Supporting Information

Table S1. Bond Distances for the Pure Boron Clusters. Refer to Figure 1 for Atom Numbering Scheme.

Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)
B_2	1	2	1.615	B_6-g	1	2	1.589	B_9	1	2	1.531
B_3	1	2	1.553		2	3	1.592		2	3	1.531
	1	3	1.553		3	6	1.525		3	4	1.531
	2	3	1.553		6	5	1.589		4	5	1.531
B_4-c	1	2	1.533		5	4	1.592		5	6	1.531
	2	4	1.533		4	1	1.525		6	7	1.531
	4	3	1.533		1	5	1.818		7	1	1.531
	3	1	1.533		5	2	1.920		1	8	1.960
	1	4	1.846		2	6	1.818		2	8	1.962
B_4-d	1	2	1.525	B_7	1	2	1.631		3	8	1.956
	2	4	1.525		2	5	1.573		4	8	1.953
	4	3	1.525		5	7	1.573		5	8	1.959
	1	3	1.525		7	6	1.630		6	8	1.962
	1	4	2.157		6	3	1.573		7	8	1.958
	2	3	2.157		3	1	1.573		9	8	1.700
B_5	1	2	1.583		1	4	1.694		1	9	1.956
	2	3	1.583		2	4	1.694		2	9	1.954
	3	5	1.568		3	4	1.732		3	9	1.960
	5	4	1.563		5	4	1.732		4	9	1.964
	4	1	1.568		6	4	1.694		5	9	1.958
	2	4	1.840		7	4	1.694		6	9	1.955
	2	5	1.841	B_8	1	2	1.559		7	9	1.957
B_6-f	1	2	1.617		2	3	1.559	B_{10}	1	2	1.619
	2	4	1.617		3	6	1.559		2	3	1.621
	4	5	1.617		6	8	1.559		3	7	1.590
	5	3	1.617		8	7	1.559		7	10	1.590
	3	1	1.617		7	4	1.559		10	9	1.621
	1	6	1.666		4	1	1.559		9	8	1.619
	2	6	1.666		1	5	1.797		8	4	1.589
	3	6	1.666		2	5	1.796		4	1	1.589
	4	6	1.666		3	5	1.797		1	5	1.663
	5	6	1.666		4	5	1.797		2	5	1.766
					6	5	1.796		4	5	1.647
					7	5	1.796		8	5	1.662
					8	5	1.796		9	5	1.766
									5	6	1.622
									2	6	1.757
									3	6	1.659
									7	6	1.644
									10	6	1.659
									9	6	1.757

Table S2. Bond Distances for the Monoxide Clusters. Refer to Figure 2 for Atom Numbering Scheme.

Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)
BO	1	2	1.215	B_7O	1	2	1.581	B_9O-m	1	3	1.535
B_2O	1	2	1.327		2	6	1.615		3	7	1.531
	2	3	1.327		6	8	1.580		7	9	1.535
B_3O	1	2	1.533		8	7	1.579		9	10	1.502
	2	3	1.616		7	3	1.847		1	2	1.502
	3	4	1.215		3	1	1.579		1	5	1.836
B_4O-d	1	2	1.540		1	4	1.713		3	5	1.899
	2	3	1.520		2	4	1.650		7	5	1.898
	3	4	1.618		6	4	1.650		9	5	1.836
	4	5	1.216		8	4	1.713		10	5	1.889
B_4O-e	1	2	1.537		7	4	1.733		2	5	1.888
	2	4	1.536		3	4	1.733		2	4	1.515
	4	3	1.704		3	5	1.398		4	8	1.925
	1	3	1.705		7	5	1.398		8	10	1.516
	1	4	1.649	B_8O	1	2	1.518		4	6	1.361
	3	5	1.245		2	5	1.564		8	6	1.361
B_4O-f	1	2	1.714		5	8	1.564	B_9O-n	1	2	1.543
	2	3	1.420		8	9	1.517		2	8	1.570
	3	5	1.391		9	7	1.528		8	10	1.589
	5	4	1.626		7	3	1.885		10	9	1.551
	4	1	1.511		3	1	1.528		9	3	2.221
	2	4	1.644		1	6	1.842		3	1	1.604
	2	5	1.667		2	6	1.774		1	4	1.728
B_5O-g	1	2	1.556		5	6	1.747		2	4	1.775
	2	3	1.417		8	6	1.773		8	4	1.722
	3	6	1.372		9	6	1.824		10	4	1.727
	5	6	1.626		7	6	1.908		9	4	1.805
	4	5	1.565		3	6	1.908		3	4	1.785
	4	1	1.540		3	4	1.374		3	5	1.591
	1	5	1.732		7	4	1.373		5	9	1.616
	2	5	1.762	B_9O-l	1	2	1.584		5	6	1.639
	2	6	1.698		2	3	1.615		6	7	1.215
B_5O-h	1	2	1.543		3	4	1.668				
	2	4	1.543		4	8	1.540				
	4	3	1.603		8	7	1.591				
	3	1	1.603		7	6	1.614				
	1	4	1.716		6	5	1.571				
	3	5	1.631		5	1	1.516				
	5	6	1.214		1	6	1.749				
B_6O	1	2	1.553		2	6	1.802				
	2	3	1.623		2	7	1.773				
	3	5	1.605		3	7	1.721				
	5	4	1.554		3	8	1.669				
	4	1	1.543		4	9	1.628				
	3	6	1.630		9	10	1.215				
	6	7	1.214								
	2	4	1.909								
	2	5	1.787								

Table S2. Bond Distances for the Dioxide Clusters. Refer to Figure 3 for Atom Numbering Scheme.

Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)
B_2O_2	1	2	1.207	B_6O_2	1	2	1.592	B_8O_2	1	3	1.507
	2	3	1.631		2	3	1.618		3	8	1.816
	3	4	1.207		3	6	1.567		8	10	1.540
B_3O_2	1	2	1.220		6	5	1.554		10	9	1.502
	2	3	1.594		5	4	1.432		9	6	1.540
	3	4	1.594		4	1	1.360		6	2	1.816
	4	5	1.220		1	5	1.667		2	1	1.507
B_4O_2	1	2	1.214		2	5	1.754		1	7	1.801
	2	3	1.617		2	6	1.712		2	7	1.825
	3	4	1.526		3	7	1.628		3	7	1.824
	4	5	1.616		7	8	1.215		6	7	1.921
	5	6	1.214	B_7O_2	1	2	1.562		8	7	1.920
B_5O_2-d	1	2	1.455		2	6	1.846		9	7	1.818
	2	3	1.630		6	8	1.850		10	7	1.818
	3	5	1.534		8	7	1.561		2	4	1.405
	5	4	1.604		7	4	1.601		6	4	1.353
	4	1	1.355		4	1	1.601		3	5	1.405
	2	4	1.685		1	5	1.678		8	5	1.353
	2	5	1.686		2	5	1.725				
	3	6	1.630		6	5	1.713				
	6	7	1.214		8	5	1.726				
B_5O_2-e	1	2	1.583		7	5	1.679				
	2	3	1.747		4	5	1.624				
	3	7	1.634		2	3	1.435				
	7	6	1.545		6	3	1.383				
	6	5	1.457		6	9	1.383				
	5	1	1.352		8	9	1.434				
	1	6	1.668								
	2	6	1.671								
	2	7	1.645								
	3	4	1.247								

Table S4. Bond Distances for the Trioxide Clusters. Refer to Figure 5 for Atom Numbering Scheme.

Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)	Molecule	Atom 1	Atom 2	Dist (Å)
B2O3	1	2	1.215	B6O3-2	1	2	1.511	B7O3-2	1	2	1.210
	2	3	1.326		2	3	1.511		2	3	1.666
	3	4	1.327		3	7	1.763		3	4	1.737
	4	5	1.215		7	6	1.610		4	5	1.615
B3O3-1	1	2	1.219		6	1	1.315		5	10	1.560
	2	3	1.624		3	4	1.624		10	9	1.583
	3	4	1.331		4	5	1.213		9	8	1.376
	4	5	1.330		7	8	1.620		8	3	1.420
	5	6	1.215		8	9	1.214		3	9	1.750
B3O3-2	1	2	1.269		2	6	1.648		4	9	1.710
	2	3	1.706		2	7	1.663		4	10	1.703
	3	4	1.209	B6O3-3	1	2	1.212		5	6	1.630
	2	5	1.705		2	3	1.624		6	7	1.214
	5	6	1.209		3	4	1.760	B7O3-3	1	2	1.224
B4O3-1	1	2	1.212		4	6	1.919		2	3	1.622
	2	3	1.654		6	5	1.627		3	4	1.685
	3	4	1.654		5	3	1.480		4	10	1.538
	3	6	1.654		4	5	1.578		10	9	1.600
	4	5	1.212		4	8	1.635		9	2	2.151
	6	7	1.212		8	9	1.211		3	9	1.681
B4O3-2	1	2	1.210		6	7	1.222		3	10	1.630
	2	3	1.646	B6O3-4	1	2	1.461		9	8	1.628
	3	4	1.395		2	3	1.552		8	7	1.212
	4	5	1.395		3	4	1.376		4	5	1.627
	3	5	1.578		4	7	1.442		5	6	1.213
	5	6	1.646		7	6	1.687	B7O3-4	1	2	1.669
	6	7	1.210		6	5	1.563		2	3	1.539
B5O3	1	2	1.211		5	1	1.364		3	8	1.720
	2	3	1.641		2	5	1.628		8	7	1.600
	3	4	1.494		2	6	1.664		7	6	1.402
	4	5	1.338		3	6	1.708		6	1	1.374
	5	6	1.572		3	7	1.760		1	7	1.703
	6	3	1.706		7	8	1.667		2	7	1.689
	3	5	1.687		8	9	1.211		2	8	1.693
	6	7	1.612	B7O3-1	1	2	1.214		8	9	1.628
	7	8	1.216		2	3	1.622		9	10	1.214
B6O3-1	1	2	1.214		3	4	1.536		3	4	1.622
	2	3	1.626		4	6	1.535		4	5	1.214
	3	4	1.713		6	5	1.760				
	4	5	1.353		5	3	1.761				
	5	7	1.485		4	5	1.618				
	7	6	1.683		5	9	1.628				
	6	3	1.503		9	10	1.215				
	4	6	1.628		6	7	1.621				
	4	7	1.684		7	8	1.214				
	7	8	1.655								
	8	9	1.209								