crystals

MDPI

Symmetric fluoroborate and its boron modification – crystal and electronic structures

Błażej Dziuk [1,2], Borys Ośmiałowski [3], Bartosz Zarychta [1], Krzysztof Ejsmont [1] and Lilianna Chęcińska [4,*]

[1] Faculty of Chemistry, Opole University, Oleska 48, 45-052 Opole, Poland; bdziuk@uni.opole.pl (B.D.); Bartosz.Zarychta@uni.opole.pl (BZ); Krzysztof.Ejsmont@uni.opole.pl (K.E.)

[2] Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, Wrocław, 50-370, Poland, bdziuk@pwr.edu.pl (B.D.)

[3] Faculty of Chemistry, Nicolaus Copernicus University, Gagarina 7, 87-100 Toruń, Poland; borys.osmialowski@umk.pl (B.O.)

[4] Faculty of Chemistry, University of Lodz, Pomorska 163/165, 90-236 Łódź, Poland; lilianna.checinska@chemia.uni.lodz.pl (L.C)

* Correspondence: lilianna.checinska@chemia.uni.lodz.pl; Tel.: +48-42 635 42 73 (L.C.)

Received: date; Accepted: date; Published: date

SUPLEMENTARY MATERIALS

Table of contents:

Table S1. Selected geometrical parameters [Å,°] for structures **1** – **4**.

	1	**2**	**3**	**4**
Bond lengths				
N2–B1	1.543(2)	1.542(3)	1.576(3)	1.574(3)
O1–B1	1.4477(19)	1.462(3)	1.4751(19)	1.477(2)
O1A–B1	1.4571(19)	1.447(3)		1.477(2)
F1–B1/ C11–B1	1.3893(18)	1.389(3)	1.605(4)	1.594(3)
N2–C2	1.3627(17)	1.363(3)	1.3603(16)	1.362(2)
N2–C2A	1.3655(17)	1.366(3)		1.362(2)
N1–C1	1.2988(17)	1.286(3)	1.302(2)	1.302(2)
N1A–C1A	1.3011(17)	1.306(3)		1.302(2)
N1–C2	1.3807(18)	1.391(3)	1.3863(19)	1.390(2)
N1A–C2A	1.3810(17)	1.372(3)		1.384(2)
O1–C1	1.3346(16)	1.335(3)	1.3277(18)	1.331(2)
O1A–C1A	1.3318(16)	1.339(3)		1.331(2)
Bond angles				
O1–B1–O1A	110.00(12)	110.3(2)	108.8(2)	108.97(17)
C1/F1–B1-N2	109.57(12)	108.6(2)	112.03(19)	112.45(16)
O1–B1–N2	108.70(12)	107.8(2)	105.57(14)	105.02(16)
O1A–B1–N2	107.75(12)	108.8(2)		105.38(16)
B1–O1–C1	118.64(11)	115.87(19)	117.46(14)	
B1–O1A–C1A	117.33(11)	117.90(19)		
O1–C1–N1	125.38(13)	127.0(2)	125.78(14)	
O1A–C1A–N1A	125.62(13)	124.7(2)		
C1–N1–C2	119.40(13)	118.2(2)	118.26(13)	118.13(17)
C1A–N1A–C2A	118.63(12)	119.6(2)		
N1–C2–N2	119.72(13)	119.4(2)	120.28(28)	
N1A–C2A–N2	119.75(13)	120.2(2)		
B1–N2–C2	119.49(12)	119.0(2)	118.71(9)	119.47(17)
B1–N2–C2A	118.08(12)	118.3(2)		118.95(17)
C2–N2–C2A	122.40(12)	122.6(2)	122.54(18)	121.55(17)

Table S2. Puckering and asymmetry parameters [Å,°] for structures **1** – **4**.

structure	ring	Puckering parameters	Asymmetry parameters	Conformation
1	O1/C1/N1/C2/N2/B1	Q=0.28(2)Å, ϕ=311.7(3)°, θ=64.7(3)°	ΔCs(B1)=7.82(16), ΔC_2(B1-O1)=10.43(19)	E/S
1	O1A/C1A/N1A/C2A/N2/B1	Q=0.358(2)Å, ϕ=125.4(2)°, θ=113.0(2)°	ΔCs(B1)=4.58(16)	E
2	O1/C1/N1/C2/N2/B1	Q=0.355(3)Å, ϕ=313.6(4)°, θ=66.0(5)°	ΔCs(B1)=10.5(3), ΔC_2(B1-O1)=11.5(3)	E/S
2	O1A/C1A/N1A/C2A/N2/B1	Q=0.317(3)Å, ϕ=130.3(5)°, θ=116.0(5)°	ΔCs(B1)=7.6(3), ΔC_2(B1-O1A)=12.4(3)	E/S
3	O1/C1/N1/C2/N2/B1	Q=0.373(2)Å, ϕ=133.6(3)°, θ=114.8(3)°	ΔCs(B1)=11.8(2), ΔC_2(B1-O1)=11.0(3)	E/S
4	O1/C1/N1/C2/N2/B1	Q=0.391(2)Å, ϕ=316.6(3)°, θ=66.8(3)°	ΔCs(B1)=14.6(2), ΔC_2(B1-O1)=9.1(3)	E/S
4	O1A/C1A/N1A/C2A/N2/B1	Q=0.371(2)Å, ϕ=130.2(3)°, θ=113.0(3)°	ΔCs(B1)=9.0(2), ΔC_2(B1-O1A)=14.5(3)	E/S

Table S3: Intermolecular interactions [Å,°] for structure **2**.

Comp.	H–Bond	D–H	H···A	D···A	D–H···A
2	C3–H3···F5^{i}	0.93	2.27	3.179 (3)	165
	C11–H11B···F2^{ii}	0.96	2.46	3.317 (3)	148
	C11A–H11AE···O1^{iii}	0.96	2.54	3.456 (3)	160

Symmetry codes: **2** (i) -½ -x, ½ +y, ½ -z; (ii) 1-x,-y,1-z; (iii) ½ +x,- ½ -y, ½ +z.

Table S4: Aromatic π···π interactions [Å,°] for structures **1 – 4.**

Compound	Interaction	*Cg*(I)···*Cg*(J)	α	*Cg*(I)$_{perp}$	*Cg*(J)$_{perp}$	Slippage
1	*Cg*(C)···*Cg*(E)^{i}	3.949(1)	20.4(1)	3.629(1)	3.943(1)	
	Cg(D)···*Cg*(E)^{ii}	3.890(1)	20.6(1)	3.476(1)	3.775(1)	
2	*Cg*(C)···*Cg*(C)^{i}	3.537(1)	0.0(1)	3.413(1)	3.413(1)	0.929
	Cg(C)···*Cg*(C)^{ii}	3.763(1)	0.0(1)	3.354(1)	3.354(1)	1.707
	Cg(D)···*Cg*(E)^{iii}	3.610(1)	5.8(1)	3.409(1)	3.353(1)	1.339
	Cg(C)···*Cg*(E)^{iv}	3.594(1)	5.8(1)	3.291(1)	3.380(1)	1.223
3	*Cg*(C)···*Cg*(C)^{i}	3.812(1)	16.5(1)	3.739(1)	3.795(1)	0.356
	Cg(C)···*Cg*(C)^{ii}	3.812(1)	16.5(1)	3.795(1)	3.739(1)	0.739
4	*Cg*(C)···*Cg*(E)^{i}	4.073(1)	21.2(1)	3.329(1)	3.952(1)	

Cg···*Cg* – distance between ring centroids; α - dihedral angle between planes I and J; *Cg*(I)$_{perp}$ and *Cg*(J)$_{perp}$ - (interplanar spacing) perpendicular distance of *Cg*(I) on ring J and *Cg*(J) on ring I, respectively; slippage - distance between *Cg*(I) and perpendicular projection of *Cg*(J) on ring I.

Symmetry codes: **1** (i) ½ -x, ½ +y, ½ -z; (ii) -½ +x, ½ -y, ½ +z;
Symmetry codes: **2** (i) -x,-y,1-z; (ii) -x,1-y,1-z; (iii) - ½ +x,- ½ -y,- ½ +z; (iv) -½ +x, ½ -y,-½ +z;
Symmetry codes: **3** (i) 1-x,1-y,- ½ +z; (ii) 1-x,1-y, ½ +z;
Symmetry codes: **4** (i) x,-1+y,z.

Table S5: Aromatic C-H···π interactions [Å,°] for structures **3 – 4.**

Comp.	H–Bond	H···Cg	H···Cg	X–H···Cg
3	C4–H4···*Cg*(F)^{i}	2.68	3.373(3)	132
	C4–H4···*Cg*(F)^{ii}	2.68	3.373(3)	132
	C14–H14···*Cg*(F)^{iii}	2.87	3.714(3)	151
	C14–H14···*Cg*(F)^{iv}	2.87	3.714(3)	151
4	C7–H7A···*Cg*(F)^{i}	2.61	3.494(2)	158
	C15–H15A···*Cg*(E)^{ii}	2.82	3.731(3)	159

Symmetry codes: **3** (i) 1-x,1-y,- ½ +z; (ii) x,1-y,- ½ +z; (iii) 1-x,-y, ½ +z; (iv) x,-y, ½ +z;

Symmetry codes: **4** (i) x,,1+y,z; (ii) 1-x,1-y,1-z.

Table S6. Real-space bonding indicators [a] for N(amine)–C(phenyl) bond.

	Bond	*d*	ρ_{bcp}	$\nabla^2\rho_{bcp}$	G/ρ_{bcp}	H/ρ_{bcp}	ε	δ	V_{001}^{ELI}	ELI_{pop}	Δ_{ELI}	*RJI*
2	N3–C8A	1.372	2.12	-23.4	0.53	-1.30	0.16	1.12	2.16	1.91	0013	66.6
4	N3–C14	1.393	2.04	-21.6	0.47	-1.21	0.14	1.08	2.38	1.98	0.031	68.0
5	N3–C8A	1.374	2.11	-23.2	0.52	1.29	0.15	1.12	2.17	1.92	0.016	66.7

a - bond length (*d* in Å), electron density (ρ_{bcp} in eÅ^{-3}), Laplacian of the electron density ($\nabla^2\rho_{bcp}$ in eÅ^{-5}), kinetic and total energy density over ρ_{bcp} ratios (G/ρ_{bcp} and H/ρ_{bcp} in he^{-1}), the bond ellipticity (ε), the delocalization index (δ), volume of the ELI-D basin cut at 0.001au (V_{001}^{ELI} in Å^3), the electron population within the ELI-D basin (ELI_{pop} in *e*), the distance of the attractor position perpendicular to the *xy* axis (Δ_{ELI} in Å) and the Raub-Jansen index (*RJI* in %).

Table S7: Pairwise model energies [kJ/mol] for structure **1.**

	N	Symmetry operations	*R*	*E*ele	*E*pol	*E*dis	*E*rep	*E*tot
	2	-x+1/2, y+1/2, -z+1/2	8.05	-11.0	-2.9	-39.7	21.9	-34.8
	1	-x, -y, -z	15.33	-3.0	-0.4	-10.8	10.7	-6.2
	2	x+1/2, -y+1/2, z+1/2	9.73	-5.2	-1.3	-30.5	18.1	-21.9
	1	-x, -y, -z	8.89	-1.9	-1.0	-23.6	10.2	-17.0
	2	-x+1/2, y+1/2, -z+1/2	9.78	-9.1	-2.4	-25.2	17.1	-22.7
	2	x, y, z	11.17	-2.2	-0.6	-8.7	6.4	-6.4
	2	x, y, z	12.58	-4.5	-1.2	-16.4	13.1	-11.9
	1	-x, -y, -z	3.88	-13.1	-2.7	-111.3	66.6	-71.5
	1	-x, -y, -z	13.24	-1.4	-0.4	-11.7	4.7	-9.1

N- number of molecules;

R is the distance between molecular centroids (mean atomic position) in Å;

Total energies (E_{tot}) are the sum of the four energy components, scaled appropriately

Table S8: Pairwise model energies [kJ/mol] for structure **2.**

	N	Symmetry operations	*R*	*E*ele	*E*pol	*E*dis	*E*rep	*E*tot
	1	-x, -y, -z	14.39	1.2	-0.2	-6.6	1.2	-3.9
	2	x+1/2, -y+1/2, z+1/2	10.91	-15.3	-3.0	-53.0	34.1	-43.6
	1	-x, -y, -z	6.51	-10.5	-2.0	-83.3	45.6	-57.1
	2	-x+1/2, y+1/2, -z+1/2	12.09	-4.1	-0.5	-7.4	11.7	-3.9
	2	x+1/2, -y+1/2, z+1/2	10.24	-16.6	-4.0	-65.8	40.7	-52.6
	2	-x+1/2, y+1/2, -z+1/2	8.52	0.1	-0.8	-12.5	5.4	-8.0
	1	-x, -y, -z	8.84	-14.2	-2.3	-38.7	20.6	-37.6
	2	-x+1/2, y+1/2, -z+1/2	12.60	0.9	-1.0	-12.9	7.1	-6.6
	1	-x, -y, -z	10.60	-24.9	-6.1	-45.7	30.1	-52.1
	2	-x+1/2, y+1/2, -z+1/2	19.29	2.0	-0.8	-6.9	2.1	-3.1

Table S9: Pairwise model energies [kJ/mol] for structure **3.**

	N	Symmetry operations	*R*	*Eele*	*Epol*	*Edis*	*Erep*	*Etot*
	4	-x+1/2, -y+1/2, z+1/2	11.30	-4.3	-1.1	-28.0	16.0	-19.9
	2	-x, -y, z+1/2	6.92	-8.4	-3.1	-56.0	31.2	-40.7
	4	x+1/2, y+1/2, z	12.18	-4.2	-1.0	-18.5	12.6	-13.4
	2	x, y, z	7.61	-1.9	-1.4	-29.9	21.5	-15.7
	2	-x, -y, z+1/2	7.19	-16.2	-3.4	-56.8	31.9	-49.4

Table S10: Pairwise model energies [kJ/mol] for structure **4.**

	N	Symmetry operations	*R*	*Eele*	*Epol*	*Edis*	*Erep*	*Etot*
	1	-x, -y, -z	9.89	-12.5	-2.9	-29.0	21.6	-27.2
	2	x+1/2, -y+1/2, z+1/2	10.31	-4.9	-1.3	-23.6	17.0	-16.1
	1	-x, -y, -z	6.15	-7.0	-3.8	-108.3	55.6	-70.2
	2	x+1/2, -y+1/2, z+1/2	13.90	-1.7	-0.2	-11.0	8.5	-6.3
	2	-x+1/2, y+1/2, -z+1/2	10.65	-1.3	-0.4	-17.0	6.3	-12.6
	2	x, y, z	8.62	-11.2	-2.5	-41.4	29.2	-31.7
	2	-x+1/2, y+1/2, -z+1/2	9.31	-10.7	-2.9	-43.2	22.5	-37.2
	1	-x, -y, -z	12.07	-6.6	-1.2	-25.0	13.3	-21.4
	1	-x, -y, -z	9.26	-18.2	-4.0	-60.8	46.7	-46.3
	2	x+1/2, -y+1/2, z+1/2	10.98	0.1	-0.3	-9.1	3.2	-6.0

Table S11. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase structure of **1** optimized at the B3LYP/6-311++G(2d,2p) level of theory.

Atom	X	Y	Z
F	-0.085598	1.999435	0.000000
O	-0.663837	0.079960	1.201938
O	-0.663837	0.079960	-1.201938
N	1.450395	0.160042	0.000000
N	1.358198	0.028279	2.361010
N	1.358198	0.028279	-2.361010
C	0.056247	0.016951	2.310962
C	3.455387	-0.219495	1.208351
H	3.952024	-0.325880	2.159131
C	0.056247	0.016951	-2.310962
C	-0.724383	-0.106567	3.556850
C	4.131669	-0.314506	0.000000
H	5.199511	-0.486040	0.000000
C	3.455387	-0.219495	-1.208351
H	3.952024	-0.325880	-2.159131
C	-0.724383	-0.106567	-3.556850
C	-2.121162	-0.037059	-3.523959
H	-2.620524	0.110788	-2.578906
C	2.078379	0.003480	-1.198515
C	-0.073069	-0.290311	-4.782065
H	1.004841	-0.341164	-4.796920
C	2.078379	0.003480	1.198515
C	-0.073069	-0.290311	4.782065
H	1.004841	-0.341164	4.796920
C	-2.853099	-0.152016	4.698424
H	-3.932352	-0.096155	4.666079
C	-2.121162	-0.037059	3.523959
H	-2.620524	0.110788	2.578906
C	-2.853099	-0.152016	-4.698424
H	-3.932352	-0.096155	-4.666079
C	-0.808705	-0.402412	5.952213
H	-0.299662	-0.543673	6.895631
C	-0.808705	-0.402412	-5.952213
H	-0.299662	-0.543673	-6.895631
C	-2.199917	-0.334435	-5.913489
H	-2.771511	-0.422479	-6.827454
C	-2.199917	-0.334435	5.913489
H	-2.771511	-0.422479	6.827454
B	-0.029414	0.616417	0.000000

Table S12. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase structure of **2** optimized at the B3LYP/6-311++G(2d,2p) level of theory.

Atom	X	Y	Z
C	-1.163093	2.745926	0.248064
C	-1.087586	4.138644	0.112061
H	-2.008518	4.693073	0.029618
C	0.152297	4.750045	0.070686
H	0.213415	5.824617	-0.035266
C	1.325059	4.000909	0.136330
H	2.303655	4.447009	0.065580
C	1.229723	2.623259	0.275728
C	-2.389646	0.792315	0.135567
C	2.216119	0.549383	0.166639
C	-3.658566	0.098602	-0.038793
C	3.431361	-0.289015	-0.009348
C	-3.721083	-1.301643	-0.059143
H	-2.811492	-1.870469	0.060583
C	3.631699	-1.442590	0.751406
C	-4.920327	-1.964541	-0.219360
H	-4.919162	-3.042505	-0.220475
C	4.766160	-2.226547	0.603456
C	-6.132382	-1.251082	-0.371445
C	5.729236	-1.872100	-0.329884
C	-6.063174	0.163128	-0.341668
H	-6.959247	0.753737	-0.444144
C	5.553401	-0.735998	-1.106225
C	-4.857674	0.811501	-0.182440
H	-4.825642	1.890440	-0.163697
C	4.418021	0.042772	-0.939644
C	-8.570050	-1.150081	-0.597276
H	-8.568587	-0.438433	-1.425397
H	-8.757586	-0.596789	0.328050
H	-9.394965	-1.838351	-0.752691
C	-7.384318	-3.354065	-0.488005
H	-8.403923	-3.676489	-0.674935
H	-7.077373	-3.742691	0.487912
H	-6.746341	-3.805509	-1.250311
N	0.000588	2.047033	0.379142
N	-2.358887	2.100336	0.221289
N	2.356333	1.830218	0.264768
O	-1.314352	0.012900	0.164617
O	1.086162	-0.128408	0.176474
N	-7.327332	-1.902378	-0.542347
F	-0.094799	0.407570	2.123030
F	2.749788	-1.803647	1.682845
F	4.943051	-3.311572	1.360187
F	6.819056	-2.621259	-0.481709
F	6.471615	-0.406899	-2.017934
F	4.280379	1.103220	-1.736600
B	-0.093298	0.544065	0.747574

Table S13. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase structure of **3** optimized at the B3LYP/6-311++G(2d,2p) level of theory.

Atom	X	Y	Z
O	-1.201605	-0.668907	-0.334467
N	0.000004	1.437089	-0.524062
N	-2.357577	1.315275	-0.730393
C	-0.000006	0.128042	1.787408
C	-1.193904	2.033443	-0.795260
C	-3.524312	-0.788068	-0.734121
C	-2.295491	0.019991	-0.589300
C	1.199894	0.296970	3.908458
H	2.141101	0.332798	4.441190
C	-1.205879	3.369194	-1.197967
H	-2.157850	3.838957	-1.385602
C	-3.489757	-2.170289	-0.521193
H	-2.557258	-2.638465	-0.245925
C	-4.645637	-2.927204	-0.661857
H	-4.611611	-3.995103	-0.496085
C	0.000006	4.032709	-1.373016
H	0.000007	5.068821	-1.683086
C	-0.000016	0.357038	4.608699
H	-0.000020	0.442026	5.687168
C	1.193759	0.182464	2.521733
H	2.146196	0.126367	2.012255
C	-4.732869	-0.176562	-1.086969
H	-4.748547	0.890303	-1.249115
C	-5.844359	-2.313294	-1.012201
H	-6.743870	-2.904106	-1.120156
C	-5.885070	-0.936563	-1.222887
H	-6.815727	-0.457913	-1.494874
B	0.000001	0.029518	0.175564
O	1.201610	-0.668910	-0.334457
N	2.357583	1.315266	-0.730412
C	1.193913	2.033438	-0.795270
C	3.524315	-0.788079	-0.734119
C	2.295495	0.019983	-0.589311
C	-1.199921	0.296839	3.908459
H	-2.141130	0.332564	4.441193
C	1.205890	3.369189	-1.197978
H	2.157861	3.838948	-1.385621
C	3.489762	-2.170296	-0.521163
H	2.557263	-2.638466	-0.245884
C	4.645642	-2.927213	-0.661816
H	4.611616	-3.995108	-0.496023
C	-1.193775	0.182334	2.521734
H	-2.146206	0.126130	2.012257
C	4.732871	-0.176580	-1.086982
H	4.748548	0.890282	-1.249149
C	5.844362	-2.313309	-1.012176
H	6.743873	-2.904123	-1.120122
C	5.885071	-0.936582	-1.222889
H	6.815727	-0.457937	-1.494888

Table S14. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase structure of **4** optimized at the B3LYP/6-311++G(2d,2p) level of theory.

Atom	X	Y	Z
O	-1.155919	-1.092148	-0.708153
O	1.239407	-1.050911	-0.691386
N	0.032120	-1.292679	1.405272
N	-2.321824	-1.514880	1.262561
N	2.397488	-1.368779	1.303223
C	-1.160387	-1.611667	1.979326
C	2.343022	-1.214205	0.007979
C	1.232068	-1.535652	2.001364
C	-2.256046	-1.336640	-0.029688
C	-3.488613	-1.437049	-0.838824
C	3.592156	-1.252982	-0.780632
C	-3.451153	-1.193845	-2.215703
H	-2.513237	-0.928513	-2.678563
C	0.004401	1.027908	0.144342
C	1.246174	-2.003746	3.316003
H	2.199138	-2.174798	3.789915
C	3.558125	-1.070024	-2.166907
H	2.610286	-0.896962	-2.652702
C	0.040028	-2.254316	3.955377
H	0.042325	-2.615374	4.974994
C	-1.167657	-2.080078	3.294589
H	-2.116178	-2.310697	3.751938
C	-4.610252	-1.292320	-2.974379
H	-4.573483	-1.103095	-4.038353
C	4.820261	-1.474885	-0.147459
H	4.835694	-1.615658	0.922389
C	4.732872	-1.111689	-2.906473
H	4.698333	-0.971268	-3.978059
C	-0.194216	1.727021	1.337614
H	-0.328444	1.184725	2.265844
C	5.991642	-1.509525	-0.889414
H	6.937358	-1.678518	-0.393061
C	-4.704010	-1.777741	-0.234474
H	-4.722146	-1.964019	0.828374
C	-5.816002	-1.630117	-2.367227
H	-6.718197	-1.705076	-2.959138
C	5.951218	-1.329780	-2.270482
H	6.865705	-1.359466	-2.847332
N	-0.049241	5.287131	0.293649
C	-0.059196	3.895471	0.241699
C	-0.233030	3.115057	1.398717
H	-0.396412	3.584390	2.356055
C	0.160226	1.817387	-1.003584
H	0.311719	1.336897	-1.962910
C	-5.859766	-1.871055	-0.995645
H	-6.795725	-2.133282	-0.521787
C	-0.525602	5.945211	1.497342
H	-0.418603	7.020319	1.378220
H	0.069199	5.651999	2.362218
H	-1.578447	5.724927	1.717930
C	0.126301	3.202500	-0.971748
H	0.248144	3.743957	-1.896729
C	-0.161607	6.036523	-0.945411
H	0.660981	5.799491	-1.619801
H	-0.102833	7.098666	-0.721974
H	-1.103328	5.847257	-1.477449
B	0.028938	-0.569110	0.025107

Table S15. Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase structure of **5** optimized at the B3LYP/6-311++G(2d,2p) level of theory.

Atom	X	Y	Z
C	0.193083	2.474425	-0.002382
C	0.452024	3.826109	-0.251733
H	-0.385311	4.497479	-0.352829
C	1.764822	4.250976	-0.377826
H	1.969801	5.295370	-0.570831
C	2.822248	3.353071	-0.286614
H	3.849288	3.652887	-0.417499
C	2.547345	2.010783	-0.035867
C	-1.293817	0.708285	0.070233
C	3.244772	-0.189605	-0.001235
C	-2.655473	0.189272	-0.010091
C	4.314633	-1.200400	-0.123268
C	-2.911780	-1.186155	0.061095
H	-2.084567	-1.869338	0.180557
C	4.007686	-2.563703	-0.063820
C	-4.198041	-1.682383	-0.009083
H	-4.345111	-2.748141	0.058385
C	5.016054	-3.511963	-0.177826
C	-5.305676	-0.816315	-0.157767
C	6.337346	-3.110001	-0.347416
C	-5.040553	0.572878	-0.217678
H	-5.850375	1.277483	-0.318084
C	6.649049	-1.753146	-0.404697
C	-3.750142	1.053574	-0.149454
H	-3.568498	2.116643	-0.198826
C	5.645270	-0.802415	-0.295435
C	-7.716020	-0.387119	-0.260748
H	-7.664871	0.290681	-1.114920
H	-7.772782	0.216537	0.650817
H	-8.635183	-0.958534	-0.346681
C	-6.841931	-2.723419	-0.071257
H	-7.900770	-2.914531	-0.216985
H	-6.564644	-3.076911	0.927376
H	-6.293173	-3.315200	-0.805996
N	1.252379	1.629201	0.149319
N	-1.082211	2.000546	0.057564
N	3.548454	1.076508	-0.012219
O	-0.337482	-0.211199	0.121564
O	2.018511	-0.680113	0.084107
N	-6.587508	-1.303026	-0.244166
F	0.991071	0.145637	2.013942
B	0.970649	0.184939	0.628401
H	5.871722	0.251888	-0.339181
H	7.675319	-1.438491	-0.535346
H	7.121758	-3.849766	-0.433463
H	4.771388	-4.564144	-0.130362
H	2.981700	-2.867923	0.074722