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SUPPORTING INFORMATION

Towards monomeric structure of phebylboronic acid: the influence of *ortho*-alkoxy substituents on the crystal structure

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Table 1. Bond lengths in [Å] for 2-methoxyphenylboronic acid (**1**), 2-ethoxyphenylboronic acid (**2**) and 2-isobutoxyphenylboronic acid (**3**).

Compound/Parameter	**(1)**	**(2)**	(**3**)	
			A	B
B(1)-O(11)	1.3717(15)	1.378(1)	1.370(2)	1.377(2)
B(1)-O(12)	1.3514(16)	1.356(1)	1.360(2)	1.352(2)
C(1)-B(1)	1.5768(16)	1.579(1)	1.566(2)	1.564(2)
O(11)-H(11)	0.86(2)	0.87(2)	0.86(2)	0.83(2)
O(12)-H(12)	0.859(19)	0.89(2)	0.88(2)	0.89(2)
C(1)-C(2)	1.4022(16)	1.408(1)	1.405(2)	1.405(2)
C(1)-C(6)	1.3968(15)	1.399(1)	1.394(2)	1.398(2)
C(2)-O(2)	1.3804(13)	1.377(1)	1.381(2)	1.384(2)
C(2)-C(3)	1.3935(16)	1.400(1)	1.384(2)	1.385(2)
C(3)-C(4)	1.3847(17)	1.391(1)	1.391(2)	1.385(2)
C(4)-C(5)	1.3823(18)	1.385(2)	1.379(2)	1.379(2)
C(5)-C(6)	1.3923(17)	1.394(1)	1.384(2)	1.384(2)
C(6)-O(6)				
O(2)-C(21)	1.4309(14)	1.439(1)	1.438(2)	1.442(2)
C(21)-C(22)		1.509(1)	1.511(2)	1.508(2)
C(22)-C(23)			1.518(2)	1.519(3)
C(22)-C(24)			1.521(2)	1.521(2)

Table 2. Bond lengths in [Å] for 2,6-dimethoxyphenylboronic acid, polymorph I (**4A**), 2,6-dimethoxyphenylboronic acid, polymorph II (**4B**) and 2,6-diethoxyphenylboronic acid, polymorph I (**5A**).

Compound/Parameter	(**4A**)	**(4B)**		**(5A)**
		A	B	
B(1)-O(11)	1.352(1)	1.352(3)	1.359(2)	1.349(2)
B(1)-O(12)	1.352(1)	1.370(3)	1.359(2)	1.364(2)
C(1)-B(1)	1.580(2)	1.574(3)	1.583(4)	1.583(2)
O(11)-H(11)	0.86(3)	0.82(3)	0.90(2)	0.98(2)
O(12)-H(12)	0.86(3)	0.82(2)	0.90(2)	0.84(2)
C(1)-C(2)	1.399(1)	1.402(3)	1.399(2)	1.399(2)
C(1)-C(6)	1.399(1)	1.408(3)	1.399(2)	1.401(2)
C(2)-O(2)	1.375(1)	1.374(2)	1.376(2)	1.369(2)
C(2)-C(3)	1.394(2)	1.390(3)	1.394(3)	1.396(2)
C(3)-C(4)	1.384(2)	1.376(3)	1.380(3)	1.383(2)
C(4)-C(5)	1.384(2)	1.384(3)	1.380(3)	1.389(2)
C(5)-C(6)	1.394(2)	1.390(3)	1.394(3)	1.394(2)
C(6)-O(6)	1.375(1)	1.380(2)	1.376(2)	1.371(2)
O(2)-C(21)	1.422(2)	1.435(2)	1.433(2)	1.440(2)
C(21)-C(22)				1.420(3) / 1.404(3)
C(22)-C(23)				
C(22)-C(24)				
O(6)-C(61)				1.438(2)
C(61)-C(62)				1.505(2)

Table 3. Bond lengths in [Å] for 2,6-diethoxyphenylboronic acid, polymorph II (**5B**) and 2-isobutoxy-6-methoxyphenylboronic acid (**6**).

Compound/Parameter	**(5B)**				**(6)**
	A	B	C	D	
B(1)-O(11)	1.361(2)	1.364(2)	1.358(3)	1.360(3)	1.355(2)
B(1)-O(12)	1.363(2)	1.355(2)	1.354(3)	1.353(2)	1.357(2)
C(1)-B(1)	1.586(3)	1.595(3)	1.590(3)	1.592(3)	1.586(2)
O(11)-H(11)	0.87(2)	0.83(3)	0.85(2)	0.81(2)	0.85(2)
O(12)-H(12)	0.84(2)	0.85(2)	0.86(3)	0.86(2)	0.87(2)
C(1)-C(2)	1.408(2)	1.407(2)	1.402(2)	1.408(2)	1.403(2)
C(1)-C(6)	1.410(2)	1.407(2)	1.412(2)	1.408(2)	1.409(2)
C(2)-O(2)	1.387(2)	1.379(2)	1.388(2)	1.374(2)	1.377(2)
C(2)-C(3)	1.392(2)	1.399(2)	1.395(2)	1.399(2)	1.390(2)
C(3)-C(4)	1.384(2)	1.381(2)	1.383(3)	1.381(3)	1.378(2)
C(4)-C(5)	1.384(2)	1.384(2)	1.383(3)	1.381(2)	1.381(2)
C(5)-C(6)	1.400(2)	1.394(2)	1.396(2)	1.393(2)	1.388(2)
C(6)-O(6)	1.373(2)	1.385(2)	1.379(2)	1.384(2)	1.375(2)
O(2)-C(21)	1.438(2)	1.443(2)	1.443(2)	1.443(2)	1.437(2)
C(21)-C(22)	1.507(3)	1.499(3)	1.510(3)	1.495(3)	1.512(2)
C(22)-C(23)					1.519(2)
C(22)-C(24)					1.522(2)
O(6)-C(61)	1.441(2)	1.441(2)	1.435(2)	1.436(2)	1.429(2)
C(61)-C(62)	1.501(3)	1.508(3)	1.496(3)	1.507(3)	

Table 4. Bond angles [°] for 2-methoxyphenylboronic acid (**1**), 2-ethoxyphenylboronic acid (**2**) and 2-isobutoxyphenylboronic acid (**3**).

Compound/Parameter	**(1)**	**(2)**	(**3**)	
			A	B
O(12)-B(1)-O(11)	119.65(10)	119.4(1)	118.4(2)	119.5(2)
O(12)-B(1)-C(1)	118.72(10)	118.6(1)	119.6(2)	118.0(2)
O(11)-B(1)-C(1)	121.63(11)	122.0(1)	121.9(1)	122.5(1)
B(1)-O(11)-H(11)	112.3(11)	111(1)	112(1)	110(1)
B(1)-O(12)-H(12)	110.6(13)	112(1)	112(1)	111(1)
C(6)-C(1)-C(2)	117.10(10)	117.2(1)	116.5(1)	116.6(1)
C(2)-C(1)-B(1)	119.43(10)	123.4(1)	122.8(1)	123.8(1)
C(6)-C(1)-B(1)	123.46(10)	119.4(1)	120.6(1)	119.6(1)
O(2)-C(2)-C(3)	121.94(11)	122.7(1)	122.3(1)	122.8(1)
O(2)-C(2)-C(1)	116.12(9)	115.8(1)	115.7(1)	115.4(1)
C(3)-C(2)-C(1)	121.92(11)	121.6(1)	122.0(1)	121.8(1)
C(4)-C(3)-C(2)	118.99(11)	119.1(1)	119.1(2)	119.2(1)
C(5)-C(4)-C(3)	120.75(10)	120.9(1)	120.8(2)	121.0(2)
C(4)-C(5)-C(6)	119.52(11)	119.2(1)	119.0(2)	118.9(2)
O(6)-C(6)-C(5)				
O(6)-C(6)-C(1)				
C(5)-C(6)-C(1)	121.65(11)	122.1(1)	122.6(2)	122.5(2)
C(2)-O(2)-C(21)	118.53(9)	119.2(1)	119.6(1)	118.3(1)
O(2)-C(21)-C(22)		107.0(1)	107.3(1)	109.3(1)
C(21)-C(22)-C(23)			108.8(1)	112.2(2)
C(21)-C(22)-C(24)			111.8(1)	108.3(1)
C(23)-C(22)-C(24)			111.2(2)	110.6(2)
C(6)-O(6)-C(61)				
O(6)-C(61)-C(62)				

Table 5. Bond angles [°] for 2,6-dimethoxyphenylboronic acid, polymorph I (**4A**), 2,6-dimethoxyphenylboronic acid, polymorph II (**4B**) and 2,6-diethoxyphenylboronic acid, polymorph I (**5A**).

Compound/Parameter	**(4A)**	**(4B)**		(**5A**)
		A	B	
O(12)-B(1)-O(11)	117.0(2)	114.0(2)	115.2(2)	118.4(1)
O(12)-B(1)-C(1)	121.5(1)	123.7(2)	122.4(1)	123.0(1)
O(11)-B(1)-C(1)	121.5(1)	122.3(2)	122.4(1)	118.6(1)
B(1)-O(11)-H(11)	119(2)	109(2)	115(1)	114(1)
B(1)-O(12)-H(12)	122(2)	109(2)	115(1)	119(1)
C(6)-C(1)-C(2)	117.3(1)	115.8(2)	116.5(2)	117.6(1)
C(2)-C(1)-B(1)	121.4(1)	121.7(2)	121.7(1)	121.3(1)
C(6)-C(1)-B(1)	121.4(1)	122.5(2)	121.7(1)	121.1(1)
O(2)-C(2)-C(3)	115.1(1)	115.1(2)	114.7(2)	123.4(1)
O(2)-C(2)-C(1)	122.9(1)	122.2(2)	123.0(2)	115.2(1)
C(3)-C(2)-C(1)	122.0(1)	122.8(2)	122.3(2)	121.4(1)
C(4)-C(3)-C(2)	118.3(1)	118.2(2)	118.6(2)	119.0(1)
C(5)-C(4)-C(3)	122.1(1)	122.4(2)	121.5(3)	121.6(1)
C(4)-C(5)-C(6)		117.9(2)		118.4(1)
O(6)-C(6)-C(5)		121.9(2)		123.1(1)
O(6)-C(6)-C(1)		115.2(2)		114.9(1)
C(5)-C(6)-C(1)		123.0(2)		122.0(1)
C(2)-O(2)-C(21)	117.9(1)	119.6(2)	117.3(2)	118.5(1)
O(2)-C(21)-C(22)				113.4(2)/ 112.5(2)
C(21)-C(22)-C(23)				
C(21)-C(22)-C(24)				
C(23)-C(22)-C(24)				
C(6)-O(6)-C(61)				117.8(1)
O(6)-C(61)-C(62)				107.0(1)

Table 6. Bond angles [°] for 2,6-diethoxyphenylboronic acid, polymorph II (**5B**) and 2-isobutoxy-6-methoxyphenylboronic acid (**6**).

Compound/Parameter	(**5B**)				(**6**)
	A	B	C	D	
O(12)-B(1)-O(11)	114.0(2)	114.9(2)	114.6(2)	114.3(2)	114.4(1)
O(12)-B(1)-C(1)	122.4(2)	122.3(2)	123.7(2)	122.4(2)	122.6(1)
O(11)-B(1)-C(1)	123.6(2)	122.8(2)	121.7(2)	123.3(2)	123.0(1)
B(1)-O(11)-H(11)	111(1)	110(2)	110(2)	112(2)	110(1)
B(1)-O(12)-H(12)	112(1)	110(1)	108(2)	110(1)	113(1)
C(6)-C(1)-C(2)	115.6(1)	115.5(1)	115.6(2)	115.8(1)	115.5(1)
C(2)-C(1)-B(1)	122.5(1)	122.2(1)	122.6(2)	121.9(2)	122.2(1)
C(6)-C(1)-B(1)	121.9(1)	122.2(2)	121.7(2)	122.3(2)	122.2(1)
O(2)-C(2)-C(3)	115.5(1)	115.8(1)	115.6(1)	115.7(1)	115.6(1)
O(2)-C(2)-C(1)	121.6(1)	121.4(1)	121.4(2)	121.6(2)	121.6(1)
C(3)-C(2)-C(1)	122.9(2)	122.8(2)	123.0(2)	122.7(2)	122.8(1)
C(4)-C(3)-C(2)	118.6(2)	118.6(2)	118.3(2)	118.3(2)	118.6(1)
C(5)-C(4)-C(3)	121.8(2)	121.4(2)	122.0(2)	121.9(2)	121.7(1)
C(4)-C(5)-C(6)	118.3(2)	118.7(2)	118.1(2)	118.6(2)	118.5(1)
O(6)-C(6)-C(5)	121.5(1)	121.5(1)	121.6(2)	121.7(2)	121.5(1)
O(6)-C(6)-C(1)	115.7(1)	115.6(1)	115.5(2)	115.6(1)	115.6(1)
C(5)-C(6)-C(1)	122.8(2)	122.9(2)	122.9(2)	122.7(2)	122.9(1)
	119.4(1)	118.3(1)	119.4(1)	118.4(1)	
C(2)-O(2)-C(21)	107.0(2)	107.3(2)	106.2(2)	107.3(1)	119.1(1)
O(2)-C(21)-C(22)					108.9(1)
C(21)-C(22)-C(23)					108.2(1)
C(21)-C(22)-C(24)					111.7(1)
C(23)-C(22)-C(24)					110.9(1)
C(6)-O(6)-C(61)	118.8(1)	119.7(1)	118.5(1)	119.4(1)	118.3(1)
O(6)-C(61)-C(62)	107.0(1)	106.8(2)	107.4(2)	107.2(2)	

Table 7. Torsion angles [°] for 2-methoxyphenylboronic acid (**1**), 2-ethoxyphenylboronic acid (**2**) and 2-isobutoxyphenylboronic acid (**3**).

Compound/Parameter	**(1)**	**(2)**	(**3**)	
			A	B
C(2)-C(1)-B(1)-O(11)	-2.45(17)	-6.4(1)	1.8(2)	2.6(2)
C(6)-C(1)-B(1)-O(11)	177.60(10)	174.2(1)	-178.9(1)	-177.8(1)
C(2)-C(1)-B(1)-O(12)	176.56(10)	172.1(1)	-178.7(1)	-177.4(1)
C(6)-C(1)-B(1)-O(12)	-3.39(16)	-7.3(1)	0.6(2)	2.1(2)
C(6)-C(1)-C(2)-O(2)	-178.15(9)	-178.8(1)	178.1(1)	178.7(1)
B(1)-C(1)-C(2)-O(2)	1.90(16)	1.7(1)	-2.6(2)	-1.8(2)
C(6)-C(1)-C(2)-C(3)	2.81(17)	1.0(1)	-1.0(2)	-1.4(2)
B(1)-C(1)-C(2)-C(3)	-177.15(10)	-178.4(1)	178.3(1)	178.2(1)
O(2)-C(2)-C(3)-C(4)	179.04(10)	178.5(1)	-177.9(1)	-178.2(1)
C(1)-C(2)-C(3)-C(4)	-1.97(17)	-1.4(1)	1.2(2)	1.9(2)
C(2)-C(3)-C(4)-C(5)	-0.46(18)	0.8(1)	-0.5(2)	-1.0(2)
C(3)-C(4)-C(5)-C(6)	1.91(19)	0.1(1)	-0.2(2)	-0.4(2)
C(4)-C(5)-C(6)-C(1)	-1.00(18)	-0.5(1)	0.4(2)	0.9(2)
C(2)-C(1)-C(6)-C(5)	-1.31(17)	-0.1(1)	0.2(2)	0.0(2)
B(1)-C(1)-C(6)-C(5)	178.65(10)	179.4(1)	-179.1(1)	-179.6(1)
B(1)-C(1)-C(6)-O(6)				
C(2)-C(1)-C(6)-O(6)				
C(4)-C(5)-C(6)-O(6)				
C(1)-C(2)-O(2)-C(21)	172.22(10)	-176.4(1)	168.2(1)	-178.4(1)
C(3)-C(2)-O(2)-C(21)	-8.73(16)	3.7(1)	-12.7(2)	1.7(2)
C(2)-O(2)-C(21)-C(22)		178.1(1)	-178.8(1)	175.9(1)
O(2)-C(21)-C(22)-C(23)			169.7(1)	176.1(1)
O(2)-C(21)-C(22)-C(24)			-67.2(2)	-61.5(2)
C(1)-C(6)-O(6)-C(61)				
C(5)-C(6)-O(6)-C(61)				
C(6)-O(6)-C(61)-C(62)				

Table 8. Torsion angles [°] for 2,6-dimethoxyphenylboronic acid, polymorph I (**4A**), 2,6-dimethoxyphenylboronic acid, polymorph II (**4B**) and 2,6-diethoxyphenylboronic acid, polymorph I (**5A**).

Compound/Parameter	**(4A)**	**(4B)**		**(5A)**
		A	B	
C(2)-C(1)-B(1)-O(11)	-46.2(1)	5.0(3)	-120.2(1)	50.6(2)
C(6)-C(1)-B(1)-O(11)	133.8(1)	-172.4(2)	59.8(1)	-130.0(1)
C(2)-C(1)-B(1)-O(12)	133.8(1)	-175.5(2)	59.8(1)	-128.3(1)
C(6)-C(1)-B(1)-O(12)	-46.2(1)	7.1(3)	-120.2(1)	51.1(2)
C(6)-C(1)-C(2)-O(2)	178.6(1)	-178.6(2)	-179.4(2)	179.8(1)
B(1)-C(1)-C(2)-O(2)	-1.4(1)	3.9(3)	0.6(2)	-0.8(2)
C(6)-C(1)-C(2)-C(3)	0.2(1)	1.3(3)	-0.3(1)	-0.4(2)
B(1)-C(1)-C(2)-C(3)	-179.8(1)	-176.2(2)	179.7(1)	179.1(1)
O(2)-C(2)-C(3)-C(4)	-178.6(1)	179.2(2)	179.6(1)	179.9(1)
C(1)-C(2)-C(3)-C(4)	-0.3(2)	-0.7(3)	0.6(3)	0.0(2)
C(2)-C(3)-C(4)-C(5)	0.2(1)	0.1(3)	-0.3(1)	0.3(2)
C(3)-C(4)-C(5)-C(6)		-0.1(3)		-0.4(2)
C(4)-C(5)-C(6)-C(1)		0.8(3)		0.0(2)
C(2)-C(1)-C(6)-C(5)		-1.4(3)		0.3(2)
B(1)-C(1)-C(6)-C(5)		176.1(2)		-179.1(1)
B(1)-C(1)-C(6)-O(6)		-4.3(3)		2.5(2)
C(2)-C(1)-C(6)-O(6)		178.2(2)		-178.1(1)
C(4)-C(5)-C(6)-O(6)		-178.7(2)		178.3(1)
C(1)-C(2)-O(2)-C(21)	178.0(1)	-174.2(2)	-174.7(2)	176.7(1)
C(3)-C(2)-O(2)-C(21)	-3.6(2)	5.9(3)	6.3(3)	-3.1(2)
C(2)-O(2)-C(21)-C(22)				-173.6(2)/ -86.0(2)
O(2)-C(21)-C(22)-C(23)				
O(2)-C(21)-C(22)-C(24)				
C(1)-C(6)-O(6)-C(61)	-177.2(1)	174.2(2)		-179.5(1)
C(5)-C(6)-O(6)-C(61)	2.4(2)	-6.2(3)		2.1(2)
C(6)-O(6)-C(61)-C(62)				-178.8(1)

Table 9. Torsion angles [°] for 2,6-diethoxyphenylboronic acid, polymorph II (**5B**) and 2-isobutoxy-6-methoxyphenylboronic acid (**6**).

Compound/Parameter	**(5B)**				**(6)**
	A	B	C	D	
C(2)-C(1)-B(1)-O(11)	-4.7(3)	3.2(3)	-7.1(3)	-9.9(3)	178.8(1)
C(6)-C(1)-B(1)-O(11)	176.4(2)	-176.5(2)	169.4(2)	171.7(2)	-2.8(2)
C(2)-C(1)-B(1)-O(12)	173.4(2)	-177.3(2)	174.5(2)	170.0(2)	-2.5(2)
C(6)-C(1)-B(1)-O(12)	-5.5(3)	3.0(3)	-8.9(3)	-8.5(3)	175.9(1)
C(6)-C(1)-C(2)-O(2)	-178.6(1)	-179.1(1)	-179.4(1)	179.8(1)	177.5(1)
B(1)-C(1)-C(2)-O(2)	2.4(2)	1.2(2)	-2.6(3)	1.3(2)	-3.9(2)
C(6)-C(1)-C(2)-C(3)	1.5(2)	0.7(2)	0.0(3)	0.0(3)	-2.9(2)
B(1)-C(1)-C(2)-C(3)	-177.5(2)	-179.0(2)	176.8(2)	-178.5(2)	175.6(1)
O(2)-C(2)-C(3)-C(4)	179.5(2)	179.6(1)	177.7(2)	-179.7(2)	-177.9(1)
C(1)-C(2)-C(3)-C(4)	-0.7(3)	-0.2(3)	-1.7(3)	0.1(3)	2.6(2)
C(2)-C(3)-C(4)-C(5)	0.1(3)	-0.1(3)	2.1(3)	-0.5(3)	-0.4(2)
C(3)-C(4)-C(5)-C(6)	-0.4(3)	-0.2(3)	-0.9(3)	0.7(3)	-1.2(2)
C(4)-C(5)-C(6)-C(1)	1.4(3)	0.8(3)	-0.9(3)	-0.7(3)	0.8(2)
C(2)-C(1)-C(6)-C(5)	-1.9(2)	-1.0(2)	1.3(3)	0.3(3)	1.2(2)
B(1)-C(1)-C(6)-C(5)	177.1(2)	178.7(2)	-175.5(2)	178.8(2)	-177.3(1)
B(1)-C(1)-C(6)-O(6)	-1.9(2)	-1.6(2)	3.5(3)	-0.5(2)	2.2(2)
C(2)-C(1)-C(6)-O(6)	179.1(1)	178.7(1)	-179.8(1)	-179.1(1)	-179.2(1)
C(4)-C(5)-C(6)-O(6)	-179.7(1)	-179.0(1)	-179.8(2)	178.6(2)	-178.8(1)
C(1)-C(2)-O(2)-C(21)	179.2(1)	177.1(1)	-178.5(2)	-170.3(1)	-170.8(1)
C(3)-C(2)-O(2)-C(21)	-0.9(2)	-2.7(2)	2.1(2)	9.5(2)	9.7(2)
C(2)-O(2)-C(21)-C(22)	179.0(2)	-176.6(2)	-177.0(2)	175.7(2)	166.3(1)
O(2)-C(21)-C(22)-C(23)					176.3(1)
O(2)-C(21)-C(22)-C(24)					-61.3(2)
C(1)-C(6)-O(6)-C(61)	-168.5(1)	-178.4(1)	173.4(2)	-178.2(2)	
C(5)-C(6)-O(6)-C(61)	12.5(2)	1.4(2)	-7.6(3)	2.5(2)	
C(6)-O(6)-C(61)-C(62)	176.0(1)	179.3(1)	-175.0(2)	-175.2(2)	

Table 10. Weak interactions in the crystal structure of 2-methoxyphenylboronic acid (**1**). The contact lengths given in [Å]

Type of contact	Symmetry code	Contact Length
B1...H12	1-x,-y,2-z	2.966
B1...O11	1-x,-y,2-z	3.511
B1...C1	1-x,-y,1-z	3.560
B1...C2	1-x,-y,1-z	3.284
B1...C3	1-x,-y,1-z	3.564
C2...H3	x,1/2-y,1/2+z	2.853
O12...H6	-x,-y,1-z	2.687
O12...H222	1-x,-y,1-z	2.682
O21...H3	x,1/2-y,1/2+z	2.639

Table 11. Weak interactions in the crystal structure of 2-ethoxyphenylboronic acid (**2**). The contact lengths given in [Å].

Type of contact	Symmetry code	Contact Length
B1...H12	1-x,1-y,1-z	2.939
B1...C5	1+x,y,z	3.547
B1...B1	-x,1-y,1-z	3.573
B1...O12	-x,1-y,1-z	3.127
C3...H81	-1+x,y,z	2.813
O12...H71	1/2-x,1/2+y,1/2-z	2.641

Table 12. Weak interactions in the crystal structure of 2-isobutoxyphenylboronic acid (**3**). The contact lengths given in [Å].

Type of contact	Symmetry code	Contact Length
B1A...H12B	x,1.5-y,-1/2+z	2.946
B1B...H3A	1-x,1-y,1-z	3.107
B1B...O11A	x,1.5-y,1/2+z	3.450
B1B...H12A	x,1.5-y,1/2+z	3.023
B1B...C3A	1-x,1-y,1-z	3.637
C5A...H92B	x,y,-1+z	2.861
C5A...H72A	-1+x,1/2-y,-1/2+z	2.837
C6A...H72A	-1+x,1/2-y,-1/2+z	2.888
H11A...H12B	x,1.5-y,-1/2+z	2.386

Table 13. Weak interactions in the crystal structure of 2,6-dimethoxyphenylboronic acid, polymorph I (**4A**). The contact lengths given in [Å].

Type of contact	Symmetry codes	Contact Length
O11...H4	y,1-x,-z	2.758
H11...H4	y,1-x,-z	2.299
O2...H3	Y, 2-x, -z	2.737

Table 14. Weak interactions in the crystal structure of 2,6-dimethoxyphenylboronic acid, polymorph II (**4B**). The contact lengths given in [Å].

Type of contact	Symmetry code	Contact Length
B1B..H4B	x,1+y,z	3.169
B1B...H81A	1-x,1-y,1-z	2.944
B1B...C61A	1-x,1-y,1-z	3.551
C21B...O11B	-1/2+x,-1/2+y,z	3.163
C4B...H73A	-1/2+x,-1/2+y,z	2.858
H11A...H11A	2-x,-y,1-z	2.319
H11B...B1A	1.5-x,1/2-y,1-z	2.841
H3B...H71B	1/2-x,-1/2+y,1.5-z	2.298
O11A...O11A	2-x,-y,1-z	3.008
O11A...H82A	1/2+x,-1/2+y,z	2.578
O11A...H11A	2-x,-y,1-z	2.557
O11B...H4B	x,1+y,z	2.698
O12A...H73B	1-x,-y,1-z	2.676

Table 15. Weak interactions in the crystal structure of 2,6-diethoxyphenylboronic acid, polymorph I (**5A**). The contact lengths given in [Å].

Type of contact	Symmetry code	Contact lengths
B1...H11	1.5-x,1/2+y,1/2-z	2.884
B1...H22A	x,1+y,z	3.118
B1...H12	x,-1+y,z	3.155
B1...H62A	x,-1+y,z	3.021
B1...H22C	2-x,1-y,1-z	3.090
B1...C22A	2-x,1-y,1-z	3.651
C21B...C2	x,y,z	2.413
C21B...C3	x,y,z	2.825
C21B...H3	x,y,z	2.521
H11...H12	1.5-x,-1/2+y,1/2-z	2.210
O2...H22C	2-x,1-y,1-z	2.681

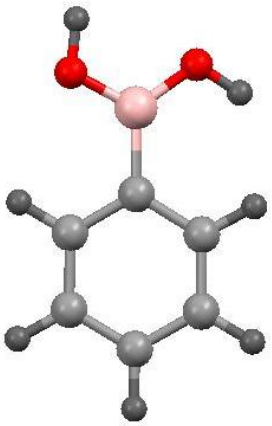
Table 16. Weak interactions in the crystal structure of 2,6-diethoxyphenylboronic acid, polymorph II (**5B**). The contact lengths given in [Å].

Type of contact	Symmetry code	Contact lengths
B1A...O6B	1-x,-1/2+y,1.5-z	3.499
B1A...H10B	1-x,1-y,2-z	3.024
B1A...H5A	1-x,-1/2+y,1.5-z	3.161
B1B...H3D	x,1.5-y,1/2+z	3.190
B1B...O2A	1-x,1/2+y,1.5-z	3.450
B1B...H72A	1-x,1-y,2-z	2.994
B1C...H91D	x,y,1+z	3.171
B1C...H5C	-x,-1/2+y,1.5-z	3.150
B1D...H81C	x,y,-1+z	3.079
C1D...H72C	x,y,-1+z	2.885
C2D...H20C	-x,1-y,1-z	2.740
C4A...H71D	1-x,1-y,1-z	2.760
C4C...H92D	-x,1-y,1-z	2.892
C5C...H92D	-x,1-y,1-z	2.782
C6D...H92C	-x,1-y,1-z	2.830
C6D...H72C	x,y,-1+z	2.867
H10C...H71B	-x,1-y,1-z	2.351
H30D...H91C	-x,-1/2+y,1/2-z	2.348
H3A...H3C	1-x,1-y,2-z	2.388
H5D...H5D	-x,1-y,-z	2.378
H83A...H72D	1-x,-1/2+y,1.5-z	2.346
O11A...H5A	1-x,-1/2+y,1.5-z	2.406
O11A...H92A	1-x,-1/2+y,1.5-z	2.707
O11C...H5C	-x,-1/2+y,1.5-z	2.403
O12B...H71D	x,1.5-y,1/2+z	2.673
O12B...H3D	x,1.5-y,1/2+z	2.484
O12D...H3B	x,1/2-y,-1/2+z	2.496

Table 17. Weak interactions in the crystal structure of 2-isobutoxy-6-methoxyphenylboronic acid (**6**). The contact lengths given in [Å].

Type of contact	Symmetry code	Contact lengths
B1...C24	1-x,1-y,2-z	3.588
B1...H5	1/2-x,1/2+y,1.5-z	3.035
B1...H10	-x,1-y,2-z	3.140
B1...H82	1-x,1-y,2-z	2.891
C6...H91	-1/2+x,1/2-y,-1/2+z	2.886
H11...H72	x,y,-1+z	2.366
H12...H12	-x,1-y,2-z	2.399
O11...H4	1/2-x,1/2+y,1.5-z	2.715
O12...O12	-x,1-y,2-z	2.911
O12...H10	-x,1-y,2-z	2.704
O12...H12	-x,1-y,2-z	2.523
O12...H5	1/2-x,1/2+y,1.5-z	2.522
O2...H612	-1/2+x,1/2-y,1/2+z	2.699

Symmetry, number of imaginary frequencies, absolute electronic energy at MP2/6-31+G* (in Hartree), absolute electronic energy corrected for zero point energy (in Hartree) and Cartesian coordinates at MP2/6-31+G* for the molecules studied.

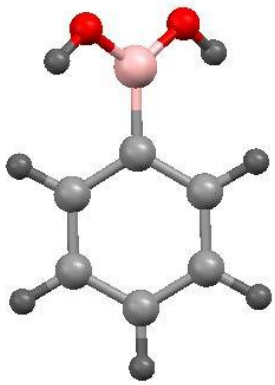


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	1	-407.0332855	-406.90971
C_1	0	-407.0334917	-406.909269

Cartesian coordinates for C_1 structure at MP2/6-31+G*

C	0.177342	0.011584	-0.013593
C	-0.531044	-1.197188	0.127951
C	-1.928265	-1.214149	0.140729
C	-2.645647	-0.019367	0.012245
C	-1.960157	1.190731	-0.136311
C	-0.562240	1.201993	-0.145187
B	1.744316	-0.000340	-0.008358
O	2.389305	-1.183798	-0.277034
O	2.528237	1.107490	0.259491
H	-0.052526	2.156637	-0.283076
H	0.024529	-2.128251	0.220287

H	2.016345	1.893696	0.511184
H	-2.513638	2.121257	-0.246640
H	-3.733806	-0.031783	0.020792
H	3.356704	-1.083625	-0.208402
H	-2.459463	-2.157390	0.252988



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2v}	1	-407.0262476	-406.902874
C_1	0	-407.0286325	-406.904221

Cartesian coordinates for C_1 structure at MP2/6-31+G*

C	-0.820332	0.889931	1.930740
C	0.000000	0.000000	2.632215
C	0.820332	-0.889931	1.930740
C	0.812999	-0.892399	0.532445
C	0.000000	0.000000	-0.193618
C	-0.812999	0.892399	0.532445
B	0.000000	0.000000	-1.769825
O	0.000000	1.161110	-2.507200
H	1.468923	-1.583488	0.002261
H	-1.468923	1.583488	0.002261

O	0.000000	-1.161110	-2.507200
H	-0.094336	-1.949899	-1.948012
H	1.464845	-1.579211	2.472858
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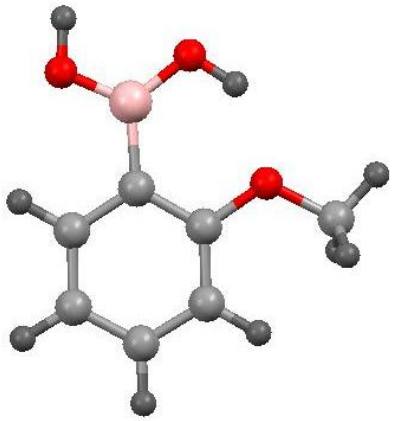
H	0.094336	1.949899	-1.948012
H	-1.464845	1.579211	2.472858

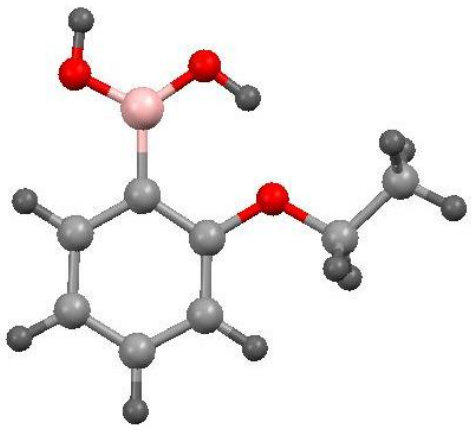


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	1	-521.2373433	-521.080081
C_1	0	-521.2373634	-521.079493

Cartesian coordinates for C_1 structure at MP2/6-31+G*

C	-0.441484	-0.475619	-0.000087
B	-1.913775	0.072267	-0.000027
O	-2.235615	1.400415	-0.000561
H	-1.435794	1.944213	-0.000858
O	-2.936620	-0.841407	0.000575
H	-3.798386	-0.411511	0.000520
C	0.699541	0.354415	-0.000297
O	0.465523	1.713723	-0.000586
C	1.569024	2.614430	0.000860

H	2.185584	2.485604	-0.893927
H	2.184573	2.483913	0.896092
H	1.138003	3.614321	0.001537
C	1.988852	-0.180325	-0.000302
H	2.860282	0.459824	-0.000508
C	2.158079	-1.565142	-0.000109
H	3.162584	-1.973977	-0.000124
C	1.055033	-2.411920	0.000082
H	1.188767	-3.487281	0.000231
C	-0.224300	-1.860465	0.000099
H	-1.091516	-2.510535	0.000280

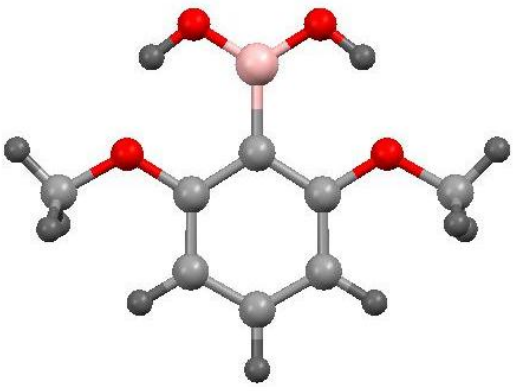


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	2	-560.4103124	-560.224718
C_1	0	-560.410438	-560.223284

Cartesian coordinates for C_1 structure at MP2/6-31+G*

C	-0.976424	0.236149	-0.030497
B	-0.897128	1.808479	-0.009308
O	0.278116	2.520504	-0.010779

H	1.033426	1.899360	-0.045135
O	-2.088947	2.500753	0.016882
H	-1.927751	3.461732	0.034897
C	0.160773	-0.598274	-0.078216
O	1.386677	0.047713	-0.168942
C	2.579469	-0.723865	0.059562
H	2.706259	-1.445940	-0.756025
H	2.475381	-1.269374	1.005406
C	3.734696	0.252309	0.101141
H	3.797473	0.809935	-0.837116
H	4.674308	-0.291062	0.244272
H	3.614724	0.958664	0.926879
C	0.047361	-1.993441	-0.083165
H	0.922521	-2.633327	-0.134214
C	-1.221130	-2.576694	0.014001
H	-1.306389	-3.661771	0.021216
C	-2.365809	-1.779283	0.068281
H	-3.350044	-2.236604	0.140126
C	-2.232824	-0.388312	0.056570
H	-3.117709	0.242700	0.102893

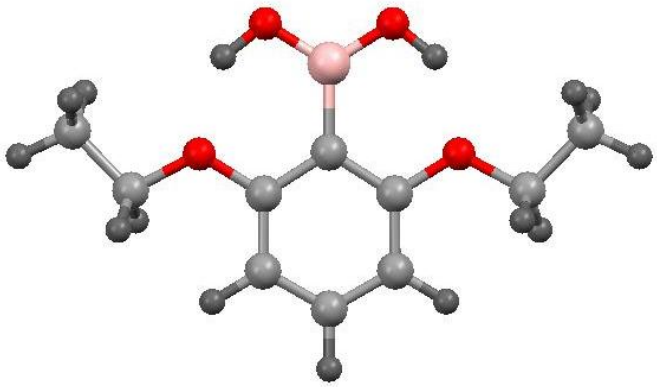


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]

C_{2v}	3	-635.4307773	-635.240239
C_1	0	-635.4309827	-635.239047

Cartesian coordinates for C_1 structure at MP2/6-31+G*

B	0.000543	1.884566	0.000062
O	1.151977	2.611799	0.147781
H	1.922463	2.014851	0.181741
O	-1.150811	2.611982	-0.147376
H	-1.921665	2.015495	-0.181813
C	0.000320	0.278663	-0.000242
C	1.195179	-0.477139	-0.043803
O	2.369334	0.254627	-0.109141
C	1.211368	-1.877258	-0.048046
H	2.138375	-2.437645	-0.093006
C	-0.000857	-2.563085	0.000202
H	-0.001338	-3.651194	0.000251
C	-1.212362	-1.876135	0.048356
H	-2.139489	-2.436275	0.093290
C	-1.195314	-0.475880	0.043445
O	-2.369478	0.255879	0.108346
C	3.612470	-0.441892	0.029195
H	3.635536	-1.011889	0.963271
H	3.786623	-1.103953	-0.824666
H	4.375065	0.336366	0.047510
C	-3.612422	-0.441346	-0.028962
H	-3.785747	-1.103017	0.825365
H	-3.635638	-1.011954	-0.962661
H	-4.375377	0.336520	-0.047350

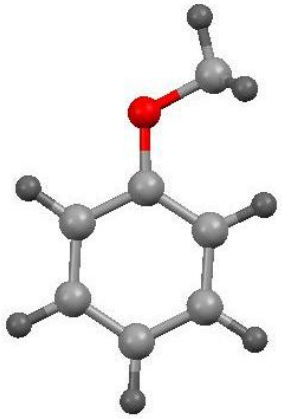


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2v}	4	-713.7767671	-713.529059
C_1	0	-713.7772947	-713.527496

Cartesian coordinates for C_1 structure at MP2/6-31+G*

B	-0.001374	-1.768466	-0.002043
O	1.159972	-2.495327	0.020251
H	1.925683	-1.891957	0.070140
O	-1.163337	-2.494541	-0.027387
H	-1.928964	-1.890992	-0.073598
C	-0.000993	-0.162207	0.001838
C	1.191538	0.592348	0.102687
O	2.365412	-0.132129	0.236985
C	1.207574	1.992753	0.119666
H	2.133181	2.548106	0.224387
C	0.002243	2.681855	-0.003673
H	0.003171	3.770061	-0.003559
C	-1.204890	1.994975	-0.122562
H	-2.129426	2.551766	-0.229418
C	-1.191586	0.594587	-0.106410
O	-2.366264	-0.128947	-0.237068
C	3.613486	0.530347	-0.042960

H	3.521416	1.075964	-0.989718
H	3.834160	1.243067	0.760728
C	4.674524	-0.545933	-0.115751
H	4.468518	-1.238657	-0.935878
H	5.654503	-0.088157	-0.285592
H	4.713056	-1.107627	0.821394
C	-3.613691	0.532201	0.048197
H	-3.838696	1.244826	-0.754357
H	-3.518390	1.077618	0.994776
C	-4.672895	-0.545692	0.125125
H	-4.459686	-1.240836	0.941387
H	-5.652298	-0.090065	0.303721
H	-4.717496	-1.104648	-0.813386

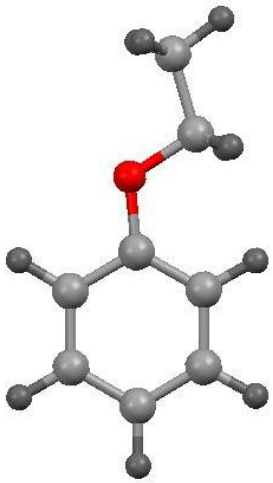


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	0	-345.6672316	-345.534469

Cartesian coordinates for C_s structure at MP2/6-31+G*

C	1.374756	0.249416	0.000000
H	2.074843	1.081562	0.000000

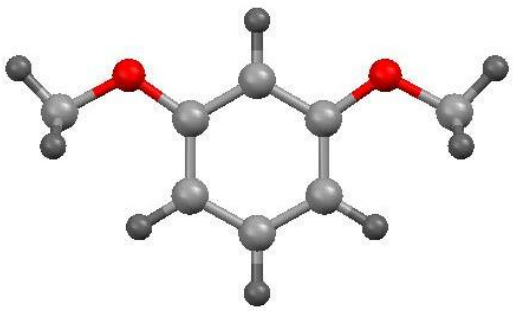
C	0.000000	0.529424	0.000000
O	-0.325237	1.865130	0.000000
C	-1.713747	2.196892	0.000000
H	-2.211121	1.810904	0.896866
H	-2.211121	1.810904	-0.896866
H	-1.748841	3.285952	0.000000
C	-0.931799	-0.516207	0.000000
H	-2.000173	-0.324824	0.000000
C	-0.472840	-1.841336	0.000000
H	-1.200125	-2.650957	0.000000
C	0.892338	-2.128252	0.000000
H	1.236895	-3.159600	0.000000
C	1.814445	-1.072437	0.000000
H	2.882622	-1.279984	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	1	-384.8398607	-384.678853
C_1	0	-384.8398912	-384.677759

Cartesian coordinates for C_1 structure at MP2/6-31+G*

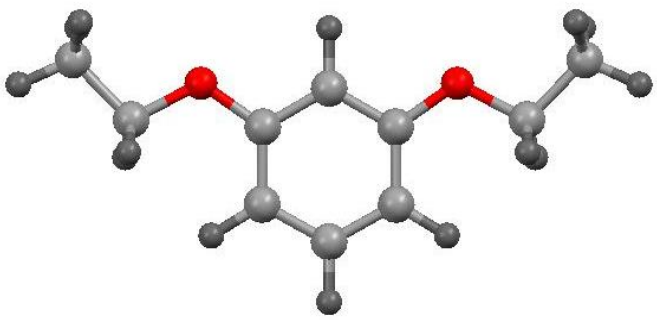
C	-0.947483	-1.300972	-0.013359
H	-0.541320	-2.309819	-0.008121
C	-0.054162	-0.218857	-0.018994
O	1.277943	-0.558318	-0.038140
C	2.234353	0.508236	0.029723
H	2.071472	1.086943	0.948527
H	2.103763	1.174551	-0.832877
C	3.605375	-0.131496	0.016749
H	3.722902	-0.798667	0.874268
H	4.378934	0.641993	0.065245
H	3.745798	-0.710074	-0.899634
C	-0.542064	1.094394	-0.039443
H	0.128221	1.947945	-0.047126
C	-1.926785	1.310946	0.006978
H	-2.300594	2.333102	0.004567
C	-2.820836	0.240031	0.017807
H	-3.892849	0.419723	0.048825
C	-2.320864	-1.069533	0.020586
H	-3.005072	-1.915651	0.031171



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2v}	0	-459.8618396	-459.695926

Cartesian coordinates for C_{2v} structure at MP2/6-31+G*

H	0.000000	0.000000	-2.008905
C	0.000000	0.000000	-0.922138
C	0.000000	1.209230	-0.223663
O	0.000000	2.335811	-1.012498
C	0.000000	1.222326	1.179419
H	0.000000	2.147731	1.745197
C	0.000000	0.000000	1.857342
H	0.000000	0.000000	2.945720
C	0.000000	-1.222326	1.179419
H	0.000000	-2.147731	1.745197
C	0.000000	-1.209230	-0.223663
O	0.000000	-2.335811	-1.012498
C	0.000000	3.597219	-0.343906
H	-0.896928	3.716124	0.274131
H	0.896928	3.716124	0.274131
H	0.000000	4.342854	-1.138596
C	0.000000	-3.597219	-0.343906
H	-0.896928	-3.716124	0.274131
H	0.896928	-3.716124	0.274131
H	0.000000	-4.342854	-1.138596

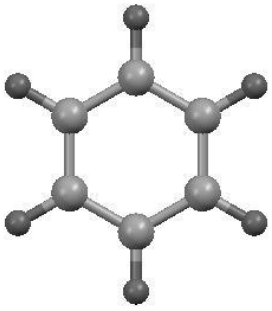


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2v}	2	-538.2070836	-537.984562
C_s	0	-538.2071568	-537.982821

Cartesian coordinates for C_s structure at MP2/6-31+G*

H	-1.725724	-0.079830	0.000000
C	-0.638708	-0.068907	0.000000
C	0.057858	-0.034760	1.210160
O	-0.731276	-0.051580	2.336700
C	1.461321	-0.022584	1.222310
H	2.026231	0.008321	2.147661
C	2.138329	0.016776	0.000000
H	3.226596	0.038016	0.000000
C	1.461321	-0.022584	-1.222310
H	2.026231	0.008321	-2.147661
C	0.057858	-0.034760	-1.210160
O	-0.731276	-0.051580	-2.336700
C	-0.073506	0.058572	3.606268
H	0.616137	-0.785314	3.737888
H	0.502946	0.992397	3.640068
C	-1.156835	0.042203	4.662564
H	-1.726357	-0.888894	4.608221
H	-0.708637	0.121918	5.658494
H	-1.842436	0.880924	4.518512
C	-0.073506	0.058572	-3.606268
H	0.616137	-0.785314	-3.737888
H	0.502946	0.992397	-3.640068
C	-1.156835	0.042203	-4.662564
H	-1.842436	0.880924	-4.518512
H	-0.708637	0.121918	-5.658494

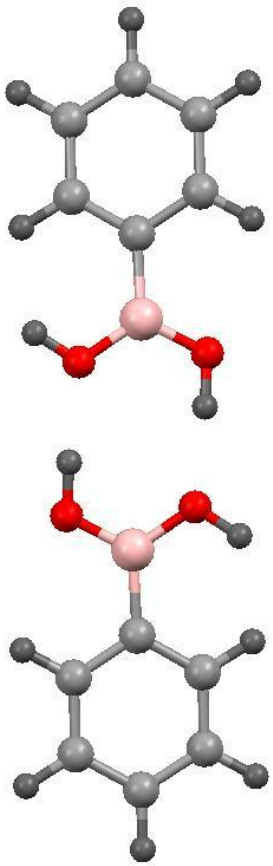
H	-1.726357	-0.888894	-4.608221



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D_{6h}	0	-231.4720259	-231.372819

Cartesian coordinates for D_{6h} structure at MP2/6-31+G*

C	0.000000	1.399496	0.000000
H	0.000000	2.487106	0.000000
C	1.211999	0.699748	0.000000
H	2.153897	1.243553	0.000000
C	1.211999	-0.699748	0.000000
H	2.153897	-1.243553	0.000000
C	0.000000	-1.399496	0.000000
H	0.000000	-2.487106	0.000000
C	-1.211999	-0.699748	0.000000
H	-2.153897	-1.243553	0.000000
C	-1.211999	0.699748	0.000000
H	-2.153897	1.243553	0.000000

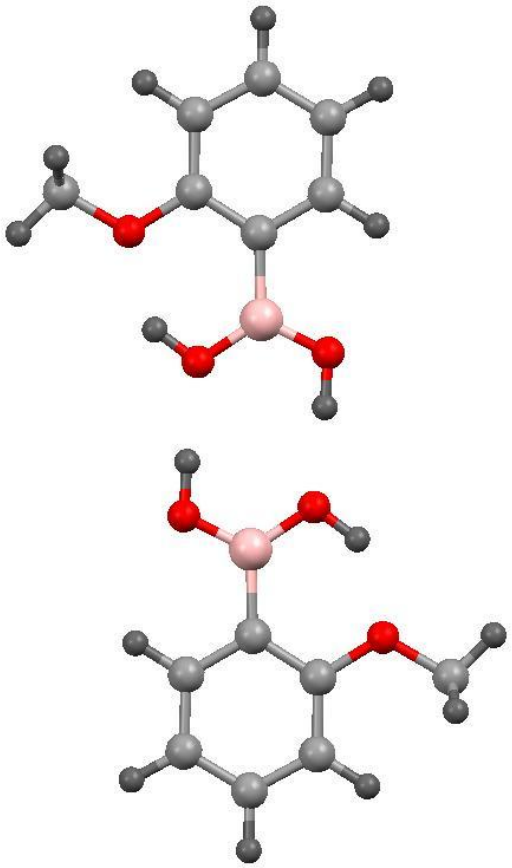


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_2	0	-814.088462	-813.837535
C_i	0	-814.0883669	-813.837547
C_1	0	-814.088462	-813.837535

Cartesian coordinates for C_2 structure at MP2/6-31+G*

B	-0.077339	2.104871	-0.130344
O	-1.282055	1.482648	-0.025335
H	-1.236916	0.507808	-0.159036
C	0.001635	3.664349	0.000606
C	-1.154386	4.436492	-0.223603
C	-1.118491	5.829988	-0.127034

H	-2.021087	6.411046	-0.306538
C	0.077339	6.479723	0.199639
H	0.106140	7.564893	0.276593
H	-2.086741	3.931681	-0.468610
O	1.059436	1.321679	-0.369310
H	1.865906	1.848924	-0.501268
C	1.192834	4.336339	0.334208
C	1.234287	5.730163	0.435790
H	2.163513	6.230132	0.702222
H	2.104014	3.775237	0.547877
O	-1.059436	-1.321679	-0.369310
O	1.282055	-1.482648	-0.025335
B	0.077339	-2.104871	-0.130344
H	1.236916	-0.507808	-0.159036
C	-0.001635	-3.664349	0.000606
C	1.154386	-4.436492	-0.223603
C	1.118491	-5.829988	-0.127034
H	2.021087	-6.411046	-0.306538
C	-0.077339	-6.479723	0.199639
H	-0.106140	-7.564893	0.276593
H	2.086741	-3.931681	-0.468610
H	-1.865906	-1.848924	-0.501268
C	-1.192834	-4.336339	0.334208
C	-1.234287	-5.730163	0.435790
H	-2.163513	-6.230132	0.702222
H	-2.104014	-3.775237	0.547877

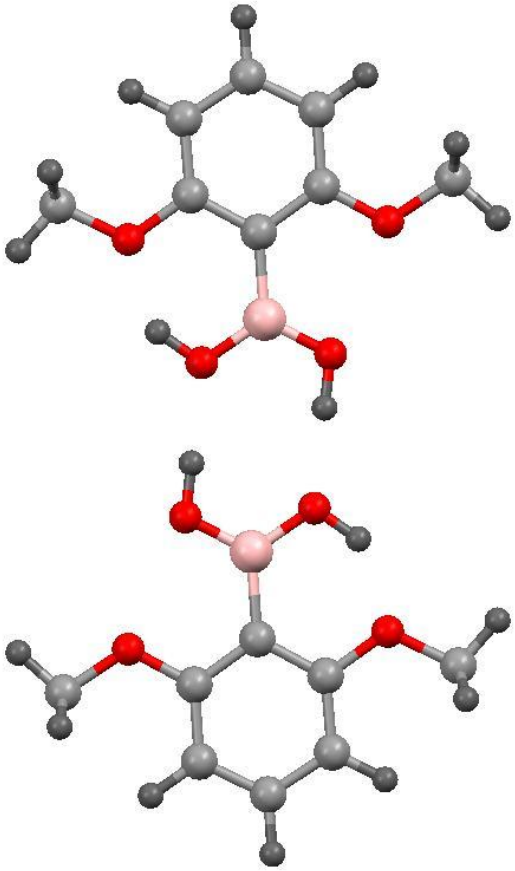


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}		-1042.498121	
C_s		-1042.498121	

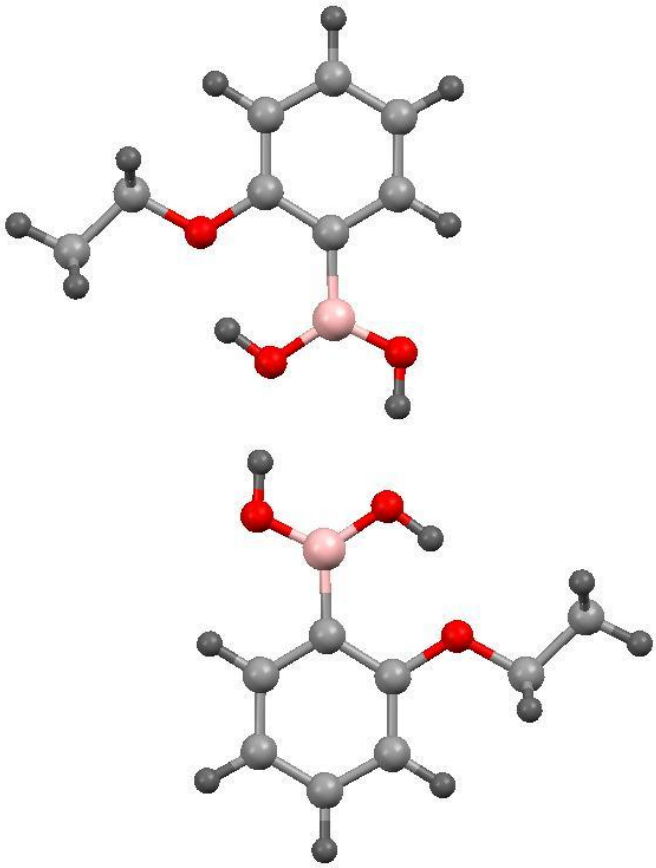
Cartesian coordinates for C_{2h} structure at MP2/6-31+G*

C	-2.201055	-5.497791	0.000000
C	-1.133407	-6.396729	0.000000
C	0.187072	-5.931959	0.000000
C	0.425161	-4.553402	0.000000
C	-0.630535	-3.616967	0.000000
C	-1.940915	-4.124715	0.000000
B	-0.425161	-2.053259	0.000000

O	-1.532469	-1.259722	0.000000
O	1.707305	-4.018475	0.000000
C	2.816548	-4.922541	0.000000
H	-2.763815	-3.413336	0.000000
O	0.838614	-1.472624	0.000000
O	1.532469	1.259722	0.000000
B	0.425161	2.053259	0.000000
O	-0.838614	1.472624	0.000000
C	0.630535	3.616967	0.000000
C	1.940915	4.124715	0.000000
C	2.201055	5.497791	0.000000
C	1.133407	6.396729	0.000000
C	-0.187072	5.931959	0.000000
C	-0.425161	4.553402	0.000000
H	2.763815	3.413336	0.000000
O	-1.707305	4.018475	0.000000
C	-2.816548	4.922541	0.000000
H	1.317581	0.296658	0.000000
H	3.225550	5.863105	0.000000
H	1.317304	7.469487	0.000000
H	-1.521465	2.175468	0.000000
H	-0.999993	6.650865	0.000000
H	-2.806993	5.548575	0.897765
H	-2.806993	5.548575	-0.897765
H	-3.703981	4.290089	0.000000
H	1.521465	-2.175468	0.000000
H	0.999993	-6.650865	0.000000
H	-1.317304	-7.469487	0.000000
H	2.806993	-5.548575	0.897765
H	2.806993	-5.548575	-0.897765
H	3.703981	-4.290089	0.000000
H	-1.317581	-0.296658	0.000000
H	-3.225550	-5.863105	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}		No convergence	
C_s		No convergence	
C_2		No convergence	
C_i		No convergence	



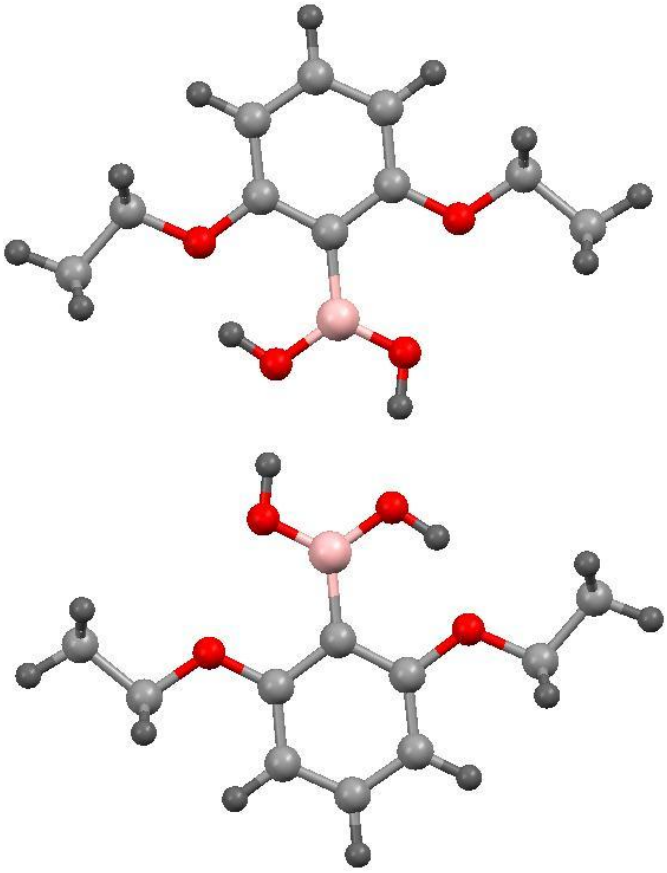
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}		-1120.844217	
C_s		No convergence	

Cartesian coordinates for C_{2h} structure at MP2/6-31+G*

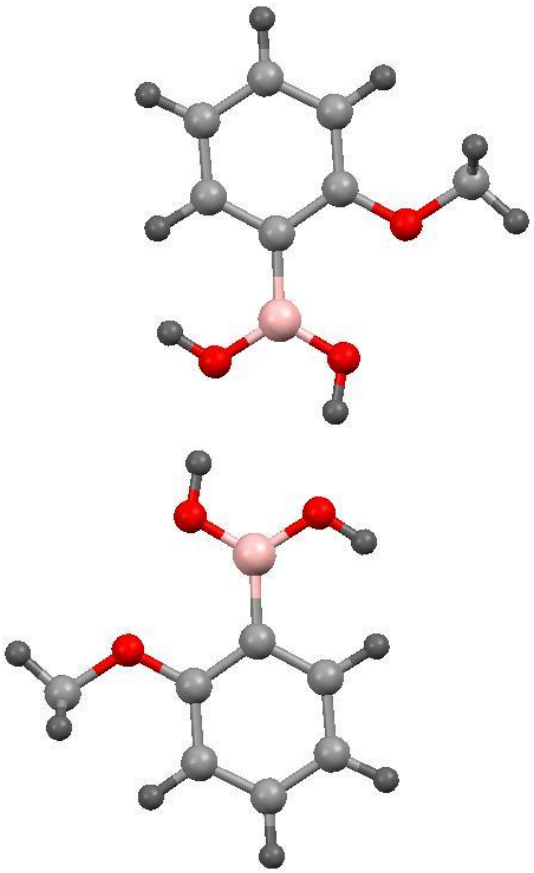
C	-2.728323	-5.257467	0.000000
C	-1.751970	-6.254717	0.000000
C	-0.392910	-5.919881	0.000000
C	-0.021996	-4.570460	0.000000
C	-0.983790	-3.537169	0.000000
C	-2.336958	-3.916055	0.000000
B	-0.628376	-2.000692	0.000000

O	-1.652866	-1.102481	0.000000
O	1.305227	-4.160909	0.000000
C	2.336958	-5.162212	0.000000
H	-3.087445	-3.128620	0.000000
O	0.686236	-1.546024	0.000000
O	1.652866	1.102481	0.000000
B	0.628376	2.000692	0.000000
O	-0.686236	1.546024	0.000000
C	0.983790	3.537169	0.000000
C	2.336958	3.916055	0.000000
C	2.728323	5.257467	0.000000
C	1.751970	6.254717	0.000000
C	0.392910	5.919881	0.000000
C	0.021996	4.570460	0.000000
H	3.087445	3.128620	0.000000
O	-1.305227	4.160909	0.000000
C	-2.336958	5.162212	0.000000
H	1.344151	0.165378	0.000000
H	3.783244	5.522646	0.000000
H	2.038453	7.304790	0.000000
H	-1.296592	2.313029	0.000000
H	-0.347061	6.713604	0.000000
H	-2.228541	5.790005	0.892655
H	-2.228541	5.790005	-0.892655
H	1.296592	-2.313029	0.000000
H	0.347061	-6.713604	0.000000
H	-2.038453	-7.304790	0.000000
H	2.228541	-5.790005	0.892655
H	2.228541	-5.790005	-0.892655
H	-1.344151	-0.165378	0.000000
H	-3.783244	-5.522646	0.000000
C	-3.660634	4.429298	0.000000
H	-3.752639	3.800993	0.889817

H	-4.483418	5.151556	0.000000
H	-3.752639	3.800993	-0.889817
C	3.660634	-4.429298	0.000000
H	3.752639	-3.800993	0.889817
H	4.483418	-5.151556	0.000000
H	3.752639	-3.800993	-0.889817



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}		No convergence	
C_s		No convergence	
C_2		No convergence	
C_i		No convergence	



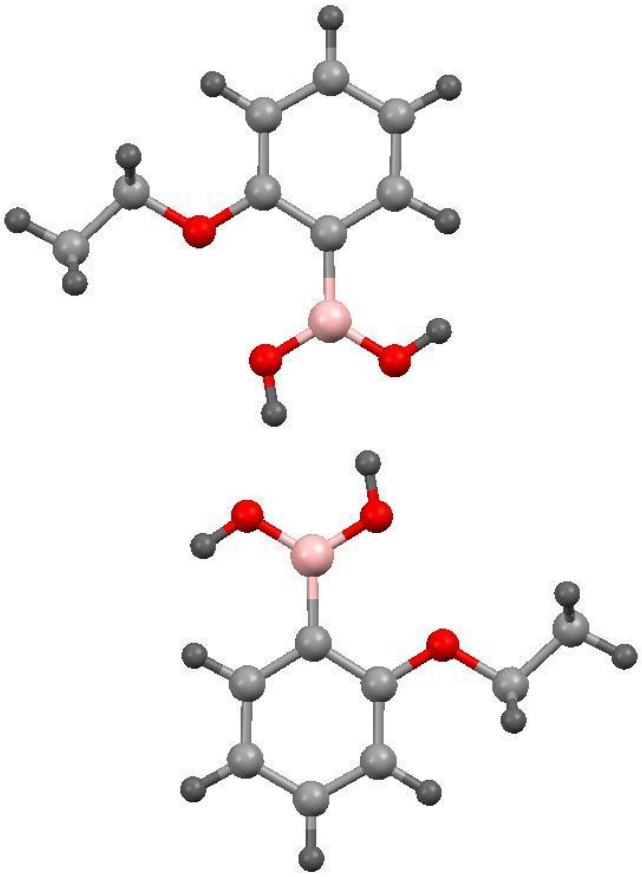
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}		-1042.466455	
C_s		No convergence	
C_2		No convergence	
C_i		No convergence	

Cartesian coordinates for C_{2h} structure at MP2/6-31+G*

C	-5.881794	-0.349855	0.000000
C	-6.329646	-1.669911	0.000000
C	-5.413133	-2.725145	0.000000

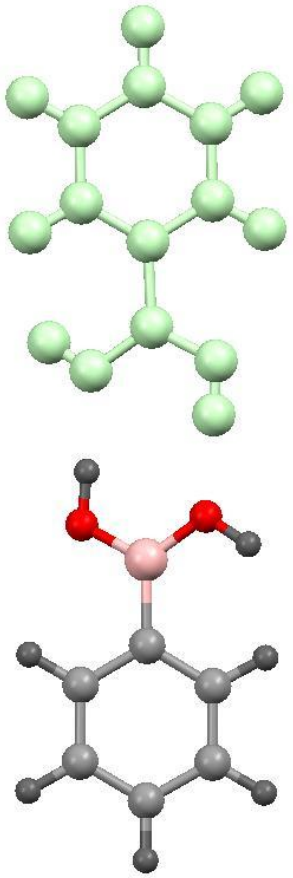
C	-4.034262	-2.461166	0.000000
C	-3.543641	-1.130400	0.000000
C	-4.506434	-0.104272	0.000000
B	-2.004724	-0.775953	0.000000
O	-1.578393	0.562333	0.000000
O	-3.093543	-3.450864	0.000000
C	-3.543641	-4.804236	0.000000
H	-4.193128	0.939999	0.000000
O	-1.031335	-1.721700	0.000000
O	1.578393	-0.562333	0.000000
B	2.004724	0.775953	0.000000
O	1.031335	1.721700	0.000000
C	3.543641	1.130400	0.000000
C	4.506434	0.104272	0.000000
C	5.881794	0.349855	0.000000
C	6.329646	1.669911	0.000000
C	5.413133	2.725145	0.000000
C	4.034262	2.461166	0.000000
H	4.193128	-0.939999	0.000000
O	3.093543	3.450864	0.000000
C	3.543641	4.804236	0.000000
H	2.297823	-1.213845	0.000000
H	6.588814	-0.476363	0.000000
H	7.395617	1.889944	0.000000
H	0.131122	1.322170	0.000000
H	5.787130	3.743570	0.000000
H	4.132577	5.027832	0.897105
H	4.132577	5.027832	-0.897105
H	2.632698	5.402034	0.000000
H	-0.131122	-1.322170	0.000000
H	-5.787130	-3.743570	0.000000
H	-7.395617	-1.889944	0.000000
H	-4.132577	-5.027832	0.897105

H	-4.132577	-5.027832	-0.897105
H	-2.632698	-5.402034	0.000000
H	-2.297823	1.213845	0.000000
H	-6.588814	0.476363	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}		No convergence	
C_s		No convergence	
C_2		No convergence	
C_i		No convergence	

Absolute electronic energy at MP2/6-31+G* (in Hartree) and Cartesian coordinates at MP2/6-31+G* for calculation of the Interaction Energy.



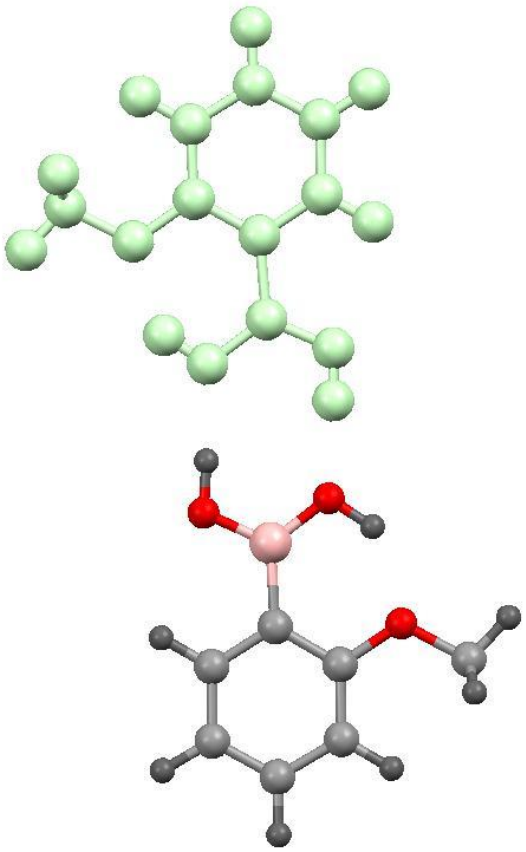
Absolute Electronic Energy [Hartree] HF= -407.0334917

Absolute Electronic Energy [Hartree] + ZPE = -406.909267

Cartesian coordinates at MP2/6-31+G*

B	0.018339	2.120661	-0.041293
O	1.188971	1.483442	-0.376526
H	1.097460	0.515074	-0.308566
C	-0.001257	3.687538	-0.036059
C	1.209961	4.401161	0.045542
C	1.220959	5.798355	0.066094
H	2.166303	6.333653	0.131418

C	0.017668	6.510437	0.005762
H	0.025406	7.598577	0.020444
H	2.147211	3.849737	0.084852
O	-1.070029	1.329488	0.279941
H	-1.844013	1.836010	0.576486
C	-1.200471	4.421879	-0.099608
C	-1.195376	5.819756	-0.082614
H	-2.133049	6.369194	-0.139857
H	-2.158673	3.908174	-0.189817
Bq	1.021574	-1.325335	-0.256144
Bq	-1.257873	-1.505556	0.378134
Bq	-0.087244	-2.120234	0.060136
Bq	-1.215636	-0.521899	0.332041
Bq	-0.014460	-3.685440	0.039135
Bq	-1.196400	-4.432151	-0.129176
Bq	-1.165548	-5.828651	-0.164750
Bq	-2.088354	-6.389723	-0.299676
Bq	0.050619	-6.507114	-0.025249
Bq	0.075518	-7.594779	-0.051654
Bq	-2.144009	-3.905906	-0.227792
Bq	1.788694	-1.841078	-0.557775
Bq	1.197520	-4.386480	0.185636
Bq	1.234192	-5.783847	0.153846
Bq	2.180552	-6.307460	0.275071
Bq	2.131447	-3.847480	0.352019



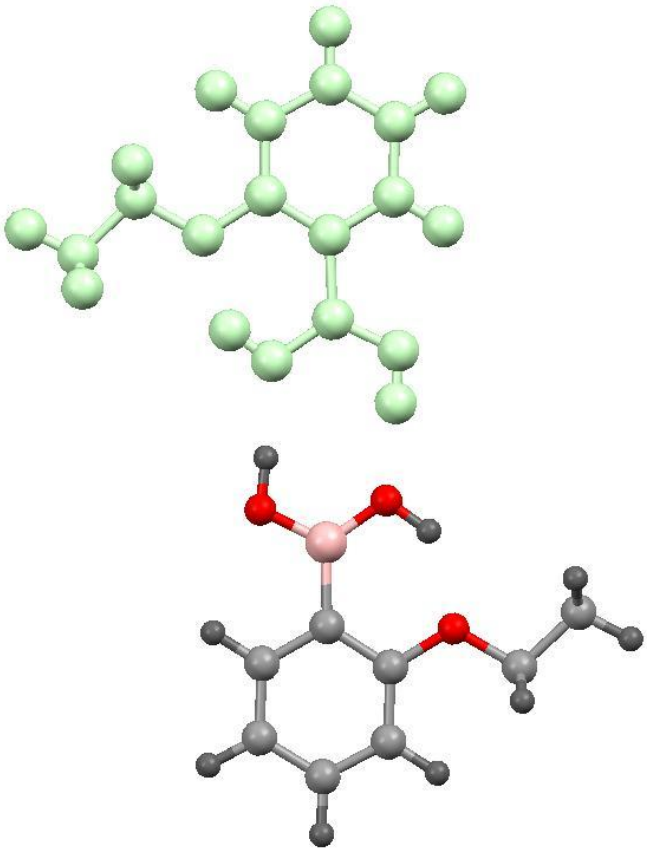
Absolute Electronic Energy [Hartree] HF= -521.2373434

Absolute Electronic Energy [Hartree] + ZPE = -521.080079

Cartesian coordinates at MP2/6-31+G*

C	-2.212920	-5.469035	0.000000
C	-1.159047	-6.383920	-0.000002
C	0.168638	-5.940197	-0.000002
C	0.429299	-4.565429	0.000000
C	-0.613037	-3.613552	0.000002
C	-1.931371	-4.100165	0.000002
B	-0.370187	-2.057828	0.000004
O	-1.484617	-1.246336	0.000005
O	1.717789	-4.049877	0.000000
C	2.811315	-4.972546	-0.000003
H	-2.744706	-3.377905	0.000004

O	0.870996	-1.468385	0.000004
Bq	1.544534	1.275252	0.000002
Bq	0.431896	2.061687	0.000001
Bq	-0.827939	1.473047	0.000001
Bq	0.626946	3.626775	0.000001
Bq	1.933972	4.143209	0.000001
Bq	2.184972	5.517945	0.000001
Bq	1.111373	6.409771	-0.000001
Bq	-0.206001	5.936265	-0.000001
Bq	-0.434962	4.556157	-0.000001
Bq	2.761676	3.437231	0.000002
Bq	-1.713448	4.012767	-0.000001
Bq	-2.828610	4.909473	-0.000003
Bq	1.336771	0.310121	0.000003
Bq	3.207006	5.890053	0.000001
Bq	1.288133	7.483723	-0.000001
Bq	-1.515500	2.171042	0.000000
Bq	-1.023647	6.649749	-0.000002
Bq	-2.823266	5.535524	0.897774
Bq	-2.823265	5.535523	-0.897780
Bq	-3.711802	4.271177	-0.000003
H	1.563943	-2.158250	0.000003
H	0.969818	-6.672132	-0.000003
H	-1.359647	-7.453650	-0.000003
H	2.791972	-5.598566	0.897745
H	2.791970	-5.598563	-0.897752
H	3.709309	-4.355145	-0.000002
H	-1.225423	-0.306680	0.000006
H	-3.242931	-5.818333	0.000001



Absolute Electronic Energy [Hartree] HF= -560.4103125

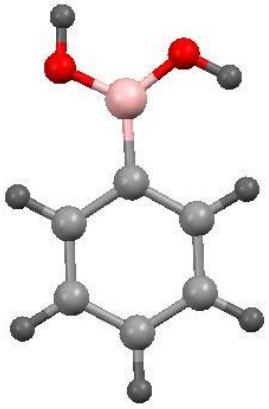
Cartesian coordinates at MP2/6-31+G*

C	-2.734533	-5.222356	0.000002
C	-1.772992	-6.233960	-0.000002
C	-0.408929	-5.919611	-0.000002
C	-0.016702	-4.575887	0.000002
C	-0.964183	-3.529029	0.000007
C	-2.323185	-3.886793	0.000006
B	-0.573095	-2.003873	0.000010
O	-1.604011	-1.088221	0.000011
O	1.314893	-4.185668	0.000001
C	2.329083	-5.204480	-0.000007
H	-3.063627	-3.089923	0.000010
O	0.719546	-1.537177	0.000009

Bq	1.665931	1.124756	0.000007
Bq	0.635033	2.015922	0.000004
Bq	-0.676257	1.552211	0.000002
Bq	0.979591	3.554934	0.000005
Bq	2.330077	3.943414	0.000004
Bq	2.711879	5.287540	0.000001
Bq	1.728466	6.277828	-0.000001
Bq	0.371816	5.933370	-0.000002
Bq	0.010461	4.581357	-0.000001
Bq	3.086218	3.161252	0.000007
Bq	-1.313759	4.162423	-0.000002
Bq	-2.352518	5.156387	-0.000005
Bq	1.364494	0.184790	0.000008
Bq	3.764879	5.560203	0.000004
Bq	2.007478	7.329904	-0.000003
Bq	-1.292094	2.314655	0.000001
Bq	-0.373749	6.721814	-0.000005
Bq	-2.248605	5.784914	0.892646
Bq	-2.248602	5.784911	-0.892658
H	1.340808	-2.292718	0.000013
H	0.318486	-6.724807	-0.000006
H	-2.075117	-7.279628	-0.000006
H	2.210578	-5.830583	0.892623
H	2.210573	-5.830573	-0.892642
H	-1.254755	-0.178137	0.000010
H	-3.793271	-5.471514	0.000002
Bq	-3.670979	4.414116	-0.000007
Bq	-3.758494	3.785213	0.889815
Bq	-4.498856	5.130530	-0.000009
Bq	-3.758491	3.785210	-0.889826
C	3.665322	-4.494865	-0.000006
H	3.767848	-3.868312	0.889889
H	4.475503	-5.231233	-0.000012

H	3.767844	-3.868303	-0.889895

Symmetry, number of imaginary frequencies, absolute electronic energy at B3LYP/6-311+G (in Hartree), absolute electronic energy corrected for zero point energy (in Hartree) and Cartesian coordinates at B3LYP/6-311+G** for the molecules studied.**

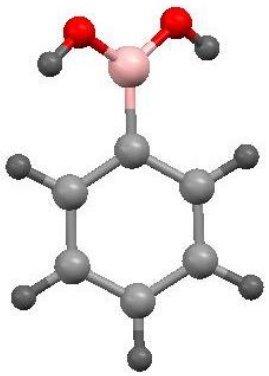


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	0	-408.3952449	-408.270673
C_1	0	-408.3952637	-408.270629

Cartesian coordinates for C_1 structure at B3LYP/6-311+G**

C	0.176924	0.014735	-0.000103
C	-0.534605	-1.197259	0.000293
C	-1.926720	-1.217730	0.000412
C	-2.642337	-0.020642	0.000094
C	-1.959528	1.194742	-0.000361
C	-0.566678	1.205615	-0.000467
B	1.743213	-0.001678	-0.000038
O	2.385840	-1.209065	-0.000742
O	2.532155	1.124029	0.000749
H	-0.063872	2.169795	-0.000938
H	0.018701	-2.129294	0.000529
H	2.051223	1.955070	0.001478
H	-2.510799	2.128521	-0.000657

H	-3.726768	-0.034209	0.000195
H	3.344243	-1.113140	-0.000423
H	-2.455091	-2.164826	0.000740

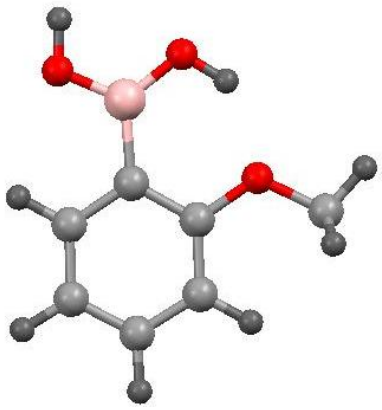


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2v}	1	-408.3891875	-408.265008
C_1	0	-408.3902305	-408.265471

Cartesian coordinates for C_1 structure at B3LYP/6-311+G**

C	-0.638661	1.022623	1.929323
C	0.000000	0.000000	2.629165
C	0.638661	-1.022623	1.929323
C	0.630341	-1.021997	0.536201
C	0.000000	0.000000	-0.193697
C	-0.630341	1.021997	0.536201
B	0.000000	0.000000	-1.769873
O	0.000000	1.153554	-2.504926
H	1.145524	-1.821917	0.011552
H	-1.145524	1.821917	0.011552
O	0.000000	-1.153554	-2.504926
H	-0.095477	-1.946699	-1.972315

H	1.142801	-1.817007	2.468561
H	0.000000	0.000000	3.713503
H	0.095477	1.946699	-1.972315
H	-1.142801	1.817007	2.468561

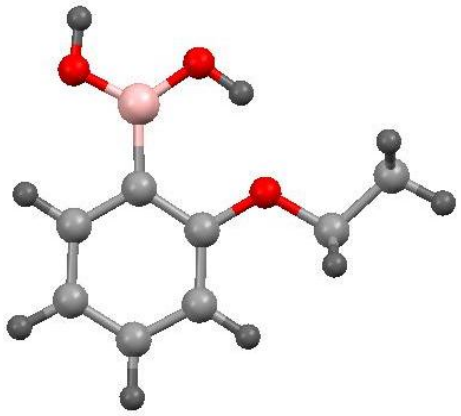


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	0	-522.9585493	-522.800733
C_1	0	-522.95852	-522.800789

Cartesian coordinates for C_S structure at B3LYP/6-311+G**

C	0.000000	0.648956	0.000000
B	-1.451782	1.249048	0.000000
O	-2.591250	0.494573	0.000000
H	-2.374150	-0.448088	0.000000
O	-1.579797	2.614591	0.000000
H	-2.503994	2.885516	0.000000
C	0.271804	-0.735671	0.000000
O	-0.824378	-1.572833	0.000000
C	-0.629043	-2.983775	0.000000
H	-0.089562	-3.308193	0.895100

H	-0.089562	-3.308193	-0.895100
H	-1.625507	-3.422781	0.000000
C	1.580538	-1.221005	0.000000
H	1.782897	-2.283206	0.000000
C	2.646534	-0.320993	0.000000
H	3.661078	-0.704316	0.000000
C	2.413942	1.050064	0.000000
H	3.243631	1.747192	0.000000
C	1.101177	1.516329	0.000000
H	0.907760	2.582753	0.000000

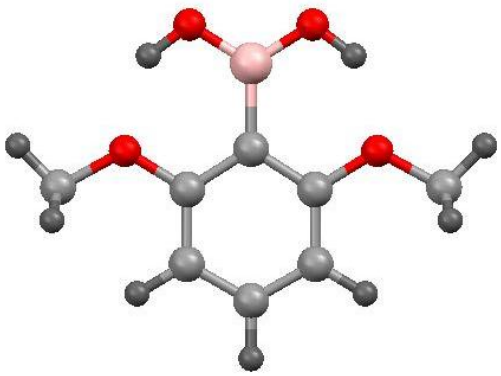


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	0	-562.2882951	-562.102384
C_1	0	-562.28826	-562.102357

Cartesian coordinates for C_S structure at B3LYP/6-311+G**

C	-0.883819	-0.485956	0.000000
B	-0.405306	-1.982014	0.000000
O	0.906882	-2.364305	0.000000
H	1.484364	-1.587994	0.000000

O	-1.364685	-2.962671	0.000000
H	-0.973044	-3.842515	0.000000
C	0.000000	0.614826	0.000000
O	1.346068	0.318105	0.000000
C	2.312113	1.377695	0.000000
H	2.165460	2.001509	0.888833
H	2.165460	2.001509	-0.888833
C	3.692451	0.749697	0.000000
H	3.839897	0.130382	0.887738
H	4.454339	1.533450	0.000000
H	3.839897	0.130382	-0.887738
C	-0.476265	1.927590	0.000000
H	0.202988	2.768715	0.000000
C	-1.851726	2.160429	0.000000
H	-2.213595	3.182865	0.000000
C	-2.749142	1.098060	0.000000
H	-3.817178	1.281512	0.000000
C	-2.257250	-0.205176	0.000000
H	-2.946354	-1.041759	0.000000

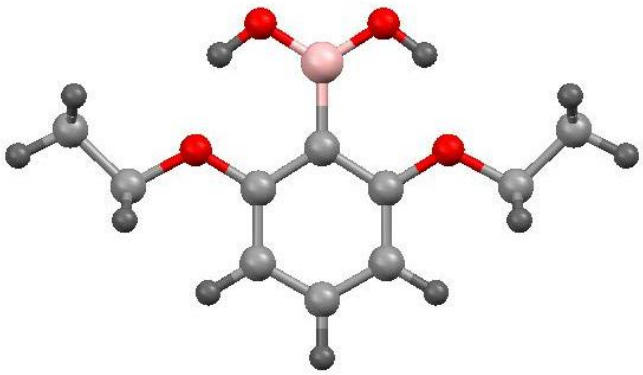


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2V}	0	-637.5126084	-637.322324

C_1	0	-637.51257	-637.322243

Cartesian coordinates for C_{2V} structure at B3LYP/6-311+G**

B	0.000000	0.000000	-1.881612
O	0.000000	1.153947	-2.607090
H	0.000000	1.925313	-2.027487
O	0.000000	-1.153947	-2.607090
H	0.000000	-1.925313	-2.027487
C	0.000000	0.000000	-0.281066
C	0.000000	1.195305	0.474312
O	0.000000	2.368537	-0.243660
C	0.000000	1.208089	1.872117
H	0.000000	2.135928	2.425318
C	0.000000	0.000000	2.556460
H	0.000000	0.000000	3.640621
C	0.000000	-1.208089	1.872117
H	0.000000	-2.135928	2.425318
C	0.000000	-1.195305	0.474312
O	0.000000	-2.368537	-0.243660
C	0.000000	3.620347	0.436856
H	-0.895582	3.734569	1.054740
H	0.895582	3.734569	1.054740
H	0.000000	4.379673	-0.343482
C	0.000000	-3.620347	0.436856
H	-0.895582	-3.734569	1.054740
H	0.895582	-3.734569	1.054740
H	0.000000	-4.379673	-0.343482

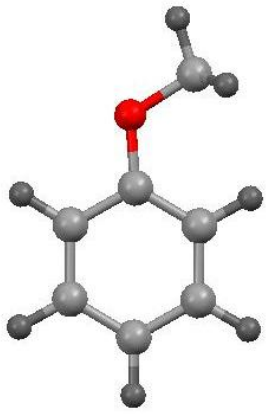


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2V}	0	-716.1721948	-715.925663
C_1	0	-716.1721956	-715.925669

Cartesian coordinates for C_{2V} structure at B3LYP/6-311+G**

B	0.000000	0.000000	-1.773088
O	0.000000	1.154094	-2.499128
H	0.000000	1.924062	-1.917449
O	0.000000	-1.154094	-2.499128
H	0.000000	-1.924062	-1.917449
C	0.000000	0.000000	-0.173201
C	0.000000	1.196876	0.581235
O	0.000000	2.369908	-0.135901
C	0.000000	1.208313	1.979632
H	0.000000	2.135474	2.533477
C	0.000000	0.000000	2.663306
H	0.000000	0.000000	3.747553
C	0.000000	-1.208313	1.979632
H	0.000000	-2.135474	2.533477
C	0.000000	-1.196876	0.581235
O	0.000000	-2.369908	-0.135901
C	0.000000	3.634980	0.540795

H	-0.889143	3.705065	1.177009
H	0.889143	3.705065	1.177009
C	0.000000	4.724206	-0.514262
H	-0.887380	4.655191	-1.147489
H	0.000000	5.704524	-0.030609
H	0.887380	4.655191	-1.147489
C	0.000000	-3.634980	0.540795
H	-0.889143	-3.705065	1.177009
H	0.889143	-3.705065	1.177009
C	0.000000	-4.724206	-0.514262
H	0.887380	-4.655191	-1.147489
H	0.000000	-5.704524	-0.030609
H	-0.887380	-4.655191	-1.147489

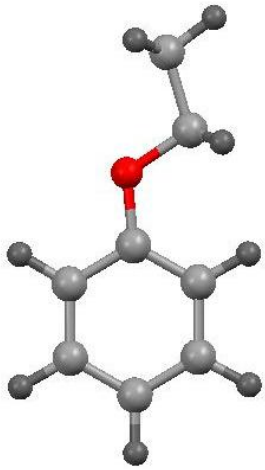


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	0	-346.8675584	-346.735116

Cartesian coordinates for C_S structure at B3LYP/6-311+G**

C	1.372036	0.245403	0.000000
H	2.070940	1.073268	0.000000

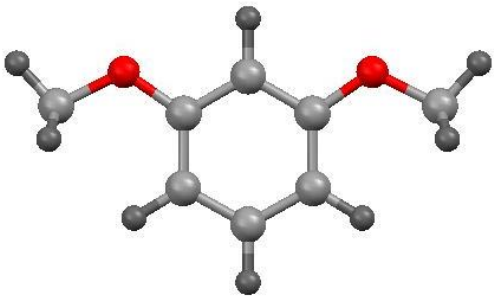
C	0.000000	0.527729	0.000000
O	-0.332496	1.852785	0.000000
C	-1.707852	2.208251	0.000000
H	-2.218195	1.833796	0.894208
H	-2.218195	1.833796	-0.894208
H	-1.733973	3.296782	0.000000
C	-0.925306	-0.519401	0.000000
H	-1.989286	-0.324548	0.000000
C	-0.468498	-1.840270	0.000000
H	-1.193019	-2.647232	0.000000
C	0.891899	-2.126160	0.000000
H	1.236789	-3.153287	0.000000
C	1.809528	-1.071636	0.000000
H	2.874056	-1.278344	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_s	0	-386.1972581	-386.036786
C_1	0	-386.19725	-386.036755

Cartesian coordinates for C_S structure at B3LYP/6-311+G**

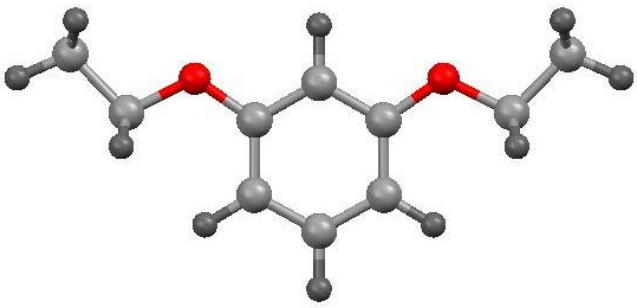
C	0.588813	1.494668	0.000000
H	-0.057850	2.364037	0.000000
C	0.000000	0.223145	0.000000
O	-1.365208	0.202159	0.000000
C	-2.040523	-1.057400	0.000000
H	-1.749485	-1.631840	0.888224
H	-1.749485	-1.631840	-0.888224
C	-3.532012	-0.781741	0.000000
H	-3.819886	-0.211898	0.886132
H	-4.085251	-1.724803	0.000000
H	-3.819886	-0.211898	-0.886132
C	0.810348	-0.916037	0.000000
H	0.379289	-1.907994	0.000000
C	2.200441	-0.771653	0.000000
H	2.821212	-1.661009	0.000000
C	2.788949	0.487769	0.000000
H	3.867668	0.589628	0.000000
C	1.970823	1.621171	0.000000
H	2.414304	2.610805	0.000000



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2V}	0	-461.423669	-461.259024

Cartesian coordinates for C_{2V} structure at B3LYP/6-311+G**

H	0.000000	0.000000	-1.998819
C	0.000000	0.000000	-0.916639
C	0.000000	1.207462	-0.220818
O	0.000000	2.331303	-0.998132
C	0.000000	1.217648	1.180136
H	0.000000	2.143011	1.738342
C	0.000000	0.000000	1.856472
H	0.000000	0.000000	2.940805
C	0.000000	-1.217648	1.180136
H	0.000000	-2.143011	1.738342
C	0.000000	-1.207462	-0.220818
O	0.000000	-2.331303	-0.998132
C	0.000000	3.600105	-0.359025
H	-0.894258	3.737888	0.258063
H	0.894258	3.737888	0.258063
H	0.000000	4.335682	-1.161664
C	0.000000	-3.600105	-0.359025
H	-0.894258	-3.737888	0.258063
H	0.894258	-3.737888	0.258063
H	0.000000	-4.335682	-1.161664

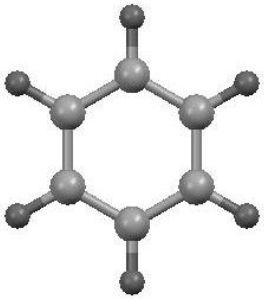


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]

C_{2V}	0	-540.0830701	-539.862403
C_S	0	-540.08306	-539.862322

Cartesian coordinates for C_{2V} structure at B3LYP/6-311+G**

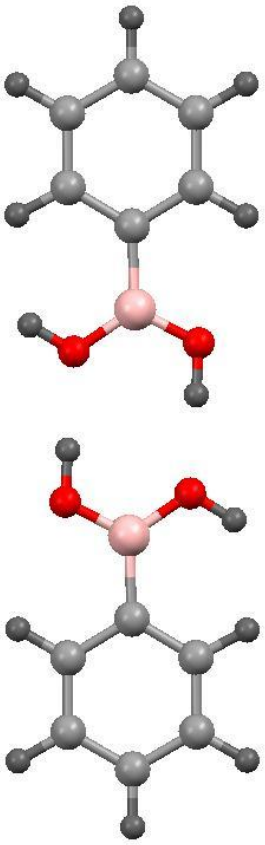
H	0.000000	0.000000	-1.713433
C	0.000000	0.000000	-0.631174
C	0.000000	1.208600	0.063532
O	0.000000	2.331788	-0.714144
C	0.000000	1.217891	1.464956
H	0.000000	2.142696	2.023841
C	0.000000	0.000000	2.140756
H	0.000000	0.000000	3.225204
C	0.000000	-1.217891	1.464956
H	0.000000	-2.142696	2.023841
C	0.000000	-1.208600	0.063532
O	0.000000	-2.331788	-0.714144
C	0.000000	3.613776	-0.081426
H	-0.888050	3.711487	0.554508
H	0.888050	3.711487	0.554508
C	0.000000	4.665290	-1.174309
H	-0.885960	4.567425	-1.805263
H	0.000000	5.664285	-0.730332
H	0.885960	4.567425	-1.805263
C	0.000000	-3.613776	-0.081426
H	-0.888050	-3.711487	0.554508
H	0.888050	-3.711487	0.554508
C	0.000000	-4.665290	-1.174309
H	0.885960	-4.567425	-1.805263
H	0.000000	-5.664285	-0.730332
H	-0.885960	-4.567425	-1.805263



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
D_{6h}	0	-408.3952449	-408.270673

Cartesian coordinates for C_1 structure at B3LYP/6-311+G**

C	0.000000	1.394278	0.000000
H	0.000000	2.478556	0.000000
C	1.207480	0.697139	0.000000
H	2.146493	1.239278	0.000000
C	1.207480	-0.697139	0.000000
H	2.146493	-1.239278	0.000000
C	0.000000	-1.394278	0.000000
H	0.000000	-2.478556	0.000000
C	-1.207480	-0.697139	0.000000
H	-2.146493	-1.239278	0.000000
C	-1.207480	0.697139	0.000000
H	-2.146493	1.239278	0.000000

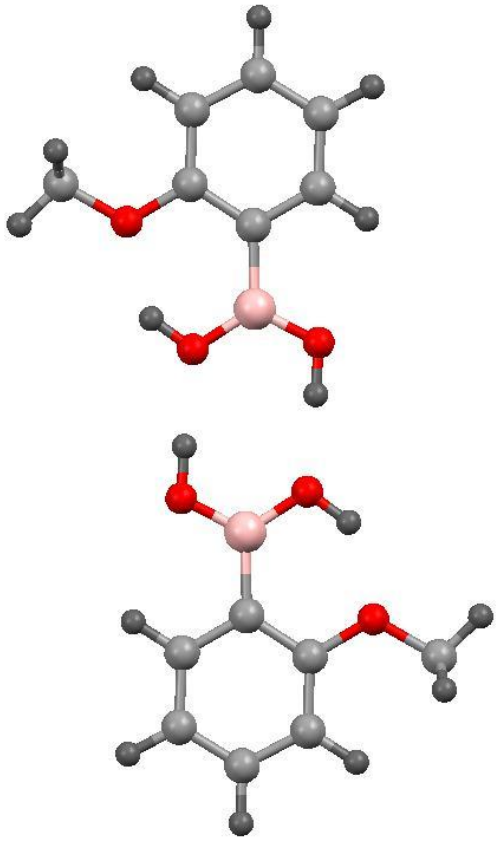


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}	2	-816.80588	-816.555126
C_s	2	-816.8058746	-816.555201
C_2	1	-816.8058804	-816.555058
C_i	0	-816.8058831	-816.554859

Cartesian coordinates for C_i structure at B3LYP/6-311+G**

B	0.055937	2.121539	-0.014372
O	1.252126	1.492494	-0.062770
H	1.205477	0.518645	-0.052373
C	0.000852	3.687638	-0.008651
C	1.200615	4.419179	0.015198

C	1.198491	5.811281	0.024840
H	2.136673	6.354977	0.044747
C	-0.009990	6.507464	0.008162
H	-0.014335	7.591950	0.015226
H	2.140447	3.879367	0.026909
O	-1.092153	1.333448	0.029889
H	-1.913886	1.827786	0.092650
C	-1.201583	4.412103	-0.027471
C	-1.213715	5.805066	-0.018746
H	-2.156276	6.340910	-0.034623
H	-2.158781	3.896270	-0.054769
O	1.092153	-1.333448	-0.029889
O	-1.252126	-1.492494	0.062770
B	-0.055937	-2.121539	0.014372
H	-1.205477	-0.518645	0.052373
C	-0.000852	-3.687638	0.008651
C	-1.200615	-4.419179	-0.015198
C	-1.198491	-5.811281	-0.024840
H	-2.136673	-6.354977	-0.044747
C	0.009990	-6.507464	-0.008162
H	0.014335	-7.591950	-0.015226
H	-2.140447	-3.879367	-0.026909
H	1.913886	-1.827786	-0.092650
C	1.201583	-4.412103	0.027471
C	1.213715	-5.805066	0.018746
H	2.156276	-6.340910	0.034623
H	2.158781	-3.896270	0.054769

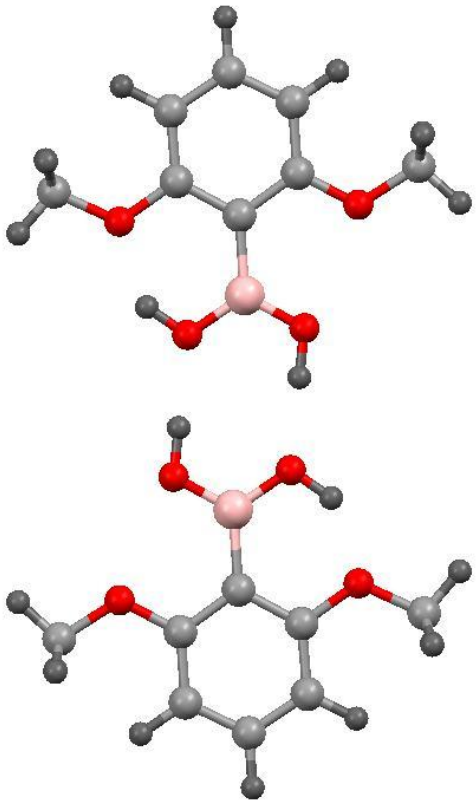


Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}	0	-1045.934266	-1045.616641
C_s	0	-1045.93418	-1045.616839

Cartesian coordinates for C_{2h} structure at B3LYP/6-311+G**

C	-2.215789	-5.475446	0.000000
C	-1.159297	-6.379703	0.000000
C	0.160495	-5.927231	0.000000
C	0.415362	-4.555139	0.000000
C	-0.631565	-3.610030	0.000000
C	-1.941131	-4.109617	0.000000
B	-0.415362	-2.051186	0.000000

O	-1.501396	-1.242548	0.000000
O	1.698737	-4.044940	0.000000
C	2.809553	-4.936841	0.000000
H	-2.754581	-3.393451	0.000000
O	0.849110	-1.487252	0.000000
O	1.501396	1.242548	0.000000
B	0.415362	2.051186	0.000000
O	-0.849110	1.487252	0.000000
C	0.631565	3.610030	0.000000
C	1.941131	4.109617	0.000000
C	2.215789	5.475446	0.000000
C	1.159297	6.379703	0.000000
C	-0.160495	5.927231	0.000000
C	-0.415362	4.555139	0.000000
H	2.754581	3.393451	0.000000
O	-1.698737	4.044940	0.000000
C	-2.809553	4.936841	0.000000
H	1.295481	0.287417	0.000000
H	3.240220	5.828958	0.000000
H	1.351381	7.447099	0.000000
H	-1.529252	2.177601	0.000000
H	-0.967987	6.646449	0.000000
H	-2.810465	5.566177	0.895057
H	-2.810465	5.566177	-0.895057
H	-3.697841	4.307177	0.000000
H	1.529252	-2.177601	0.000000
H	0.967987	-6.646449	0.000000
H	-1.351381	-7.447099	0.000000
H	2.810465	-5.566177	0.895057
H	2.810465	-5.566177	-0.895057
H	3.697841	-4.307177	0.000000
H	-1.295481	-0.287417	0.000000
H	-3.240220	-5.828958	0.000000



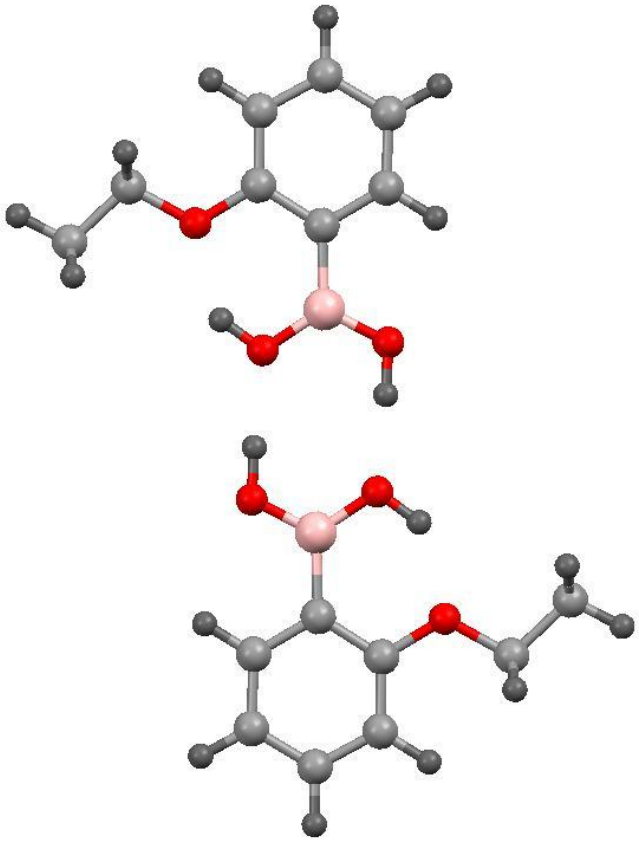
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}	2	-1275.030271	-1274.648969
C_s	2	-1275.030321	-1274.649136
C_2	2	-1275.030248	-1274.648815
C_i	0	-1275.030254	-1274.648582

Cartesian coordinates for C_i structure at B3LYP/6-311+G**

C	1.057698	-5.934013	-0.017368
C	-0.194151	-6.530761	-0.032895
C	-1.352226	-5.763445	-0.020767
C	-1.235760	-4.371790	0.002022
C	0.008719	-3.701456	0.008522

C	1.156297	-4.535039	0.006507
B	0.114056	-2.115779	0.012671
O	1.291786	-1.470314	-0.136823
O	-2.363134	-3.573283	0.017156
C	-3.657968	-4.165616	-0.002472
O	2.357099	-3.908786	0.037449
C	3.550956	-4.673846	0.016029
O	-1.023131	-1.335800	0.167523
O	-1.291786	1.470314	0.136823
B	-0.114056	2.115779	-0.012671
O	1.023131	1.335800	-0.167523
C	-0.008719	3.701456	-0.008522
C	-1.156297	4.535039	-0.006507
C	-1.057698	5.934013	0.017368
C	0.194151	6.530761	0.032895
C	1.352226	5.763445	0.020767
C	1.235760	4.371790	-0.002022
O	-2.357099	3.908786	-0.037449
C	-3.550956	4.673846	-0.016029
O	2.363134	3.573283	-0.017156
C	3.657968	4.165616	0.002472
H	-1.192305	0.498159	0.136378
H	-1.943328	6.552562	0.021566
H	0.271157	7.612296	0.051347
H	-3.627589	5.277352	0.895201
H	-3.629752	5.326016	-0.893122
H	-4.361407	3.946887	-0.034710
H	1.819711	1.885346	-0.206454
H	2.317104	6.248531	0.028969
H	3.820629	4.792754	-0.879086
H	3.808357	4.755942	0.911029
H	4.362634	3.335499	-0.009206
H	-1.819711	-1.885346	0.206454

H	-2.317104	-6.248531	-0.028969
H	-0.271157	-7.612296	-0.051347
H	-3.808357	-4.755942	-0.911029
H	-3.820629	-4.792754	0.879086
H	-4.362634	-3.335499	0.009206
H	1.192305	-0.498159	-0.136378
H	1.943328	-6.552562	-0.021566
H	3.629752	-5.326016	0.893122
H	3.627589	-5.277352	-0.895201
H	4.361407	-3.946887	0.034710



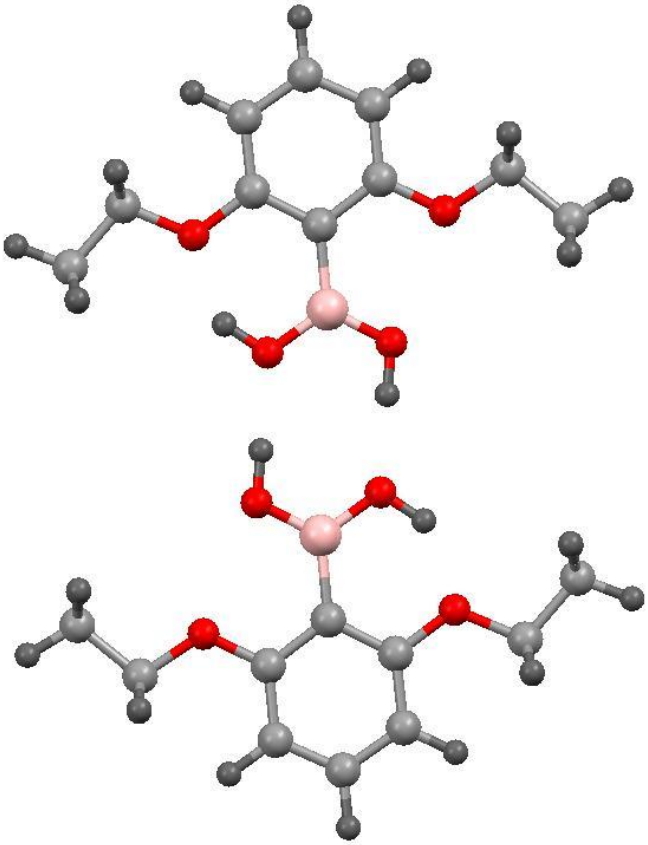
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]

C_{2h}	0	-1124.593774	-1124.219995
C_s	0	-1124.593713	-1124.220075

Cartesian coordinates for C_{2h} structure at B3LYP/6-311+G**

C	-2.736486	-5.237307	0.000000
C	-1.770457	-6.237771	0.000000
C	-0.413604	-5.913474	0.000000
C	-0.027916	-4.571513	0.000000
C	-0.981689	-3.531491	0.000000
C	-2.333060	-3.903937	0.000000
B	-0.617227	-2.000322	0.000000
O	-1.619681	-1.089574	0.000000
O	1.297223	-4.186171	0.000000
C	2.333060	-5.177742	0.000000
H	-3.074873	-3.113726	0.000000
O	0.695836	-1.561497	0.000000
O	1.619681	1.089574	0.000000
B	0.617227	2.000322	0.000000
O	-0.695836	1.561497	0.000000
C	0.981689	3.531491	0.000000
C	2.333060	3.903937	0.000000
C	2.736486	5.237307	0.000000
C	1.770457	6.237771	0.000000
C	0.413604	5.913474	0.000000
C	0.027916	4.571513	0.000000
H	3.074873	3.113726	0.000000
O	-1.297223	4.186171	0.000000
C	-2.333060	5.177742	0.000000
H	1.319100	0.159829	0.000000
H	3.789896	5.491929	0.000000
H	2.063496	7.282052	0.000000
H	-1.304032	2.316388	0.000000

H	-0.321128	6.706794	0.000000
H	-2.228692	5.809698	0.888857
H	-2.228692	5.809698	-0.888857
H	1.304032	-2.316388	0.000000
H	0.321128	-6.706794	0.000000
H	-2.063496	-7.282052	0.000000
H	2.228692	-5.809698	0.888857
H	2.228692	-5.809698	-0.888857
H	-1.319100	-0.159829	0.000000
H	-3.789896	-5.491929	0.000000
C	-3.667966	4.457981	0.000000
H	-3.773976	3.830185	0.887611
H	-4.480777	5.188754	0.000000
H	-3.773976	3.830185	-0.887611
C	3.667966	-4.457981	0.000000
H	3.773976	-3.830185	0.887611
H	4.480777	-5.188754	0.000000
H	3.773976	-3.830185	-0.887611



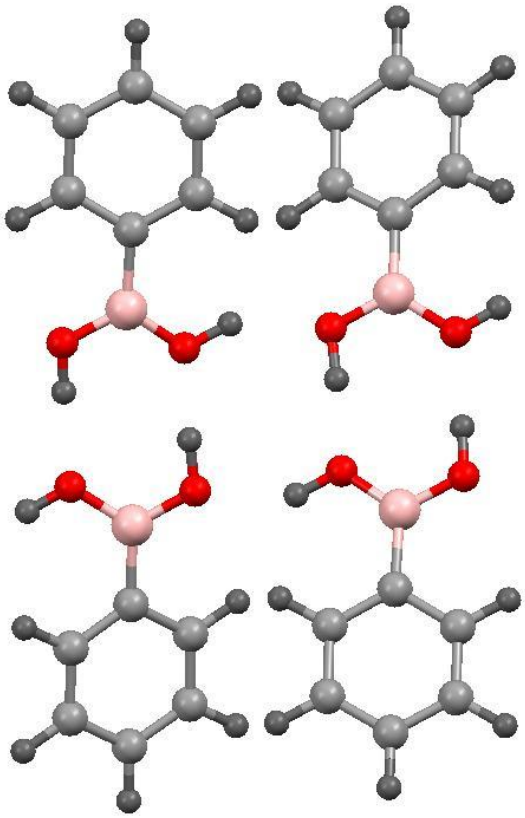
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}	3	-1432.349005	-1431.855513
C_s	No convergence		
C_2	1	-1432.348849	-1431.855209
C_i	0	-1432.348934	-1431.855077

Cartesian coordinates for C_i structure at B3LYP/6-311+G**

C	0.911628	-5.961331	0.012430
C	-0.354810	-6.525968	0.028163
C	-1.493366	-5.730237	0.021078
C	-1.343434	-4.341188	0.000736
C	-0.081109	-3.702583	-0.009044

C	1.046307	-4.564822	-0.007767
B	0.063889	-2.120102	-0.015715
O	1.263206	-1.501074	0.066492
O	-2.451211	-3.516777	-0.009307
C	-3.773367	-4.071119	0.002740
O	2.262589	-3.970277	-0.031933
C	3.450161	-4.761164	-0.019249
O	-1.060116	-1.311028	-0.103833
O	-1.263206	1.501074	-0.066492
B	-0.063889	2.120102	0.015715
O	1.060116	1.311028	0.103833
C	0.081109	3.702583	0.009044
C	-1.046307	4.564822	0.007767
C	-0.911628	5.961331	-0.012430
C	0.354810	6.525968	-0.028163
C	1.493366	5.730237	-0.021078
C	1.343434	4.341188	-0.000736
O	-2.262589	3.970277	0.031933
C	-3.450161	4.761164	0.019249
O	2.451211	3.516777	0.009307
C	3.773367	4.071119	-0.002740
H	-1.183647	0.527035	-0.068080
H	-1.780861	6.602394	-0.014728
H	0.458910	7.605369	-0.044199
H	-3.467868	5.422019	0.895081
H	-3.470926	5.387460	-0.881440
H	1.869928	1.842525	0.121741
H	2.469642	6.191348	-0.031452
H	3.903006	4.679250	-0.904487
H	3.905039	4.715655	0.873107
H	-1.869928	-1.842525	-0.121741
H	-2.469642	-6.191348	0.031452
H	-0.458910	-7.605369	0.044199

H	-3.905039	-4.715655	-0.873107
H	-3.903006	-4.679250	0.904487
H	1.183647	-0.527035	0.068080
H	1.780861	-6.602394	0.014728
H	3.470926	-5.387460	0.881440
H	3.467868	-5.422019	-0.895081
C	4.758779	2.917947	0.019855
H	5.780327	3.306781	0.008876
H	4.633363	2.313617	0.921162
H	4.628269	2.274653	-0.853202
C	-4.629282	3.806525	0.039785
H	-4.605429	3.185726	0.937554
H	-5.565904	4.371107	0.028619
H	-4.605591	3.148911	-0.831256
C	4.629282	-3.806525	-0.039785
H	4.605591	-3.148911	0.831256
H	5.565904	-4.371107	-0.028619
H	4.605429	-3.185726	-0.937554
C	-4.758779	-2.917947	-0.019855
H	-4.633363	-2.313617	-0.921162
H	-5.780327	-3.306781	-0.008876
H	-4.628269	-2.274653	0.853202



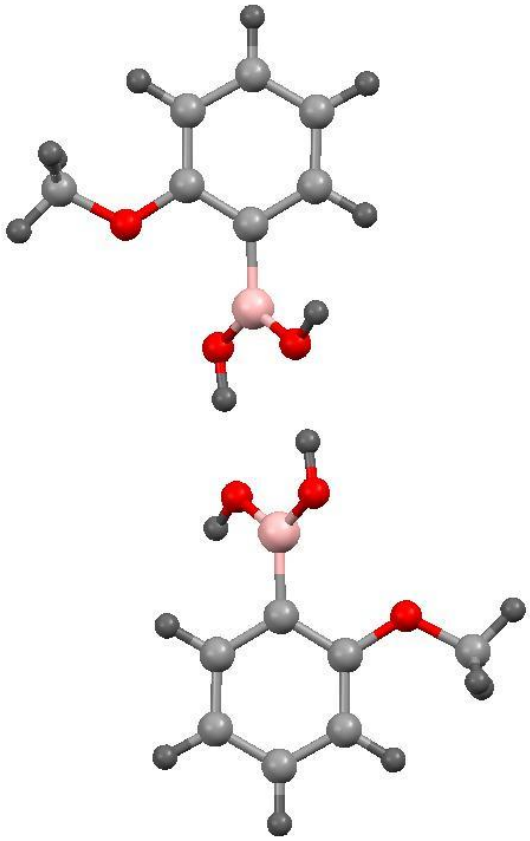
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_2	0	-1633.628565	-1633.123713

Cartesian coordinates for C_2 structure at B3LYP/6-311+G**

B	1.718571	2.675849	-0.602953
O	3.067642	2.515714	-0.647215
H	3.372770	1.646706	-0.336632
C	1.099163	4.038375	-1.064596
C	1.949248	5.119496	-1.356218
C	1.440487	6.346825	-1.771880
H	2.114544	7.168319	-1.989498
C	0.063018	6.519065	-1.911570

H	-0.335941	7.473699	-2.237445
H	3.020012	4.985152	-1.253494
O	0.963291	1.606899	-0.144686
H	0.002898	1.718689	-0.045961
C	-0.282799	4.235316	-1.214614
C	-0.799362	5.459976	-1.633397
H	-1.870770	5.586849	-1.742088
H	-0.976139	3.425567	-1.011104
O	-1.736430	0.968751	0.339150
O	3.895281	-0.059769	0.339755
O	1.736430	-0.968751	0.339150
B	-3.067642	1.151261	0.559636
H	-1.489790	0.034722	0.138821
C	-3.622879	2.530047	1.046365
C	-2.781952	3.447774	1.697683
C	-3.266419	4.668318	2.160931
H	-2.600172	5.358835	2.665721
C	-4.606432	5.003958	1.971090
H	-4.984498	5.955865	2.327390
H	-1.738352	3.196515	1.849041
O	-3.895281	0.059769	0.339755
H	-4.811756	0.199734	0.594169
C	-4.969094	2.891512	0.867052
C	-5.459018	4.114457	1.318424
H	-6.499596	4.374983	1.160150
H	-5.650564	2.223781	0.345866
O	-0.963291	-1.606899	-0.144686
O	-3.067642	-2.515714	-0.647215
B	-1.718571	-2.675849	-0.602953
H	-0.002898	-1.718689	-0.045961
C	-1.099163	-4.038375	-1.064596
C	0.282799	-4.235316	-1.214614
C	0.799362	-5.459976	-1.633397

H	1.870770	-5.586849	-1.742088
C	-0.063018	-6.519065	-1.911570
H	0.335941	-7.473699	-2.237445
H	0.976139	-3.425567	-1.011104
H	-3.372770	-1.646706	-0.336632
C	-1.949248	-5.119496	-1.356218
C	-1.440487	-6.346825	-1.771880
H	-2.114544	-7.168319	-1.989498
H	-3.020012	-4.985152	-1.253494
B	3.067642	-1.151261	0.559636
H	1.489790	-0.034722	0.138821
C	3.622879	-2.530047	1.046365
C	2.781952	-3.447774	1.697683
C	3.266419	-4.668318	2.160931
H	2.600172	-5.358835	2.665721
C	4.606432	-5.003958	1.971090
H	4.984498	-5.955865	2.327390
H	1.738352	-3.196515	1.849041
H	4.811756	-0.199734	0.594169
C	4.969094	-2.891512	0.867052
C	5.459018	-4.114457	1.318424
H	6.499596	-4.374983	1.160150
H	5.650564	-2.223781	0.345866



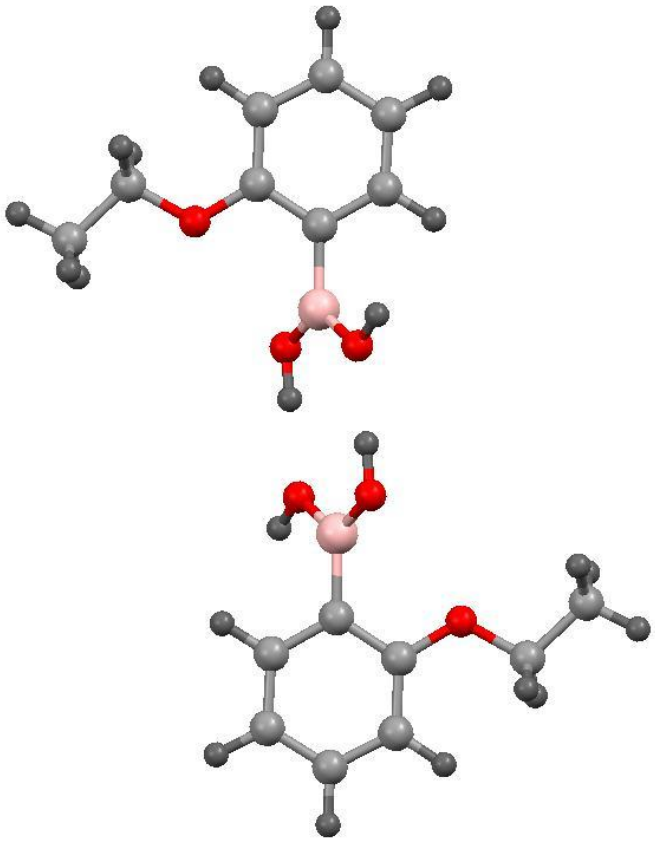
Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}	3	-1045.906233	-1045.59159
C_s	3	-1045.906254	-1045.591613
C_2	0	-1045.910317	-1045.594341
C_i	0	-1045.910269	-1045.594444

Cartesian coordinates for C_i structure at B3LYP/6-311+G**

C	-5.477861	2.104929	-0.242573
C	-6.408468	1.076513	-0.158513
C	-5.992055	-0.249780	-0.035189
C	-4.626907	-0.550032	-0.004005
C	-3.659061	0.472249	-0.099566

C	-4.118318	1.790796	-0.206110
B	-2.112515	0.182443	-0.117691
O	-1.269199	0.912795	0.722063
O	-4.140683	-1.814296	0.147292
C	-5.049113	-2.904268	0.194056
H	-3.393856	2.596322	-0.289539
O	-1.550056	-0.702243	-0.963635
O	1.269199	-0.912795	-0.722063
B	2.112515	-0.182443	0.117691
O	1.550056	0.702243	0.963635
C	3.659061	-0.472249	0.099566
C	4.118318	-1.790796	0.206110
C	5.477861	-2.104929	0.242573
C	6.408468	-1.076513	0.158513
C	5.992055	0.249780	0.035189
C	4.626907	0.550032	0.004005
H	3.393856	-2.596322	0.289539
O	4.140683	1.814296	-0.147292
C	5.049113	2.904268	-0.194056
H	1.742276	-1.475932	-1.341871
H	5.800798	-3.134632	0.340246
H	7.470089	-1.296971	0.184387
H	0.580824	0.774599	0.880611
H	6.734221	1.033134	-0.039285
H	5.648513	2.964703	0.720515
H	5.713943	2.837524	-1.062794
H	4.433411	3.798129	-0.280775
H	-0.580824	-0.774599	-0.880611
H	-6.734221	-1.033134	0.039285
H	-7.470089	1.296971	-0.184387
H	-5.713943	-2.837524	1.062794
H	-5.648513	-2.964703	-0.720515
H	-4.433411	-3.798129	0.280775

H	-1.742276	1.475932	1.341871
H	-5.800798	3.134632	-0.340246



Symmetry	Number of Imaginary Frequencies	Absolute Electronic Energy [Hartree]	Absolute Electronic Energy + ZPE [Hartree]
C_{2h}	2	-1124.565638	-1124.194692
C_s	2	-1124.565712	-1124.194897
C_2	0	-1124.569803	-1124.197735
C_i	0	-1124.569766	-1124.19781

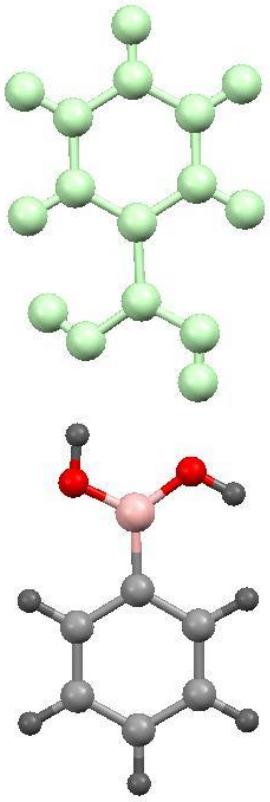
Cartesian coordinates for C_i structure at B3LYP/6-311+G**

C	5.229242	2.664401	-0.174124

C	6.260614	1.734768	-0.118928
C	5.983547	0.369369	-0.038511
C	4.656480	-0.071907	-0.020879
C	3.589003	0.848979	-0.088557
C	3.909446	2.210730	-0.152069
B	2.080825	0.400446	-0.118047
O	1.171072	1.006141	0.751361
O	4.302290	-1.382429	0.091340
C	5.314508	-2.390450	0.099696
H	3.105494	2.939240	-0.212590
O	1.610349	-0.504060	-0.998493
O	-1.171072	-1.006141	-0.751361
B	-2.080825	-0.400446	0.118047
O	-1.610349	0.504060	0.998493
C	-3.589003	-0.848979	0.088557
C	-3.909446	-2.210730	0.152069
C	-5.229242	-2.664401	0.174124
C	-6.260614	-1.734768	0.118928
C	-5.983547	-0.369369	0.038511
C	-4.656480	0.071907	0.020879
H	-3.105494	-2.939240	0.212590
O	-4.302290	1.382429	-0.091340
C	-5.314508	2.390450	-0.099696
H	-1.590728	-1.591914	-1.388475
H	-5.444451	-3.724477	0.237953
H	-7.293892	-2.064179	0.134058
H	-0.655210	0.685684	0.918917
H	-6.802801	0.334634	-0.014872
H	-5.980614	2.240415	-0.958715
H	-5.914721	2.316324	0.815414
H	0.655210	-0.685684	-0.918917
H	6.802801	-0.334634	0.014872
H	7.293892	2.064179	-0.134058

H	5.914721	-2.316324	-0.815414
H	5.980614	-2.240415	0.958715
H	1.590728	1.591914	1.388475
H	5.444451	3.724477	-0.237953
C	-4.620439	3.736581	-0.183229
H	-4.027227	3.809558	-1.097316
H	-5.363215	4.538971	-0.187185
H	-3.956329	3.880058	0.671371
C	4.620439	-3.736581	0.183229
H	3.956329	-3.880058	-0.671371
H	5.363215	-4.538971	0.187185
H	4.027227	-3.809558	1.097316

Absolute electronic energy at B3LYP/6-311+G (in Hartree) and Cartesian coordinates at B3LYP/6-311+G** for calculation of the Interaction Energy.**



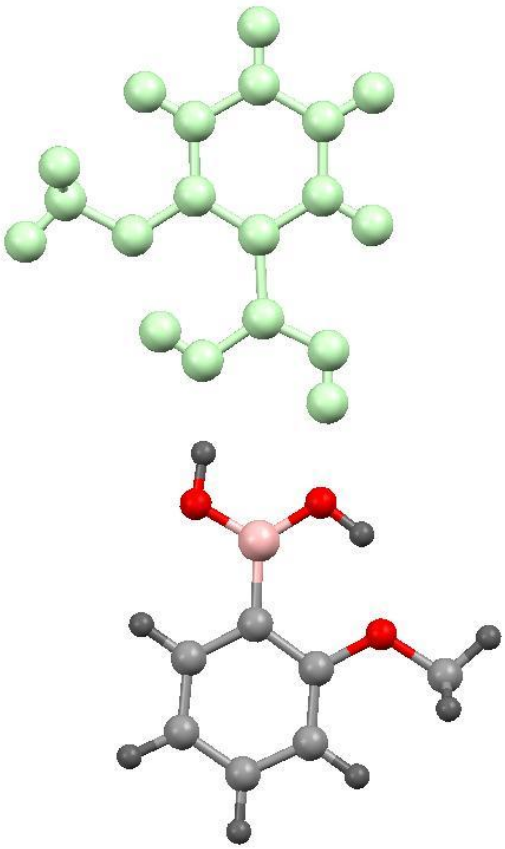
Absolute Electronic Energy [Hartree] HF= -408.3952698

Absolute Electronic Energy [Hartree] + ZPE = -408.270608

Cartesian coordinates at B3LYP/6-311+G**

B	0.052338	2.088343	0.270055
O	1.266893	1.473768	0.403728
H	1.185155	0.518438	0.495361
C	0.013360	3.645324	0.102455
C	1.214355	4.373531	0.053213
C	1.214257	5.757772	-0.096723
H	2.153173	6.299323	-0.133041
C	0.007038	6.448567	-0.199504

H	0.004541	7.526835	-0.315748
H	2.154125	3.839544	0.134061
O	-1.060299	1.281295	0.291935
H	-1.895878	1.741710	0.183387
C	-1.188084	4.364125	-0.002186
C	-1.197806	5.748971	-0.151758
H	-2.139423	6.281027	-0.229959
H	-2.144405	3.847897	0.034371
Bq	0.998920	-1.261941	-0.335022
Bq	-1.246749	-1.469243	0.397401
Bq	-0.095782	-2.073878	0.023087
Bq	-1.202959	-0.494615	0.347491
Bq	-0.023523	-3.639223	-0.009658
Bq	-1.210739	-4.385319	-0.122422
Bq	-1.181629	-5.781060	-0.165483
Bq	-2.109987	-6.342179	-0.253665
Bq	0.040086	-6.458932	-0.096811
Bq	0.063563	-7.546431	-0.129759
Bq	-2.159604	-3.860965	-0.171853
Bq	1.741705	-1.788847	-0.689046
Bq	1.195741	-4.339325	0.067541
Bq	1.231249	-5.735799	0.022213
Bq	2.182627	-6.259199	0.090357
Bq	2.137741	-3.799512	0.185981



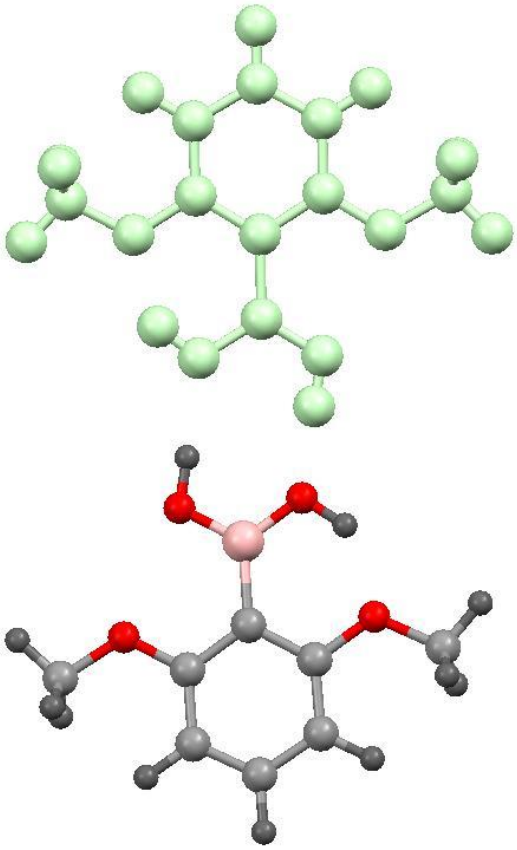
Absolute Electronic Energy [Hartree] HF= -522.9585924

Absolute Electronic Energy [Hartree] + ZPE = -522.800701

Cartesian coordinates at B3LYP/6-311+G**

C	-2.258710	-5.355517	0.000005
C	-1.250774	-6.313683	-0.000001
C	0.090916	-5.931482	-0.000006
C	0.418283	-4.574502	-0.000004
C	-0.578738	-3.576232	0.000002
C	-1.913118	-4.005993	0.000007
B	-0.267281	-2.036545	0.000005
O	-1.329754	-1.169190	0.000009
O	1.724563	-4.132349	-0.000005
C	2.785687	-5.082435	-0.000012
H	-2.690155	-3.250484	0.000012
O	0.994134	-1.510593	0.000008

Bq	1.579098	1.289006	0.000010
Bq	0.465344	2.067523	0.000004
Bq	-0.780908	1.467878	-0.000001
Bq	0.632405	3.633258	0.000004
Bq	1.926425	4.173888	0.000010
Bq	2.157399	5.547652	0.000010
Bq	1.072357	6.418169	0.000004
Bq	-0.232614	5.924343	-0.000001
Bq	-0.444054	4.544815	-0.000002
Bq	2.763751	3.482520	0.000014
Bq	-1.710123	3.994541	-0.000007
Bq	-2.848268	4.851187	-0.000013
Bq	1.404414	0.320897	0.000009
Bq	3.169941	5.933487	0.000014
Bq	1.230234	7.491051	0.000004
Bq	-1.483200	2.133372	-0.000005
Bq	-1.062373	6.617569	-0.000006
Bq	-2.869847	5.479686	0.895269
Bq	-2.869838	5.479685	-0.895296
Bq	-3.716032	4.194045	-0.000016
H	1.656969	-2.214755	0.000009
H	0.859479	-6.692251	-0.000010
H	-1.498948	-7.369443	-0.000003
H	2.753503	-5.711134	0.895021
H	2.753497	-5.711128	-0.895050
H	3.706327	-4.501069	-0.000014
H	-1.039830	-0.250770	0.000012
H	-3.300161	-5.655016	0.000008



Absolute Electronic Energy [Hartree] HF= -637.5074663

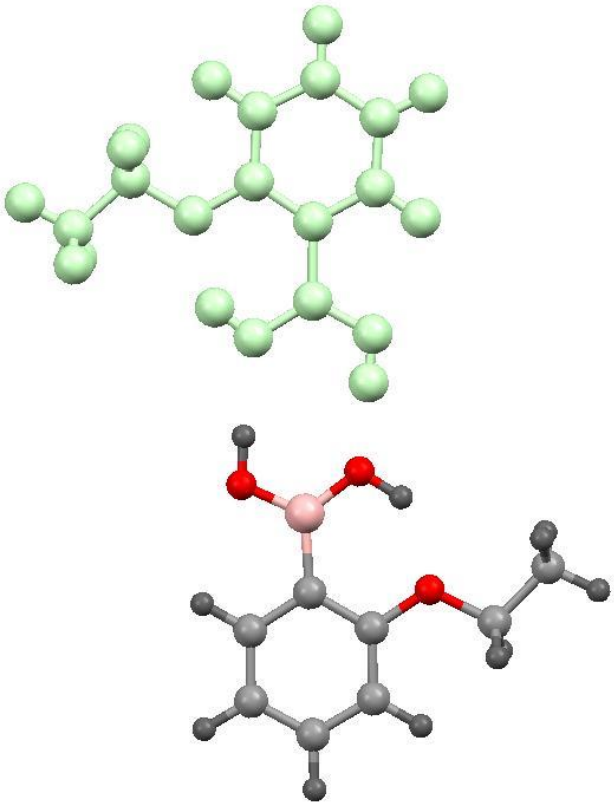
Absolute Electronic Energy [Hartree] + ZPE = -637.317524

Cartesian coordinates at B3LYP/6-311+G**

C	1.013269	-5.931031	-0.118323
C	-0.256393	-6.474996	-0.243861
C	-1.388041	-5.670031	-0.202511
C	-1.227901	-4.293163	-0.030094
C	0.037607	-3.677370	0.107168
C	1.156879	-4.546900	0.055045
B	0.183041	-2.112199	0.306449
O	1.405489	-1.521515	0.480373
O	-2.325166	-3.457685	0.014110
C	-3.637061	-3.998971	-0.106315
O	2.375034	-3.968048	0.179734
C	3.545025	-4.769783	0.139852

O	-0.898510	-1.269383	0.317159
Bq	-1.216214	1.411587	0.234792
Bq	-0.068520	2.077990	0.024968
Bq	1.083093	1.316253	-0.142224
Bq	-0.005912	3.663670	-0.021221
Bq	-1.174009	4.466351	0.000024
Bq	-1.113298	5.867263	-0.022691
Bq	0.120944	6.496857	-0.072726
Bq	1.298054	5.760221	-0.106017
Bq	1.218956	4.366072	-0.082219
Bq	-2.354076	3.809181	0.031707
Bq	-3.568429	4.542493	0.076299
Bq	2.367143	3.596891	-0.116396
Bq	3.645451	4.222891	-0.164094
Bq	-1.087821	0.457559	0.255179
Bq	-2.014658	6.461928	-0.003027
Bq	0.168515	7.580169	-0.089586
Bq	-3.628960	5.170471	0.972537
Bq	-3.698921	5.164731	-0.815818
Bq	-4.358206	3.794238	0.108814
Bq	1.861114	1.890756	-0.233098
Bq	2.249039	6.270527	-0.149401
Bq	3.756677	4.826433	-1.070471
Bq	3.812284	4.846336	0.718529
Bq	4.371938	3.410897	-0.176797
H	-1.723684	-1.759617	0.201284
H	-2.366689	-6.115438	-0.303582
H	-0.368588	-7.545304	-0.377217
H	-3.773823	-4.495353	-1.071540
H	-3.851604	-4.700244	0.705385
H	-4.314476	-3.149165	-0.037900
H	1.291575	-0.569858	0.585352
H	1.877095	-6.578532	-0.155814

H	3.561617	-5.500799	0.955661
H	3.645520	-5.289948	-0.819084
H	4.375604	-4.076432	0.261603



Absolute Electronic Energy [Hartree] HF= -562.2883332

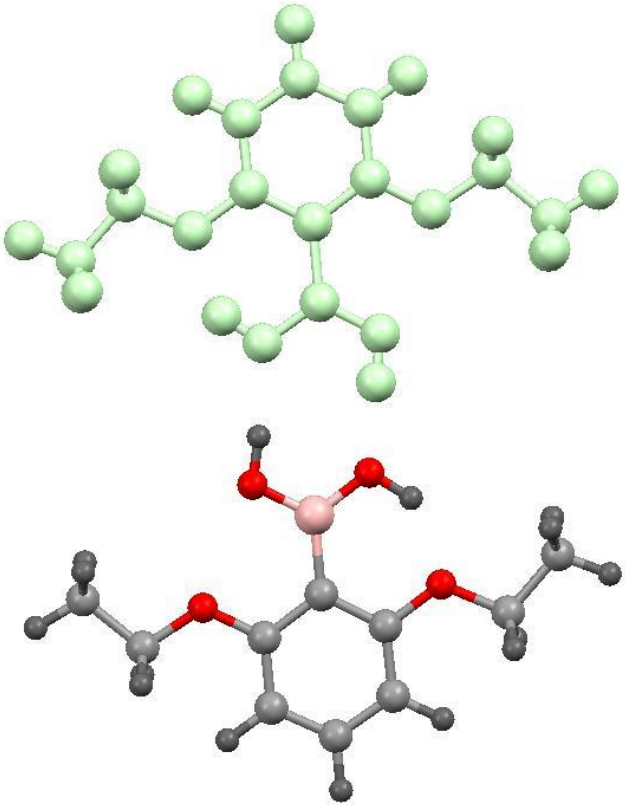
Absolute Electronic Energy [Hartree] + ZPE = -562.102319

Cartesian coordinates at B3LYP/6-311+G**

C	-2.701731	-5.361126	0.000032
C	-1.695459	-6.321082	0.000035
C	-0.352988	-5.942007	0.000032
C	-0.021016	-4.585407	0.000025
C	-1.017579	-3.585763	0.000017
C	-2.352973	-4.012534	0.000024
B	-0.704209	-2.046733	0.000004

O	-1.765079	-1.176978	0.000022
O	1.285120	-4.145924	0.000017
C	2.359262	-5.095501	0.000027
H	-3.128318	-3.255249	0.000020
O	0.558143	-1.522655	0.000002
Bq	1.521958	1.039972	-0.000009
Bq	0.552862	1.976232	-0.000015
Bq	-0.774129	1.576294	-0.000010
Bq	0.967000	3.493692	-0.000027
Bq	2.328557	3.821779	-0.000037
Bq	2.776067	5.141120	-0.000054
Bq	1.844091	6.172475	-0.000039
Bq	0.477502	5.892834	-0.000027
Bq	0.048087	4.564366	-0.000025
Bq	3.042068	3.009679	-0.000036
Bq	-1.289401	4.222658	-0.000015
Bq	-2.292194	5.247474	-0.000012
Bq	1.193427	0.129540	-0.000007
Bq	3.837458	5.360821	-0.000052
Bq	2.171781	7.206572	-0.000047
Bq	-1.356086	2.353980	-0.000006
Bq	-0.230723	6.709887	-0.000029
Bq	-2.166353	5.875971	0.888694
Bq	-2.166364	5.875966	-0.888722
H	1.218816	-2.229074	0.000005
H	0.413135	-6.704983	0.000034
H	-1.945750	-7.376401	0.000041
H	2.280879	-5.731358	0.888877
H	2.280866	-5.731384	-0.888804
H	-1.472711	-0.259376	0.000021
H	-3.743824	-5.658452	0.000034
Bq	-3.648953	4.572126	-0.000002
Bq	-3.776605	3.947462	0.887363

Bq	-4.437356	5.329156	0.000000
Bq	-3.776614	3.947456	-0.887363
C	3.664306	-4.322818	0.000007
H	3.744543	-3.691237	0.887719
H	4.505954	-5.020203	0.000013
H	3.744532	-3.691265	-0.887726



Absolute Electronic Energy [Hartree] HF= -716.1668558

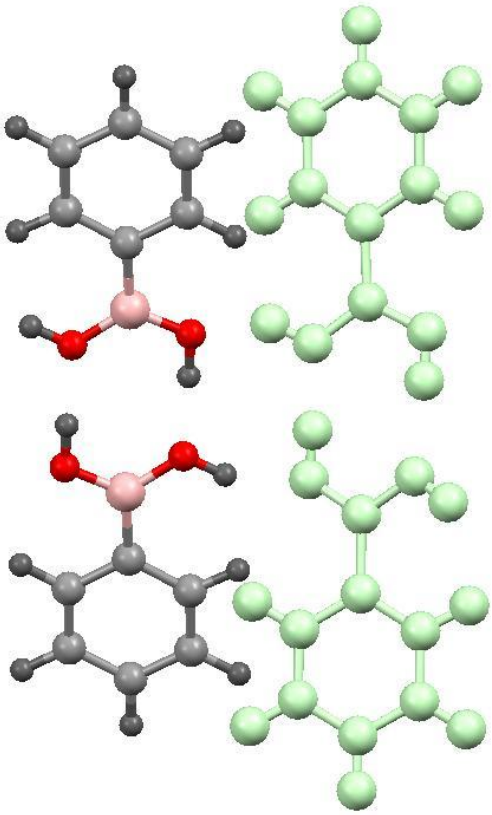
Absolute Electronic Energy [Hartree] + ZPE = -715.920642

Cartesian coordinates at B3LYP/6-311+G**

C	0.900998	-5.921377	0.213942
C	-0.367991	-6.477515	0.275498
C	-1.504501	-5.685116	0.172806

C	-1.351245	-4.306749	0.001377
C	-0.085204	-3.679667	-0.075224
C	1.039964	-4.535961	0.043045
B	0.053928	-2.115319	-0.280810
O	1.274434	-1.515987	-0.444218
O	-2.452986	-3.483477	-0.101976
C	-3.776294	-4.033898	-0.061237
O	2.256683	-3.944447	-0.012694
C	3.444482	-4.729867	0.094211
O	-1.032472	-1.278772	-0.310654
Bq	-1.246137	1.472991	-0.143386
Bq	-0.050754	2.090832	-0.048348
Bq	1.077624	1.282605	-0.016164
Bq	0.087010	3.672118	0.018749
Bq	-1.043725	4.527135	0.079295
Bq	-0.915928	5.923675	0.123805
Bq	0.347160	6.495367	0.112107
Bq	1.489158	5.706367	0.060592
Bq	1.345815	4.317172	0.017043
Bq	-2.255379	3.925994	0.097801
Bq	-3.447257	4.709883	0.143529
Bq	2.457454	3.499139	-0.032065
Bq	3.776749	4.060286	-0.040364
Bq	-1.164303	0.506938	-0.191633
Bq	-1.787948	6.559276	0.168053
Bq	0.445879	7.574903	0.145934
Bq	-3.452992	5.328219	1.049970
Bq	-3.487194	5.377896	-0.725874
Bq	1.884563	1.819565	0.015229
Bq	2.462999	6.172640	0.054784
Bq	3.887763	4.711511	-0.914081
Bq	3.920417	4.663409	0.862845
H	-1.856258	-1.776323	-0.216844

H	-2.481814	-6.140958	0.227185
H	-0.475973	-7.548485	0.407815
H	-3.890086	-4.762427	-0.871265
H	-3.926062	-4.549963	0.893381
H	1.152566	-0.566213	-0.557222
H	1.767826	-6.559918	0.299584
H	3.447904	-5.271156	1.048425
H	3.476486	-5.467241	-0.717457
Bq	4.767436	2.912523	-0.089359
Bq	5.786831	3.306898	-0.099275
Bq	4.660626	2.264900	0.783957
Bq	4.624646	2.310626	-0.989859
Bq	-4.621733	3.748723	0.139269
Bq	-4.578799	3.086407	1.006097
Bq	-5.561141	4.307927	0.171344
Bq	-4.610047	3.133546	-0.762133
C	4.624484	-3.780179	0.008280
H	4.588073	-3.047804	0.817079
H	5.559937	-4.341262	0.085960
H	4.616975	-3.242160	-0.941547
C	-4.759512	-2.889839	-0.219244
H	-4.610236	-2.374918	-1.170947
H	-5.781396	-3.277159	-0.196379
H	-4.651504	-2.165318	0.591269



Absolute Electronic Energy [Hartree] HF= -816.8059249

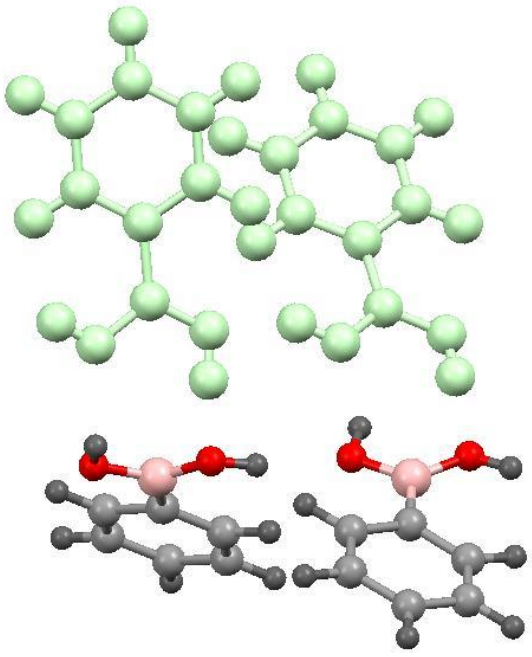
Absolute Electronic Energy [Hartree] + ZPE = -816.554637

Cartesian coordinates at B3LYP/6-311+G**

B	1.721739	2.909224	-0.761102
O	2.964027	2.742118	-0.253739
H	3.185773	1.826661	-0.001803
C	1.256082	4.331219	-1.226677
C	2.177722	5.392108	-1.230355
C	1.807894	6.669152	-1.643217
H	2.536588	7.472379	-1.640569
C	0.499680	6.916702	-2.058819
H	0.208986	7.910970	-2.379933
H	3.193815	5.201467	-0.904707
O	0.898438	1.788813	-0.851461
H	0.044615	1.954906	-1.260223

C	-0.054947	4.607193	-1.646452
C	-0.434847	5.882390	-2.058963
H	-1.454391	6.070093	-2.376896
H	-0.810938	3.825106	-1.650124
Bq	-1.736476	0.864499	0.220226
O	3.580208	0.075177	0.468050
O	1.514507	-0.878078	-0.129347
Bq	-3.015080	0.954778	0.717988
Bq	-1.448601	-0.064754	0.077845
Bq	-3.603572	2.323922	1.197631
Bq	-2.751756	3.373936	1.574722
Bq	-3.257509	4.589015	2.027105
Bq	-2.580914	5.383354	2.318800
Bq	-4.636622	4.781449	2.107059
Bq	-5.034012	5.727159	2.458505
Bq	-1.676356	3.232824	1.517237
Bq	-3.750749	-0.220683	0.768985
Bq	-4.607580	-0.135503	1.198030
Bq	-4.988986	2.545911	1.279569
Bq	-5.504038	3.758246	1.727386
Bq	-6.576499	3.907740	1.777742
Bq	-5.686717	1.769349	0.974218
Bq	-0.826847	-1.661641	-0.160589
Bq	-2.871058	-2.794680	-0.151940
Bq	-1.536438	-2.828117	-0.369294
Bq	0.116499	-1.684597	-0.219662
Bq	-0.879215	-4.173323	-0.817060
Bq	0.459963	-4.265839	-1.219788
Bq	1.017148	-5.477730	-1.627039
Bq	2.055348	-5.521968	-1.936960
Bq	0.237724	-6.632864	-1.628325
Bq	0.667404	-7.578686	-1.941858
Bq	1.087120	-3.384817	-1.228581

Bq	-3.196172	-1.930963	0.143877
Bq	-1.644080	-5.350618	-0.836750
Bq	-1.097506	-6.566961	-1.233779
Bq	-1.708534	-7.463211	-1.236986
Bq	-2.681690	-5.300433	-0.531957
B	2.756828	-1.045190	0.377946
H	1.292824	0.037357	-0.381425
C	3.222423	-2.467145	0.843707
C	2.300738	-3.527993	0.847483
C	2.670505	-4.805010	1.260485
H	1.941777	-5.608207	1.257907
C	3.978701	-5.052572	1.676133
H	4.269352	-6.046818	1.997354
H	1.284658	-3.337345	0.521803
H	4.434075	-0.090953	0.876703
C	4.533433	-2.743130	1.263531
C	4.913272	-4.018297	1.676187
H	5.932801	-4.206011	1.994162
H	5.289463	-1.961078	1.267146



Absolute Electronic Energy [Hartree] HF= -816.7986347

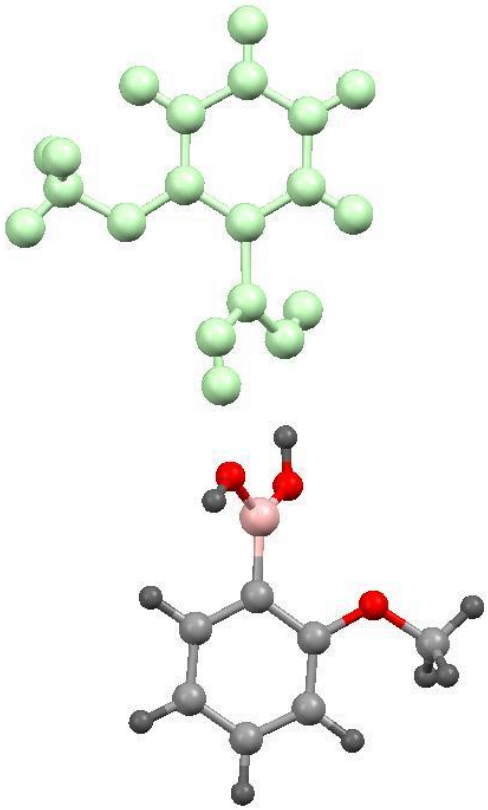
Absolute Electronic Energy [Hartree] + ZPE = -816.547472

Cartesian coordinates at B3LYP/6-311+G**

B	1.451852	2.699529	-0.046894
O	2.710362	2.892565	0.466414
H	2.778232	2.570611	1.371603
C	1.194779	3.135687	-1.532540
C	2.280227	3.474442	-2.358717
C	2.088857	3.860172	-3.683028
H	2.942023	4.112797	-4.303400
C	0.799422	3.925770	-4.210796
H	0.647154	4.229496	-5.240912
H	3.283118	3.431680	-1.949417
O	0.522580	2.134666	0.782651
H	-0.346168	1.918655	0.411703
C	-0.094170	3.211141	-2.085580
C	-0.293818	3.604004	-3.407880
H	-1.299183	3.662066	-3.811053
H	-0.960408	2.973768	-1.476415
O	-2.098013	1.193870	0.075936
Bq	3.373715	0.658116	1.467291
Bq	1.325228	-0.317794	0.890621
B	-3.355910	1.271647	0.638443
H	-2.066425	0.535247	-0.628838
C	-3.616572	2.226983	1.845445
C	-2.552533	2.758653	2.594829
C	-2.787558	3.596659	3.682153
H	-1.952027	3.991485	4.249240
C	-4.093153	3.930376	4.039550
H	-4.275689	4.585447	4.884282

H	-1.530729	2.511458	2.331737
O	-4.308539	0.470612	0.064276
H	-5.162331	0.482048	0.504352
C	-4.923340	2.579650	2.224674
C	-5.164576	3.422252	3.306237
H	-6.181697	3.684732	3.574856
H	-5.776437	2.210037	1.661204
Bq	-1.211429	-0.935891	-0.202404
Bq	-3.143942	-1.782638	-1.268522
Bq	-1.799128	-1.894827	-1.024997
Bq	-0.268498	-1.026090	0.033582
Bq	-1.002924	-3.085985	-1.668833
Bq	0.400390	-3.181807	-1.619778
Bq	1.073633	-4.249480	-2.214152
Bq	2.155598	-4.299278	-2.163249
Bq	0.355487	-5.246607	-2.872051
Bq	0.876600	-6.076419	-3.335671
Bq	0.986877	-2.413296	-1.118696
Bq	-3.563650	-1.012736	-0.845372
Bq	-1.711336	-4.106089	-2.343675
Bq	-1.038371	-5.176010	-2.930449
Bq	-1.600861	-5.950834	-3.441348
Bq	-2.792222	-4.044743	-2.397085
Bq	2.614825	-0.492051	1.286200
Bq	1.046867	0.617297	0.866849
Bq	3.199946	-1.923467	1.530463
Bq	2.344810	-3.007733	1.795834
Bq	2.850459	-4.282182	2.041958
Bq	2.172802	-5.101900	2.250424
Bq	4.227975	-4.503317	2.016736
Bq	4.623561	-5.495389	2.202147
Bq	1.271979	-2.846436	1.816252
Bq	4.244957	0.493823	1.845408

Bq	4.583427	-2.172647	1.509916
Bq	5.096532	-3.446477	1.743191
Bq	6.167116	-3.615468	1.711433
Bq	5.280248	-1.369853	1.283003



Absolute Electronic Energy [Hartree] HF= -522.9477017

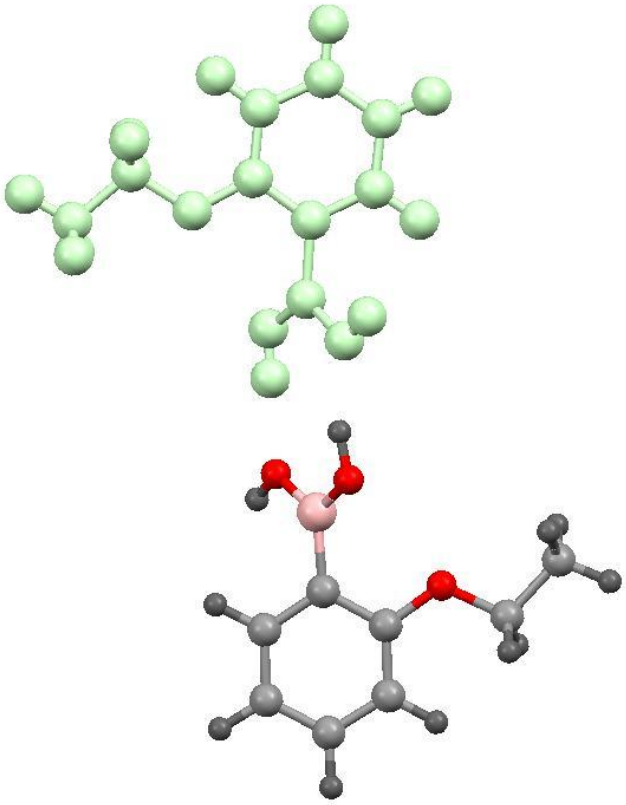
Absolute Electronic Energy [Hartree] + ZPE = -522.790652

Cartesian coordinates at B3LYP/6-311+G**

C	-5.411178	2.152921	-0.080055
C	-6.370943	1.147977	-0.072214
C	-5.992984	-0.195130	-0.049846
C	-4.636863	-0.535819	-0.044268
C	-3.640072	0.462799	-0.063354

C	-4.061522	1.798280	-0.068879
B	-2.102353	0.136564	-0.097037
O	-1.214535	0.781934	0.736036
O	-4.188148	-1.821640	0.009243
C	-5.129009	-2.884619	-0.021442
H	-3.314121	2.586546	-0.090805
O	-1.584135	-0.743805	-0.998083
Bq	1.289314	-1.075424	-0.604229
Bq	2.123555	-0.256410	0.171440
Bq	1.545177	0.663521	0.950819
Bq	3.678169	-0.490907	0.160843
Bq	4.185645	-1.781227	0.361660
Bq	5.555599	-2.043565	0.407700
Bq	6.447816	-0.991603	0.238565
Bq	5.982745	0.305608	0.020081
Bq	4.607533	0.554424	-0.020182
Bq	3.491261	-2.603810	0.512319
Bq	4.074780	1.784127	-0.260942
Bq	4.942748	2.900523	-0.397041
Bq	1.786223	-1.667545	-1.180613
Bq	5.916323	-3.050395	0.580837
Bq	7.516867	-1.171286	0.271081
Bq	0.582385	0.696008	0.871304
Bq	6.695473	1.107439	-0.119790
Bq	5.545730	3.051106	0.504508
Bq	5.603135	2.792820	-1.265299
Bq	4.294255	3.763055	-0.544835
H	-0.628726	-0.831664	-0.905539
H	-6.757204	-0.960429	-0.033379
H	-7.425741	1.400214	-0.079748
H	-5.790170	-2.862138	0.852077
H	-5.731242	-2.859253	-0.936010
H	-4.540405	-3.800397	-0.003671

H	-1.640781	1.345379	1.387529
H	-5.704605	3.195819	-0.098781



Absolute Electronic Energy [Hartree] HF= -562.2774379

Absolute Electronic Energy [Hartree] + ZPE = -562.092303

Cartesian coordinates at B3LYP/6-311+G**

C	5.424284	2.614782	-0.051776
C	6.377472	1.603657	-0.032095
C	5.991366	0.263039	-0.006537
C	4.632843	-0.070671	-0.009317
C	3.643080	0.935294	-0.041070
C	4.072587	2.268289	-0.049264
B	2.103643	0.620197	-0.086036
O	1.213726	1.275921	0.736963

O	4.175595	-1.352422	0.047283
C	5.105736	-2.436660	0.020214
H	3.330095	3.060921	-0.080740
O	1.584494	-0.259943	-0.987388
Bq	-1.073815	-0.904729	-0.697187
Bq	-2.009444	-0.312516	0.147669
Bq	-1.583815	0.650620	0.995726
Bq	-3.493397	-0.839075	0.133131
Bq	-3.743997	-2.211677	0.247570
Bq	-5.039071	-2.731189	0.285911
Bq	-6.116509	-1.858546	0.194332
Bq	-5.909664	-0.484560	0.062650
Bq	-4.606894	0.023138	0.029390
Bq	-2.904033	-2.895027	0.336216
Bq	-4.320130	1.345651	-0.131714
Bq	-5.382625	2.298493	-0.179589
Bq	-1.456639	-1.533680	-1.314148
Bq	-5.199808	-3.797889	0.388881
Bq	-7.131557	-2.239885	0.220803
Bq	-0.633745	0.877884	0.913402
Bq	-6.763734	0.173780	-0.018265
Bq	-6.037678	2.081930	-1.032860
Bq	-5.980972	2.228151	0.736931
H	0.627508	-0.337329	-0.901824
H	6.751034	-0.506283	0.019536
H	7.433898	1.849293	-0.032789
H	5.720615	-2.370914	-0.885628
H	5.771010	-2.376371	0.890645
H	1.639311	1.839381	1.388894
H	5.724356	3.655755	-0.073016
Bq	-4.758478	3.673986	-0.313523
Bq	-4.167204	3.742670	-1.229123
Bq	-5.541527	4.436271	-0.348647

Bq	-4.105297	3.883488	0.535773
C	4.307569	-3.726429	0.038989
H	3.645304	-3.781294	-0.827222
H	4.985389	-4.584059	0.015223
H	3.699113	-3.791444	0.943624

Dependences between hydrogen bond energies estimated based on systems optimised at two levels of theory: B3LYP/6-311+G and MP2/6-31+G*.**

Figure 1. Based on ZPE uncorrected energy values

The following systems are taken into account:
Systems with intramolecular hydrogen bond:
1. 2-methoxyprenylboronic acid
2. 2-ethoxyprenylboronic acid
3. 2,6-di methoxyprenylboronic acid
4. 2,6-di ethoxyprenylboronic acid
Systems with intermolecular hydrogen bond:
5. Phenylboronic acid dimer (basis-set superposition error (BSSE) corrected interaction energy).
6. 2-methoxyprenylboronic acid dimer (basis-set superposition error (BSSE) corrected interaction energy).
7. 2-ethoxyprenylboronic acid dimer (basis-set superposition error (BSSE) corrected interaction energy).
dimer (basis-set superposition error (BSSE) corrected interaction energy).

Correlation coefficient R=0.9987

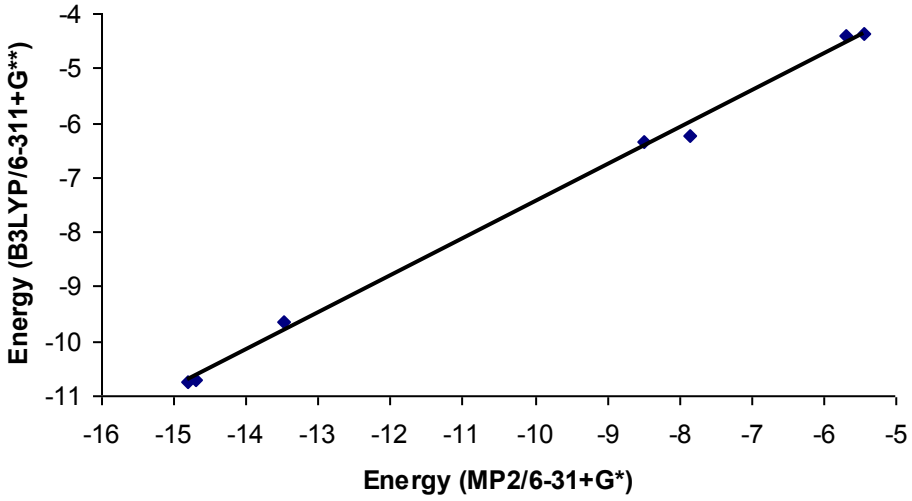


Figure 2. Based on ZPE corrected energy values

The following systems are taken into account:
1. 2-methoxyprenylboronic acid
2. 2-ethoxyprenylboronic acid
3. 2,6-di methoxyprenylboronic acid
4. 2,6-di ethoxyprenylboronic acid
5. Phenylboronic acid dimer (basis-set superposition error (BSSE) corrected interaction energy).

Correlation coefficient R=0.9896