

Electronic Supplementary Information

A DFT Study on the Mechanism of the Sulfonic Acid + Alcohol Esterification Reaction

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1. Relative stability of **5** and related pseudorotamers

Structure **5** as well as all possible related pseudorotamers (depending on the position occupied by every substituent around the pentacoordinated sulfur) were optimized in both gas phase and methanol solution. Interestingly, no energy minima for structures bearing an apical oxo group could be located after several extensive searches. Codes for all optimized pseudorotamers are gathered in Table S1.

Table S1 Pseudorotamers of **5**

Pseudorotamer	O=	Ph-	HO-	HO-	MeO-
5	eq	eq	eq	ap	ap
5a	eq	eq	ap	ap	eq
5b	eq	ap	eq	eq	ap
5c	eq	ap	eq	eq	ap

eq: equatorial; ap: apical

Structures of all optimized pseudorotamers and the corresponding relative Gibbs free energies (kJ mol^{-1}) in gas phase and solution are shown in Figure S1. As can be observed, structure **5** (bearing phenyl, oxo, and one hydroxy groups in equatorial positions) is clearly favored over all related pseudorotamers in gas phase and solution (by at least 22.7 kJ mol^{-1} and 16.4 kJ mol^{-1} , respectively).

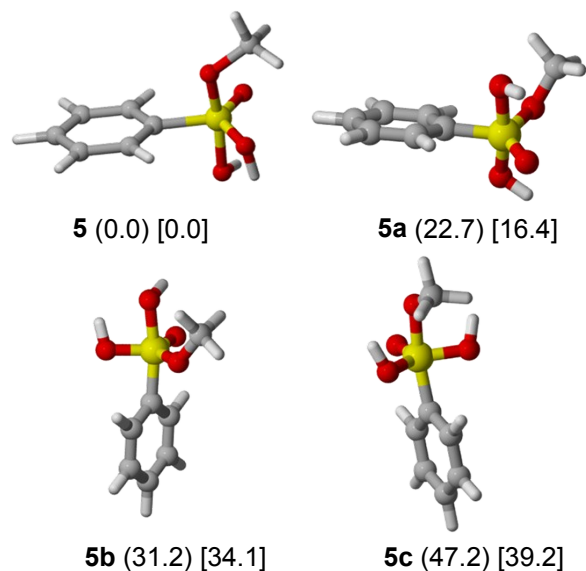


Figure S1 Structure of **5** and related pseudorotamers. Relative Gibbs free energies (kJ mol^{-1}) in gas phase (in parenthesis) and methanol solution (in square brackets) are also shown.

2. Methanol assistance on neutral and acid-catalyzed Ad-E pathways

The participation of one or several water molecules (i. e., water assistance) can lower the free energy barriers for some reactions (such as neutral and acid-promoted hydrolysis of formamide).^{S1} In order to assess the possible role of methanol assistance on the neutral and acid-catalyzed Ad-E mechanism

for the sulfonic acid + alcohol esterification has been studied here through discrete and continuum solvent models. Results on the one methanol molecule-assisted neutral Ad-E path are shown in Figure S2.

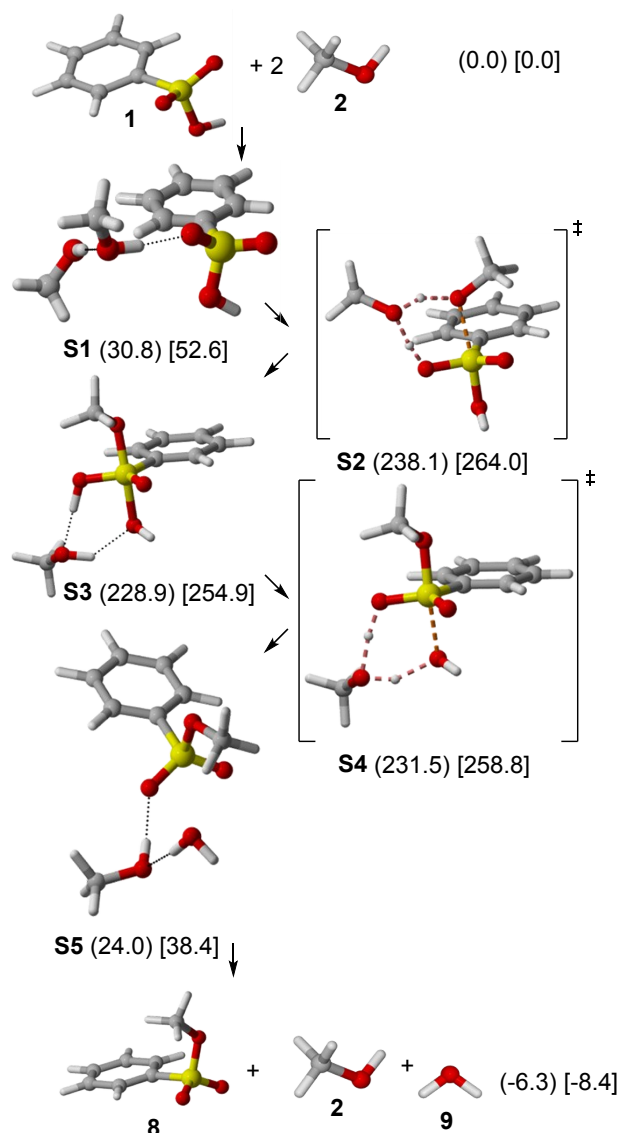


Figure S2 One methanol molecule-assisted neutral Ad-E mechanism. Relative Gibbs free energies (kJ mol^{-1}) in gas phase (in parenthesis) and methanol solution (in square brackets) of involved structures are shown.

Thus, the methanol (**2**) attack to benzenesulfonic acid (**1**) can be assisted by an additional methanol molecule. Interestingly, the pre-reactive hydrogen-bonded benzenesulfonic acid-(methanol)₂ complex (**S1**) is disfavored in Gibbs free energy terms.

The water-assisted methanol addition to benzenesulfonic acid TS (**S2**) shows a concerted proton transfer from methanol to an oxo group through a further methanol molecule. A very high activation barrier ($207.3 \text{ kJ mol}^{-1}$ in gas phase, $211.3 \text{ kJ mol}^{-1}$ in methanol solution) is found for the methanol-assisted pathway, similarly to that found for the non-assisted step ($205.8 \text{ kJ mol}^{-1}$ in gas phase, $223.7 \text{ kJ mol}^{-1}$ in solution). The lack of methanol assistance in such a pathway contrasts with the water-assisted

acceleration reported for the hydration of metaphosphoric acid.¹⁴

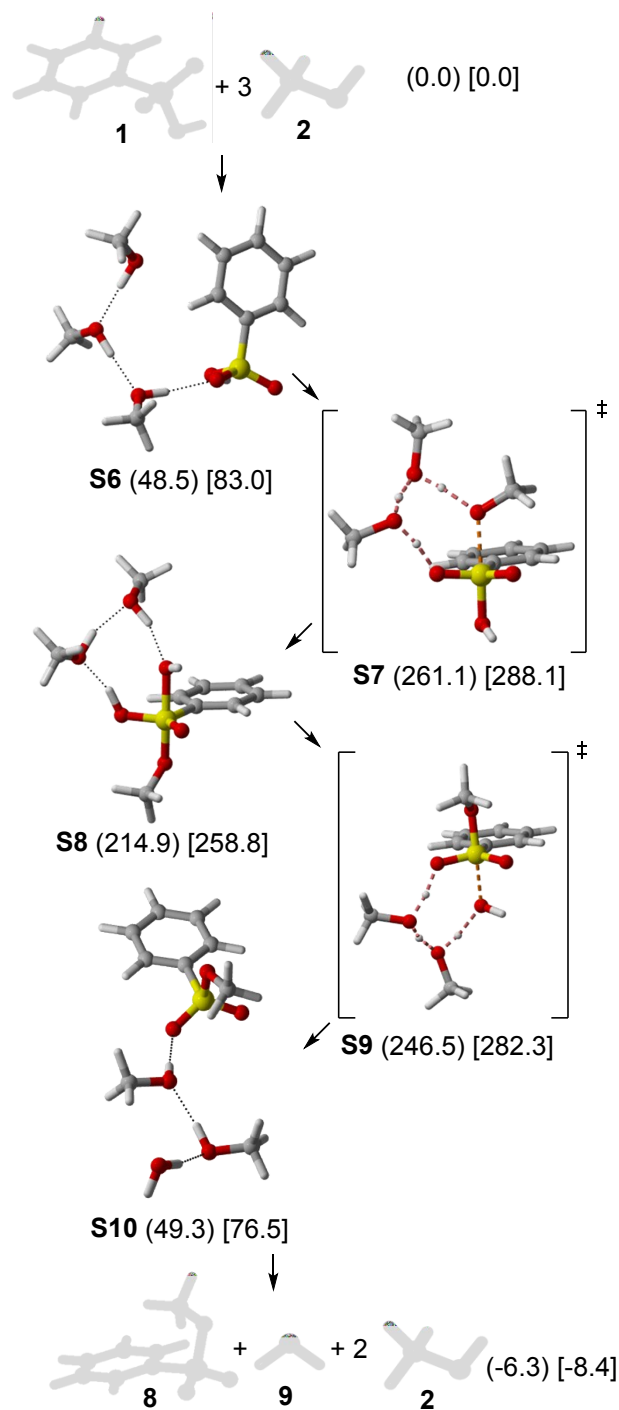


Figure S3 Two water molecules-assisted neutral Ad-E mechanism. Relative Gibbs free energies (kJ mol^{-1}) in gas phase (in parenthesis) and solution (in square brackets) of involved structures are shown.

The high activation barrier of the methanol-assisted pathway can be attributed to the instability of the resulting methanol-coordinated methyl dihydrogen benzeneorthosulfonate (**S3**), in agreement with the low stability of the pentacoordinate sulfur

species. A very low activation barrier is found for the subsequent water elimination step through TS **S4** (2.6 kJ mol^{-1} in gas phase, 3.9 kJ mol^{-1} in methanol solution).

As a result, a hydrogen-bonded (methanol)₂-methyl benzenesulfonate complex (**S5**) is obtained. The final dissociation of such a hydrogen-bonded complex yields methyl benzenesulfonate and two methanol molecules. The reaction energy for the whole methanol-assisted process is obviously identical to that corresponding to the non-assisted mechanism. Results on the two methanol molecules-assisted neutral Ad-E path are shown in Figure S3. The formation of the (methanol)₃-benzenesulfonic acid hydrogen-bonded complex (**S6**) is largely disfavored in Gibbs free energy terms.

The subsequent two methanol molecules-assisted methanol addition (through TS **S7**) involves a significant activation barrier ($212.6 \text{ kJ mol}^{-1}$ in gas phase, $205.1 \text{ kJ mol}^{-1}$ in solution).

The two methanol molecules-coordinated pentacoordinate sulfur species (**S8**) is again rather unstable, as previously found for both non-coordinated and one water molecule-coordinated analogs.

A low activation barrier is found for the subsequent water elimination step through TS **S9** (31.4 kJ mol^{-1} in gas phase, 13.5 kJ mol^{-1} in solution).

As a result, a water-(methanol)₂-methyl benzenesulfonate hydrogen-bonded complex (**S10**) is obtained. The final dissociation of that species yields methyl benzenesulfonate (**8**), methanol (**9**) and two water molecules (**2**).

Results on the one methanol molecule-assisted acid-catalyzed Ad-E mechanism are shown in Figure S4. Thus, the formation of a cyclic benzenesulfonic acid-methanol-methyloxonium cation hydrogen-bonded complex (**S11**) is thermodynamically favored. Instead, a large energy is required for the addition step through TS **S12** ($260.4 \text{ kJ mol}^{-1}$ in gas phase, $247.5 \text{ kJ mol}^{-1}$ in solution). Such an activation energy is similar to that of the non-assisted acid mechanism ($256.8 \text{ kJ mol}^{-1}$ in gas phase, $260.1 \text{ kJ mol}^{-1}$ in solution).

The lack of a significant role of methanol assistance in the methanol addition to sulfonic acid contrasts with a previous theoretical study on the formamide hydration showing a little effect in the neutral mechanism, but a more important role in the pathway involving the H_3O^+ cation.⁵¹

As a result of the addition step, a methanol-coordinated protonated methyl dihydrogen benzenesulfonate cation (**S13**) is obtained. Such a species is rather unstable (in comparison with the cyclic complex **S11**) (by $230.1 \text{ kJ mol}^{-1}$ in gas phase, by $228.6 \text{ kJ mol}^{-1}$ in solution).

A very low activation barrier is required for the subsequent water elimination through TS **S14** (4.8 kJ mol^{-1} in gas phase, 6.6 kJ mol^{-1} in solution).

As a consequence a stable hydrogen-bonded methyl benzenesulfonate-oxonium cation-water complex (**S15**) is formed. The final dissociation yields methyl benzenesulfonate (**8**), methyloxonium cation (**16**) and water (**9**) as the reaction products.

As a general conclusion for all considered methanol-assisted mechanisms, very similar activation barriers are found. Thus,

methanol assistance cannot avoid the unfeasibility of both neutral and acid-catalyzed Ad-E mechanisms.

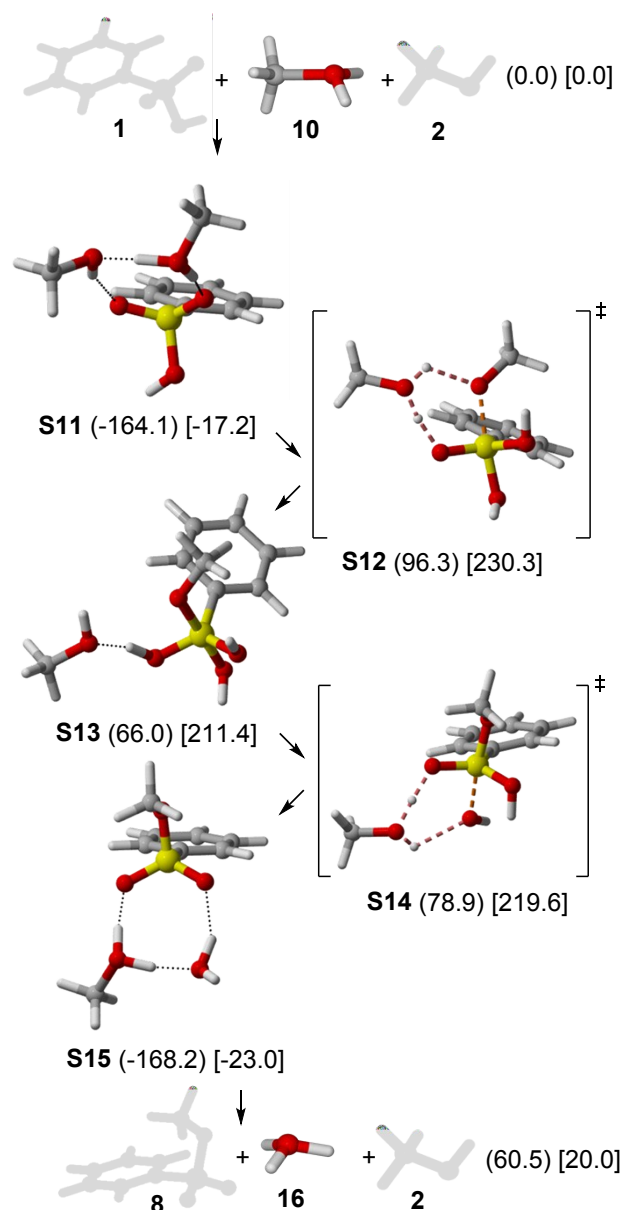


Figure S4 Acid-catalyzed water-assisted Ad-E mechanism. Relative Gibbs free energies (kJ mol⁻¹) in gas phase (in parenthesis) and solution (in square brackets) of involved structures are shown.

Notes and references

- S1 S. Antonczak, M. F. Ruiz-López and J. L. Rivail, *J. Am. Chem. Soc.*, 1994, **116**, 3912–3921; S. Antonczak, M. Ruiz-López and J.-L. Rivail, *J. Mol. Model.*, 1997, **3**, 434–442.

3. Electronic and Gibbs free energies (calculated as the sum of electronic and thermal free energies, in Hartrees) in gas phase and methanol (IEF-PCM continuum model) for structures at B3LYP/aug-cc-pVTZ level.

Code	Structure	Electronic energy (gas phase)	Electronic energy (methanol)	Gibbs free energy (gas phase)	Gibbs free energy (methanol)
1	benzenesulfonic acid	-856.288421036	-856.300488755	-856.208354	-856.220474
2	methanol	-115.776759287	-115.781603679	-115.748529	-115.753465
3	benzenesulfonic acid···methanol HB complex	-972.072865556	-972.072865556	-971.949354	-971.965605
4	benzenesulfonic acid + methanol addition TS	-971.995930573	-972.005249828	-971.870969	-971.880413
5	methyl dihydrogen benzeneorthosulfonate, pseudorotamer 5	-972.004708623	-972.013709889	-971.874941	-971.884971
5a	methyl dihydrogen benzeneorthosulfonate, pseudorotamer 5a	-971.995633913	-972.006703388	-971.866286	-971.866286
5b	methyl dihydrogen benzeneorthosulfonate, pseudorotamer 5b	-971.994046252	-972.001965584	-971.863066	-971.863066
5c	methyl dihydrogen benzeneorthosulfonate, pseudorotamer 5c	-971.986013374	-972.998475217	-971.856968	-971.856968
6	methyl dihydrogen benzeneorthosulfonate, water elimination TS	-971.997968843	-972.007518690	-971.871091	-971.881055
7	methyl benzenesulfonate···water HB complex	-972.077302355	-972.090571508	-971.952733	-971.970000
8	methyl benzenesulfonate	-895.602843373	-895.613990999	-895.496695	-895.508123
9	water	-76.466196562	-76.4724927575	-76.462601	-76.469017
10	methyloxonium cation	-116.074455952	-116.179571300	-116.033814	-116.138579
11	benzenesulfonic acid···methyloxonium cation HB complex	-972.421245845	-972.496927459	-972.287624	-972.361047
12	protonated benzenesulfonic acid + methanol addition TS	-972.326672897	-972.398826479	-972.189785	-972.261966
13	protonated methyl dihydrogen benzeneorthosulfonate	-972.346667234	-972.418515215	-972.203865	-972.276590
14	protonated methyl dihydrogen benzeneorthosulfonate, water elimination TS	-972.332743157	-972.402441009	-972.196717	-972.265543
15	protonated methyl benzenesulfonate···water HB complex	-972.426461045	-972.496159846	-972.290991	-972.361632
16	oxonium cation	-76.738518512	-76.859943078	-76.722411	-76.843298
17	protonated benzenosulfonic acid	-856.605184042	-856.684858610	-856.514464	-856.594174
	benzenesulfonylium cation	-780.103490061	-780.184203921	-780.035948	-780.116779
18	benzenesulfonylium cation···water complex	-856.596154636	-856.674927631	-856.507585	-856.584637
19	methanol···benzenesulfonylium cation···water complex	-972.395201205	-972.466053836	-972.261626	-972.332525
20	benzenesulfonylium cation···methanol complex	-895.916245998	-895.991546256	-895.800527	-895.874553
21	protonated methyl benzenesulfonate	-895.929485740	-896.002119587	-895.812955	-895.885404
22	methyloxonium cation···water pre-reactive complex	-192.556362559	-192.653773709	-192.499404	-192.598637
23	methyloxonium cation + water S _N 2 TS	-192.543183489	-192.634586902	-192.484527	-192.574690
S1	benzenesulfonic acid···2 methanol HB complex	-1087.86148989	-1087.87448037	-1087.693681	-1087.707364
S2	one methanol molecule-assisted benzenesulfonic acid + methanol addition TS	-1087.78736497	-1087.79798744	-1087.614734	-1087.626869

Code	Structure	Electronic energy (gas phase)	Electronic energy (methanol)	Gibbs free energy (gas phase)	Gibbs free energy (methanol)
S3	methyl dihydrogen benzeneorthosulfonate...methanol HB complex	-1087.79448342	-1087.80478467	-1087.618247	-1087.630316
S4	one methanol molecule-assisted methyl dihydrogen benzeneorthosulfonate, water elimination TS	-1087.79089812	-1087.80091180	-1087.617241	-1087.628845
S5	methyl benzenesulfonate...methanol...water HB complex	-1087.86504757	-1087.87800856	-1087.696258	-1087.712787
S6	benzenesulfonic acid...3 methanol HB complex	-1203.65038737	-1203.66419537	-1203.435454	-1203.449262
S7	two methanol molecules-assisted benzenesulfonic acid + methanol addition TS	-1203.57563991	-1203.59228955	-1203.354489	-1203.371138
S8	methyl dihydrogen benzeneorthosulfonate...2 methanol HB complex	-1203.58701804	-1203.59721421	-1203.372085	-1203.382281
S9	two methanol molecules-assisted methyl dihydrogen benzeneorthosulfonate, water elimination TS	-1203.58118694	-1203.59449520	-1203.360036	-1203.373344
S10	methyl benzenesulfonate...2 methanol...water HB complex	-1203.65009250	-1203.66666734	-1203.435159	-1203.451734
S11	benzenesulfonic acid...methyloxonium cation...methanol HB complex	-1088.23683266	-1088.30304591	-1088.053218	-1088.119085
S12	methanol-assisted protonated benzenesulfonic acid + methanol addition TS	-1088.14247653	-1088.21323000	-1087.954031	-1088.024784
S13	protonated methyl dihydrogen benzeneorthosulfonate...methanol HB complex	-1088.15095930	-1088.21742133	-1087.965553	-1088.032015
S14	methanol-assisted protonated methyl dihydrogen benzeneorthosulfonate, water elimination TS	-1088.14908666	-1088.21669035	-1087.960641	-1088.028245
S15	methyl benzenesulfonate...oxonium cation...methanol HB complex	-1088.23993022	-1088.30554635	-1088.054757	-1088.121267

4. Cartesian coordinates (Å) for all structures.

1 [benzenesulfonic acid], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -0.380391048, -0.1006175553, 0.1980938282
O, -1.8351763102, -0.5262045357, -0.4070400718
H, -1.68264961, -1.0278473281, -1.2207769991
O, 0.6097520625, -0.9113413282, -0.4841084438
O, -0.5388358907, -0.1290897369, 1.6304222881
C, -0.2208654873, 1.5965515125, -0.333333359
C, -0.8139950116, 2.5986059856, 0.4265745152
C, 0.4985060348, 1.882743581, -1.4873520229
C, -0.6905119816, 3.9167667703, 0.0085484095
H, -1.348612709, 2.3465837657, 1.3305218917
C, 0.6160429271, 3.2067249741, -1.8923691037
H, 0.9686324321, 1.0845887113, -2.0427892086
C, 0.0207565755, 4.2195839869, -1.1484623643
H, -1.1443612111, 4.7073111626, 0.5897803849
H, 1.1779369344, 3.4458326224, -2.784515451
H, 0.117068373, 5.2486514917, -1.4667557636

1 [benzenesulfonic acid], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.4772464396, 0.001626565, -0.1605367138
O, -1.9404152543, -0.1912880526, 1.3803117973
H, -1.8864323292, 0.6547958883, 1.8528794131
O, -1.9470095536, 1.2976678284, -0.615736063
O, -1.9331193494, -1.2092923639, -0.8106910627
C, 0.3008808042, 0.0077930121, -0.0778755787
C, 0.975348706, -1.2076104313, -0.0069092473
C, 0.9750839027, 1.2237175549, -0.0814375291
C, 2.3614895185, -1.1968815724, 0.0667921918
H, 0.428844427, -2.1388607201, -0.0167917467
C, 2.3627317527, 1.2172900898, -0.0075957534
H, 0.4277091638, 2.1518194061, -0.1479918459
C, 3.05243534, 0.0118352707, 0.0677714334
H, 2.9010119808, -2.1318023408, 0.1196899449
H, 2.9020551746, 2.1537961496, -0.0127961981
H, 4.1321341559, 0.0130547163, 0.1234049583

2 [methanol], in gas phase (at B3LYP/aug-cc-pVTZ level)

H, 0.7625156054, -1.1572189366, 0.
O, -0.1052374465, -0.7448541863, 0.
C, 0.0539201827, 0.6696260877, 0.
H, -0.9463722232, 1.0976781284, 0.
H, 0.5818659758, 1.0228333684, 0.8907874089
H, 0.5818659758, 1.0228333684, -0.8907874089

2 [methanol], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

H, 0.766393827, -1.1526794175, 0.
O, -0.1065551923, -0.7483694584, 0.
C, 0.0514987171, 0.6722615014, 0.
H, -0.9477290516, 1.1024006096, 0.
H, 0.5824748849, 1.0186422973, 0.8898190699
H, 0.5824748849, 1.0186422973, -0.8898190699

3 [benzenesulfonic acid...methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0.2596971931, 1.5329858944, 0.6011520699
O, 0.5895582175, 1.9693852082, -0.9330105266

H, 0.0501715678, 2.7438402771, -1.14946169
O, 1.4847663297, 0.9297767142, 1.0790528838
C, -0.9898147692, 0.2746735197, 0.407257274
C, -0.6172086766, -1.0014512664, -0.0052511028
C, -2.3121887224, 0.6043188798, 0.6822126353
C, -1.6079427706, -1.9636875192, -0.1495043166
H, 0.4180925344, -1.2456985829, -0.2003728828
C, -3.289129042, -0.3724000502, 0.534365764
H, -2.5620464905, 1.5997137915, 1.0180769523
C, -2.9374417415, -1.6513690396, 0.1176000728
H, -1.3363391319, -2.9612043313, -0.4653814545
H, -4.3212412759, -0.1341353703, 0.7505007204
H, -3.7008375181, -2.409361775, 0.0060545054
O, -0.3136480945, 2.6858544238, 1.2642691711
H, 2.5560112511, -0.6444168342, 0.4470650323
O, 2.7336008241, -1.4899626202, 0.0150525581
C, 4.0465647841, -1.4753813527, -0.5259212072
H, 4.8068418962, -1.360476019, 0.2527060593
H, 4.2030802043, -2.4329240764, -1.0200007619
H, 4.1764204306, -0.6788028714, -1.2650547562

3 [benzenesulfonic acid···methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.3586479082, -0.8533262115, -0.0660902088
O, 0.814279543, -0.8702226843, 1.484800039
H, 0.3948239843, -1.6120674663, 1.9499458493
O, 1.3214398557, 0.036073328, -0.6920835619
C, -1.2401537375, -0.0754933617, -0.049891867
C, -1.3139360023, 1.30941231, 0.0701109681
C, -2.3775119665, -0.8682850063, -0.1545327755
C, -2.5654256234, 1.9088965093, 0.0888873727
H, -0.4152880495, 1.9041013737, 0.139291169
C, -3.6227377816, -0.2516652622, -0.135789447
H, -2.2898131845, -1.9393223716, -0.2563938198
C, -3.7155211777, 1.1305100621, -0.0131198779
H, -2.6418255081, 2.983110052, 0.1785241941
H, -4.5170699999, -0.8522532138, -0.2208442753
H, -4.687073185, 1.6045683384, -0.0006404784
O, 0.2355597715, -2.2225226584, -0.5265731781
H, 2.9822654293, 0.9445748494, -0.1974208525
O, 3.7867639054, 1.4444494894, -0.0007037794
C, 4.9059700499, 0.5711911896, -0.1272096537
H, 4.9933981099, 0.1677648792, -1.1398120324
H, 5.7992685742, 1.1537956156, 0.0910596794
H, 4.8530870847, -0.2612637605, 0.5799115363

4 [benzenesulfonic acid + methanol addition TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -1.0978100838, -0.5401754786, 0.200403021
O, -1.7918181023, -0.9447055863, -1.1488672973
O, -1.8423927785, -0.006998761, 1.3277385002
H, -1.6164203666, -2.4184528091, 1.1270539019
O, -0.8219337969, -2.1048679235, 0.6722060804
C, 0.6544044784, -0.1909193349, 0.0699701189
C, 1.232961584, 0.5581951506, 1.0820480601
C, 1.3793691822, -0.6887934739, -1.0010539321

C, 2.5963033503, 0.8184459079, 1.0103918078
H, 0.6345848358, 0.9277271764, 1.9018192368
C, 2.7403017514, -0.4154644542, -1.05610376
H, 0.8962963494, -1.2699319455, -1.7722529281
C, 3.3474809665, 0.33559989, -0.0551902916
H, 3.0684033345, 1.4002920226, 1.7898096176
H, 3.3248327069, -0.7914534557, -1.8842792637
H, 4.4072399505, 0.544030039, -0.1058772006
C, -1.8547855545, 2.3732695105, -0.3433126405
H, -1.1627156632, 2.8611548658, 0.3524958939
H, -2.0796209987, 3.0838885243, -1.1441247853
H, -2.7803018649, 2.1535954461, 0.1976297965
H, -1.8722758146, 0.0725315155, -1.4783367578
O, -1.2727534659, 1.223758174, -0.9049641781

4 [benzenesulfonic acid + methanol addition TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.0825871714, -0.524968231, 0.2225085067
O, -1.8076916836, -0.9317205496, -1.1170835061
O, -1.8199072257, 0.0245740083, 1.3473197162
H, -1.6531525085, -2.4920078628, 0.9450513748
O, -0.8110772516, -2.0859304619, 0.6862120077
C, 0.6699239466, -0.1843285587, 0.0813642398
C, 1.2512682217, 0.5963445998, 1.0686562916
C, 1.3898507181, -0.7206097474, -0.9756714266
C, 2.616382252, 0.8467637136, 0.986762785
H, 0.6602071655, 0.9975330382, 1.8783579589
C, 2.7521454246, -0.4532458343, -1.0418035382
H, 0.907906189, -1.3262904121, -1.7284687099
C, 3.3633796373, 0.3268960692, -0.0650420822
H, 3.0918095389, 1.4500471194, 1.7471345043
H, 3.3333048667, -0.8581074516, -1.858219693
H, 4.4237114544, 0.5287794799, -0.123597318
C, -1.8852765683, 2.3774060561, -0.325270748
H, -1.2650853349, 2.8165183431, 0.4644273495
H, -2.0274040691, 3.1380402528, -1.0992678296
H, -2.8643022154, 2.1433946062, 0.1057278268
H, -1.8921879434, 0.0586595965, -1.4661358385
O, -1.2618674431, 1.2529772264, -0.8957588711

5 [methyl dihydrogen benzeneorthosulfonate, pseudorotamer 5], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 1.0913186785, -0.3794896262, 0.0341241951
O, 1.5887543656, 1.1496178368, -0.4891459742
O, 2.6419763506, -0.8622250398, -0.104010902
H, 2.6196698475, -1.7942126718, 0.1770118209
O, 0.0518575276, -0.6312716954, -0.9691515451
H, 0.111170301, -2.3774565406, 0.3804921198
O, 0.8573909014, -1.9760405558, 0.8398611684
C, 0.7001575333, 0.390202492, 1.6224127332
C, -0.6362336384, 0.6240804102, 1.9025869349
C, 1.7115474542, 0.7204748468, 2.5085548032
C, -0.9663418973, 1.2097278883, 3.1190489872
H, -1.4006835407, 0.3591102295, 1.18629438
C, 1.3635688806, 1.2978683381, 3.7246303656
H, 2.7458131953, 0.5390801786, 2.2572025818
C, 0.0297036492, 1.5428025763, 4.0302459473

H, -2.0042751615, 1.4038277023, 3.3520232708
H, 2.1400212489, 1.560332513, 4.4300197632
H, -0.2332500045, 1.9951269378, 4.9765396366
C, 1.8912703786, 1.3319860085, -1.8740385617
H, 1.0359801348, 1.0729235124, -2.4965400012
H, 2.1214896138, 2.3893977895, -1.9866484443
H, 2.7591858617, 0.7407407696, -2.1699877697

5 [methyl dihydrogen benzeneorthosulfonate, pseudorotamer **5**], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.0528346688, 0.3689351758, 0.0287321655
O, -1.2559363257, -1.2725778348, -0.363467126
O, -1.7640123989, 0.048332625, 1.4525320382
H, -1.7750251359, 0.8975983432, 1.9285988499
O, -1.7525295817, 0.9458664311, -1.127769047
H, -1.0311832026, 2.6191788948, 0.1214428445
O, -0.6864424803, 1.973087544, 0.7493425201
C, 0.7290461277, 0.0586696492, 0.0028874921
C, 1.4278669671, 0.444957005, -1.1300434253
C, 1.34711654, -0.5359109146, 1.0912338691
C, 2.8002002645, 0.2224199695, -1.1691390962
H, 0.9192250184, 0.9074797523, -1.9635727424
C, 2.721402826, -0.7452302727, 1.0372602836
H, 0.778623467, -0.8316329501, 1.9603538376
C, 3.4463233669, -0.3688879414, -0.0885006837
H, 3.3607147424, 0.5137411397, -2.0464265467
H, 3.2211590817, -1.2064420278, 1.8776576625
H, 4.5136319521, -0.5370461818, -0.1239673614
C, -2.5698812031, -1.7459207128, -0.6817903251
H, -2.9786101961, -1.2162587387, -1.541016815
H, -2.4527644568, -2.7995811448, -0.9252800409
H, -3.2437947036, -1.6463078097, 0.1694546463

5a [methyl dihydrogen benzeneorthosulfonate, pseudorotamer **5a**], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -1.016799732, 0.1107703252, 0.7436740641
O, -1.8672110853, 1.2487792279, -0.0681468765
O, -1.2303032892, -1.0404489886, -0.5563359723
H, -1.8007548966, -1.7267430048, -0.1911457717
O, -1.665663894, -0.7538407783, 1.7463735235
C, 0.7486502367, 0.1083998902, 0.3010102466
C, 1.4809073026, -1.0416182149, 0.5494047048
C, 1.3244965478, 1.2435226821, -0.2459547128
C, 2.836793973, -1.0471062688, 0.2472692434
H, 1.004494663, -1.9144300868, 0.9709064268
C, 2.6777190465, 1.2141189327, -0.5665899319
H, 0.735043758, 2.1322724956, -0.4115444962
C, 3.434054718, 0.0756120665, -0.3161043152
H, 3.422997725, -1.9339120119, 0.4454155663
H, 3.1394042076, 2.0890271729, -1.0034090621
H, 4.4877521521, 0.0624262675, -0.5589471256
C, -2.7646879702, 0.9481285212, -1.1582079409
H, -3.5055645476, 0.2076670015, -0.8682803185
H, -3.2538362641, 1.9016510715, -1.3461268382
H, -2.2228457218, 0.612859879, -2.0357950279

O, -0.6095186667, 1.3655783415, 1.8360660479
H, -1.3217004826, 1.4067348487, 2.4864685664

5a [methyl dihydrogen benzeneorthosulfonate, pseudorotamer **5a**], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.0105808207, 0.0356708431, 0.7030518878
O, -1.8720721055, 1.2448075163, 0.035651154
O, -1.1835610338, -0.9637535873, -0.7146156805
H, -1.8633662102, -1.6192809093, -0.5133912853
O, -1.657791509, -0.9337920519, 1.6067519683
C, 0.7617995992, 0.069510907, 0.2941669663
C, 1.5429895209, -0.9946722564, 0.7165915508
C, 1.2852027695, 1.1388262232, -0.4133527869
C, 2.9014625706, -0.9786435143, 0.4206310784
H, 1.1079533442, -1.8186333648, 1.2638431648
C, 2.6448373901, 1.133000307, -0.7122586481
H, 0.6565453708, 1.9591919084, -0.7259273907
C, 3.4515762784, 0.0805559961, -0.2947505163
H, 3.5262580443, -1.7980269056, 0.7478350221
H, 3.0692401846, 1.957154109, -1.2686271715
H, 4.5076339376, 0.0848958304, -0.5260576378
C, -2.7911772025, 1.0613607316, -1.0723058008
H, -3.5161989354, 0.2821505282, -0.8561368355
H, -3.2937149174, 2.0228964076, -1.135608958
H, -2.2562255577, 0.8455162789, -1.9896046135
O, -0.6006015636, 1.1728416613, 1.9346028598
H, -1.3767813743, 1.2878727115, 2.4995116727

5b [methyl dihydrogen benzeneorthosulfonate, pseudorotamer **5b**], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -0.6403552423, -0.5913159715, -0.818095312
O, -2.2287047078, -1.3909998332, -1.1984376348
O, -0.8963377442, -0.9039684617, 0.7700259754
O, -0.0278292998, -1.8468049231, -1.6823935986
H, -0.8101626948, -2.3051873848, -2.0356967338
C, 1.0975698731, -0.153133873, -0.3572801587
C, 1.5527557996, 1.1354160986, -0.5938955761
C, 1.9367293798, -1.1017051089, 0.2211751731
C, 2.8589019899, 1.4766690894, -0.2496507284
H, 0.8948138411, 1.8606977316, -1.0449170655
C, 3.2356887764, -0.7536738479, 0.5632196635
H, 1.582381785, -2.1050845773, 0.4033014497
C, 3.7005567629, 0.5372249046, 0.3283473349
H, 3.2124526606, 2.4814798456, -0.4378097334
H, 3.8860596443, -1.4921612876, 1.0124320977
H, 4.7141271033, 0.8053584597, 0.5944259599
O, -1.0700432299, 0.6799255289, -1.414643689
C, -2.1945659414, -1.0847264946, 1.375457307
H, -2.6107763585, -2.0540427946, 1.1245691411
H, -1.9880146499, -1.0147037443, 2.4415233714
H, -2.8780350631, -0.2938814555, 1.0790311453
H, -2.7248529944, -0.6913455705, -1.6375897888

5b [methyl dihydrogen benzeneorthosulfonate, pseudorotamer **5b**], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.6534955461, -0.5736583006, -0.8263761011
O, -2.2211795655, -1.362872771, -1.2017256375
O, -0.9072435222, -0.8522778786, 0.7646761225
O, -0.0278139561, -1.8191491525, -1.6980930811
H, -0.7920153819, -2.2911108877, -2.0720389815
C, 1.0905869851, -0.1390358306, -0.360208893
C, 1.5681517043, 1.1376538323, -0.6196180736
C, 1.9136786645, -1.0870235837, 0.2442973884
C, 2.8778332393, 1.4678959372, -0.2736541869
H, 0.9279879763, 1.8676631742, -1.0880804669
C, 3.2164061048, -0.7512889698, 0.5875612176
H, 1.5448156982, -2.0810540469, 0.4488956973
C, 3.7026267759, 0.5281156986, 0.329019715
H, 3.2462502986, 2.4638222543, -0.4792183159
H, 3.8519211319, -1.4897664619, 1.0572519008
H, 4.7179887134, 0.7869404209, 0.596753963
O, -1.0645359674, 0.7016595321, -1.4394962637
C, -2.1910591109, -1.1206969837, 1.382433907
H, -2.5322118681, -2.1212818908, 1.1432697157
H, -1.9804908014, -1.0300527925, 2.4453578569
H, -2.9299694035, -0.383162967, 1.0858125982
H, -2.7558724792, -0.6572820022, -1.5837214813

5c [methyl dihydrogen benzeneorthosulfonate, pseudorotamer **5c**], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -0.849407167, 0.2492896436, 0.5259812119
O, -2.661302277, 0.0638290455, 0.4031075643
O, -0.8390737832, -1.3482206185, 0.9943277815
O, -0.9336547921, 0.8656811198, -1.018313832
H, -1.8422874727, 1.186606928, -1.1314108165
C, 0.9627483897, 0.0670309687, 0.2400480891
C, 1.4468273764, -0.8002776088, -0.732214638
C, 1.8257173593, 0.8190521991, 1.0203206214
C, 2.8171749364, -0.9129856099, -0.9225570587
H, 0.767904874, -1.3838704193, -1.3370266927
C, 3.1992553793, 0.6990615116, 0.8218745049
H, 1.4279342652, 1.4860336578, 1.7692481621
C, 3.6957561964, -0.1633115444, -0.145688117
H, 3.1985166737, -1.586627806, -1.677953423
H, 3.8769070543, 1.2842229526, 1.4286903474
H, 4.7629818008, -0.2532733061, -0.2963795646
O, -0.9404828716, 1.2213141407, 1.5988091217
C, -3.2380392747, -0.835635802, -0.5351747518
H, -4.3174296576, -0.7045798184, -0.4580595728
H, -2.9360329794, -0.629320521, -1.5667872665
H, -3.0023456267, -1.8838232317, -0.3239504578
H, -1.7247114636, -1.5353058511, 1.3431087873

5c [methyl dihydrogen benzeneorthosulfonate, pseudorotamer **5c**], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.8639402606, 0.2457209553, 0.5236477427
O, -2.643506074, 0.0665664667, 0.407712665
O, -0.830805534, -1.3431353707, 1.0146048545
O, -0.9247283851, 0.880299617, -1.0128290619
H, -1.8329981731, 1.1793938218, -1.1796889075

C, 0.9551300372, 0.0686800984, 0.2444854798
C, 1.4376996764, -0.8025787467, -0.7265318507
C, 1.821395549, 0.8221958487, 1.0207948962
C, 2.8084885466, -0.9169104656, -0.9185073902
H, 0.7587737314, -1.3881624297, -1.3295960764
C, 3.1956344232, 0.7007341888, 0.8208849424
H, 1.4319283495, 1.49356813, 1.7698350443
C, 3.6899499042, -0.1654076134, -0.1451618491
H, 3.1873835205, -1.5932410167, -1.6724507727
H, 3.8740295208, 1.2874589239, 1.4251337014
H, 4.7566436248, -0.2568181059, -0.2973249784
O, -0.9461983091, 1.2256493459, 1.6019493323
C, -3.2301222004, -0.8326219219, -0.5391648579
H, -4.3068779107, -0.7200821565, -0.4261884403
H, -2.9591546955, -0.5927142166, -1.5694447128
H, -2.965687019, -1.8748347489, -0.3475152193
H, -1.7160813823, -1.5788705737, 1.3353554586

6 [methyl dihydrogen benzeneorthosulfonate, water elimination TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -1.1203444735, -0.4565453109, 0.1578967297
O, -1.7914224741, -0.953999404, -1.1801249368
O, -1.887070055, 0.1974039281, 1.2051817021
O, -0.8742562899, -1.9715708114, 0.7526016554
C, 0.6435650557, -0.1549235468, 0.0539905376
C, 1.2067353868, 0.6904641466, 0.9954765835
C, 1.3889373587, -0.7792221878, -0.9325105105
C, 2.5772621507, 0.9121390372, 0.9441227195
H, 0.5891254081, 1.1655404986, 1.743376281
C, 2.7571253994, -0.5392864439, -0.972999207
H, 0.9167327072, -1.4321970492, -1.6511821617
C, 3.3500434782, 0.3016732286, -0.0378271093
H, 3.0381794602, 1.5666855907, 1.6707684341
H, 3.3578122171, -1.0127399466, -1.7371660148
H, 4.4154532077, 0.4825237105, -0.0750941655
H, -1.832522046, 0.0320618794, -1.581684653
O, -1.2292088475, 1.2366356122, -1.0611476031
H, -1.819665767, 1.855803412, -0.6192931069
C, -2.0317279743, -2.7127758752, 1.1803995898
H, -1.6401619431, -3.6382690353, 1.5933170236
H, -2.5752652453, -2.1626503202, 1.9463214628
H, -2.682969274, -2.9299583428, 0.3346781394

6 [methyl dihydrogen benzeneorthosulfonate, water elimination TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 1.0520656475, 0.2668327608, -0.0570838015
O, 1.7354860687, 0.3964018829, 1.3631145394
O, 1.669075037, 0.8355955319, -1.2450520686
O, 1.3438444318, -1.3379193175, -0.1942644211
C, -0.7209662591, 0.0128122177, -0.0264002251
C, -1.4309059455, 0.3048649996, -1.1803948133
C, -1.3189678573, -0.4895229526, 1.118846918
C, -2.8022699746, 0.0780829136, -1.1809130018
H, -0.9318653634, 0.6999117481, -2.0527897554
C, -2.692677838, -0.7025792776, 1.0999167484

H,-0.7375858217,-0.708211606,2.0019889695
C,-3.4313285092,-0.421119032,-0.0448085964
H,-3.3760425444,0.2953998437,-2.0706924923
H,-3.181539822,-1.0905993047,1.9823220472
H,-4.4988255018,-0.5911371752,-0.0514577059
H,1.464620137,1.3908744112,1.4988853301
O,0.52812823,2.203412878,0.62891055
H,0.964345838,2.8158984169,0.0265552283
C,2.7121266953,-1.7676795274,-0.389540811
H,2.6538947908,-2.8457073897,-0.5017390998
H,3.1253461012,-1.3197029413,-1.2901244683
H,3.3187924597,-1.5150090804,0.4774669297

7 [methyl benzenesulfonate···water HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S,-0.875976914,-1.969670581,-0.3649975313
O,0.2305536059,-1.1058775502,-0.7228704495
H,0.4682669533,0.8257653731,-0.3572854264
O,-0.8282458495,-3.3854739242,-0.663912387
O,-1.010692513,-1.7692608182,1.23427924
C,-2.4012863686,-1.2919501274,-1.0009048608
C,-3.3383719064,-2.1545561647,-1.5579577804
C,-2.6145678888,0.0829744164,-0.9353874999
C,-4.5221191603,-1.6255673637,-2.0594726776
H,-3.1327762937,-3.2134945371,-1.6066497623
C,-3.8032806416,0.5934247117,-1.438936663
H,-1.8679613889,0.7424312459,-0.5140519126
C,-4.7536706824,-0.2564742384,-1.9979224211
H,-5.2577455443,-2.2834728441,-2.5009438951
H,-3.982359606,1.6588704498,-1.4001757951
H,-5.6748496372,0.1516063858,-2.3912781575
O,0.2520506195,1.7566202124,-0.1978018685
H,0.8888801401,2.0601975576,0.4544097308
C,-1.8908131075,-2.6588443182,1.9550355197
H,-1.622527097,-3.6946362604,1.7619328502
H,-1.7396311,-2.4161238415,3.0023601393
H,-2.9291137694,-2.4747651438,1.6788060381

7 [methyl benzenesulfonate···water HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S,0.8390480677,0.0236846062,-0.3155102468
O,1.2287784489,1.3718351929,-0.6996024496
H,2.7521566451,2.4949777013,-0.2632413368
O,1.2826019901,-1.1009641532,-1.1181736775
O,1.4189955055,-0.1162796615,1.1757766106
C,-0.9279383222,-0.045697011,-0.1193564485
C,-1.6203991325,-1.1583553963,-0.5825038814
C,-1.5773371614,1.0235555485,0.4933926616
C,-3.0014366578,-1.1974251344,-0.4266404066
H,-1.0910732862,-1.969098223,-1.0593879367
C,-2.9551695086,0.9677374979,0.6439659405
H,-1.0192803725,1.8812932085,0.8390341901
C,-3.6646242985,-0.1397224101,0.1848478131
H,-3.5551774288,-2.0534126426,-0.7850926497
H,-3.4751057668,1.7891341047,1.1160733189
H,-4.7386793758,-0.1752118844,0.3030323416

O, 3.4534407351, 3.1196551319, -0.0207887978
H, 4.1319080999, 3.0057192183, -0.6937488466
C, 1.3445853297, -1.4126828264, 1.8310246148
H, 1.8659017923, -1.2758368955, 2.7720730316
H, 0.3062978073, -1.6822569519, 2.0137504121
H, 1.8408538893, -2.1661020198, 1.2260467429

8 [methyl benzenesulfonate], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -1.5293036387, 0.0210391228, -0.3427997297
O, -2.0547797889, -0.1507700301, 1.1821042112
O, -1.9607247736, 1.3120455735, -0.8408808657
O, -1.9202913761, -1.2082308966, -0.9878636495
C, 0.2484579914, 0.0464924661, -0.152190815
C, 0.9136066147, -1.1494107158, 0.1016768318
C, 0.9331384018, 1.2499933823, -0.2679957069
C, 2.2930187304, -1.1309149414, 0.2509884576
H, 0.3577169719, -2.0733971202, 0.1666823596
C, 2.3157169042, 1.254143724, -0.1175543267
H, 0.3907210015, 2.1575811576, -0.4879125001
C, 2.9921308938, 0.0684932279, 0.1432783962
H, 2.8234572098, -2.0528584544, 0.4448317306
H, 2.8618029907, 2.18265535, -0.2102446809
H, 4.0676504152, 0.0758699552, 0.2569068882
C, -2.0473611514, 1.0118689296, 2.0359220804
H, -2.6137354571, 1.8207359757, 1.5810121907
H, -2.5214871456, 0.6880864899, 2.957645882
H, -1.0250047442, 1.3317507339, 2.239464256

8 [methyl benzenesulfonate], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0, 1.2538833456, 0.3596886919, -0.4246991001
O, 0, 1.8947773508, 0.0047823716, 1.0104544403
O, 0, 1.732017187, -0.5955688187, -1.4096272421
O, 0, 1.5482402991, 1.7697754956, -0.5888380112
C, 0, -0.4973427456, 0.1321628719, -0.1884135082
C, 0, -1.2023539286, 1.0801102917, 0.5494387396
C, 0, -1.1227717309, -0.9797767431, -0.7406828799
C, 0, -2.5657069779, 0.9019415552, 0.7355705839
H, 0, -0.6967278306, 1.9407264879, 0.9619575094
C, 0, -2.4897682033, -1.1437740905, -0.5463830391
H, 0, -0.5539038193, -1.6946412047, -1.3154727842
C, 0, -3.2070800906, -0.2073128214, 0.1892040744
H, 0, -3.1276890858, 1.6299596636, 1.3031725829
H, 0, -2.990699063, -2.0015564154, -0.9720795856
H, 0, -4.2700972299, -0.338864254, 0.3362132261
C, 0, 1.9226436355, -1.385779875, 1.4289848342
H, 0, 2.4662261473, -1.9842719196, 0.7034132647
H, 0, 2.4415703253, -1.3785593118, 2.3814494836
H, 0, 0.9093064151, -1.7610919753, 1.5586804116

9 [water], in gas phase (at B3LYP/aug-cc-pVTZ level)

H, 0.7634939049, 0., -0.4641537136
H, -0.7634939049, 0., -0.4641537136
O, 0., 0., 0.1208598971

9 [water], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

H, 0., 0.7620989914, -0.4693792381
H, 0., -0.7620989914, -0.4693792381
O, 0., 0., 0.1197394762

10 [methyloxonium cation], in gas phase (at B3LYP/aug-cc-pVTZ level)

H, -0.2670366005, -1.1506144944, 0.7996494277
H, -0.2670366005, -1.1506144944, -0.7996494277
O, 0.0879944285, -0.7201125046, 0.
C, -0.0180094119, 0.7982185473, 0.
H, 0.5045316508, 1.1049239762, 0.8982291696
H, 0.5045316508, 1.1049239762, -0.8982291696
H, -1.0695900971, 1.0625723637, 0.

10 [methyloxonium cation], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

H, -0.8312679086, -0.3747393882, 0.2340822704
H, -0.0001213504, 0.9745711116, 0.1711151964
O, 0.0037736008, 0.0290159248, -0.0656147506
C, 1.2231199706, -0.6992128413, 0.4242957545
H, 1.1158757945, -1.7055459322, 0.0424638547
H, 2.0562227456, -0.1789550246, -0.0287767603
H, 1.2330668347, -0.6548518216, 1.5061795689

11 [benzenesulfonic acid···methyloxonium cation HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0.6089184469, -0.6058736706, 0.2794296759
O, 1.0446131972, -0.0445169274, 1.5363889001
H, 2.593942251, 2.3377010871, 0.2356880207
H, 1.872691154, -2.3341766055, 0.463297136
O, 0.9580126639, -2.1574309634, 0.1819824026
C, -1.1356474537, -0.6429771455, 0.0857128984
C, -1.6831938142, -0.7599689125, -1.1904370916
C, -1.9144280417, -0.5653275657, 1.2377799633
C, -3.0642406361, -0.8004187486, -1.3051410125
H, -1.0515869706, -0.814834008, -2.0645230557
C, -3.2941436345, -0.6050418167, 1.0963567227
H, -1.4550999178, -0.4690566523, 2.2104453602
C, -3.8636726276, -0.7238050564, -0.1674541583
H, -3.516103449, -0.890063876, -2.2824500321
H, -3.9220067418, -0.5420777036, 1.9733234501
H, -4.9395738722, -0.754741899, -0.2680543389
C, 3.3372496972, 2.492333544, -1.6677927506
H, 2.8806447611, 2.3138431577, -2.6344608124
H, 3.5924375732, 3.5402923516, -1.5541754899
H, 4.1980687008, 1.8485055045, -1.512575747
O, 2.2962465407, 2.1834725326, -0.6727312385
O, 1.2300867129, 0.0241043118, -0.9328565647
H, 1.8061259905, 1.1742443517, -0.7713476578

11 [benzenesulfonic acid···methyloxonium cation HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.4020332905, 0.8814083549, 0.111664529
O, 0.6933854495, 1.7124819853, -1.0343222895
H, 3.5364193711, -0.5012659838, -1.6317680018
H, 0.9984142865, 2.2229075375, 1.682759057
O, 0.1742800118, 1.7766593867, 1.4187405098

C,-1.1868360792,0.1203866468,-0.0103065669
C,-1.491178658,-0.9544785476,0.8205873916
C,-2.0872532692,0.6207696864,-0.9443313517
C,-2.7446483329,-1.5378290974,0.7082992777
H,-0.7684001007,-1.3272685424,1.5307255698
C,-3.3359842279,0.0211097203,-1.0429803158
H,-1.8164060493,1.4508886498,-1.5788640957
C,-3.6622542464,-1.0510424438,-0.2192261577
H,-3.0029395655,-2.3736334766,1.3423453921
H,-4.0500632002,0.3917425229,-1.7640491168
H,-4.636106777,-1.5129897378,-0.3014815316
C,4.4832460279,-1.3283512922,-0.0063922408
H,4.1218587402,-1.9888267869,0.7714715821
H,5.2117726866,-1.8238826425,-0.6356049989
H,4.857646307,-0.3933359961,0.3949301399
O,3.3092699374,-1.0529021096,-0.8659839053
O,1.4106318538,-0.1363580282,0.4778162236
H,2.5101225439,-0.6313178059,-0.3490201

12 [protonated benzenesulfonic acid + methanol addition TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S,1.1614403424,-0.4981646803,0.2785543204
O,1.9806834411,0.3035588619,1.310058668
H,2.1002763277,1.1611468428,0.609552543
H,1.8894129961,-2.1884007283,1.4233059381
O,1.0305853055,-1.861940175,1.1006849438
C,-0.5856566537,-0.235733815,0.1034415192
C,-1.2150425488,-0.702569423,-1.0432759164
C,-1.2459157595,0.3970476928,1.1499884165
C,-2.5900085659,-0.524820265,-1.1320009224
H,-0.6690876473,-1.2009826809,-1.8305356969
C,-2.6194742967,0.5622031504,1.0288031332
H,-0.7212043447,0.7384521239,2.0305611025
C,-3.2852134163,0.1042648423,-0.1041416609
H,-3.1140721753,-0.8839550435,-2.0059749714
H,-3.1661891312,1.0453782897,1.8257543734
H,-4.3548678868,0.2360707175,-0.1850775609
C,0.7705213912,2.2240340555,-1.213424468
H,0.0765928726,2.5906671915,-0.4566840068
H,1.3979329045,3.0480497709,-1.5513276711
H,0.2133878975,1.8340530759,-2.0646072206
O,1.6474106293,1.2225198608,-0.6862963106
O,1.8996470595,-1.1535840285,-0.9539927592
H,2.1965585786,-0.4022026465,-1.5159850429

12 [protonated benzenesulfonic acid + methanol addition TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S,-1.0825871714,-0.524968231,0.2225085067
O,-1.8076916836,-0.9317205496,-1.1170835061
O,-1.8199072257,0.0245740083,1.3473197162
H,-1.6531525085,-2.4920078628,0.9450513748
O,-0.8110772516,-2.0859304619,0.6862120077
C,0.6699239466,-0.1843285587,0.0813642398
C,1.2512682217,0.5963445998,1.0686562916
C,1.3898507181,-0.7206097474,-0.9756714266

C, 2.616382252, 0.8467637136, 0.986762785
H, 0.6602071655, 0.9975330382, 1.8783579589
C, 2.7521454246, -0.4532458343, -1.0418035382
H, 0.907906189, -1.3262904121, -1.7284687099
C, 3.3633796373, 0.3268960692, -0.0650420822
H, 3.0918095389, 1.4500471194, 1.7471345043
H, 3.3333048667, -0.8581074516, -1.858219693
H, 4.4237114544, 0.5287794799, -0.123597318
C, -1.8852765683, 2.3774060561, -0.325270748
H, -1.2650853349, 2.8165183431, 0.4644273495
H, -2.0274040691, 3.1380402528, -1.0992678296
H, -2.8643022154, 2.1433946062, 0.1057278268
H, -1.8921879434, 0.0586595965, -1.4661358385
O, -1.2618674431, 1.2529772264, -0.8957588711

13 [protonated methyl dihydrogen benzeneorthosulfonate], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 1.0415524435, -0.2570622902, 0.0826568688
O, 1.5986211769, 1.2456067054, -0.0898554421
O, 1.7111746215, -0.3767608332, 1.531658218
H, 1.5888487881, -1.2868840449, 1.8554189857
H, -0.3935213087, -1.9789690814, 0.5386343314
O, 0.524784021, -1.924552256, 0.2408647831
C, -0.6537974721, 0.3385679063, -0.0854432471
C, -1.4859305819, -0.2753745442, -1.0178751756
C, -1.069006297, 1.3943054837, 0.719841692
C, -2.7845843806, 0.200291248, -1.1443414682
H, -1.1377226249, -1.0788795592, -1.6496943868
C, -2.3825944679, 1.826121891, 0.596118286
H, -0.3985197716, 1.8624831596, 1.423005593
C, -3.232883784, 1.2384636617, -0.3348809036
H, -3.4418813903, -0.2449870854, -1.8772381631
H, -2.7342760427, 2.6326137216, 1.2234108471
H, -4.248844985, 1.5939466668, -0.4328359664
C, 3.0155553983, 1.590673189, -0.0186022967
H, 3.5724696736, 1.0469320589, -0.7754022445
H, 3.0361235067, 2.6546973193, -0.2290031274
H, 3.3990353572, 1.3925737022, 0.9775054264
O, 1.8871782941, -0.7593792808, -1.173589104
H, 1.7392548158, -1.7151756882, -1.2929813158

13 [protonated methyl dihydrogen benzeneorthosulfonate], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.9980959687, -0.3300356981, 0.0977934137
O, 1.2610818488, 1.1384260971, -0.553196372
O, 1.7985451062, 0.0915780172, 1.4137232774
H, 1.8954365706, -0.6851893939, 1.9930951579
H, 0.0166002098, -1.9803060704, 1.303915163
O, 0.7960951016, -1.9229480403, 0.7326141188
C, -0.7825649291, -0.0401158541, 0.0050103707
C, -1.583149561, -1.0031033931, -0.5990818258
C, -1.2925687164, 1.13335803, 0.5497048639
C, -2.9498838635, -0.7646388936, -0.667212167
H, -1.1660637518, -1.9049295061, -1.0195057209
C, -2.6655249643, 1.3306191544, 0.4984310686
H, -0.6470741545, 1.8661173521, 1.0065264228

C,-3.4889077803,0.3913472256,-0.1141124914
H,-3.5886602624,-1.4901803579,-1.1493155756
H,-3.0865443447,2.2264484031,0.9313344822
H,-4.5551097097,0.5617015857,-0.1604893747
C,2.5945500894,1.6906229599,-0.7235620755
H,3.228037078,0.999569914,-1.2716776052
H,2.4377581743,2.593635379,-1.3043869892
H,3.0257475553,1.9323862283,0.2429646838
O,1.7914824189,-1.0209896601,-1.0972920072
H,1.8191859164,-1.9846314788,-0.9530298181

14 [protonated methyl dihydrogen benzeneorthosulfonate, water elimination TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S,-1.1548043301,-0.5328182173,0.002879573
O,-2.0388503639,0.2265542225,-1.0087780683
H,-2.0467948238,1.1449047489,-0.4164263112
O,-1.1261331421,-1.9547136781,-0.6623867828
C,0.5988562444,-0.2503381089,0.0006170498
C,1.3272406766,-0.6005680535,1.1302627115
C,1.1609134351,0.2803617376,-1.1542748582
C,2.7014580748,-0.4035995412,1.0871100655
H,0.8544688958,-1.0178741645,2.0069052634
C,2.5372372931,0.4667586929,-1.1638993044
H,0.560023392,0.5348683736,-2.0151424473
C,3.3003871255,0.1280473766,-0.0508167215
H,3.3005971238,-0.669033154,1.9461861812
H,3.008786753,0.8757781159,-2.045832824
H,4.3704335406,0.278486556,-0.0707413428
O,-1.476262903,1.3419488878,0.8594059232
O,-1.7884456844,-0.9721459907,1.3752636271
H,-1.9546024918,-0.1288625234,1.8627919289
C,-2.3696655713,-2.6888086404,-0.974646738
H,-2.0135733888,-3.6014272972,-1.437764819
H,-2.9025209929,-2.9019699858,-0.053424257
H,-2.9670080371,-2.1050234554,-1.6671064085
H,-0.7309772354,1.9436741985,0.9738131193

14 [protonated methyl dihydrogen benzeneorthosulfonate, water elimination TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S,1.0044418843,0.1885330054,-0.0004445305
O,1.7175021551,0.4823309301,1.334343072
H,1.4368237934,1.5488516348,1.3068863208
O,1.3596416816,-1.3356590378,-0.1709773204
C,-0.7627020426,-0.01161225,-0.018752099
C,-1.454744454,0.272438768,-1.1878505945
C,-1.3608954623,-0.4697875889,1.1477004361
C,-2.8291986116,0.0740954254,-1.1772020887
H,-0.9530381978,0.6271670296,-2.0751690907
C,-2.7375013191,-0.651117011,1.1279303699
H,-0.7861325483,-0.6776647281,2.0375659442
C,-3.4650346772,-0.3817986713,-0.0268186584
H,-3.3983801927,0.2788698624,-2.0720414413
H,-3.2358371572,-1.0046536479,2.0186351123
H,-4.5356743305,-0.527837418,-0.0303465067
O,0.7764514998,2.2274174011,0.2865834938

O, 1.6560598529, 0.6801397511, -1.3432733667
H, 1.5915853814, 1.6616923508, -1.3445813665
C, 2.7573568968, -1.8001070717, -0.1321242976
H, 2.6756867504, -2.8661072253, -0.3054531773
H, 3.321057334, -1.319528248, -0.924834697
H, 3.1767745378, -1.5931018567, 0.8461865797
H, -0.1246477741, 2.5283055959, 0.4578589065

15 [protonated methyl dihydrogen benzeneorthosulfonate···water HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0.86947, -0.24301, 0.22884
O, 1.35612, 0.06083, 1.54566
H, 2.709, 3.15231, 0.5021
O, 1.13622, -1.70323, -0.25328
C, -0.86723, -0.09585, 0.05817
C, -1.4444, -0.14554, -1.21111
C, -1.61175, 0.06048, 1.22518
C, -2.82205, -0.03464, -1.30087
H, -0.83935, -0.26514, -2.09781
C, -2.9901, 0.17089, 1.10663
H, -1.12748, 0.0974, 2.18957
C, -3.58898, 0.12241, -0.14765
H, -3.29828, -0.06959, -2.27002
H, -3.5928, 0.29454, 1.99465
H, -4.66342, 0.2086, -0.23013
O, 2.10566, 2.96739, -0.22739
H, 2.2711, 3.62602, -0.91222
C, 2.5176, -2.23135, -0.22844
H, 2.39659, -3.27163, -0.5053
H, 3.1151, -1.69629, -0.95986
H, 2.91846, -2.1376, 0.77614
O, 1.5577, 0.58909, -0.88532
H, 1.79539, 1.55868, -0.59744

15 [protonated methyl dihydrogen benzeneorthosulfonate···water HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.8243200405, -0.2851401934, 0.1958930341
O, 1.2507054108, -0.3934171937, 1.5721953869
H, 3.6864261575, 2.5224790396, 0.2602167454
O, 0.9866435819, -1.6522592047, -0.5834545849
C, -0.9151757034, -0.0336524687, 0.0487900721
C, -1.4357299559, 0.4713656209, -1.1397427598
C, -1.7155423856, -0.353388187, 1.1406012878
C, -2.8078328739, 0.6552353155, -1.2291126952
H, -0.7889855919, 0.7182585794, -1.9682344905
C, -3.086045693, -0.1600296839, 1.0308080772
H, -1.2777878363, -0.7359307455, 2.050100447
C, -3.6278905511, 0.3401318685, -0.1487305652
H, -3.2351302598, 1.0473110778, -2.1406424333
H, -3.7269112488, -0.3982270838, 1.8672896064
H, -4.6957594797, 0.4887618933, -0.2264645278
O, 2.7235617893, 2.6389827792, 0.3003843583
H, 2.4916114987, 3.4566811708, -0.1687104707
C, 2.3346504558, -2.2220671192, -0.6967781866
H, 2.1852881079, -3.14667483, -1.2410813102

H, 2.9706894505, -1.5425774241, -1.2562335819
H, 2.7324829686, -2.4174681639, 0.2945314859
O, 1.5382172021, 0.7371338831, -0.6291094629
H, 2.1788889159, 1.7563580698, -0.107435432

16 [oxonium cation], in gas phase (at B3LYP/aug-cc-pVTZ level)

H, -0.8163045293, -0.4712936476, 0.2265398663
H, -0.0000000006, 0.942587282, 0.2265398663
H, 0.8163045353, -0.4712936372, 0.2265398663
O, 0., -0.0000000009, -0.0429598951

16 [oxonium cation], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

H, -0.0000000787, 0.927998, -0.224395
H, -0.8036698033, -0.4639990681, -0.224395
H, 0.803669882, -0.4639989319, -0.224395
O, 0., 0., 0.084148

17 [protonated benzenesulfonic acid], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -0.5852039241, -0.0503841858, -0.0338463939
O, -1.48401212, -0.5793111132, -1.2052162305
H, -1.6797606104, -1.5340381703, -1.1375997944
O, 0.7216489738, -0.8990251792, -0.3438826182
H, 1.3139567483, -0.9401718218, 0.4296884145
O, -1.0825136037, -0.2664298453, 1.288401436
C, -0.3055177812, 1.6112312966, -0.4667721521
C, -0.6837263904, 2.5770923553, 0.4675775344
C, 0.2731308257, 1.9192849468, -1.7016864325
C, -0.469222094, 3.907391667, 0.1393497486
H, -1.1292089925, 2.2968421576, 1.4105807149
C, 0.4724822191, 3.2555334373, -1.9994010519
H, 0.5552511757, 1.147052855, -2.4024434671
C, 0.1030325964, 4.2414587594, -1.0840289795
H, -0.7512079453, 4.6799012449, 0.8397973337
H, 0.9163741887, 3.5302739973, -2.9452128213
H, 0.2648798238, 5.2816768282, -1.3299671108

17 [protonated benzenesulfonic acid], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.394006, 0.135164, -0.004735
O, -1.788859, -0.714577, -1.254127
H, -2.753723, -0.844219, -1.345164
O, -1.960427, -0.810832, 1.122618
H, -1.964542, -0.377488, 1.99733
O, -1.921693, 1.464224, 0.044763
C, 0.348924, 0.039139, -0.007605
C, 1.052456, 1.241138, -0.018957
C, 0.967284, -1.211874, 0.016747
C, 2.438186, 1.177929, -0.010027
H, 0.535331, 2.188107, -0.034549
C, 2.351124, -1.243639, 0.023413
H, 0.39208, -2.1255, 0.029557
C, 3.080282, -0.055525, 0.010285
H, 3.011962, 2.092694, -0.018912
H, 2.860986, -2.195471, 0.040864
H, 4.160309, -0.094285, 0.017479

benzenesulfonylium cation, in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0., 0., -1.61417517
O, 0., -1.27672928, -2.25724307
O, 0., 1.27672928, -2.25724307
C, 0., 0., 0.09584283
C, 0., 1.24325997, 0.75924073
C, 0., -1.24325997, 0.75924073
C, 0., 1.22135308, 2.13772673
H, 0., 2.17038592, 0.20560365
C, 0., -1.22135308, 2.13772673
H, 0., -2.17038592, 0.20560365
C, 0., 0., 2.81944483
H, 0., 2.15127812, 2.68755165
H, 0., -2.15127812, 2.68755165
H, 0., 0., 3.90104583

benzenesulfonylium cation, in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0., 0., -1.6037517081
O, 0., -1.271725796, -2.2585171267
O, 0., 1.271725796, -2.2585171267
C, 0., 0., 0.0981379241
C, 0., 1.2429480331, 0.7594483948
C, 0., -1.2429480331, 0.7594483948
C, 0., 1.220720597, 2.1366374138
H, 0., 2.1684329153, 0.2056929471
C, 0., -1.220720597, 2.1366374138
H, 0., -2.1684329153, 0.2056929471
C, 0., 0., 2.8173914543
H, 0., 2.1499375066, 2.6857700446
H, 0., -2.1499375066, 2.6857700446
H, 0., 0., 3.8980766824

18 [benzenesulfonylium cation···water complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0.4273739318, -1.3401186303, 0.
O, 0.7104010754, -1.9198403317, 1.2750341299
O, 0.7104010754, -1.9198403317, -1.2750341299
H, -1.9909060085, -2.4610889867, -0.7783158583
H, -1.9909060085, -2.4610889867, 0.7783158583
O, -1.748183763, -1.9379031033, 0.
C, 0.1763387614, 0.3645499519, 0.
C, 0.0874251197, 1.0218655666, -1.2353603329
C, 0.0874251197, 1.0218655666, 1.2353603329
C, -0.0839296123, 2.393023718, -1.2168656031
H, 0.1647892612, 0.4758988102, -2.1635419521
C, -0.0839296123, 2.393023718, 1.2168656031
H, 0.1647892612, 0.4758988102, 2.1635419521
C, -0.1710045628, 3.0711979373, 0.
H, -0.1469651037, 2.9362981489, -2.14845328
H, -0.1469651037, 2.9362981489, 2.14845328
H, -0.3064190307, 4.1440055338, 0.

18 [benzenesulfonylium cation···water complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.011046376, 0.5788324566, -0.5475078812
O, -1.6379235644, -0.2678388326, -1.5158409946

O, -1.3785941051, 1.9366874955, -0.2863110771
H, -2.5702561708, 0.3267341155, 1.4982175299
O, -1.8337987636, -0.2266742269, 1.1870422936
C, 0.6386028052, 0.1864401316, -0.1969907082
C, 1.389811446, 1.0979436703, 0.5507440029
C, 1.1510724532, -1.0168247078, -0.6906619474
C, 2.7144391112, 0.7841135884, 0.7957676164
H, 0.9528348047, 2.01483554, 0.9144452797
C, 2.4792267508, -1.3011990798, -0.4273983192
H, 0.5344724897, -1.6924507339, -1.2627565192
C, 3.2526071094, -0.40734307, 0.3112515513
H, 3.3276641955, 1.4679464914, 1.3633819689
H, 2.911282517, -2.2183153444, -0.7989967971
H, 4.2884310431, -0.6416803176, 0.5115722864
H, -2.182281046, -1.1234413363, 1.047482805

19 [methanol···benzenesulfonylium cation···water complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

O, -1.6656020005, 0.5765246191, -1.1732232402
O, -1.4375708634, 1.0816140386, 1.3235828862
S, -1.0113095295, 0.4874600221, 0.0943147561
H, -2.358892153, -1.3063085443, 1.4136509297
H, -0.2679447356, 3.3740156349, -1.342851166
H, -0.0392878232, 3.6644253233, 0.1451858226
O, -1.8122170163, -1.4683149834, 0.6310453316
O, -0.0200053406, 2.9579167052, -0.5098029827
C, 0.6423913978, -0.0302827375, 0.0449013676
C, 1.3772347377, -0.0128502906, 1.2327465634
C, 1.1721823571, -0.4376766089, -1.1817961162
C, 2.6990258269, -0.4186563632, 1.1755214788
H, 0.929848989, 0.3159281472, 2.1585273435
C, 2.4967078315, -0.8383966082, -1.2073376331
H, 0.5717280077, -0.423413406, -2.0787243062
C, 3.2527499865, -0.8299223778, -0.0361113915
H, 3.2990314822, -0.4122243947, 2.0738728717
H, 2.9420005084, -1.1524572803, -2.1401763838
H, 4.286623882, -1.144522997, -0.0685106132
C, -2.5674927274, -2.2199885028, -0.3623503098
H, -2.9153758782, -3.1397730764, 0.102303391
H, -3.4015937202, -1.6311172801, -0.7357434082
H, -1.875547219, -2.453319039, -1.1643051914

19 [methanol···benzenesulfonylium cation···water complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

O, -1.6568690302, 0.6226530068, -1.1552499042
O, -1.4143365596, 1.0906544286, 1.3355026204
S, -1.0370823377, 0.4306764726, 0.1209108961
H, -2.321227775, -1.2548158011, 1.4176779582
H, -0.2121343764, 3.4645066861, -1.2446396247
H, 0.2075328704, 3.6425003149, 0.2133663281
O, -1.8358742534, -1.3799456465, 0.5853997443
O, 0.2163417447, 3.0081838364, -0.5119899165
C, 0.6224738871, -0.0890265648, 0.0549811204
C, 1.3611977529, -0.0898522878, 1.2383507255
C, 1.1471975079, -0.4745376437, -1.1786240915

C, 2.6848971147, -0.4898767491, 1.1690282392
H, 0.9172301347, 0.2188643686, 2.1720118532
C, 2.4738786593, -0.8696036667, -1.2172421115
H, 0.5416542751, -0.4565779733, -2.0714160919
C, 3.2354089018, -0.8780113217, -0.050773451
H, 3.2869225519, -0.4972467663, 2.0655245655
H, 2.9134650836, -1.1679801516, -2.1574677165
H, 4.2696714187, -1.1887951369, -0.0928579451
C, -2.6773507527, -2.058890798, -0.4051272664
H, -3.0337787751, -2.9707489432, 0.064285657
H, -3.5005456837, -1.415124571, -0.6971243178
H, -2.036466359, -2.2913470924, -1.2466092706

20 [benzenesulfonylium cation···methanol complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -1.0127616064, 0.5395309646, -0.545250952
O, -1.620658554, -0.3184137027, -1.5160932818
O, -1.3892882369, 1.8941029098, -0.2724339854
H, -2.4577495372, 0.4601456679, 1.5138073876
O, -1.897061497, -0.2524590347, 1.1679865311
C, 0.6430010522, 0.1644636335, -0.1940869776
C, 1.3841744526, 1.0772590903, 0.5645169357
C, 1.1767959103, -1.0237524812, -0.7056825273
C, 2.7134402404, 0.7796285741, 0.8063669208
H, 0.9361307037, 1.9879390661, 0.9326608677
C, 2.509288969, -1.292238958, -0.4464303717
H, 0.5735538923, -1.6939064126, -1.2995044465
C, 3.2694693307, -0.3975046841, 0.3059047175
H, 3.3184979766, 1.4662365579, 1.3803956704
H, 2.9579035148, -2.1945999296, -0.8357477031
H, 4.309880303, -0.6179618675, 0.5008116245
C, -2.6555489816, -1.5026365366, 1.0624870488
H, -3.0748345574, -1.7094574307, 2.0437921724
H, -3.4323329741, -1.40938181, 0.3089237882
H, -1.939738401, -2.2710496165, 0.7932015806

20 [benzenesulfonylium cation···methanol complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.0424498831, 0.5050745973, -0.5246483382
O, -1.630594995, -0.3472124605, -1.5154307599
O, -1.3931350355, 1.8813077951, -0.3229931389
H, -2.4246923493, 0.4989666047, 1.4821152808
O, -1.8726953546, -0.2151029323, 1.1178188457
C, 0.6247165888, 0.1407283469, -0.1796754354
C, 1.353789661, 1.044100496, 0.5966522035
C, 1.1731043638, -1.0248293546, -0.7185472143
C, 2.6879345629, 0.7593689675, 0.8305948528
H, 0.893864598, 1.9361688698, 0.9928112728
C, 2.5108204284, -1.2814516433, -0.4693253455
H, 0.5748861584, -1.6952964703, -1.3156785405
C, 3.2604723792, -0.3958447965, 0.3010994701
H, 3.2818751302, 1.4395002117, 1.4228233149
H, 2.967556654, -2.1702357147, -0.8786778804
H, 4.3036176912, -0.6065594429, 0.4895907237
C, -2.6217472115, -1.4828381491, 1.0622736113
H, -3.0284531976, -1.6326555343, 2.0572198956

H, -3.4046938876, -1.4120118727, 0.3152226808
H, -1.9020143018, -2.2552335178, 0.8223795009

21 [protonated methyl benzenesulfonate], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 1.3876690021, 0.1274267395, -0.0647568026
O, 1.8276809386, -0.695320576, 1.1726342671
O, 1.9214358549, -0.8274257949, -1.2226471131
H, 2.0176669387, -0.3451123344, -2.0634840499
O, 1.9176607103, 1.4534393763, -0.1751852309
C, -0.3537700158, 0.0291790384, -0.0338720001
C, -1.0523372414, 1.2345941353, 0.0330501902
C, -0.9802133634, -1.2188012468, -0.0756671821
C, -2.4382141794, 1.1761243785, 0.0598824164
H, -0.5303244566, 2.1794608787, 0.0620349772
C, -2.3636875544, -1.2449103628, -0.0464881387
H, -0.4096789208, -2.1343204094, -0.1307032388
C, -3.0864356178, -0.0540431614, 0.0209694388
H, -3.008317024, 2.0922717672, 0.1111276108
H, -2.8797252005, -2.1935219978, -0.077798259
H, -4.166740658, -0.088393901, 0.0419814686
C, 3.27326514, -0.8212978379, 1.506536703
H, 3.2616712968, -1.3067743338, 2.4745733665
H, 3.7506591337, -1.4407179491, 0.754604048
H, 3.7096223369, 0.1706206711, 1.5656359989

21 [protonated methyl benzenesulfonate], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.0581927766, 0.3392372943, 0.2050994615
O, -1.6618221213, -0.6082558027, -0.8599883335
O, -1.5506031569, -0.3868219639, 1.5202112844
H, -1.4491355283, 0.1778725662, 2.309065134
O, -1.4663315845, 1.7121302634, 0.1406578994
C, 0.6638949042, 0.0849382694, 0.0439782624
C, 1.4472783763, 1.1986211513, -0.2471081708
C, 1.1885306628, -1.1962198924, 0.2160520283
C, 2.8162664737, 1.0110986444, -0.3730270061
H, 1.0017953491, 2.1738029745, -0.3690916716
C, 2.5577014915, -1.3541785494, 0.0833673909
H, 0.5536283992, -2.0383144274, 0.4466724805
C, 3.3650849469, -0.2562846487, -0.2093174564
H, 3.4500527678, 1.8560142291, -0.5981147758
H, 2.9949422157, -2.3335084874, 0.2101580221
H, 4.4326108025, -0.3924112132, -0.30864487
C, -3.1375414437, -0.7144558143, -1.0085526128
H, -3.2531634574, -1.3158565909, -1.9007466114
H, -3.5372575694, -1.2137174941, -0.1334076428
H, -3.5515517517, 0.2786934917, -1.1433188124

22 [oxonium cation···water pre-reactive complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

H, 2.399109552468, 0.532467058737, 0.675787423451
H, 2.405335102424, -0.806112559943, -0.188594970774
O, 1.979996717090, 0.061113349565, -0.065980940643
H, 0.138722236322, 1.039956912885, 0.057730335356
H, 0.145995597874, -0.477124348137, -0.910593373414
H, 0.179469209965, -0.563443356603, 0.898399022573

C, 0.436941847840, 0.002240491799, 0.013108982377
H, -2.818456368566, 0.451061693450, -0.659170862314
H, -2.865547791118, -0.475970915657, 0.551653918193
O, -2.253696104567, -0.017210326083, -0.034459534996

22 [oxonium cation···water pre-reactive complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

H, 2.449413114582, -0.120485576863, -0.824275364966
H, 2.416198141786, 0.672199915266, 0.547749386105
O, 2.026463000932, -0.070157558808, 0.051782552382
H, 0.232690227419, -0.909409360730, -0.544633248906
H, 0.193043838764, -0.015671946977, 1.010465731774
H, 0.241599268835, 0.894084848737, -0.546093471901
C, 0.517541220654, -0.009310662041, -0.019609924378
H, -2.916682158176, -0.745462844136, 0.217640617726
H, -2.956490165056, 0.632888562230, -0.434876690303
O, -2.372140489744, 0.027709623343, 0.034414412479

23 [methyloxonium cation + water S_N2 TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

H, -0.1352263049, -2.4464583896, -0.8115795118
H, 0.6218678378, -2.4308039582, 0.5468017398
O, -0.0737573232, -1.9898255038, 0.0390708792
H, -0.9340440425, -0.0044056505, -0.5419002496
H, 0.9340440425, 0.0044056505, -0.5419002496
H, 0., 0., 1.0636430404
C, 0., 0., -0.0109394367
H, 0.1352263049, 2.4464583896, -0.8115795118
H, -0.6218678378, 2.4308039582, 0.5468017398
O, 0.0737573232, 1.9898255038, 0.0390708792

23 [methyloxonium cation + water S_N2 TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

H, -0.0776711829, -2.3482211619, -0.8470353256
H, 0.6126014604, -2.3639604729, 0.5345448199
O, -0.1314628724, -1.9829671527, 0.0472342009
H, -0.9313693958, 0.0282543121, -0.5228626849
H, 0.9313693958, -0.0282543121, -0.5228626849
H, 0., 0., 1.0837001062
C, 0., 0., 0.0100282607
H, 0.0776711829, 2.3482211619, -0.8470353256
H, -0.6126014604, 2.3639604729, 0.5345448199
O, 0.1314628724, 1.9829671527, 0.0472342009

S1 [benzenesulfonic acid···2 methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -0.727038, -1.559813, 0.283788
O, 0.530163, -1.611484, -0.433374
H, 2.3736, -1.092495, -0.407136
O, -1.673757, -2.651588, 0.194906
H, -0.998905, -1.772958, 2.394573
O, -0.291837, -1.406961, 1.843271
C, -1.552765, -0.021172, -0.071937
C, -2.923424, -0.043313, -0.304235
C, -0.811118, 1.155866, -0.122971
C, -3.569937, 1.151635, -0.595853
H, -3.463302, -0.977719, -0.26782
C, -1.476325, 2.339669, -0.412646

H, 0.256267, 1.168998, 0.056981
C, -2.848068, 2.338662, -0.648456
H, -4.63432, 1.151563, -0.785257
H, -0.913916, 3.261658, -0.457556
H, -3.355142, 3.266283, -0.877171
C, 3.159803, 2.44285, 1.344766
H, 2.692972, 3.382712, 1.638073
H, 3.152163, 1.769593, 2.208137
H, 4.2007, 2.648399, 1.073979
O, 3.241011, -0.662672, -0.438616
H, 2.811607, 1.063902, -0.011149
O, 2.422317, 1.917969, 0.253514
C, 3.91559, -1.055303, -1.630164
H, 4.098657, -2.132465, -1.645308
H, 3.352902, -0.776609, -2.524925
H, 4.873612, -0.539323, -1.644671

S1 [benzenesulfonic acid···2 methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.7115414693, -1.545255032, 0.08524894
O, 0.4923074426, -1.5500629441, -0.7294469252
H, 2.3217485618, -1.0550612437, -0.504576372
O, -1.6407970797, -2.6533330707, -0.0112506763
H, -0.8414050058, -1.6800003879, 2.2323469409
O, -0.1388855824, -1.4741471241, 1.5944698573
C, -1.5789669349, -0.0086035447, -0.1347372387
C, -2.9690191547, -0.0228190794, -0.1602638278
C, -0.8477283478, 1.1682431496, -0.2773504891
C, -3.6444523364, 1.1789043658, -0.3364143034
H, -3.507503585, -0.9519719216, -0.0524043285
C, -1.5399801893, 2.3589278579, -0.4496114817
H, 0.2332928338, 1.1650890085, -0.2563556052
C, -2.9322326797, 2.3644482341, -0.4797497334
H, -4.7247619163, 1.1850964797, -0.3634660349
H, -0.9901872641, 3.2824156657, -0.5632861667
H, -3.4624655176, 3.2965323849, -0.6175248682
C, 3.0688370353, 2.4431465954, 1.2774229611
H, 2.8067675901, 3.4936315201, 1.3958560494
H, 2.5464144251, 1.8685390731, 2.0482935858
H, 4.1464212549, 2.3372459925, 1.4346522827
O, 3.2061604336, -0.6747937978, -0.3894629075
H, 2.9194427995, 1.1063499842, -0.1573628438
O, 2.6827613963, 2.0453959085, -0.0328708073
C, 4.0598639112, -1.1449634903, -1.4361300294
H, 4.1677719461, -2.2306190295, -1.3974124179
H, 3.6835212103, -0.8568763559, -2.4200028703
H, 5.0361262223, -0.6895751984, -1.28586769

S2 [one methanol molecule-assisted benzenesulfonic acid + methanol addition TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 1.4176704598, 1.5265194415, -0.4420805809
O, 2.4792351065, 1.0286046943, -1.446197421
H, 2.8241033624, -0.0285617011, -1.3539928305
O, 1.6987641661, 1.6578895868, 0.978805639
H, 2.3211221897, 3.496757416, -0.4719829964

O, 1.5543687836, 3.1221388091, -0.927542836
C, -0.2693961808, 1.5020565025, -1.0687830385
C, -1.2796033099, 1.8939199457, -0.2053125397
C, -0.5136194463, 1.1555781093, -2.3884544173
C, -2.5857723211, 1.9219431553, -0.6842607349
H, -1.0531713503, 2.1791676242, 0.8114595107
C, -1.8223452643, 1.1948531959, -2.850439899
H, 0.2970838676, 0.8648758468, -3.039218065
C, -2.8578538145, 1.5731736909, -2.0009317738
H, -3.3871623507, 2.2233519569, -0.0238844765
H, -2.0315798481, 0.9299188024, -3.8777278007
H, -3.8745944727, 1.5999802275, -2.3678665646
C, 0.3840245861, -0.8736936069, 1.0378303601
H, -0.6130884641, -0.4316590086, 1.1489939255
H, 0.262242302, -1.9611982792, 1.0507426067
H, 0.9865747096, -0.5788827768, 1.9011185253
O, 3.0608549834, -1.3095532226, -1.1383582464
H, 2.1515842396, -1.2497827872, -0.629724114
O, 0.9812489413, -0.49571434, -0.1796773091
C, 2.9777464643, -2.1633406661, -2.2796366081
H, 2.0803066094, -1.9570670236, -2.8676073159
H, 3.8580981987, -1.9963957618, -2.8976240613
H, 2.9632466125, -3.205745131, -1.9606286577

S2 [one methanol molecule-assisted benzenesulfonic acid + methanol addition TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.3651891203, -1.0715787658, -0.2860678434
O, -1.4714871667, -0.4917627896, -1.1870351865
H, -2.327556281, 0.0927605291, -0.6939532583
O, -0.6184291908, -2.1798915799, 0.6304460281
H, -0.2060365926, -2.6822535946, -1.758683357
O, 0.3548949322, -1.9195872872, -1.5548438639
C, 1.1308096379, -0.07239733, -0.1642527447
C, 2.166548176, -0.5531176325, 0.6212251864
C, 1.2284906367, 1.1106112852, -0.8819046979
C, 3.3402475939, 0.1922828206, 0.6974060539
H, 2.0707469288, -1.4870792296, 1.1549125121
C, 2.4094032337, 1.8374938713, -0.7985675722
H, 0.4072234052, 1.4591422198, -1.4899400925
C, 3.4622230828, 1.3827482652, -0.0086173355
H, 4.1574874649, -0.1663961461, 1.3073963234
H, 2.5042504639, 2.7608256174, -1.3528332914
H, 4.3770272212, 1.9555442198, 0.052547867
C, -0.7341001019, -0.0094918351, 2.4622964164
H, 0.3451350313, -0.06031221, 2.6446821672
H, -1.1353419957, 0.8016808911, 3.0760303648
H, -1.1808083296, -0.9503769733, 2.7947729158
O, -3.1610778127, 0.7401146421, 0.0174137867
H, -2.4194937593, 0.7256971795, 0.7287404966
O, -1.0200101317, 0.2667091548, 1.1096198187
C, -3.4548154402, 2.0756515072, -0.431648771
H, -2.541859987, 2.6024138338, -0.7101482162
H, -4.1105282659, 1.9994371799, -1.294836431
H, -3.963108633, 2.6176281566, 0.3631187246

S3 [methyl dihydrogen benzeneorthosulfonate···methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0, -0.5781230803, -0.218591301, -1.5572490795
O, 0, -1.0450873081, 0.181536716, -0.0832208919
H, 0, -1.8566866802, 0.766789084, -0.0696511813
O, 0, -1.2118875408, -1.2648235734, -2.3649992475
O, 0, 0.6684631527, -1.1356843433, -0.8788904179
C, 0, 0.7183182797, 0.8432815597, -2.2391394667
C, 0, 1.1057364598, 0.616740482, -3.5495578855
C, 0, 1.292595153, 1.8320740671, -1.4585606603
C, 0, 2.1014672578, 1.4183546059, -4.0954958706
H, 0, 0.6442948991, -0.1703703768, -4.128557937
C, 0, 2.2846559799, 2.6278222927, -2.0207445953
H, 0, 0.9823760609, 1.9738821686, -0.4340384887
C, 0, 2.6883347489, 2.4238810886, -3.3354122172
H, 0, 2.4178705449, 1.2529442403, -5.1162286945
H, 0, 2.7450888533, 3.4041627382, -1.4250732775
H, 0, 3.4619090769, 3.0449583903, -3.7656153032
O, 0, -3.1495807484, 1.8289293248, -0.0354703442
H, 0, -2.9403446085, 1.8818015388, -0.9866848501
O, 0, -1.7625513946, 1.0592139745, -2.1781661339
H, 0, -2.2148542518, 0.600841986, -2.8948754827
C, 0, 0.332942157, -2.3663330067, -0.2346059792
H, 0, 1.2813735317, -2.8127393325, 0.0570034568
H, 0, -0.1924915576, -3.0331771749, -0.9172776037
H, 0, -0.2736504967, -2.1918624582, 0.6551928673
C, 0, -3.0653531892, 3.1175969503, 0.5695623148
H, 0, -3.8532237869, 3.7755575951, 0.1972061472
H, 0, -2.0942955, 3.5864288066, 0.3910618627
H, 0, -3.2001829027, 2.9825426575, 1.6405110795

S3 [methyl dihydrogen benzeneorthosulfonate···methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.325643624, 0.8027037905, 0.3328705209
O, -1.5132943806, 0.4243430893, -0.6597656788
H, -2.1735747133, -0.2238388882, -0.260267204
O, -0.4427831513, 1.7871129094, 1.4202940754
O, 0.2747779093, 1.8650901465, -0.8664761288
C, 1.1961716903, -0.1458069598, 0.0805947191
C, 2.2706180305, 0.1309134402, 0.9110504544
C, 1.2555634101, -1.1129034417, -0.910259916
C, 3.4458995682, -0.5935067061, 0.7399083654
H, 2.1979421195, 0.8930148111, 1.67357151
C, 2.4381126873, -1.8283122304, -1.0675874439
H, 0.4059766432, -1.3071489691, -1.5480922629
C, 3.5306386609, -1.5712513971, -0.2455866303
H, 4.29380678, -0.3886292805, 1.3786197735
H, 2.5019226109, -2.5856937918, -1.8365311552
H, 4.4466540826, -2.1308490313, -0.3741350699
O, -3.3050671128, -1.2646859008, 0.2790457909
H, -2.7128360951, -1.5352545218, 0.9953437366
O, -0.8875057207, -0.5585244367, 1.3846021001
H, -0.8348683898, -0.2069891339, 2.2808525333
C, -0.4473988542, 3.0696797832, -1.1337523041
H, 0.121004182, 3.5952380497, -1.8985155467

H, -0.5172095565, 3.6924382943, -0.2423039233
H, -1.4477328301, 2.857317475, -1.5131817589
C, -3.7027571074, -2.407236449, -0.4938472242
H, -4.2843853918, -3.0978458327, 0.1167323439
H, -2.8371681436, -2.9263063538, -0.9077081903
H, -4.3232103038, -2.0401804647, -1.3070304864

**S4 [one methanol molecule-assisted methyl dihydrogen benzeneorthosulfonate, water elimination TS],
in gas phase (at B3LYP/aug-cc-pVTZ level)**

S, -0.4285728833, 0.636769663, -1.5095033854
O, -0.8687899708, 0.7948502272, -0.0346172547
H, -1.6206716017, 1.5893226429, 0.1986999791
O, -1.3226168821, 0.1321130292, -2.5435911255
O, 0.5099848324, -0.7034747935, -1.1994514559
C, 1.0679616256, 1.5366432287, -1.9518351199
C, 1.4225551696, 1.5816458378, -3.2898600866
C, 1.841399243, 2.1130424995, -0.9589931711
C, 2.5940735544, 2.24080134, -3.6417762738
H, 0.7982635633, 1.1153877984, -4.0381698162
C, 3.0086805297, 2.7711988374, -1.328878615
H, 1.5443690899, 2.0481256432, 0.0770572588
C, 3.3848291428, 2.8371637875, -2.6656423973
H, 2.8866320978, 2.2865388368, -4.6817628142
H, 3.6250722641, 3.2289328648, -0.5673320375
H, 4.2945348303, 3.3499368233, -2.9461024861
O, -2.4579546292, 2.6011903634, 0.291103185
H, -2.1085045559, 2.8129347459, -0.671985549
O, -1.242750551, 2.5220631028, -1.8152094982
H, -1.7374011052, 2.3980048094, -2.6311832625
C, -0.1668440536, -1.9246932451, -0.8722708171
H, 0.6166669217, -2.6721191882, -0.775427492
H, -0.8547765089, -2.2098548647, -1.6668746524
H, -0.7026782023, -1.8300485541, 0.0722574956
C, -2.1090484568, 3.6260770522, 1.221459733
H, -1.0616554257, 3.9194011106, 1.1182063872
H, -2.7406369966, 4.5000868618, 1.0613518982
H, -2.2783891815, 3.2485250499, 2.2283609837

**S4 [one methanol molecule-assisted methyl dihydrogen benzeneorthosulfonate, water elimination TS],
in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)**

S, 0, -0.4543730956, 0.8025967085, 0.2646759875
O, 0, -1.58253351, 0.3538372629, -0.6892692361
H, 0, -2.3026358669, -0.4387704887, -0.3252923411
O, 0, -0.7186641476, 1.5995210772, 1.461659419
O, 0, 0.1039752484, 1.9842756306, -0.779071444
C, 0, 1.1149583393, -0.0603175655, 0.0565782372
C, 0, 2.1287460756, 0.2108081705, 0.961470262
C, 0, 1.2801247174, -0.9283721911, -1.0102774671
C, 0, 3.3544746251, -0.4228503972, 0.7888807473
H, 0, 1.9701018645, 0.8948976689, 1.7823397095
C, 0, 2.5124227576, -1.5544047802, -1.1660411576
H, 0, 0.4735082356, -1.1162613481, -1.7031288297
C, 0, 3.546686456, -1.3042903217, -0.2701293247
H, 0, 4.1573509522, -0.2241457951, 1.4849986295
H, 0, 2.6602884141, -2.2361589577, -1.9919451216

H,0,4.5018371552,-1.7941565835,-0.3980675024
O,0,-3.0063972738,-1.3699588268,0.2395331482
H,0,-2.2290403097,-1.4157561805,0.9113976852
O,0,-0.8748805436,-0.8840107352,1.3656302336
H,0,-0.884106408,-0.5468433897,2.2673595056
C,0,-0.7313172649,3.1329474813,-1.0003255803
H,0,-0.1678053932,3.7768753396,-1.67030702
H,0,-0.926321668,3.6557101659,-0.0655074065
H,0,-1.6701666288,2.8458852458,-1.4724096171
C,0,-3.146270406,-2.5910005808,-0.5060795685
H,0,-2.1899362067,-2.9052621466,-0.9256208149
H,0,-3.5321769711,-3.371567614,0.1469661763
H,0,-3.854330147,-2.4118158489,-1.3110653091

S5 [methyl benzenesulfonate···methanol···water HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S,0,-0.2447948224,-0.3483526649,-0.2676157863
O,0,-0.9655252422,0.9190373879,-0.2690695761
H,0,-2.693414698,1.5861908168,-0.6896784096
O,0,-0.3490011304,-1.2086834184,-1.4284801709
O,0,-0.6491234329,-1.1755168668,1.0497995587
C,0,1.4611869766,-0.0382358978,0.130995359
C,0,2.4287517272,-0.9133869242,-0.3472509987
C,0,1.7911133408,1.0747885423,0.8951554314
C,0,3.7612583516,-0.6671101761,-0.0425231943
H,0,2.139431276,-1.7590544876,-0.9534931422
C,0,3.1271282912,1.3070384446,1.1939661896
H,0,1.0172717199,1.7454048663,1.2379001242
C,0,4.1082645786,0.4380567171,0.7274244552
H,0,4.5269721709,-1.3358953395,-0.4100275045
H,0,3.401327188,2.1686148636,1.7865857949
H,0,5.1475057446,0.6259645741,0.9604531674
O,0,-3.6065929949,1.9075984488,-0.7468925184
H,0,-4.5433745153,0.6563734543,0.1984720276
O,0,-4.8992209181,-0.0793980592,0.734849388
H,0,-5.6691753682,-0.3956778155,0.2552777559
C,0,-1.9437678509,-1.8498292417,1.034892426
H,0,-1.984920681,-2.3705737302,1.9859841472
H,0,-1.9747928483,-2.5597698995,0.2114825387
H,0,-2.758869925,-1.1331544518,0.9621152849
C,0,-3.6367390048,3.2896747229,-0.4087769017
H,0,-3.0457818076,3.8833618867,-1.1108863803
H,0,-4.6736715947,3.6153469996,-0.4655797119
H,0,-3.2696259605,3.467291648,0.6057656963

S5 [methyl benzenesulfonate···methanol···water HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S,-0.1907563671,-0.3090231824,-0.1956684504
O,-0.9528161893,0.9192323354,0.0168206209
H,-2.6920147274,1.4862454028,-0.4501130032
O,-0.3460457679,-0.9851547081,-1.4722366421
O,-0.5296872916,-1.3356222724,0.9933302832
C,1.5210038082,-0.0203937388,0.1662803
C,2.4765223844,-0.8404844284,-0.4245211608
C,1.866780007,1.0197354797,1.0224084542

C, 3.8163889913, -0.6098406235, -0.1420356065
H, 2.178503519, -1.6338691652, -1.093406755
C, 3.2111769829, 1.2366932343, 1.2945254781
H, 1.1037814917, 1.6466428792, 1.4585658042
C, 4.1810651505, 0.4242972608, 0.7149050206
H, 4.5732255151, -1.2351008398, -0.5936977651
H, 3.4995136226, 2.0415339632, 1.9554914351
H, 5.2260879456, 0.6002709854, 0.92906282
O, -3.6041352274, 1.7649952173, -0.6295202241
H, -4.7734702062, 0.7835983812, 0.3421245599
O, -5.3731446909, 0.2445971421, 0.8973533068
H, -5.9774638242, -0.1785060685, 0.2798832222
C, -1.8725594086, -1.9044907289, 1.0115905729
H, -1.8853624152, -2.5462936445, 1.8853385318
H, -2.0405085362, -2.4875038357, 0.1097304988
H, -2.6147807349, -1.1160737771, 1.1104691722
C, -3.6736586906, 3.1925051195, -0.5924413695
H, -3.0338459164, 3.6375131512, -1.357005436
H, -4.7056093582, 3.4721046855, -0.7928693376
H, -3.386371496, 3.5824961755, 0.3864807196

S6 [benzenesulfonic acid...3 methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -1.5747863627, -1.6107316307, 0.0128310927
O, -0.3591416373, -1.8073888084, -0.7518762613
H, 1.5067200798, -2.0004696207, -0.4965815855
O, -2.7452281697, -2.4272220948, -0.2298358928
O, -1.1166426438, -1.8562416809, 1.5556918047
C, -2.0190031793, 0.1112546368, -0.0210686532
C, -3.3666572587, 0.4555420896, -0.0071461029
C, -1.0129021261, 1.0709077466, -0.0540049277
C, -3.7080378913, 1.8018737213, -0.0197105006
H, -4.1235898902, -0.3145900084, -0.0018595543
C, -1.3702680357, 2.4120138927, -0.0603383411
H, 0.0302840947, 0.7954840424, -0.0838265423
C, -2.7133885066, 2.7747074753, -0.0419081967
H, -4.7505071287, 2.0886348382, -0.0163663213
H, -0.5838183328, 3.1523282654, -0.0815127979
H, -2.9875725466, 3.8210253065, -0.0500770394
O, 2.4725996692, -2.0042665566, -0.4136966515
H, 3.0937568558, -0.4841861344, 0.2556369362
O, 3.3946838612, 0.3600990275, 0.6491596048
H, 2.4854287358, 1.8334017511, 0.1473339321
O, 1.9738015317, 2.6064201006, -0.1597911858
H, -1.8841900683, -2.1707244268, 2.0553891711
C, 2.7943505248, 3.3822489815, -1.0153205321
H, 3.1164920097, 2.8200539403, -1.8982814989
H, 2.2098490975, 4.2388291236, -1.3512820326
H, 3.6853077912, 3.7576340184, -0.5008378158
C, 3.0397181857, -2.6393109274, -1.5569456837
H, 4.1212243284, -2.6100790581, -1.4407775338
H, 2.7221748187, -3.682152712, -1.6261055144
H, 2.7706570677, -2.1216650725, -2.4808900432
C, 3.8263879164, 0.1333693034, 1.9842684378
H, 4.1109640213, 1.0954444925, 2.407319846
H, 3.0321559566, -0.2969148281, 2.6006630738

H, 4.6946952318, -0.530568194, 2.0157223095

S6 [benzenesulfonic acid...3 methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -1.076930, -1.565967, 0.147284
O, 0.0726, -1.356877, -0.718695
H, 1.931866, -1.608733, -0.498535
O, -1.825165, -2.804505, 0.058212
O, -0.449381, -1.442222, 1.630946
C, -2.182029, -0.180064, 0.012513
C, -3.552483, -0.414426, 0.025740
C, -1.648125, 1.101288, -0.102292
C, -4.414110, 0.670521, -0.082081
H, -3.933013, -1.420755, 0.111476
C, -2.525793, 2.172033, -0.206020
H, -0.579441, 1.270380, -0.111583
C, -3.901850, 1.958186, -0.196779
H, -5.482299, 0.5068, -0.078580
H, -2.132748, 3.174735, -0.296458
H, -4.576331, 2.799014, -0.280994
O, 2.896608, -1.646358, -0.398060
H, 3.482893, -0.035861, 0.025669
O, 3.748216, 0.876336, 0.269903
H, 2.304059, 1.940046, 0.137993
O, 1.503980, 2.495543, 0.045339
H, -1.079866, -1.770916, 2.292108
C, 1.822868, 3.622236, -0.761646
H, 2.159653, 3.327061, -1.760118
H, 0.919651, 4.221717, -0.868174
H, 2.597217, 4.245565, -0.303953
C, 3.457615, -2.353861, -1.507789
H, 4.535349, -2.379192, -1.363879
H, 3.083028, -3.378206, -1.548160
H, 3.238349, -1.853616, -2.453285
C, 4.474182, 0.840728, 1.497877
H, 4.739973, 1.864439, 1.754584
H, 3.874038, 0.421137, 2.309085
H, 5.391992, 0.256671, 1.397956

S7 [two methanol molecules-assisted benzenesulfonic acid + methanol addition TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0.301735, -1.404859, 0.259904
O, -0.936816, -1.448490, -0.591145
H, -2.125082, -0.903373, -0.326959
O, 0.382295, -2.005180, 1.586875
H, 1.063260, -3.384722, -0.151334
O, 1.162559, -2.549727, -0.627408
C, 1.502855, -0.146639, -0.222081
C, 2.568752, 0.099629, 0.629885
C, 1.380691, 0.482084, -1.451221
C, 3.531991, 1.023039, 0.239245
H, 2.645814, -0.421232, 1.572884
C, 2.352626, 1.401056, -1.826520
H, 0.546067, 0.259772, -2.098232
C, 3.425739, 1.673996, -0.984420

H, 4.368430, 1.228032, 0.893313
H, 2.270623, 1.901792, -2.781534
H, 4.179731, 2.389006, -1.283640
C, -0.167417, 0.670576, 2.400764
H, 0.809557, 1.178038, 2.419086
H, -0.899945, 1.362287, 2.835764
H, -0.107473, -0.201258, 3.058063
O, -0.555065, 0.311559, 1.100244
H, -1.417178, 1.337511, 0.340904
O, -2.158762, 1.834953, -0.167692
H, -2.902467, 0.580946, -0.263457
O, -3.127995, -0.439764, -0.334740
C, -2.611108, 2.954644, 0.597442
H, -3.700596, 2.989925, 0.579354
H, -2.280392, 2.881652, 1.632446
H, -2.224878, 3.879123, 0.167241
C, -3.838660, -0.768182, -1.546141
H, -4.812086, -0.287737, -1.510861
H, -3.282638, -0.433578, -2.419642
H, -3.961054, -1.846459, -1.572652

S7 [two methanol molecules-assisted benzenesulfonic acid + methanol addition TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.278571, -1.307536, 0.236084
O, -0.910435, -1.353587, -0.729097
H, -2.004793, -0.930759, -0.449424
O, 0.313347, -2.060585, 1.496653
H, 0.867390, -3.336596, -0.412233
O, 1.164087, -2.462410, -0.698624
C, 1.575856, -0.126298, -0.211208
C, 2.721111, -0.081007, 0.568744
C, 1.407800, 0.689029, -1.320736
C, 3.724945, 0.821692, 0.228032
H, 2.837921, -0.738894, 1.417511
C, 2.423053, 1.578663, -1.652621
H, 0.507294, 0.632825, -1.914032
C, 3.578339, 1.648998, -0.879059
H, 4.622338, 0.869747, 0.829196
H, 2.308102, 2.217077, -2.517698
H, 4.362847, 2.345041, -1.141664
C, -0.162126, 0.533205, 2.360060
H, 0.878620, 0.874136, 2.397192
H, -0.795924, 1.356178, 2.697043
H, -0.280462, -0.302170, 3.050710
O, -0.563134, 0.185917, 1.047450
H, -1.497709, 1.462185, 0.321669
O, -2.248709, 1.907967, -0.136037
H, -3.000063, 0.504903, -0.284701
O, -3.130421, -0.493702, -0.346928
C, -2.758188, 2.991673, 0.647495
H, -3.652881, 3.360231, 0.151340
H, -3.020984, 2.667365, 1.655955
H, -2.027523, 3.799536, 0.706979
C, -3.997295, -0.854603, -1.445981
H, -4.979828, -0.424612, -1.270845

H, -3.592059, -0.494712, -2.390346
H, -4.068288, -1.937810, -1.459685

S8 [methyl dihydrogen benzeneorthosulfonate···2 methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0, 0.20506, -1.133082, 0.327356
O, 0, -0.922492, -1.192214, -0.784874
H, 0, -1.768926, -0.669869, -0.585319
O, 0, 0.156447, -1.908233, 1.571097
O, 0, 1.154439, -2.182319, -0.595979
C, 0, 1.485247, 0.110274, 0.025716
C, 0, 2.422497, 0.324542, 1.02276
C, 0, 1.508994, 0.802139, -1.173337
C, 0, 3.416161, 1.271867, 0.806992
H, 0, 2.378724, -0.238012, 1.944273
C, 0, 2.50581, 1.752074, -1.370757
H, 0, 0.774914, 0.599981, -1.939261
C, 0, 3.45723, 1.987252, -0.385041
H, 0, 4.15858, 1.44873, 1.573136
H, 0, 2.539946, 2.301572, -2.301602
H, 0, 4.232299, 2.723763, -0.546727
O, 0, -0.746857, 0.255387, 1.107967
H, 0, -1.695356, 1.715869, 0.765349
O, 0, -2.440892, 2.285504, 0.481614
H, 0, -3.105609, 0.922928, -0.393543
O, 0, -3.216413, 0.015035, -0.752362
C, 0, 0.75953, -3.551963, -0.688764
H, 0, 1.551537, -4.049203, -1.245018
H, 0, 0.669534, -3.999524, 0.300471
H, 0, -0.181681, -3.653666, -1.231126
H, 0, -0.854828, -0.043062, 2.017431
C, 0, -4.336674, -0.615093, -0.134213
H, 0, -5.259612, -0.082066, -0.370257
H, 0, -4.405527, -1.625986, -0.530887
H, 0, -4.220228, -0.666693, 0.950989
C, 0, -1.957515, 3.529635, -0.010039
H, 0, -1.257879, 3.395186, -0.839478
H, 0, -2.8149, 4.098424, -0.365272
H, 0, -1.463483, 4.101304, 0.779536

S8 [methyl dihydrogen benzeneorthosulfonate···2 methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.1913630354, -1.1219790372, 0.3308886309
O, -0.9419817967, -1.1589926499, -0.7745939422
H, -1.7913024631, -0.636274678, -0.5624550371
O, 0.1569854066, -1.943293737, 1.5503816001
O, 1.1291749881, -2.1720169173, -0.6313324618
C, 1.4890948772, 0.1085368856, 0.0430241102
C, 2.4688848145, 0.2515666912, 1.0126424775
C, 1.4743653184, 0.8687688317, -1.1148537323
C, 3.4700946096, 1.195016006, 0.8089634661
H, 2.4548630012, -0.3556770386, 1.9062096904
C, 2.4807312705, 1.8117162361, -1.3003294361
H, 0.7030832059, 0.7327317966, -1.8583918348
C, 3.4761906541, 1.9749788235, -0.3429989195

H, 4.2440411103, 1.3176323928, 1.5538428728
H, 2.4843599435, 2.4144057697, -2.1978894917
H, 4.2565582654, 2.7076091657, -0.4948142083
O, -0.7353314541, 0.2309170435, 1.143030538
H, -1.6769986986, 1.7476838138, 0.8052115912
O, -2.4251306394, 2.317199374, 0.5373048077
H, -3.0983921276, 0.9445937648, -0.3263374736
O, -3.2165794897, 0.0453075164, -0.70634489
C, 0.7019440886, -3.5292965316, -0.7790862002
H, 1.4750615854, -4.0225262541, -1.3645929625
H, 0.6120143107, -4.0206366778, 0.1891337144
H, -0.2468986603, -3.5894030904, -1.3132689318
H, -0.8436189958, -0.0687847014, 2.0528121798
C, -4.324140387, -0.6045032421, -0.0716989638
H, -5.2496973553, -0.0623926165, -0.2682527742
H, -4.4033871125, -1.6037410873, -0.4933675909
H, -4.1733033746, -0.6830471351, 1.0065611815
C, -1.9355644002, 3.4977379406, -0.1024141137
H, -1.3206564697, 3.257329889, -0.9724116805
H, -2.7986519181, 4.0731022207, -0.430117912
H, -1.3504741428, 4.1049112325, 0.5910356962

**S9 [two methanol molecules-assisted methyl dihydrogen benzeneorthosulfonate, water elimination TS],
in gas phase (at B3LYP/aug-cc-pVTZ level)**

S, -0.4149287137, 1.0205439863, -0.4575388686
O, 0.719625815, 1.3497866966, 0.5009145006
H, 1.8823453956, 0.9283516397, 0.3742349847
O, -0.4370464877, 1.4883132459, -1.8398017001
O, -1.5185740268, 2.0682959347, 0.2501842707
C, -1.4769906328, -0.3465972212, 0.0440452516
C, -2.4440173518, -0.7799441509, -0.8482614995
C, -1.3336954116, -0.9005518805, 1.3042469374
C, -3.2876359476, -1.8138577704, -0.4620146876
H, -2.5300413731, -0.3224029653, -1.8230534248
C, -2.1838339593, -1.9363725359, 1.6750996166
H, -0.576555777, -0.5338041212, 1.9809703883
C, -3.1580071516, -2.3942108787, 0.7955114377
H, -4.0470661121, -2.1652904793, -1.1471516629
H, -2.0832282469, -2.3827540644, 2.6550409726
H, -3.8165899686, -3.1999457245, 1.0895728498
O, 0.7401709817, -0.5714237497, -1.100133292
H, 1.8797687464, -1.4506684955, -0.6000835454
O, 2.7475348831, -1.7846447728, -0.1667518109
H, 3.0562189883, -0.3850313732, 0.2064348221
O, 3.0083126596, 0.6222569814, 0.4496045256
C, -1.2787699115, 3.4691265399, 0.0957108822
H, -2.1101340621, 3.9658199278, 0.5910476201
H, -1.2585304433, 3.7471386334, -0.9578407129
H, -0.3429781175, 3.7608243893, 0.574687443
C, 3.5305849442, -2.5135612218, -1.1036771942
H, 3.0098344447, -3.4226703345, -1.411010887
H, 4.4664930266, -2.7959979028, -0.6233699577
H, 3.7574238714, -1.9187851439, -1.9933582146
C, 3.5482456663, 0.8804774615, 1.7566782948
H, 3.0601820558, 0.2613465281, 2.5094029934

H, 3.3849010752, 1.9308315783, 1.9820788717
H, 4.6161980888, 0.6740377859, 1.7424204566
H, 0.7361910523, -0.4300745422, -2.0511536612

S9 [two methanol molecules-assisted methyl dihydrogen benzeneorthosulfonate, water elimination TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.397194978, 0.9950433646, -0.5141800747
O, 0.7140243854, 1.3701290134, 0.4653489655
H, 1.8651087508, 0.9357344371, 0.3906007261
O, -0.4829095203, 1.5336703139, -1.8806651451
O, -1.5291887546, 2.0468220951, 0.2294698447
C, -1.4841867197, -0.3533885004, 0.0101032775
C, -2.4849162616, -0.7652187754, -0.8559149101
C, -1.3008605878, -0.9334759534, 1.2547074822
C, -3.3251538504, -1.7996696367, -0.4581612202
H, -2.6067290531, -0.2937008844, -1.8203976111
C, -2.1487082477, -1.9680199182, 1.6379507914
H, -0.5162222194, -0.5905202509, 1.9128882602
C, -3.1579882358, -2.4020427805, 0.7848942259
H, -4.1105825129, -2.1321138368, -1.1228309783
H, -2.0177700781, -2.4315216733, 2.6060455543
H, -3.813766193, -3.2062928381, 1.088301752
O, 0.7187539034, -0.4387050153, -1.1483264588
H, 1.8935864799, -1.521095163, -0.6031594397
O, 2.7051976696, -1.8548214657, -0.1403494385
H, 3.0432209113, -0.3778201881, 0.2736665745
O, 2.9965917942, 0.6159431566, 0.4717545444
C, -1.2889734796, 3.4509418998, 0.1305492888
H, -2.1131373313, 3.9360862653, 0.6501484513
H, -1.2766142771, 3.7775097791, -0.9097590106
H, -0.3496044802, 3.7273290948, 0.6117348033
C, 3.5395672891, -2.5735983973, -1.0542452013
H, 3.0337902307, -3.4732613445, -1.4072718162
H, 4.4417554556, -2.8624911331, -0.5200809926
H, 3.8161251344, -1.9569865352, -1.9119028577
C, 3.5887601377, 0.935421407, 1.7524977213
H, 3.0751783257, 0.4084760806, 2.5546425964
H, 3.4997979604, 2.0081614741, 1.892539718
H, 4.637595375, 0.6535212873, 1.727394003
H, 0.6808609775, -0.3414833788, -2.1053074258

S10 [methyl benzenesulfonate···2 methanol···water HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 1.078193, -0.540299, -0.078533
O, 0.204225, 0.503772, -0.600429
H, -1.679177, 0.732011, -0.34521
O, 0.949699, -1.88359, -0.6046
O, 0.922191, -0.58524, 1.52761
C, 2.765555, 0.010168, -0.165897
C, 3.774134, -0.94377, -0.233389
C, 3.038947, 1.372736, -0.180468
C, 5.092754, -0.515562, -0.308459
H, 3.524785, -1.994532, -0.238913
C, 4.362686, 1.785707, -0.254545
H, 2.230934, 2.08816, -0.145441

C, 5.385169, 0.844513, -0.316463
H, 5.889887, -1.243478, -0.36522
H, 4.594006, 2.841559, -0.268961
H, 6.413947, 1.172403, -0.377014
O, -2.587472, 0.786696, -0.012114
H, -3.963448, -0.129679, -0.72917
O, -4.81581, -0.519843, -1.00478
O, -6.468548, 1.278869, 0.380773
H, -5.987747, 0.608768, -0.143309
C, -0.300215, -1.183915, 2.040937
H, -1.167859, -0.608078, 1.724249
H, -0.192352, -1.144144, 3.119899
H, -0.376728, -2.215669, 1.704908
C, -2.904346, 2.147966, 0.293488
H, -2.781101, 2.789915, -0.581967
H, -3.945829, 2.174699, 0.605484
H, -2.274992, 2.524238, 1.103844
C, -4.808443, -1.912832, -0.726465
H, -4.67629, -2.114851, 0.340905
H, -5.771324, -2.315678, -1.036485
H, -4.021781, -2.428555, -1.284458
H, -7.13775, 1.632325, -0.210731

S10 [methyl benzenesulfonate···2 methanol···water HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 1.106314, -0.613703, -0.003004
O, 0.110495, 0.443147, -0.165638
H, -1.695429, 0.725032, 0.267392
O, 0.931339, -1.826153, -0.784290
O, 1.203459, -0.997612, 1.554420
C, 2.731721, 0.057191, -0.226945
C, 3.763730, -0.800247, -0.594482
C, 2.934487, 1.420391, -0.040118
C, 5.034720, -0.271113, -0.774383
H, 3.574876, -1.852890, -0.742779
C, 4.211853, 1.933374, -0.224339
H, 2.112324, 2.063742, 0.234656
C, 5.257124, 1.090229, -0.588870
H, 5.848455, -0.921203, -1.062411
H, 4.388049, 2.990534, -0.086276
H, 6.248764, 1.496224, -0.732543
O, -2.628838, 0.872704, 0.490489
H, -3.919029, 0.140198, -0.482878
O, -4.669835, -0.231942, -0.989678
O, -7.084058, 0.977709, -0.311699
H, -6.237402, 0.548357, -0.555997
C, 0.069412, -1.709214, 2.129043
H, -0.830926, -1.106282, 2.042343
H, 0.332620, -1.846220, 3.171805
H, -0.055820, -2.670652, 1.638025
C, -2.793533, 2.202204, 0.991296
H, -2.396653, 2.942572, 0.294261
H, -3.861249, 2.370060, 1.112204
H, -2.304311, 2.321296, 1.960006
C, -4.618975, -1.657005, -0.918040

H, -4.709286, -2.011783, 0.111623
H, -5.455154, -2.045961, -1.495834
H, -3.690265, -2.041119, -1.345778
H, -7.494314, 1.219663, -1.147554

S11 [benzenesulfonic acid···methyloxonium cation···methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0.1793975909, -0.1295415865, 0.6610105418
O, -0.5106710346, -1.3054640379, 0.1454669526
H, -2.3176211318, -1.3731835487, -0.4609457015
H, -2.0736420199, 1.40922484, 0.2133404018
O, -0.464601623, 1.1726282803, 0.5002103634
C, 1.8327089969, -0.0672136481, 0.0455243848
C, 2.5898107997, 1.0788646894, 0.2838779652
C, 2.3344440261, -1.1643210785, -0.6483871067
C, 3.891294577, 1.1157751162, -0.1914197113
H, 2.1715327903, 1.9183291738, 0.8198162507
C, 3.6408008824, -1.1046608307, -1.1166711652
H, 1.7185191886, -2.0332896733, -0.8245296127
C, 4.4137038716, 0.0281077111, -0.8875375878
H, 4.4973351123, 1.9939031127, -0.0207400991
H, 4.0505730832, -1.9424861821, -1.6622140321
H, 5.4295250036, 0.0666775171, -1.2553033311
C, -3.4351151495, 2.340097173, -1.0252552311
H, -3.2530021471, 3.3155418314, -0.5871444322
H, -4.4958845201, 2.2002373739, -1.2013437536
H, -2.8660767756, 2.2075248069, -1.941642817
O, -3.1941961975, -1.0100169843, -0.6853691082
H, -3.1919207065, 0.2927320628, -0.3392804855
O, -3.0371852331, 1.3364685891, -0.0370770178
O, 0.3123629902, -0.2648622098, 2.2556379834
H, 0.603778089, -1.1560691235, 2.5081501192
C, -4.2593724197, -1.9075024354, -0.2820467513
H, -5.1935314619, -1.4440889427, -0.5832353285
H, -4.140598286, -2.8546263869, -0.8018544794
H, -4.2479552955, -2.0593366094, 0.7957697891

S11 [benzenesulfonic acid···methyloxonium cation···methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.1640924582, -0.2211081288, 0.7050787471
O, -0.5232790766, -1.338652916, 0.0734739809
H, -2.3411948226, -1.3675253486, -0.5004554407
H, -2.0947966724, 1.3945674735, 0.2421560032
O, -0.472315563, 1.0922340849, 0.6942769628
C, 1.810637893, -0.0878669824, 0.066617919
C, 2.5196260621, 1.090553877, 0.2847883231
C, 2.351609903, -1.1644085672, -0.628410295
C, 3.8114280546, 1.1841081349, -0.2120901579
H, 2.0720025575, 1.9143544216, 0.8201523032
C, 3.6464156713, -1.0507438364, -1.1181376408
H, 1.7739725292, -2.0620503809, -0.7880151508
C, 4.3720142563, 0.1173039019, -0.9097053118
H, 4.3779640384, 2.0910399083, -0.057312744
H, 4.0837060976, -1.8739952838, -1.6643541522
H, 5.3786751017, 0.1991878697, -1.294989215

C, -3.3253279942, 2.3271835023, -1.1118410064
H, -3.1814775599, 3.3079088251, -0.6726937268
H, -4.3628521091, 2.1829174021, -1.3894725152
H, -2.6677498734, 2.1765069813, -1.962942802
O, -3.2157883654, -1.0043807536, -0.7325491108
H, -3.1842205941, 0.2901044992, -0.38781924
O, -3.0326070016, 1.3370582593, -0.0748231519
O, 0.3297019173, -0.5270217287, 2.2710354445
H, 0.5947631628, -1.4499347373, 2.4218102413
C, -4.2758635449, -1.8289852123, -0.1897095938
H, -5.2126655584, -1.3634907546, -0.4782161671
H, -4.20917699, -2.8230659358, -0.6237566176
H, -4.2028809773, -1.8823495748, 0.8947111146

S12 [methanol-assisted protonated benzenesulfonic acid + methanol addition TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -0.3432532842, -0.962785944, -0.259838285
O, -1.5036618235, -0.5148369876, -1.0966484623
H, -2.5490731274, 0.146951187, -0.5596499313
H, -0.2796253927, -2.6128604706, -1.6918016585
O, 0.3477079906, -1.9396502101, -1.386397972
C, 1.1883281641, -0.0082977844, -0.1988678885
C, 2.3757097977, -0.6571234566, 0.1083307734
C, 1.1207628206, 1.3451696595, -0.4956280596
C, 3.5422375878, 0.0983046229, 0.1300434249
H, 2.4000767882, -1.7160750085, 0.3154587069
C, 2.3034695487, 2.0735240146, -0.495146267
H, 0.1820081643, 1.8188542741, -0.7391896184
C, 3.5073425089, 1.4541223944, -0.1752056677
H, 4.4790669653, -0.381977206, 0.3737530374
H, 2.2806820559, 3.1247128705, -0.7448075698
H, 4.4220105529, 2.029866109, -0.1686564849
C, -0.2699769292, 0.2827336063, 2.3371702161
H, 0.4374461105, 1.0977888246, 2.1930553156
H, -0.971983624, 0.5532195843, 3.1252768188
H, 0.2782702072, -0.6056456565, 2.6589305483
O, -3.3047366439, 0.662790107, 0.0375271022
H, -2.7556513213, 0.8320086693, 0.8343273373
O, -1.0440926599, 0.0429758383, 1.1519095956
O, -0.5361970728, -2.2462537591, 0.6991708272
H, -1.0678301043, -1.9654096315, 1.4630105192
C, -3.907844379, 1.8613946647, -0.5524966047
H, -4.6059989609, 2.263298003, 0.1736779526
H, -3.1357149395, 2.583748329, -0.8031166123
H, -4.434295, 1.5282343564, -1.4396430933

S12 [methanol-assisted protonated benzenesulfonic acid + methanol addition TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.3519231107, -1.0016890018, -0.2819696284
O, -1.5102862002, -0.5624150618, -1.1112107387
H, -2.5996141733, 0.2124069223, -0.5477512741
H, -0.2227824925, -2.6053414653, -1.7729375052
O, 0.3880905142, -1.9206685671, -1.4606648642
C, 1.1541741217, -0.0029580568, -0.203358901
C, 2.3601509529, -0.6007993369, 0.1302343463

C, 1.0378096834, 1.3477030521, -0.4958864043
C, 3.4954368108, 0.2003997497, 0.1768477448
H, 2.4202216411, -1.655849531, 0.3490292751
C, 2.189454859, 2.1250209693, -0.4671333708
H, 0.0836927556, 1.784875578, -0.7482011564
C, 3.4116811225, 1.5551046668, -0.1258945801
H, 4.4447703961, -0.2414619656, 0.4437653428
H, 2.1251916217, 3.1765798375, -0.7074524726
H, 4.3009776765, 2.1686966505, -0.0958747246
C, -0.2804057758, 0.1071428739, 2.3378784555
H, 0.4013789618, 0.949562527, 2.2322640499
H, -0.997431905, 0.3201939125, 3.1286271402
H, 0.2888707603, -0.780886907, 2.6173495543
O, -3.2727908426, 0.7356573225, 0.063592182
H, -2.7215427519, 0.8109984023, 0.8741741477
O, -1.046337373, -0.0953166304, 1.1402339198
O, -0.4760338246, -2.3428081994, 0.6087978263
H, -1.032221975, -2.1391115804, 1.380482485
C, -3.7195425631, 2.0331826549, -0.4669166616
H, -4.3637782351, 2.4713715069, 0.2854244588
H, -2.8575006386, 2.6594204762, -0.6717327958
H, -4.2736540164, 1.8100052008, -1.3702888505

S13 [protonated methyl dihydrogen benzeneorthosulfonate···methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 1.7746843378, -1.8522071995, -1.639399134
O, 1.7753754869, -3.1949713053, -0.8652952553
H, 2.6828808774, -3.7257151526, -0.8175981184
O, 0.1647333769, -1.6674435246, -1.5088798606
C, 1.9944856282, -0.2636990198, -0.8002156401
C, 1.369935801, 0.862407254, -1.3226418219
C, 2.7842324648, -0.2266257208, 0.3435506839
C, 1.5697544548, 2.0756264649, -0.6762100565
H, 0.7476081369, 0.8015205363, -2.2018320753
C, 2.9413614456, 0.9932776638, 0.9896068647
H, 3.2472878788, -1.118974539, 0.7374758944
C, 2.3445212364, 2.1398749173, 0.4767980752
H, 1.1058801819, 2.9678163622, -1.0718711914
H, 3.5326028275, 1.0425721867, 1.8927448228
H, 2.4807731707, 3.0866454604, 0.9799931142
O, 3.7681598036, -4.676691524, -0.7196790368
H, 4.6497452742, -4.3280338707, -0.8831115094
O, 3.5214586984, -2.0281373386, -1.8360626471
O, 1.6536349254, -1.8945620261, -3.2418212623
H, 2.539526954, -2.0757219075, -3.6007201666
C, 3.8030398526, -5.8059198967, 0.1833857678
H, 2.7779710464, -6.1461052501, 0.2934277592
H, 4.404043142, -6.6029638785, -0.2487581018
H, 4.2002485165, -5.512955083, 1.1538537824
C, -0.7770217425, -2.6562554322, -2.004086882
H, -0.596191542, -3.6185120272, -1.5338629053
H, -1.7483920943, -2.2727063056, -1.7089385263
H, -0.7151951262, -2.7299407592, -3.0862506572
H, 3.9369908963, -1.1558840346, -1.842274006

S13 [protonated methyl dihydrogen benzeneorthosulfonate···methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.376416, 0.751028, 0.206880
O, 1.591958, 0.390487, -0.588706
H, 2.499382, -0.540188, -0.098609
O, -0.221130, 1.876808, -0.852526
C, -1.180247, -0.154750, 0.028003
C, -2.353355, 0.411963, 0.504159
C, -1.136587, -1.400725, -0.580178
C, -3.531375, -0.313922, 0.366977
H, -2.356225, 1.386762, 0.967662
C, -2.329537, -2.099332, -0.724717
H, -0.206912, -1.816206, -0.939253
C, -3.520347, -1.560858, -0.248541
H, -4.456633, 0.104199, 0.736953
H, -2.321942, -3.066598, -1.206437
H, -4.442157, -2.114473, -0.357987
O, 3.172339, -1.247838, 0.347119
H, 2.678709, -1.564115, 1.125624
O, 0.891027, -0.423787, 1.485174
O, 0.456052, 1.888734, 1.343048
H, 0.845967, 1.476053, 2.133900
C, 0.617244, 2.957623, -1.312715
H, 1.475596, 2.569776, -1.855771
H, -0.013656, 3.537470, -1.980109
H, 0.941826, 3.578861, -0.480754
H, 0.1257, -0.740230, 1.983229
C, 3.597269, -2.339905, -0.540154
H, 4.274893, -2.964613, 0.029198
H, 2.727892, -2.894782, -0.877460
H, 4.111037, -1.866252, -1.367678

S14 [methanol-assisted protonated methyl dihydrogen benzeneorthosulfonate, water elimination TS], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, 0.3555537652, 0.689722501, 0.1765859708
O, 1.5548805573, 0.3071706278, -0.6535989784
H, 2.4430941726, -0.4798255763, -0.1748075799
O, -0.2008409916, 1.8695932768, -0.7923605471
C, -1.2303128356, -0.1618417994, 0.0159077715
C, -2.3591812725, 0.4282775531, 0.5664165007
C, -1.2602551751, -1.3714609618, -0.6632568366
C, -3.5700719244, -0.2423531264, 0.4362934911
H, -2.3057059085, 1.3810577464, 1.0715647218
C, -2.4864717533, -2.01163141, -0.7976289801
H, -0.365753582, -1.7964507276, -1.0938132294
C, -3.6337486387, -1.4528257667, -0.2447016842
H, -4.4639356787, 0.1928312807, 0.8598615066
H, -2.5409086418, -2.9466071289, -1.3367789013
H, -4.5820071436, -1.960598736, -0.3494963257
O, 3.2126922061, -1.1500441384, 0.3282962637
H, 2.6973348066, -1.5224252482, 1.0661131322
O, 0.8732920808, -0.6042085401, 1.4198161035
O, 0.5409840252, 1.7290658462, 1.3862085444
H, 0.905531129, 1.2229397152, 2.1346304437
C, 0.6455928514, 2.9758242, -1.2011954272

H, 1.5188482525, 2.6050563671, -1.7306916309
H, 0.0220835835, 3.5607734996, -1.8694884176
H, 0.9335460832, 3.5723831892, -0.3393997336
H, 0.0896821506, -1.0088430053, 1.811458941
C, 3.8837700416, -2.158122942, -0.4911920973
H, 4.6040469092, -2.6697658475, 0.1386016672
H, 3.1568359451, -2.8530440184, -0.9037315248
H, 4.3931859859, -1.6158518302, -1.2798871641

S14 [methanol-assisted protonated methyl dihydrogen benzeneorthosulfonate, water elimination TS], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, 0.37620208, 0.75234909, 0.20833302
O, 1.59514217, 0.38877572, -0.57945750
H, 2.49331773, -0.54651032, -0.11147938
O, -0.21711630, 1.87215124, -0.85972921
C, -1.17968992, -0.15453791, 0.02847902
C, -2.35345992, 0.41249809, 0.50260802
C, -1.13624166, -1.39806156, -0.58463633
C, -3.53119992, -0.31375891, 0.36506502
H, -2.35700592, 1.38784809, 0.96493002
C, -2.32782892, -2.10016291, -0.72326498
H, -0.20510992, -1.81684791, -0.93592898
C, -3.51925392, -1.56144491, -0.24889898
H, -4.45691892, 0.10465009, 0.73356502
H, -2.31951692, -3.06802091, -1.20377998
H, -4.44081492, -2.11543291, -0.35855798
O, 3.07615803, -1.26497505, 0.45181261
H, 2.43235514, -1.42117599, 1.18610190
O, 0.89765391, -0.44161767, 1.52375099
O, 0.44950614, 1.89633623, 1.33891220
H, 0.83982455, 1.48985706, 2.13271296
C, 0.62243077, 2.95135476, -1.32151953
H, 1.48640050, 2.56142697, -1.85407046
H, -0.00415016, 3.52409179, -1.99905174
H, 0.93823581, 3.58008213, -0.49181334
H, 0.12799985, -0.80482199, 1.98005625
C, 3.50993052, -2.45761183, -0.28967490
H, 4.12148354, -3.04435175, 0.38511825
H, 2.64122118, -3.01233521, -0.62885773
H, 4.09637675, -2.09089395, -1.12315765

S15 [methyl benzenesulfonate···oxonium cation···methanol HB complex], in gas phase (at B3LYP/aug-cc-pVTZ level)

S, -0.1078760174, 0.7040932538, -0.0406640331
O, -0.7079121415, 0.8006809465, 1.2862035847
H, -3.7082150232, -0.2230708259, 2.5649965121
O, 0.3003885874, 2.1438406805, -0.5595711672
C, 1.4706936775, -0.0740972916, 0.0165596538
C, 1.993616104, -0.6249679503, -1.1508996963
C, 2.1537762421, -0.1016128952, 1.2289776347
C, 3.2440319806, -1.2220161589, -1.0919198837
H, 1.4380785548, -0.590171827, -2.0762192997
C, 3.4028206283, -0.7058338978, 1.2656539133
H, 1.7185771975, 0.3326949711, 2.1165642396
C, 3.9441053962, -1.2613944239, 0.1108313368

H, 3.6711390566, -1.6566559352, -1.9842374624
H, 3.951272373, -0.7417149698, 2.1959216197
H, 4.9179281763, -1.7293416702, 0.1477550235
O, -3.0382247052, -0.5769690586, 1.9700450231
H, -2.2397238679, -0.0192796011, 2.0338609555
H, -3.2753464944, -0.8210348162, 0.5498788745
O, -3.2454456921, -0.9423351002, -0.48824233
O, -0.9538083243, 0.0653635202, -1.0704152623
H, -2.3517861455, -0.5676052381, -0.7919730726
C, -0.7525902334, 3.1414917144, -0.7511486037
H, -1.2621766885, 3.3239351068, 0.1912783159
H, -0.2219459972, 4.0293337301, -1.0752467563
H, -1.4409630187, 2.805368165, -1.5222287054
C, -3.4746968621, -2.3200488283, -0.9360778097
H, -3.4318269645, -2.3107792352, -2.0194575837
H, -2.718624062, -2.9769489627, -0.5150643729
H, -4.4674167363, -2.5964004022, -0.5989076481

S15 [methyl benzenesulfonate···oxonium cation···methanol HB complex], in solution (at PCM(methanol)/B3LYP/aug-cc-pVTZ level)

S, -0.105171, 0.69688, -0.064933
O, -0.704598, 0.8242, 1.25839
H, -3.92636, 0.222219, 2.176858
O, 0.306221, 2.133589, -0.608169
C, 1.485848, -0.063685, 0.030341
C, 2.006034, -0.682216, -1.102563
C, 2.172061, -0.023938, 1.23979
C, 3.257798, -1.274944, -1.013562
H, 1.445803, -0.705518, -2.025043
C, 3.422381, -0.623618, 1.308899
H, 1.737708, 0.455996, 2.10367
C, 3.962085, -1.244528, 0.186719
H, 3.679885, -1.762723, -1.880344
H, 3.971237, -0.60716, 2.239402
H, 4.935479, -1.710648, 0.248347
O, -3.211516, -0.35123, 1.87453
H, -2.387696, 0.169931, 1.911373
H, -3.314518, -0.795102, 0.510616
O, -3.232564, -1.061836, -0.508839
O, -0.921559, 0.032596, -1.092217
H, -2.356087, -0.688821, -0.821726
C, -0.766697, 3.102045, -0.842765
H, -1.294876, 3.297299, 0.086216
H, -0.252887, 3.992473, -1.185078
H, -1.437804, 2.727248, -1.610364
C, -3.347514, -2.503536, -0.751582
H, -3.288322, -2.649254, -1.823645
H, -2.548814, -3.027146, -0.235338
H, -4.319855, -2.800906, -0.377231