-0.000377627
H	4.063343649	-3.304450015	-0.001400936
B	0.309846877	-4.095048441	0.885870344
H	-0.467312902	-4.763595085	1.485604944
B	0.309562576	-4.094182566	-0.886587621
H	-0.468262210	-4.761268983	-1.487470490
B	2.114225197	-1.876051239	-0.886851564
H	2.650915334	-1.041705582	-1.533201390
B	2.114130094	-1.876969551	0.887429587
H	2.651665619	-1.044120699	1.534810060
B	0.520439092	-2.414469840	-1.444744700
H	-0.081296134	-1.939125623	-2.349916336
B	1.766279949	-4.577980024	-0.001429870
H	2.131585709	-5.709981005	-0.001876932
B	1.894461609	-3.533271662	1.443555106
H	2.355896153	-3.885732604	2.481365462
B	1.893923394	-3.531204791	-1.444538556
H	2.354156595	-3.882410348	-2.483066544
B	0.521055536	-2.416308758	1.445662521
H	-0.079865939	-1.942096979	2.351403290
B	0.567595434	2.768998349	-0.886851564
H	-0.423314170	2.816612814	-1.533201390
B	2.111151358	3.405788168	-1.444538556

H	2.185187692	3.979964589	-2.483066544
B	1.330269389	4.092434514	-0.000377627
H	0.830065834	5.171183832	-0.001400936
B	3.390884822	2.315180338	-0.886587621
H	4.357510999	1.975107522	-1.487470490
B	3.081507025	3.818633319	-0.001429870
H	3.879195751	4.700997876	-0.001876932
B	3.391492541	2.315859487	0.885870344
H	4.359050808	1.977092697	1.485604944
B	2.112672213	3.407287711	1.443555106
H	2.187195071	3.983132219	2.481365462
B	1.830772673	1.657948395	-1.444744700
H	1.719980118	0.899158295	-2.349916336
B	1.832057000	1.659401710	1.445662521
H	1.721838290	0.901882558	2.351403290
B	0.568438266	2.769375143	0.887429587
H	-0.421597760	2.818470138	1.534810060

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B(C6F5)3 (2)

B	0.000000000	0.000000000	0.000000000
C	-0.780214000	-1.351369000	0.000000000
C	-0.352749000	-2.460430000	0.747614000
C	-1.954420000	-1.535705000	-0.747614000
C	-1.041285000	-3.668763000	0.769297000
C	-2.656599000	-2.736161000	-0.769297000
C	-2.198453000	-3.807832000	0.000000000
F	0.749076000	-2.374832000	1.520388000
F	-2.431202000	-0.538697000	-1.520388000
F	-0.609755000	-4.696807000	1.516803000
F	-3.762677000	-2.876467000	-1.516803000
F	-2.866647000	-4.965179000	0.000000000
C	-0.780214000	1.351369000	0.000000000
C	-0.352749000	2.460430000	-0.747614000
C	-1.954420000	1.535705000	0.747614000
C	-1.041285000	3.668763000	-0.769297000
C	-2.656599000	2.736161000	0.769297000
C	-2.198453000	3.807832000	0.000000000
F	0.749076000	2.374832000	-1.520388000
F	-2.431202000	0.538697000	1.520388000
F	-0.609755000	4.696807000	-1.516803000
F	-3.762677000	2.876467000	1.516803000
F	-2.866647000	4.965179000	0.000000000
C	1.560427000	0.000000000	0.000000000
C	2.307169000	-0.924725000	-0.747614000
C	2.307169000	0.924725000	0.747614000
C	3.697884000	-0.932602000	-0.769297000
C	3.697884000	0.932602000	0.769297000
C	4.396906000	0.000000000	0.000000000
F	1.682127000	-1.836134000	-1.520388000
F	1.682127000	1.836134000	1.520388000
F	4.372432000	-1.820340000	-1.516803000
F	4.372432000	1.820340000	1.516803000
F	5.733295000	0.000000000	0.000000000

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B(C6H5)3 (3)

B	0.000000000	0.000000000	0.000000000
C	-0.780055000	-1.351094000	0.000000000
C	-0.268093000	-2.493931000	0.650245000
C	-2.025761000	-1.479141000	-0.650245000
C	-0.969362000	-3.697979000	0.664782000
C	-2.717862000	-2.688482000	-0.664782000

C	-2.193656000	-3.799523000	0.000000000
H	0.690115000	-2.424979000	1.165087000
H	-2.445152000	-0.614832000	-1.165087000
H	-0.560806000	-4.561806000	1.189297000
H	-3.670237000	-2.766575000	-1.189297000
H	-2.738718000	-4.743599000	0.000000000
C	-0.780055000	1.351094000	0.000000000
C	-0.268093000	2.493931000	-0.650245000
C	-2.025761000	1.479141000	0.650245000
C	-0.969362000	3.697979000	-0.664782000
C	-2.717862000	2.688482000	0.664782000
C	-2.193656000	3.799523000	0.000000000
H	0.690115000	2.424979000	-1.165087000
H	-2.445152000	0.614832000	1.165087000
H	-0.560806000	4.561806000	-1.189297000
H	-3.670237000	2.766575000	1.189297000
H	-2.738718000	4.743599000	0.000000000
C	1.560109000	0.000000000	0.000000000
C	2.293854000	-1.014790000	-0.650245000
C	2.293854000	1.014790000	0.650245000
C	3.687225000	-1.009497000	-0.664782000
C	3.687225000	1.009497000	0.664782000
C	4.387311000	0.000000000	0.000000000
H	1.755036000	-1.810147000	-1.165087000
H	1.755036000	1.810147000	1.165087000
H	4.231042000	-1.795231000	-1.189297000
H	4.231042000	1.795231000	1.189297000
H	5.477437000	0.000000000	0.000000000

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B(CH₂CH₃)₃ (4)

B	-0.000007000	-0.000128000	0.000000000
C	-1.416097000	0.692401000	0.000000000
H	-1.438025000	1.386172000	0.861925000
H	-1.438025000	1.386172000	-0.861925000
C	-2.672531000	-0.185724000	0.000000000
H	-2.706093000	-0.839242000	0.883292000
H	-2.706093000	-0.839242000	-0.883292000
H	-3.594627000	0.412482000	0.000000000
C	1.307740000	0.880077000	0.000000000
H	1.919556000	0.552338000	0.861996000
H	1.919556000	0.552338000	-0.861996000
C	1.175120000	2.407212000	0.000000000
H	0.625822000	2.762998000	0.883282000
H	0.625822000	2.762998000	-0.883282000
H	2.154161000	2.906790000	0.000000000
C	0.108411000	-1.572776000	0.000000000
H	-0.481352000	-1.938763000	0.861956000
H	-0.481352000	-1.938763000	-0.861956000
C	1.497325000	-2.221369000	0.000000000
H	2.080000000	-1.923452000	0.883306000
H	2.080000000	-1.923452000	-0.883306000
H	1.440691000	-3.319067000	0.000000000

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BoCb3 (1)-MeCN

C	2.378643000	3.961531000	6.796249000
C	3.696139000	6.364212000	7.660563000
C	1.639123000	6.495059000	5.653893000
C	0.400179000	5.768488000	4.787872000
H	0.375292000	4.689414000	4.835892000
B	1.994101000	2.860088000	5.526030000
H	1.969607000	3.291781000	4.418237000

C	3.808281000	8.038188000	7.676524000
H	3.234622000	8.545839000	6.914490000
B	3.456656000	1.447911000	7.549603000
H	4.483447000	0.957066000	7.885634000
B	0.924883000	1.619113000	6.227253000
H	0.068443000	1.120819000	5.569484000
C	3.207481000	3.073816000	7.951449000
H	3.974755000	3.615746000	8.485472000
B	2.647310000	1.266480000	5.981207000
H	3.055834000	0.515526000	5.154693000
B	1.592336000	3.525831000	8.271569000
H	1.346536000	4.386964000	9.042080000
B	0.777746000	3.302944000	6.732099000
H	-0.144786000	3.998701000	6.506877000
B	1.830844000	0.754737000	7.491732000
H	1.645267000	-0.388459000	7.759113000
B	0.681410000	2.035912000	7.949344000
H	-0.336849000	1.842075000	8.531174000
B	2.252526000	1.937632000	8.754550000
H	2.451232000	1.760075000	9.910169000
B	3.552273000	2.729925000	6.339594000
H	4.599622000	3.064515000	5.905602000
B	2.817288000	5.563330000	6.443970000
B	0.657862000	8.968068000	4.724822000
H	0.788988000	10.149645000	4.731883000
B	-0.007636000	6.553901000	3.342810000
H	-0.316973000	5.870639000	2.423065000
B	-1.038749000	6.650577000	4.783147000
H	-2.059651000	6.048498000	4.835084000
B	1.029187000	8.031928000	6.174952000
H	1.367792000	8.487455000	7.205972000
B	2.086928000	7.903382000	4.760380000
H	3.230254000	8.231177000	4.796029000
B	0.013159000	6.601799000	6.227287000
H	-0.266146000	6.010928000	7.211815000
B	-0.643586000	8.122380000	3.857157000
H	-1.471340000	8.685062000	3.216425000
B	1.055497000	7.972859000	3.309586000
H	1.469517000	8.417137000	2.287335000
B	-0.640910000	8.145565000	5.639363000
H	-1.443153000	8.722794000	6.299338000
B	1.664397000	6.429027000	3.891367000
H	2.414835000	5.691410000	3.354576000
B	3.874205000	5.847813000	9.305090000
H	3.298386000	4.899032000	9.696958000
B	4.022369000	7.293821000	10.297075000
H	3.573097000	7.314405000	11.397251000
B	5.476684000	6.355914000	9.844649000
H	6.074222000	5.695798000	10.632401000
B	3.932823000	8.698886000	9.225057000
H	3.375616000	9.724233000	9.439052000
B	5.518485000	8.134142000	9.813183000
H	6.155608000	8.782380000	10.578514000
B	5.325516000	8.641058000	8.128635000
H	5.704198000	9.622018000	7.579347000
B	6.274619000	7.186997000	8.493300000
H	7.445091000	7.140425000	8.289347000
B	2.913352000	7.265017000	8.908459000
H	1.732446000	7.297216000	8.911046000
B	5.157147000	7.193513000	7.132831000
H	5.424324000	7.229945000	5.980636000

B	5.236183000	5.774689000	8.177254000
H	5.613820000	4.749017000	7.707302000
C	4.685941000	5.269961000	4.524153000
C	5.692666000	5.131775000	3.509448000
H	5.622290000	4.130162000	3.058879000
H	5.540735000	5.896616000	2.732181000
H	6.686155000	5.262614000	3.962848000
N	3.883935000	5.379580000	5.339876000

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B(C6F5)3 (2)-MeCN

B	0.066398000	0.030791000	0.626075000
C	-0.728462000	-1.352254000	0.299430000
C	-0.360142000	-2.541125000	0.935385000
C	-1.811129000	-1.460707000	-0.574289000
C	-1.014106000	-3.754553000	0.754384000
C	-2.497328000	-2.658162000	-0.788671000
C	-2.101386000	-3.811809000	-0.116953000
F	0.711228000	-2.551454000	1.775907000
F	-2.248880000	-0.394260000	-1.277951000
F	-0.611488000	-4.864085000	1.399918000
F	-3.545118000	-2.706979000	-1.631699000
F	-2.756625000	-4.967793000	-0.306776000
C	-0.751461000	1.392861000	0.249896000
C	-0.327171000	2.357376000	-0.668012000
C	-1.955007000	1.681787000	0.900922000
C	-1.030348000	3.541206000	-0.904579000
C	-2.688932000	2.844856000	0.697049000
C	-2.215262000	3.790286000	-0.215017000
F	0.801110000	2.187110000	-1.391448000
F	-2.473494000	0.783790000	1.786062000
F	-0.567505000	4.452002000	-1.783373000
F	-3.839496000	3.065219000	1.359999000
F	-2.897200000	4.927881000	-0.424634000
C	1.642671000	0.037398000	0.194728000
C	2.238569000	-0.878120000	-0.676992000
C	2.510486000	0.985845000	0.743570000
C	3.606528000	-0.875731000	-0.962849000
C	3.875971000	1.027297000	0.486413000
C	4.431507000	0.078356000	-0.373069000
F	1.509166000	-1.826333000	-1.303403000
F	2.020380000	1.948632000	1.574113000
F	4.139077000	-1.792734000	-1.792445000
F	4.658800000	1.965269000	1.049709000
F	5.750482000	0.087086000	-0.623770000
C	0.215298000	0.120041000	3.363767000
N	0.129859000	0.073013000	2.218845000
C	0.337302000	0.180180000	4.796647000
H	-0.500602000	0.753183000	5.216328000
H	0.324510000	-0.837240000	5.208340000
H	1.284892000	0.670406000	5.064261000

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B(C6H5)3 (3)-MeCN

B	0.087514000	0.045206000	0.789297000
C	-0.706560000	-1.323614000	0.437103000
C	-0.366152000	-2.545987000	1.042367000
C	-1.719514000	-1.346667000	-0.532859000
C	-1.012798000	-3.736632000	0.709028000
C	-2.366422000	-2.534763000	-0.883316000
C	-2.019834000	-3.733803000	-0.259343000
H	0.436728000	-2.572852000	1.782972000
H	-2.007702000	-0.415196000	-1.021442000

H	-0.727267000	-4.669757000	1.197176000
H	-3.147258000	-2.522732000	-1.644637000
H	-2.527128000	-4.660950000	-0.526803000
C	-0.734967000	1.385465000	0.396208000
C	-0.281541000	2.268716000	-0.594381000
C	-1.967344000	1.679004000	1.006134000
C	-1.019793000	3.398711000	-0.957400000
C	-2.707856000	2.808535000	0.659364000
C	-2.232729000	3.676421000	-0.326962000
H	0.668168000	2.068170000	-1.090100000
H	-2.366191000	0.996744000	1.760150000
H	-0.644346000	4.065921000	-1.734125000
H	-3.660147000	3.010237000	1.151196000
H	-2.807815000	4.559347000	-0.604195000
C	1.629972000	0.050961000	0.289905000
C	2.116024000	-0.897258000	-0.621762000
C	2.525827000	1.042005000	0.729365000
C	3.438275000	-0.862360000	-1.074454000
C	3.849623000	1.082030000	0.290607000
C	4.311464000	0.124235000	-0.615960000
H	1.446303000	-1.677737000	-0.983938000
H	2.174439000	1.811970000	1.420492000
H	3.787381000	-1.610415000	-1.787226000
H	4.520990000	1.863696000	0.648820000
H	5.344135000	0.150908000	-0.963825000
C	0.263598000	0.099815000	3.511806000
N	0.180459000	0.075814000	2.362294000
C	0.372458000	0.132434000	4.952274000
H	-0.422141000	0.762246000	5.372513000
H	0.277335000	-0.883698000	5.357205000
H	1.347908000	0.544362000	5.242267000
28			
BEt3-MeCN			
B	0.043254000	-0.006613000	-0.084049000
C	-1.372137000	0.696405000	-0.073142000
H	-1.334688000	1.559922000	0.606611000
H	-1.481405000	1.161561000	-1.070929000
C	-2.604480000	-0.159211000	0.235044000
H	-2.527534000	-0.596823000	1.237114000
H	-2.706967000	-0.990336000	-0.472724000
H	-3.539677000	0.417524000	0.197966000
C	1.354753000	0.868411000	-0.223210000
H	2.147117000	0.427350000	0.406779000
H	1.723102000	0.696671000	-1.258119000
C	1.247613000	2.375584000	0.043307000
H	0.927102000	2.566611000	1.077262000
H	0.507467000	2.849612000	-0.615455000
H	2.204877000	2.894859000	-0.110942000
C	0.137587000	-1.581029000	-0.204654000
H	-0.589119000	-2.037115000	0.488624000
H	-0.267506000	-1.831487000	-1.208135000
C	1.512439000	-2.234845000	-0.022378000
H	1.905776000	-2.032853000	0.988789000
H	2.248641000	-1.840685000	-0.741452000
H	1.473710000	-3.328037000	-0.153036000
C	0.435501000	-0.003254000	3.732671000
C	0.750213000	0.070439000	5.148844000
H	1.205711000	-0.870867000	5.481900000
H	1.451582000	0.891255000	5.338281000
H	-0.162723000	0.249120000	5.725661000
N	0.186851000	-0.061609000	2.603302000

BoCb3 (1)-NH3

N	3.938930000	5.367362000	5.289056000
H	4.136792000	6.260679000	4.825083000
H	3.611216000	4.699984000	4.582145000
H	4.812507000	5.010761000	5.692030000
C	2.373581000	3.971014000	6.814597000
C	3.675753000	6.374714000	7.664778000
C	1.629236000	6.485528000	5.666075000
C	0.391120000	5.764450000	4.788459000
H	0.358877000	4.685379000	4.834766000
B	1.995385000	2.870787000	5.540975000
H	1.976617000	3.307604000	4.430600000
C	3.791959000	8.051328000	7.695523000
H	3.211708000	8.568791000	6.945255000
B	3.446234000	1.443081000	7.557384000
H	4.472201000	0.951122000	7.893659000
B	0.919727000	1.627896000	6.224061000
H	0.066622000	1.137585000	5.556813000
C	3.197477000	3.069661000	7.969438000
H	3.961851000	3.604712000	8.514422000
B	2.643188000	1.272251000	5.983050000
H	3.055281000	0.531255000	5.150155000
B	1.582712000	3.523075000	8.283906000
H	1.336290000	4.377903000	9.060185000
B	0.774422000	3.310566000	6.741100000
H	-0.145031000	4.007996000	6.515584000
B	1.818513000	0.753862000	7.486336000
H	1.631464000	-0.391028000	7.744102000
B	0.669560000	2.035302000	7.947768000
H	-0.350915000	1.838147000	8.523121000
B	2.236351000	1.929009000	8.758962000
H	2.430506000	1.744833000	9.914595000
B	3.546127000	2.732876000	6.359799000
H	4.597670000	3.057955000	5.921390000
B	2.818621000	5.565006000	6.447132000
B	0.661655000	8.964823000	4.729529000
H	0.799773000	10.145584000	4.739866000
B	-0.006265000	6.552820000	3.338874000
H	-0.309462000	5.869426000	2.417427000
B	-1.044047000	6.653523000	4.774458000
H	-2.067142000	6.054959000	4.818727000
B	1.020060000	8.023323000	6.181613000
H	1.353371000	8.476084000	7.214522000
B	2.082252000	7.891518000	4.772486000
H	3.229387000	8.217618000	4.812314000
B	-0.000843000	6.598839000	6.225275000
H	-0.289035000	6.009106000	7.206725000
B	-0.637710000	8.124671000	3.852079000
H	-1.457811000	8.690939000	3.204962000
B	1.063196000	7.968932000	3.314039000
H	1.490649000	8.409233000	2.296103000
B	-0.645749000	8.146334000	5.634993000
H	-1.448618000	8.727408000	6.289972000
B	1.658271000	6.422434000	3.901239000
H	2.415214000	5.692187000	3.355904000
B	3.872962000	5.850159000	9.304535000
H	3.298634000	4.901664000	9.696450000
B	4.037716000	7.285499000	10.306697000
H	3.602578000	7.296253000	11.412119000
B	5.484874000	6.348576000	9.829268000

H	6.090525000	5.677301000	10.601254000
B	3.937484000	8.698714000	9.247619000
H	3.384386000	9.723275000	9.474616000
B	5.529452000	8.127288000	9.811951000
H	6.179638000	8.769324000	10.571595000
B	5.317498000	8.650773000	8.134715000
H	5.690110000	9.634725000	7.586121000
B	6.269546000	7.190649000	8.476219000
H	7.435961000	7.141086000	8.252870000
B	2.911339000	7.269080000	8.930225000
H	1.731186000	7.304518000	8.945781000
B	5.135408000	7.212390000	7.132222000
H	5.395227000	7.256297000	5.977026000
B	5.220400000	5.786612000	8.160697000
H	5.593323000	4.760284000	7.679353000
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BoCb3 (1)-CO			
C	3.900950000	5.374093000	5.332403000
O	4.681442000	5.233998000	4.526321000
C	2.360529000	3.966104000	6.812553000
C	3.678358000	6.369196000	7.678457000
C	1.627066000	6.499304000	5.670742000
C	0.409284000	5.761619000	4.793408000
H	0.386904000	4.682678000	4.844612000
B	1.981930000	2.878299000	5.531012000
H	1.959026000	3.327354000	4.429525000
C	3.787904000	8.038951000	7.687454000
H	3.203713000	8.547069000	6.934050000
B	3.460058000	1.461314000	7.538897000
H	4.491173000	0.977333000	7.869598000
B	0.922645000	1.627152000	6.222421000
H	0.068930000	1.130980000	5.560811000
C	3.199011000	3.082508000	7.958731000
H	3.962444000	3.625249000	8.497127000
B	2.648429000	1.286843000	5.968847000
H	3.059377000	0.549593000	5.132992000
B	1.579327000	3.521129000	8.288068000
H	1.332729000	4.375340000	9.064898000
B	0.763288000	3.307218000	6.743003000
H	-0.159383000	4.003373000	6.525435000
B	1.837774000	0.758374000	7.476525000
H	1.658890000	-0.387345000	7.735417000
B	0.678709000	2.028830000	7.949204000
H	-0.337269000	1.824764000	8.529657000
B	2.253047000	1.933011000	8.751347000
H	2.457689000	1.749610000	9.905230000
B	3.542077000	2.755030000	6.341182000
H	4.576510000	3.130316000	5.908712000
B	2.784240000	5.571337000	6.484549000
B	0.663980000	8.962884000	4.724046000
H	0.794085000	10.144383000	4.731465000
B	0.024989000	6.539998000	3.337244000
H	-0.267279000	5.850172000	2.417529000
B	-1.029970000	6.641101000	4.762508000
H	-2.048403000	6.034473000	4.799857000
B	1.014049000	8.033224000	6.185454000
H	1.338468000	8.487342000	7.221112000
B	2.092673000	7.902649000	4.783735000
H	3.237007000	8.222955000	4.838527000
B	-0.005199000	6.600289000	6.225829000
H	-0.295180000	6.011038000	7.206889000

B	-0.620984000	8.110463000	3.837262000
H	-1.440446000	8.669273000	3.183221000
B	1.086329000	7.962703000	3.316211000
H	1.518847000	8.402693000	2.301017000
B	-0.647965000	8.141198000	5.621726000
H	-1.458716000	8.720130000	6.268532000
B	1.687285000	6.422667000	3.915655000
H	2.461366000	5.678251000	3.420626000
B	3.876260000	5.846638000	9.316219000
H	3.300045000	4.901345000	9.714010000
B	4.047427000	7.292543000	10.303455000
H	3.617508000	7.311385000	11.410645000
B	5.491829000	6.350641000	9.824139000
H	6.100841000	5.685856000	10.598808000
B	3.942516000	8.698849000	9.232097000
H	3.390372000	9.725440000	9.451319000
B	5.538210000	8.128856000	9.789893000
H	6.190146000	8.776560000	10.542916000
B	5.316368000	8.637871000	8.109124000
H	5.684437000	9.617662000	7.550869000
B	6.269422000	7.179799000	8.457445000
H	7.434190000	7.127263000	8.229313000
B	2.910897000	7.269348000	8.937909000
H	1.730726000	7.303639000	8.956320000
B	5.126570000	7.189007000	7.119000000
H	5.340488000	7.205220000	5.956166000
B	5.220796000	5.771211000	8.163677000
H	5.578599000	4.744640000	7.680170000

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[Au (OTeF₅)₃] -MeCN

N	-0.379422000	-1.800858000	-0.121576000
C	-0.121868000	-2.918784000	-0.014049000
C	0.217810000	-4.309671000	0.130016000
H	-0.686367000	-4.926421000	0.085837000
H	0.901613000	-4.605598000	-0.672549000
H	0.707352000	-4.449012000	1.100125000
O	-0.700056000	0.068426000	1.951924000
Te	0.904932000	-0.089735000	3.016842000
F	2.076713000	0.115684000	1.492622000
Au	-0.466014000	0.187358000	-0.041403000
O	-0.316011000	2.144737000	0.106986000
Te	-1.974912000	3.158163000	-0.001517000
F	-3.047169000	1.558346000	-0.215448000
O	-0.618128000	0.344238000	-2.034312000
Te	1.006964000	0.228629000	-3.080255000
F	1.932109000	-0.819883000	-1.736262000
F	1.024128000	1.781540000	3.382544000
F	2.456522000	-0.326697000	4.098651000
F	-0.187898000	-0.365260000	4.559432000
F	0.977916000	-2.010173000	2.736535000
F	-2.276020000	3.065179000	1.888489000
F	-3.565663000	4.202039000	-0.107532000
F	-0.942272000	4.745222000	0.235968000
F	-1.861166000	3.333821000	-1.904518000
F	0.403401000	-1.413471000	-3.884018000
F	2.573987000	0.064185000	-4.154795000
F	0.182433000	1.221904000	-4.485906000
F	1.777087000	1.816091000	-2.331830000