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Theoretical Study on the Factors Controlling the Stability of the Borate Complexes of Ribose, Arabinose, Lyxose and Xylose

Judit E. Šponer,^{*,[a]} Bobby G. Sumpter,^[b] Jerzy Leszczynski,^[c] Jirí Šponer^[a]
and Miguel Fuentes-Cabrera^{*,[b]}

^[a] *Institute of Biophysics,
Academy of Sciences of the Czech Republic,
Královopolská 135,
CZ-61265 Brno,
Czech Republic*

^[b] *Center for Nanophase Materials Sciences,
and Computer Sciences and Mathematics Division,
Oak Ridge National Laboratory,
Oak Ridge, P. O. Box 2008,
Oak Ridge, TN 37831-6494
USA*

^[c] *Department of Chemistry,
Computational Center for Molecular Structure and Interactions,
Jackson State University,
Jackson, Mississippi 39217
USA*

** Corresponding authors.*

Cartesian coordinates of all optimized structures discussed in the paper.

Model 1, optimized at B3LYP/6-31G** level

C	-2.209215	-0.676101	-0.369227
C	-2.209211	0.676182	0.368772
H	-2.465692	1.491456	-0.341037
H	-2.953199	-0.714434	-1.185496
O	-0.909147	0.799228	0.861557
O	-0.908833	-0.799634	-0.861118
C	2.209125	0.676033	-0.369308
C	2.209229	-0.676065	0.368919
O	0.908991	0.799139	-0.861636
H	2.465316	-1.491458	-0.340851
O	0.909112	-0.798770	0.861962
H	2.953442	0.714525	-1.185288
B	-0.000013	-0.000027	0.000308
H	-2.466452	-1.491239	0.340435
H	-2.953728	0.714742	1.184569
H	2.466020	1.491284	0.340483
H	2.953804	-0.714734	1.184586

Model 2, optimized at B3LYP/6-31G** level

C	2.117957	-0.022943	0.861281
C	2.228144	-1.319771	0.021510
H	3.102336	-1.286352	-0.648476
O	2.845353	1.085486	0.295807
O	1.033543	-1.410188	-0.696821
O	0.765675	0.204109	0.976616
C	-2.117837	-0.022961	-0.861347
C	-2.228032	-1.319863	-0.021721
O	-0.765549	0.204117	-0.976549
H	-3.102481	-1.286805	0.647930
O	-1.033676	-1.409977	0.697081
O	-2.845397	1.085397	-0.295869
B	0.000017	-0.622683	0.000130
H	2.595093	-0.121751	1.848855
H	2.372406	-2.182361	0.702935
H	-2.594860	-0.121709	-1.848981
H	-2.371726	-2.182421	-0.703308
C	2.353395	1.530578	-0.958050
C	-2.353602	1.530534	0.958042
H	2.888593	2.458406	-1.193219
H	1.276285	1.722419	-0.928184
H	2.541061	0.804132	-1.763523
H	-2.888604	2.458546	1.192962
H	-1.276418	1.722071	0.928381
H	-2.541507	0.804248	1.763565

Model 3a, optimized at B3LYP/6-31G** level

C	-2.154092	-0.558778	-0.751820
C	-2.268949	0.549001	0.356105
C	-2.808845	1.775021	-0.415669
O	-2.636809	0.046892	-1.971455
O	-0.978043	0.739245	0.849299
O	-0.832697	-0.921161	-0.784863

C	2.152018	0.551259	-0.761794
C	2.269757	-0.548405	0.353886
O	0.830623	0.913765	-0.793698
C	2.807186	-1.780171	-0.410431
O	0.980216	-0.734662	0.852153
O	2.631113	-0.063463	-1.978333
B	0.000035	-0.000650	0.045975
H	-2.802696	-1.436600	-0.610983
H	-2.955655	0.259306	1.168753
H	2.801225	1.429926	-0.629252
H	2.958851	-0.252971	1.162434
H	-3.903399	1.828585	-0.340272
C	-2.406071	1.451952	-1.858512
H	-2.377246	2.701336	-0.026505
H	-3.017919	1.954364	-2.617408
H	-1.347997	1.691023	-2.032317
H	2.376504	-2.703516	-0.013278
H	3.901943	-1.833426	-0.337730
C	2.400405	-1.467589	-1.854466
H	3.010035	-1.975684	-2.611361
H	1.341807	-1.707700	-2.023558

Model 3b, optimized at B3LYP/6-31G** level

C	-2.163067	-0.663155	-0.545912
C	-2.258923	0.585729	0.381311
C	-2.608518	1.720206	-0.611629
O	-2.806824	-0.314024	-1.797353
O	-1.013853	0.710764	0.990556
O	-0.826240	-0.922982	-0.679098
C	2.131486	0.680940	-0.536937
C	2.222677	-0.568181	0.390533
O	0.795417	0.942257	-0.674848
C	2.575176	-1.702773	-0.601257
O	0.975176	-0.692097	0.994995
O	2.779214	0.331158	-1.786161
B	-0.017426	0.009541	0.168795
H	-2.704544	-1.550636	-0.172156
H	-3.053619	0.478200	1.137656
H	2.672557	1.567823	-0.161189
H	3.014570	-0.461510	1.149936
H	-3.175680	2.541272	-0.158768
C	-3.382616	0.983200	-1.702002
H	-1.666281	2.113801	-1.003552
H	-4.457097	0.913950	-1.442433
H	-3.318065	1.465703	-2.686080
H	1.634141	-2.095097	-0.997338
H	3.139502	-2.524622	-0.146283
C	3.354499	-0.966071	-1.688058
H	3.294569	-1.448538	-2.672440
H	4.427768	-0.896960	-1.423388

Model 4a, optimized at B3LYP/6-31G** level

O	3.508495	-1.080078	-1.410769
O	-3.492412	1.121867	-1.406152

C	-2.074624	-0.637357	-0.671410
C	-2.311144	0.340198	0.530501
C	-3.031585	1.549091	-0.118177
C	-2.492365	0.219923	-1.889664
O	-1.046348	0.637172	1.034599
O	-0.732133	-0.987963	-0.629064
C	2.083914	0.656737	-0.637187
C	2.311913	-0.354304	0.538308
O	0.741045	1.005854	-0.594857
C	3.039198	-1.543539	-0.138456
O	1.043375	-0.666877	1.023267
C	2.510928	-0.165843	-1.875955
B	0.001445	-0.003158	0.221775
H	-2.717916	-1.530353	-0.608284
H	-2.945750	-0.110526	1.312345
H	2.726474	1.547644	-0.544197
H	2.939468	0.074710	1.337869
H	-3.907745	1.906021	0.436187
H	-2.302476	2.368807	-0.207106
H	-1.603855	0.758991	-2.252745
H	-2.934445	-0.347559	-2.716291
H	3.912036	-1.914224	0.412120
H	2.312303	-2.361712	-0.255288
H	1.625515	-0.695280	-2.260163
H	2.958189	0.424858	-2.683305

Model 4b, optimized at B3LYP/6-31G** level

O	2.998476	-1.411770	-1.041421
O	-2.989266	1.441356	-1.027919
C	-2.228176	-0.629296	-0.112903
C	-2.252147	0.461834	1.019604
C	-3.068521	1.605504	0.386708
C	-3.023794	0.033024	-1.255505
O	-0.926719	0.795680	1.256762
O	-0.890732	-0.836336	-0.418905
C	2.229375	0.631924	-0.074151
C	2.242779	-0.491254	1.026729
O	0.894832	0.847938	-0.386611
C	3.064291	-1.616916	0.368551
O	0.915169	-0.830767	1.242602
C	3.035551	0.002536	-1.227855
B	-0.001844	-0.005747	0.418220
H	-2.720627	-1.570293	0.192710
H	-2.750668	0.107533	1.940599
H	2.718868	1.563667	0.262947
H	2.733322	-0.163877	1.961865
H	-4.126774	1.554118	0.714254
H	-2.659279	2.585757	0.644800
H	-4.073851	-0.322933	-1.254493
H	-2.574780	-0.171122	-2.230825
H	4.119443	-1.576102	0.707302
H	2.651885	-2.603798	0.594313
H	2.595819	0.235066	-2.201053
H	4.085645	0.357770	-1.206640

Model 5, optimized at B3LYP/6-31G** level

C	-2.219097	-0.555397	-0.578820
C	-2.299408	0.539742	-1.684321
C	-2.744441	1.825156	-0.917636
O	-2.779052	0.041986	0.606893
O	-1.000852	0.708522	-2.179112
O	-0.888671	-0.885043	-0.471365
C	2.131587	0.565006	-0.593067
C	2.235845	-0.565228	-1.677195
O	0.804546	0.918941	-0.545680
C	2.837308	-1.755570	-0.900144
O	0.929610	-0.807964	-2.108288
O	2.634486	-0.008373	0.630472
B	-0.030256	-0.028024	-1.329513
H	-2.837013	-1.448616	-0.751634
H	-2.994827	0.288825	-2.498356
H	2.766283	1.446097	-0.765161
H	2.877652	-0.275786	-2.525298
H	-3.820043	2.000609	-1.057449
C	-2.470534	1.434236	0.547471
O	-2.043244	2.964786	-1.362181
H	-3.108175	1.953595	1.271224
H	-1.416082	1.628222	0.787482
H	2.436070	-2.704807	-1.265659
H	3.931336	-1.766743	-0.995273
C	2.448525	-1.422259	0.544002
H	3.088729	-1.891265	1.300273
H	1.402300	-1.694290	0.741425
H	-1.219183	2.572342	-1.719492

Model 6, optimized at B3LYP/6-31G** level

O	3.966285	0.865328	0.109293
O	-3.504832	0.997383	0.107207
C	-1.663108	0.522938	-1.296985
C	-2.153455	-0.811863	-0.658958
C	-3.227277	-0.376338	0.395237
C	-2.284580	1.582248	-0.358115
O	-1.023894	-1.361561	-0.043026
O	-0.271892	0.474369	-1.295224
C	1.988633	0.029842	1.119477
C	2.464393	-1.001336	0.042168
O	0.605791	0.109674	0.998742
C	3.598643	-0.255396	-0.703759
O	1.347373	-1.266207	-0.751395
C	2.752464	1.312554	0.718356
B	0.180927	-0.509487	-0.287246
H	-2.047608	0.657286	-2.319862
H	-2.588114	-1.510008	-1.390228
H	2.277879	-0.273824	2.137907
H	2.848070	-1.929238	0.497883
H	-4.194405	-0.885676	0.289570
O	-2.741651	-0.573730	1.685632
H	-1.588239	1.778770	0.468031

H	-2.537517	2.527424	-0.850261
H	4.504906	-0.851047	-0.862954
H	3.205484	0.070613	-1.678887
H	2.128518	1.878573	0.009139
H	3.024756	1.962987	1.556536
H	-1.810094	-0.856377	1.544991

Model T1, optimized at B3LYP/6-31G** level with COSMO

C	-2.195894	-0.443791	-0.882914
C	-2.266317	0.582231	0.288029
C	-2.943118	1.815289	-0.331553
O	-2.621609	0.264505	-2.066812
O	-0.932566	0.832362	0.652822
O	-0.880820	-0.870262	-0.943820
C	2.210330	0.454604	-0.872376
C	2.268677	-0.548402	0.322301
O	0.890925	0.864414	-0.971612
C	2.924612	-1.800738	-0.281659
O	0.926782	-0.762761	0.697419
O	2.674483	-0.268187	-2.030378
B	0.003394	0.012227	-0.138725
H	-2.874457	-1.303333	-0.798546
H	-2.859490	0.218856	1.141042
H	2.876266	1.324676	-0.789651
H	2.848269	-0.155327	1.171509
O	-4.347784	1.670593	-0.129334
C	-2.549411	1.671328	-1.802756
H	-2.561996	2.745708	0.114885
H	-3.234232	2.185505	-2.486171
H	-1.530468	2.052459	-1.964897
H	2.556069	-2.717174	0.187987
H	4.013260	-1.755626	-0.159440
C	2.561322	-1.674777	-1.761439
H	3.241905	-2.201193	-2.437711
H	1.535869	-2.023609	-1.949088
H	-4.797001	2.402622	-0.601611

Model T2, optimized at B3LYP/6-31G** level with COSMO

C	1.634321	0.230392	1.206268
C	2.031217	-0.946028	0.260080
C	3.047546	-0.309670	-0.714834
O	2.319412	1.397690	0.692874
O	0.843241	-1.334903	-0.381898
O	0.257923	0.332603	1.142938
C	-2.218609	0.182950	-1.151359
C	-2.616340	-0.982989	-0.194624
O	-0.840253	0.293824	-1.078450
C	-3.694945	-0.364784	0.707373
O	-1.439321	-1.305541	0.512217
O	-2.912376	1.353743	-0.673649
B	-0.298679	-0.506812	0.048758
H	1.971045	0.139576	2.247723
H	2.499706	-1.789124	0.790170
H	-2.538561	0.063515	-2.195787

H	-2.993542	-1.861238	-0.740604
O	4.394658	-0.469196	-0.271435
C	2.610806	1.153883	-0.695034
H	2.985439	-0.769195	-1.707011
H	3.402902	1.841528	-1.005051
H	1.720360	1.312451	-1.318318
H	-3.689763	-0.805636	1.708347
H	-4.687673	-0.507903	0.264523
C	-3.322363	1.117511	0.682449
H	-4.153577	1.793970	0.904296
H	-2.498664	1.330179	1.379015
H	4.498734	0.031396	0.565366

Model T3, optimized at B3LYP/6-31G** level with COSMO

C	-2.192248	-0.397516	-0.885397
C	-2.220606	0.620694	0.288681
C	-2.946755	1.832048	-0.315359
O	-2.597321	0.338122	-2.070712
O	-0.871448	0.880565	0.586363
O	-0.896891	-0.869779	-0.958155
C	2.239827	0.396219	-0.944803
C	2.287491	-0.554216	0.290021
O	0.925944	0.816432	-1.062523
C	2.971789	-1.819317	-0.248826
O	0.941135	-0.772645	0.646471
O	2.694784	-0.380732	-2.072020
B	0.027763	0.013164	-0.194583
H	-2.901970	-1.232085	-0.807321
H	-2.749262	0.234118	1.174220
H	2.914790	1.262165	-0.898190
H	2.844442	-0.117182	1.133131
H	-4.030118	1.633717	-0.261151
C	-2.520178	1.738930	-1.785338
O	-2.614345	3.041905	0.338657
H	-3.185279	2.267664	-2.476269
H	-1.496829	2.123498	-1.903387
H	2.627864	-2.720622	0.266637
H	4.059079	-1.739663	-0.132166
C	2.604823	-1.773683	-1.732187
H	3.293276	-2.322352	-2.382309
H	1.584917	-2.148630	-1.900444
H	-3.242170	3.724280	0.021960

Model T4, optimized at B3LYP/6-31G** level with COSMO

C	-2.234653	-0.507431	-0.794878
C	-2.301370	0.529741	0.359456
C	-2.851871	1.815774	-0.311159
O	-2.748508	0.160113	-1.964748
O	-0.972931	0.738681	0.780095
O	-0.903468	-0.872075	-0.912596
C	2.164090	0.505331	-0.796711
C	2.250621	-0.561773	0.339624
O	0.834263	0.894684	-0.861872
C	2.911860	-1.771284	-0.342264

O	0.916068	-0.813335	0.722381
O	2.631392	-0.139543	-1.995201
B	-0.023047	-0.019658	-0.073303
H	-2.871211	-1.394066	-0.672022
H	-2.926660	0.204616	1.202631
H	2.810767	1.384131	-0.668293
H	2.837371	-0.209973	1.201263
H	-3.939228	1.880026	-0.175806
C	-2.535824	1.565210	-1.795688
O	-2.275814	2.992264	0.221759
H	-3.199984	2.094249	-2.485637
H	-1.494780	1.846451	-2.012131
H	2.552369	-2.716152	0.074850
H	4.000763	-1.725606	-0.222891
C	2.539886	-1.561630	-1.810019
H	3.225962	-2.035272	-2.518824
H	1.519263	-1.913963	-2.016198
H	-1.382224	2.715292	0.512683

Model T5, optimized at B3LYP/6-31G** level with COSMO

C	2.213732	0.790070	-0.947734
C	2.797403	-0.635564	-0.706510
C	3.866381	-0.416171	0.376141
O	2.809094	1.645839	0.049508
O	1.714898	-1.408940	-0.245962
O	0.838595	0.675653	-0.822048
C	-1.388092	-0.981915	1.201767
C	-1.664007	-1.688766	-0.150864
O	-0.090522	-0.511797	1.143387
C	-3.040700	-1.167151	-0.581024
O	-0.623058	-1.267952	-1.002338
O	-2.375724	0.069587	1.323753
B	0.461236	-0.631028	-0.234810
H	2.471181	1.247271	-1.913262
H	3.228629	-1.067681	-1.623380
H	-1.524651	-1.614369	2.091404
H	-1.668610	-2.785832	-0.043443
H	4.836028	-0.192622	-0.084817
C	3.335580	0.821165	1.100974
H	3.975331	-1.293366	1.020140
H	4.102127	1.398397	1.627392
H	2.544392	0.550640	1.814710
H	-3.123971	-1.107858	-1.670545
H	-3.826333	-1.837563	-0.214708
C	-3.152634	0.197898	0.113889
H	-4.181334	0.421284	0.429407
C	-2.655234	1.376745	-0.721999
H	-3.286957	1.475645	-1.613746
H	-1.623802	1.194824	-1.049979
O	-2.763331	2.606256	-0.006170
H	-2.182398	2.519338	0.775996

Model T6, optimized at B3LYP/6-31G** level with COSMO

C	2.22848	0.82749	-0.94565
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C	2.83754	-0.58838	-0.6998
C	3.85655	-0.35505	0.42897
O	2.79769	1.69497	0.05204
O	1.75637	-1.40283	-0.30959
O	0.85408	0.68609	-0.82403
C	-1.33535	-1.05424	1.18198
C	-1.61995	-1.71899	-0.19095
O	-0.04698	-0.55159	1.11715
C	-3.00015	-1.18536	-0.58939
O	-0.58493	-1.27224	-1.03994
O	-2.3374	-0.03206	1.3637
B	0.49413	-0.63825	-0.26572
H	2.48151	1.28877	-1.91027
H	3.32104	-0.99813	-1.59962
H	-1.43757	-1.72329	2.04926
H	-1.61986	-2.81855	-0.12202
H	4.84257	-0.12509	0.00839
C	3.29065	0.87981	1.12926
H	3.94745	-1.22995	1.07898
H	4.03246	1.46704	1.67898
H	2.47452	0.60903	1.81431
H	-3.09352	-1.08444	-1.67465
H	-3.78027	-1.87389	-0.24531
C	-3.11958	0.15066	0.16716
H	-4.14854	0.34369	0.50114
C	-2.6739	1.36931	-0.63943
H	-3.21222	1.36112	-1.59727
H	-1.60117	1.30072	-0.85636
O	-2.93581	2.57333	0.09245
H	-3.48689	3.1575	-0.46416

Ribose-borate 2:1 complex, optimized at B3LYP/6-31G** level with COSMO

C	1.565204	-0.379682	-1.624351
C	2.202443	-1.518110	-0.782353
C	3.374913	-0.831314	-0.042952
O	2.328176	0.808939	-1.341520
O	1.217208	-1.920739	0.143153
O	0.243237	-0.291620	-1.214330
C	-1.569628	-0.372634	1.625451
C	-2.206141	-1.514216	0.787105
O	-0.246930	-0.286815	1.217155
C	-3.375529	-0.829401	0.040880
O	-1.218855	-1.922837	-0.133501
O	-2.331981	0.815015	1.337008
B	-0.001243	-1.098385	0.003133
H	1.623312	-0.506887	-2.713218
H	2.537213	-2.372863	-1.386058
H	-1.629281	-0.495475	2.714729
H	-2.544005	-2.365470	1.394010
C	2.954602	0.650965	-0.060164
C	4.107301	1.620049	0.081251
H	2.230860	0.834180	0.749875
O	-3.596285	-1.360537	-1.250307
H	-4.306561	-0.943186	0.614072

C	-2.955127	0.652964	0.054536
C	-4.107844	1.621132	-0.092707
H	-2.229373	0.833830	-0.754160
H	-4.681884	1.324193	-0.984933
O	-3.601206	2.945829	-0.216417
H	-4.769534	1.521693	0.782844
H	-4.363009	3.548111	-0.344408
O	3.599754	2.944464	0.203906
H	4.766177	1.519275	-0.796214
H	4.684497	1.325447	0.972273
H	4.361974	3.549054	0.317750
H	-2.709874	-1.630532	-1.567044
H	4.303692	-0.947289	-0.619336
O	3.600541	-1.358047	1.249211
H	2.715187	-1.625697	1.570827

Xylose-borate 2:1 complex, optimized at B3LYP/6-31G** level with COSMO

C	1.742086	-0.270811	-1.391071
C	2.260119	-1.480918	-0.559626
C	3.456883	-0.909469	0.223767
O	2.457720	0.884206	-0.911911
O	1.193190	-1.845736	0.281483
O	0.377362	-0.203573	-1.161678
C	-1.761229	-0.294672	1.403172
C	-2.274793	-1.487945	0.545810
O	-0.391520	-0.240633	1.204216
C	-3.456749	-0.898534	-0.245224
O	-1.198748	-1.844437	-0.286601
O	-2.454915	0.874188	0.922225
B	-0.003866	-1.032881	0.009493
H	1.946143	-0.317950	-2.469169
H	2.582430	-2.326971	-1.188249
H	-1.987340	-0.352054	2.476247
H	-2.609380	-2.342083	1.157246
O	4.663480	-0.990120	-0.531397
C	3.063530	0.564186	0.353846
H	3.558910	-1.397193	1.204497
C	4.201205	1.524453	0.637344
H	2.317757	0.657108	1.158593
H	-3.549841	-1.373012	-1.233482
O	-4.673607	-0.979188	0.493127
C	-3.050477	0.573584	-0.353082
C	-4.180478	1.542801	-0.636758
H	-2.295956	0.670871	-1.148696
H	-4.750655	1.169703	-1.502796
O	-3.621100	2.827292	-0.899195
H	-4.858409	1.562885	0.226323
H	-4.362085	3.452929	-1.036525
H	-4.883287	-1.929860	0.610099
O	3.648304	2.809393	0.912060
H	4.873756	1.547515	-0.229726
H	4.774643	1.142417	1.497282
H	4.391801	3.433682	1.038030
H	4.868929	-1.940766	-0.654834

Lyxose-borate 2:1 complex, optimized at B3LYP/6-31G** level with COSMO

C	1.735238	-0.435542	-1.600570
C	2.238093	-1.524297	-0.622187
C	3.408938	-0.851502	0.160534
O	2.650620	0.661715	-1.504896
O	1.164500	-1.815652	0.239032
O	0.440617	-0.121801	-1.196886
C	-1.653519	-0.407306	1.578857
C	-2.215358	-1.479806	0.612798
O	-0.365693	-0.124850	1.139342
C	-3.457848	-0.816075	-0.043801
O	-1.213750	-1.711507	-0.349123
O	-2.543828	0.718972	1.511722
B	0.005036	-0.926624	-0.043167
H	1.746612	-0.720318	-2.661754
H	2.577721	-2.433972	-1.135005
H	-1.643477	-0.695955	2.638898
H	-2.485334	-2.413634	1.125030
H	4.366695	-1.254756	-0.192485
C	3.324050	0.645835	-0.228972
O	3.312117	-1.102691	1.550949
H	4.318281	1.073782	-0.414147
C	2.609140	1.541749	0.781020
O	-3.550039	-1.113306	-1.425504
H	-4.370007	-1.186721	0.440554
C	-3.301070	0.689104	0.284500
H	-4.266954	1.156722	0.517968
C	-2.625988	1.529141	-0.798234
H	-3.258351	1.537568	-1.691686
H	-1.651498	1.107947	-1.072576
O	-2.493145	2.884734	-0.370502
H	-2.016647	2.857333	0.483714
O	2.559519	2.890737	0.314648
H	3.178385	1.551790	1.716076
H	1.603226	1.162600	0.997188
H	2.076983	2.872038	-0.535615
H	2.372002	-1.347865	1.683253
H	-2.630208	-1.312054	-1.697500

Arabinose-borate 2:1 complex, optimized at B3LYP/6-31G** level with COSMO

C	-1.985824	-0.285168	1.420495
C	-2.394062	-1.401889	0.412022
C	-3.464574	-0.733209	-0.489464
O	-2.787124	0.861171	1.107078
O	-1.214204	-1.755710	-0.262672
O	-0.623787	-0.064722	1.230162
C	1.742270	-0.393812	-1.337040
C	2.187199	-1.473680	-0.306813
O	0.402439	-0.135830	-1.076864
C	3.456746	-0.887864	0.356184
O	1.105522	-1.623251	0.580376
O	2.615025	0.741757	-1.138608
B	-0.082220	-0.896487	0.125163

H	-2.196403	-0.498418	2.477283
H	-2.845974	-2.278052	0.897636
H	1.879623	-0.666077	-2.392157
H	2.441897	-2.434535	-0.777544
O	-4.775655	-1.075227	-0.013271
C	-3.227974	0.768379	-0.267262
H	-3.343880	-1.039595	-1.535597
H	-4.176863	1.314820	-0.324040
C	-2.203374	1.431586	-1.195279
H	3.481060	-1.136207	1.424591
O	4.623691	-1.383764	-0.310822
C	3.342051	0.624876	0.105295
H	4.339319	1.049553	-0.063216
C	2.635145	1.456912	1.177955
H	3.273295	1.538376	2.066059
H	1.689429	0.988793	1.473261
O	2.423866	2.784782	0.706577
H	2.018690	2.682575	-0.174788
O	-1.905752	2.755975	-0.729480
H	-2.644698	1.546081	-2.197284
H	-1.280956	0.828728	-1.277390
H	-1.554839	2.643683	0.172074
H	5.117713	-1.943855	0.320158
H	-5.224098	-1.591660	-0.711232

Ribose-borate complex formed via O2,O3-binding, optimized at B3LYP/6-31G** level with COSMO

O	-3.738273	0.276142	0.228802
O	3.738864	0.270717	-0.227894
C	1.907851	-0.345995	1.117715
C	2.324087	-1.580404	0.276436
C	3.433441	-1.048491	-0.686427
C	2.548936	0.831871	0.349152
O	1.158684	-1.943993	-0.434232
O	0.506104	-0.332727	1.137413
C	-1.911474	-0.346183	-1.119175
C	-2.328035	-1.578645	-0.275051
O	-0.509389	-0.336371	-1.142542
C	-3.436483	-1.044096	0.687214
O	-1.163025	-1.940925	0.435874
C	-2.547305	0.833754	-0.349509
B	-0.001786	-1.120509	-0.001061
H	2.309077	-0.384659	2.141674
H	2.694911	-2.420415	0.878908
H	-2.315897	-0.384549	-2.141849
H	-2.699463	-2.419649	-0.875928
H	4.378249	-1.602243	-0.627802
O	2.979002	-1.059960	-2.010642
H	1.856788	1.160164	-0.441310
C	2.905572	2.013976	1.222599
H	-4.382644	-1.595559	0.628241
O	-2.982037	-1.056707	2.012825
H	-1.853276	1.159515	0.440219
C	-2.901106	2.016911	-1.222593

H	2.030364	-1.303764	-1.942850
H	-2.034173	-1.307068	1.947774
H	2.003738	2.290815	1.792361
O	3.358776	3.089919	0.409282
H	3.675797	1.700792	1.945784
H	3.566642	3.845510	0.997198
H	-2.000294	2.287644	-1.797013
O	-3.343902	3.096656	-0.409234
H	-3.676628	1.707262	-1.941532
H	-3.555604	3.850572	-0.997957