

Supplementary material

Toward size-dependent thermodynamics of nanoparticles from quantum chemical calculations of small atomic clusters: A case study of $(\text{B}_2\text{O}_3)_n$

Boris I. Loukhovitski^{a,b}, Alexey V. Pelevkin^{a,c}, Alexander S. Sharipov^{a,b}
biloukhovitski@ciam.ru avpelevkin@ciam.ru assharipov@ciam.ru

^a Central Institute of Aviation Motors, Moscow, Russia

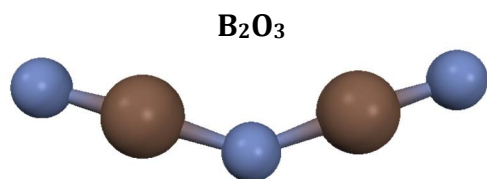
^b Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia

^c Prokhorov General Physics Institute of the Russian Academy of Sciences, Moscow, Russia

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designations:

Sym.	– group of symmetry
$\Delta_f H_0^0$	– enthalpy of formation at $T = 0$ K
$\Delta_f H_{298}^0$	– enthalpy of formation at $T = 298$ K
E_b	– binding energy calculated via the electronic energy and ZPE only
A_0, B_0, C_0	– rotational constants
$\omega_e^1, \dots, \omega_e^N$	– vibrational frequencies
E_{ZP}	– zero-point energy
XYZ	– Cartesian structure (chemical element, x, y, z)



Sym.: C_{2v}

$$\Delta_f H_0^0 = -837.6 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -822.7 \text{ kJ/mol}$$

$$E_b = 5.565 \text{ eV}$$

$$A_0, B_0, C_0 = 7.473 \times 10^{-2}, 7.704 \times 10^{-2}, 2.491 \text{ cm}^{-1}$$

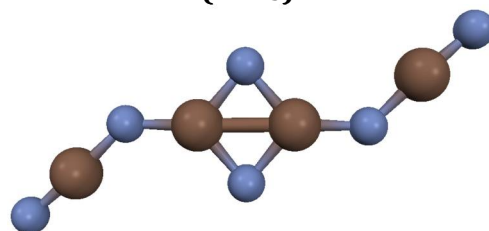
$$\omega_e^1, \dots, \omega_e^9 = 106, 471, 482, 507, 553, 761, 1228, 2105, 2114 \text{ cm}^{-1}$$

$$E_{\text{ZP}} = 0.516 \text{ eV}$$

XYZ, Å:

B	-0.16118034	0.64417299	0.42795869
B	0.35136326	-1.79917132	0.52625160
O	0.18804953	-0.54091531	0.90158559
O	0.51243397	-2.95538998	0.22780678
O	-0.47276444	1.74105059	0.03860036

$(\text{B}_2\text{O}_3)_2$



Sym.: C_{2h}

$$\Delta_f H_0^0 = -1934.5 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -1907.3 \text{ kJ/mol}$$

$$E_b = 5.834 \text{ eV}$$

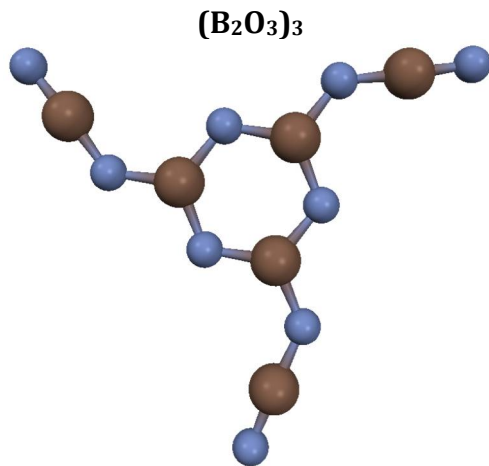
$$A_0, B_0, C_0 = 1.555 \times 10^{-2}, 1.639 \times 10^{-2}, 3.021 \times 10^{-1} \text{ cm}^{-1}$$

$$\omega_e^1, \dots, \omega_e^{24} = 37, 59, 91, 94, 146, 305, 427, 454, 514, 523, 529, 581, 632, 728, 740, 870, 964, 1075, 1106, 1350, 1448, 1644, 2094, 2105 \text{ cm}^{-1}$$

$$E_{\text{ZP}} = 1.148 \text{ eV}$$

XYZ, Å:

B	0.49077749	-2.44801217	1.07453102
B	0.65401463	-0.34399575	-0.19578022
O	0.47115235	-3.20631096	2.01253822
O	0.50234108	-1.66588814	0.00535306
O	0.64160425	0.35473729	-1.40407929
B	0.85115431	1.40461500	-0.50513404
B	1.01416986	3.50871032	-1.77541052
O	0.86367580	0.70585884	0.70315859
O	1.00247499	2.72655224	-0.70625575
O	1.03395223	4.26704233	-2.71338409



(B₂O₃)₃

Sym.: C_{3h}

$$\Delta_f H_0^0 = -3113.7 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -3073.9 \text{ kJ/mol}$$

$$E_b = 5.981 \text{ eV}$$

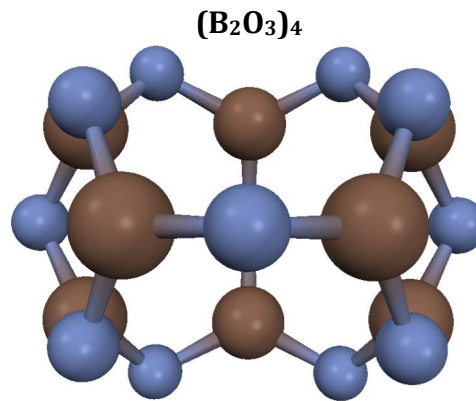
$$A_0, B_0, C_0 = 7.976 \times 10^{-3}, 1.594 \times 10^{-2}, 1.596 \times 10^{-2} \text{ cm}^{-1}$$

$$\omega_e^1, \dots, \omega_e^{39} = 39, 44, 47, 61, 64, 90, 152, 153, 156, 271, 274, 413, 415, 423, 475, 529, 529, 532, 571, 572, 653, 677, 677, 750, 811, 846, 847, 1043, 1118, 1119, 1255, 1401, 1402, 1422, 1424, 1495, 2093, 2094, 2104 \text{ cm}^{-1}$$

$$E_{ZP} = 1.800 \text{ eV}$$

XYZ, Å:

B	-0.83387990	0.45733226	1.06338523
O	-0.70867882	1.32665812	0.01209138
O	-0.38195213	-0.83247951	0.95786791
B	-1.68089732	0.34336459	3.37585010
O	-1.41615690	0.90792434	2.20940064
O	-1.94410456	-0.12454086	4.45741010
B	0.19939558	-1.24940637	-0.21035098
B	-0.30202071	2.99945328	-2.42898033
O	-0.57564877	4.14992056	-2.67286428
B	-0.12359564	0.89837749	-1.15123417
O	0.02045421	1.73444610	-2.21686285
O	0.33228214	-0.38806270	-1.26838942
B	1.22750161	-3.23532335	-1.24660264
O	0.63881819	-2.53620365	-0.29053679
O	1.76547000	-3.91710132	-2.08548092



(B₂O₃)₄

Sym.: C_{2v}

$$\Delta_f H_0^0 = -4305.9 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -4267.4 \text{ kJ/mol}$$

$$E_b = 6.061 \text{ eV}$$

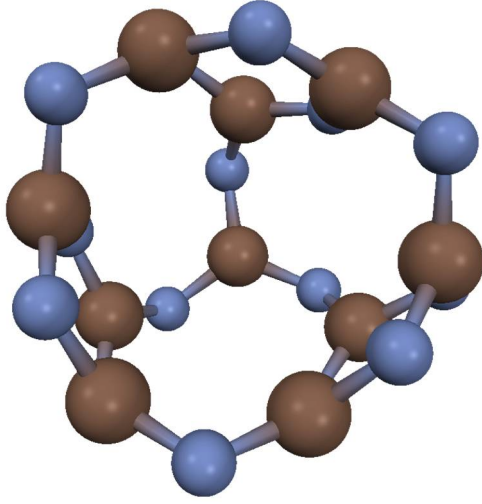
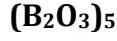
$$A_0, B_0, C_0 = 1.558 \times 10^{-2}, 1.562 \times 10^{-2}, 1.997 \times 10^{-2} \text{ cm}^{-1}$$

$$\omega_e^1, \dots, \omega_e^{54} = 92, 96, 98, 135, 190, 243, 249, 262, 314, 378, 390, 424, 431, 461, 461, 478, 480, 517, 545, 563, 591, 629, 642, 669, 694, 729, 754, 779, 780, 783, 786, 853, 877, 878, 919, 924, 975, 1014, 1110, 1113, 1124, 1126, 1140, 1251, 1295, 1326, 1331, 1331, 1367, 1371, 1379, 1387, 1401, 1431 \text{ cm}^{-1}$$

$$E_{ZP} = 2.577 \text{ eV}$$

XYZ, Å:

B	-1.72696836	-0.65068600	-0.38552069
B	1.13233290	1.82359787	-0.90085832
O	0.66452681	-1.96491623	1.35342608
O	-1.20438771	-0.42994199	-1.64428499
O	-2.14240282	0.45327414	0.34114762
B	0.12705574	-0.08969512	-1.52897102
B	-0.64785554	-1.53653078	1.34483748
O	0.94767018	-0.87130080	-0.73752138
O	-1.47867718	-1.83461885	0.28207003
O	0.59554214	1.13105202	-1.96765021
B	-1.45653178	0.62781755	1.52907346
B	2.21101699	0.93721936	0.82997711
O	1.41385730	1.58779493	1.75767062
O	0.26175284	2.53554557	-0.09154477
O	-0.95511849	1.87021176	1.85226830
B	1.41356396	-1.14632540	0.53430111
B	0.24799733	2.10422902	1.22219723
O	2.46495802	-0.40484319	1.03089081
O	-0.99009789	-0.49361321	2.19010226
O	2.38683460	1.50818441	-0.41582675



Sym.: C_3

$$\Delta_f H_0^0 = -5584.7 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -5536.0 \text{ kJ/mol}$$

$$E_b = 6.144 \text{ eV}$$

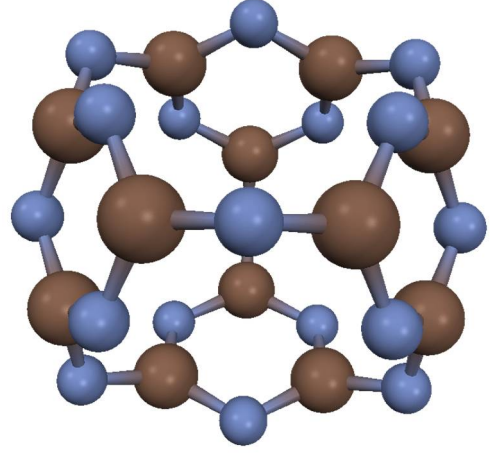
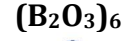
$$A_0, B_0, C_0 = 9.669 \times 10^{-3}, 1.108 \times 10^{-2}, 1.109 \times 10^{-2} \text{ cm}^{-1}$$

$\omega_e^1, \dots, \omega_e^{69} = 78, 79, 83, 143, 153, 154, 169, 170, 191, 248, 248, 303, 319, 319, 410, 420, 420, 432, 445, 462, 462, 484, 524, 524, 549, 555, 556, 624, 626, 663, 673, 694, 695, 744, 745, 770, 771, 772, 781, 823, 835, 836, 868, 889, 890, 964, 964, 1000, 1016, 1146, 1150, 1151, 1162, 1166, 1166, 1303, 1304, 1327, 1328, 1333, 1350, 1378, 1379, 1392, 1394, 1415, 1431, 1431, 1455 \text{ cm}^{-1}$

$$E_{ZP} = 3.267 \text{ eV}$$

XYZ, Å:

B	0.72423044	1.47334590	1.21501126
O	0.01012862	1.21882900	2.36589095
O	0.20360111	2.26083817	0.22410668
O	1.03410095	-0.93561121	2.48732221
B	1.87594256	-0.59603751	1.45181685
O	1.83371049	0.69333933	0.95786171
O	2.52459268	-1.56560492	0.72485835
B	-1.96834205	-0.75369247	1.42979363
O	-2.13211032	0.44169602	0.75703700
O	-2.18287315	-1.93074755	0.74827740
B	-0.09105991	-0.13624660	2.60663487
O	-1.32443857	-0.74949731	2.64404763
B	-0.12899192	1.70694700	-0.99695226
B	-2.11242524	0.44267005	-0.62296809
O	-1.45156388	1.43758401	-1.29130494
O	-2.51174981	-0.70412510	-1.27465201
O	0.10051827	-0.96781531	-2.21649315
B	-2.05621654	-1.83506050	-0.62800877
O	-1.20212391	-2.70867545	-1.26539955
B	2.09096429	-1.65339627	-0.58014336
O	1.16127478	-2.63067120	-0.89689797
O	2.31228168	-0.61566171	-1.46246400
B	0.03222677	-2.16739036	-1.53483109
B	1.12628867	-0.09051982	-1.92864345
O	0.86772701	1.25027685	-1.83749388



Sym.: T_d

$$\Delta_f H_0^0 = -6877.3 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -6816.1 \text{ kJ/mol}$$

$$E_b = 6.205 \text{ eV}$$

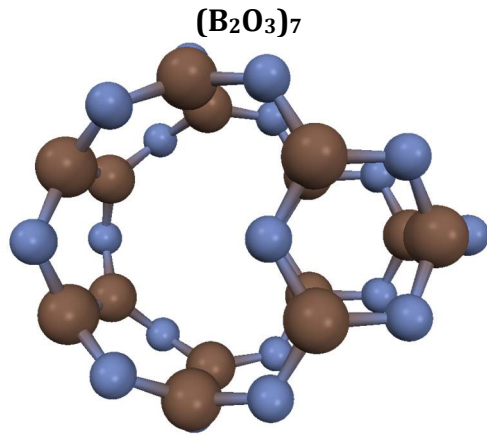
$$A_0, B_0, C_0 = 7.015 \times 10^{-3}, 7.017 \times 10^{-3}, 7.021 \times 10^{-3} \text{ cm}^{-1}$$

$\omega_e^1, \dots, \omega_e^{84} = 50, 53, 54, 71, 72, 74, 136, 136, 171, 172, 172, 177, 178, 212, 257, 258, 258, 421, 421, 422, 425, 425, 442, 443, 443, 449, 467, 468, 468, 502, 552, 552, 553, 601, 602, 602, 662, 662, 664, 726, 726, 727, 774, 774, 780, 780, 781, 785, 825, 826, 860, 880, 880, 944, 945, 947, 1012, 1013, 1013, 1180, 1181, 1181, 1182, 1197, 1198, 1199, 1311, 1311, 1341, 1342, 1342, 1360, 1361, 1361, 1399, 1415, 1416, 1416, 1438, 1439, 1444, 1445, 1445 \text{ cm}^{-1}$

$$E_{ZP} = 3.935 \text{ eV}$$

XYZ, Å:

B	0.95556182	-2.14153959	1.46214185
O	1.43606103	-2.50024968	0.22171364
B	-1.36226620	-1.90924137	1.47313880
O	-1.76781177	-0.79569606	2.17602586
O	-0.26012629	-2.61143388	1.88482700
B	2.19721372	-1.58581716	-0.47288060
B	1.09967386	-0.80071045	-2.37111122
O	2.83397884	-0.57769696	0.21730503
O	2.12608553	-1.53701035	-1.84036952
O	-0.14671099	-1.36868842	-2.52053508
B	1.38785545	1.89981775	1.45579331
O	1.44896773	2.49846748	0.21635089
B	2.34256456	-0.22548313	1.45532157
O	1.58267954	-1.13302172	2.16048084
O	2.40492531	1.07948568	1.86827281
B	0.27128360	2.69587781	-0.47080401
B	0.12813533	1.35531910	-2.37061432
O	-0.91588886	2.73749217	0.22703318
O	0.25653726	2.61135137	-1.83826627
O	1.24205379	0.56036666	-2.52960743
B	-2.32760469	0.24926958	1.47422800
O	-2.88260362	0.00785249	0.23656896
B	-0.96499444	2.13824003	1.46657544
O	0.20639915	1.93717234	2.16344252
O	-2.12191176	1.53859210	1.88987931
B	-2.47430877	-1.11190374	-0.45469795
B	-1.25359364	-0.56378534	-2.36209516
O	-1.91721531	-2.16433266	0.23831254
O	-2.40192315	-1.08109195	-1.82260424
O	-1.12301205	0.79839890	-2.52133273



Sym.: C_{2v}

$$\Delta_f H_0^0 = -8015.0 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -7942.7 \text{ kJ/mol}$$

$$E_b = 6.203 \text{ eV}$$

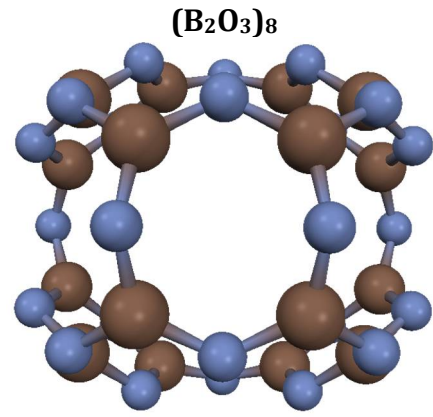
$$A_0, B_0, C_0 = 4.648 \times 10^{-3}, 5.171 \times 10^{-3}, 6.437 \times 10^{-3} \text{ cm}^{-1}$$

$\omega_e^1, \dots, \omega_e^{99} = 56, 78, 83, 86, 88, 101, 108, 108, 111, 145, 153, 165, 183, 183, 204, 217, 222, 245, 259, 281, 284, 313, 323, 331, 398, 415, 426, 428, 434, 434, 458, 472, 488, 491, 492, 506, 559, 569, 576, 587, 593, 596, 610, 629, 646, 667, 669, 680, 686, 711, 712, 723, 735, 739, 758, 772, 781, 797, 811, 813, 839, 856, 859, 874, 887, 932, 951, 976, 978, 1032, 1103, 1176, 1178, 1187, 1187, 1199, 1213, 1216, 1226, 1294, 1295, 1321, 1322, 1331, 1336, 1354, 1356, 1359, 1380, 1384, 1387, 1410, 1426, 1430, 1460, 1462, 1465, 1502, 1504 \text{ cm}^{-1}$

$$E_{ZP} = 4.577 \text{ eV}$$

XYZ, Å:

B	-1.99216101	-0.65785268	1.42068309
O	-2.33152685	-1.76487925	0.71762427
O	-1.81219095	-0.71546878	2.78142133
B	1.40513342	-1.74853019	1.34729648
O	1.27697892	-1.70783717	2.71450878
O	1.01273648	-2.83821611	0.64484051
O	2.00456995	0.55183171	2.75308228
B	1.18641054	-0.44053953	3.25321556
B	-0.97940013	0.25524090	3.29960311
O	0.11480140	-0.10913956	4.04989326
O	-1.08523709	1.54448621	2.81909154
O	1.77382796	-0.58576940	0.68247568
B	-1.25270155	1.64381931	1.45910626
O	-1.64246243	0.51078860	0.75607602
B	2.14429385	0.55312493	1.38644296
O	2.46431881	1.68938072	0.72198701
O	-0.87805724	2.76236219	0.79343505
B	2.00200096	2.02287849	-0.53303917
B	-0.35711879	2.78020945	-0.48259900
O	2.46613852	1.34876088	-1.63162358
O	0.99276556	2.94125425	-0.64322818
B	0.45410150	-2.80104270	-0.61486902
B	-1.90566518	-2.04367963	-0.56337892
O	-0.90012181	-2.95537475	-0.74189700
O	-2.40136080	-1.32341386	-1.61800390
B	0.87195028	-1.48047590	-2.56008344
B	-1.55489651	-0.70212377	-2.50724627
O	1.23385994	-2.48928570	-1.69751293
O	-0.42605817	-1.32544573	-2.96529704
O	-1.79830802	0.62026929	-2.78292846
B	1.59343841	0.76630643	-2.52203626
B	-0.83346272	1.54483110	-2.46937880
O	1.82772220	-0.54268761	-2.86196823
O	0.45193127	1.40823489	-2.91887234
O	-1.16909675	2.51542889	-1.55393564



Sym.: C_{2v}

$$\Delta_f H_0^0 = -9288.2 \text{ kJ/mol}$$

$$\Delta_f H_{298}^0 = -9207.6 \text{ kJ/mol}$$

$$E_b = 6.236 \text{ eV}$$

$$A_0, B_0, C_0 = 3.486 \times 10^{-3}, 3.771 \times 10^{-3}, 4.267 \times 10^{-3} \text{ cm}^{-1}$$

$\omega_e^1, \dots, \omega_e^{114} = 25, 32, 35, 59, 66, 86, 92, 101, 111, 114, 127, 140, 151, 166, 169, 183, 189, 190, 191, 197, 202, 220, 260, 269, 280, 304, 328, 362, 387, 399, 403, 415, 422, 427, 449, 454, 482, 482, 491, 505, 516, 518, 531, 544, 545, 593, 618, 621, 623, 638, 657, 657, 669, 673, 680, 714, 714, 721, 734, 744, 753, 757, 764, 769, 775, 777, 815, 815, 821, 831, 838, 846, 848, 866, 926, 947, 952, 963, 1006, 1008, 1026, 1084, 1189, 1194, 1197, 1200, 1207, 1214, 1217, 1224, 1227, 1304, 1311, 1313, 1334, 1341, 1342, 1347, 1360, 1365, 1379, 1393, 1400, 1410, 1413, 1417, 1440, 1440, 1450, 1458, 1467, 1470, 1470, 1474 \text{ cm}^{-1}$

$$E_{ZP} = 5.259 \text{ eV}$$

XYZ, Å:

B	-0.50544656	1.51608782	1.89231952
O	-0.23904294	0.58431331	2.85064279
B	-2.22782468	2.42192588	0.56220408
O	-1.32004141	2.81079722	-0.40013396
O	-1.77550952	2.03782152	1.80420602
B	1.49606815	-2.08385369	1.09502463
B	0.09531938	-0.72618293	2.61799373
O	2.36136321	-1.92831945	0.04117235
O	1.23723055	-1.01014832	1.91072876
O	-0.77987903	-1.71043971	2.99281228
B	2.17714237	-1.08546562	-1.01380552
O	2.00416444	0.26565202	-0.83195070
B	1.18505741	-0.90902522	-3.14619897
O	0.82558332	-3.26962913	1.23224831
O	1.96938338	-1.61842894	-2.26528419
B	-0.03804133	2.31958054	-0.30017420
B	1.32249027	1.00163495	-1.77447223
O	0.39945904	1.80480921	0.89933374
O	0.71018420	2.17691464	-1.43586903
O	1.08900825	0.46050012	-3.01847097
B	-1.04182943	-3.75394939	-1.58882554
O	-0.46914302	-4.27522761	-0.46723584
B	-0.61453622	-2.39909434	-3.46863732
O	-1.94537610	-2.04890251	-3.55482533
O	-0.24201776	-3.45432734	-2.66765490
B	-1.79505393	-2.28675077	2.27732544
B	-0.39877588	-3.64943220	0.75212675
O	-3.05245487	-1.74206991	2.35131546
O	-1.56247751	-3.31701285	1.40029083
O	0.33081771	-1.55939694	-3.99819850
B	-3.71457527	-1.13663696	1.32530391
O	-3.93938251	-1.78315744	0.13392010
B	-4.02928969	0.93300798	0.24399476
O	-3.53296185	2.21022203	0.20027845
O	-3.99282864	0.20794672	1.41340678
B	-2.76016745	-2.37852004	-2.49525775
B	-4.11384196	-1.05338786	-1.02008917
O	-2.35337884	-3.34335090	-1.60181415
O	-3.86416865	-1.61140842	-2.24343683
O	-4.35386664	0.29946453	-0.93714860