Supporting information (SI) for:

Modelling CH_3SOH-aromatic complexes to probe cysteine sulfenic acid–aromatic interactions in proteins

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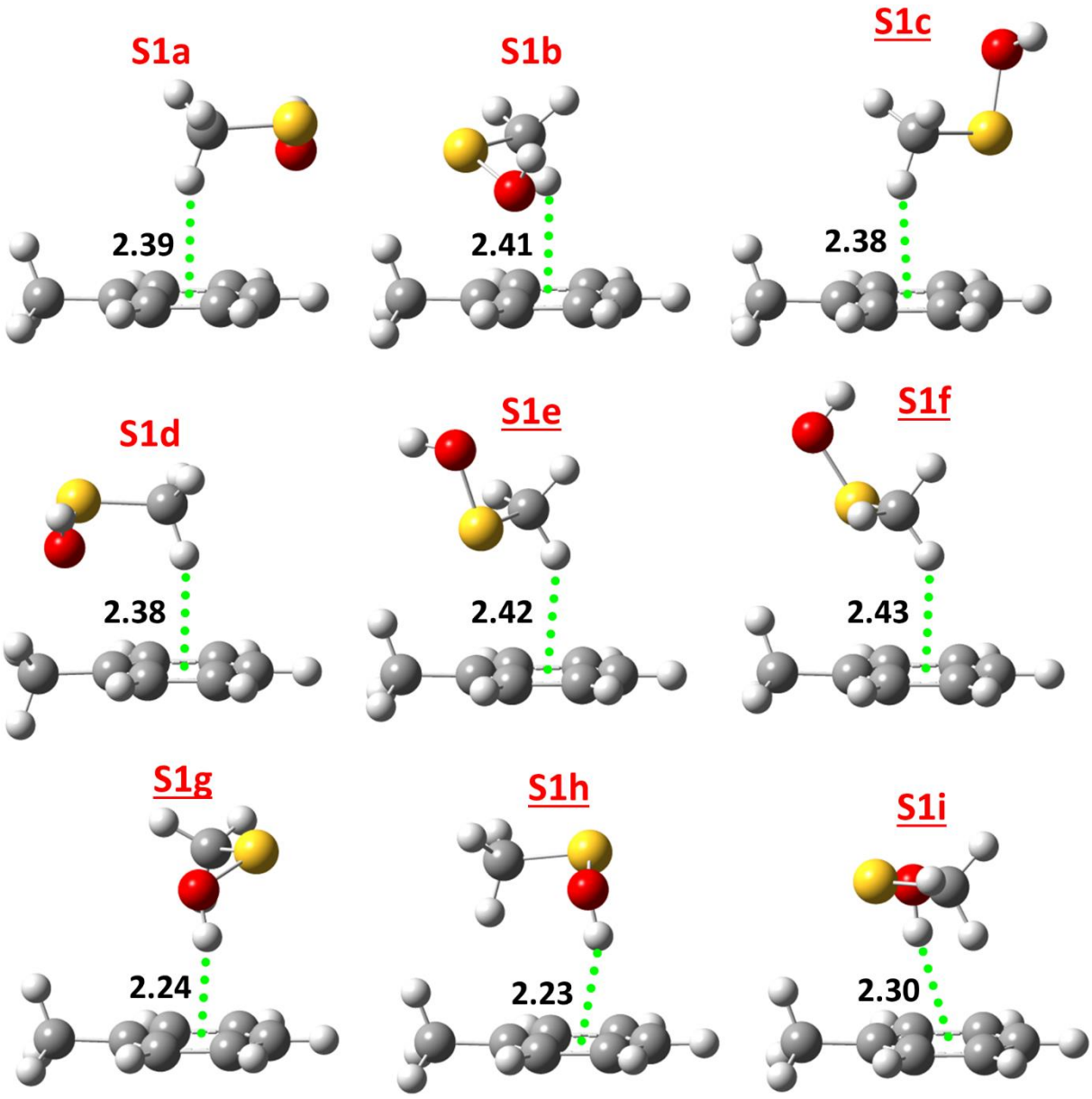

Fig. S1. Optimized geometries of the **CH_3SOH–toluene** conformers (models for **CysOH–Phe** interactions) at the MP2(full)/6-311++G(d,p) level of theory. Atom color code: hydrogen (white), carbon (gray), nitrogen (blue), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds and dotted green lines show intermolecular π-type H-bonds. Structures in which CH_3SOH is partially or fully oxidized are indicated with red and underlined red labels, respectively. The atomic coordinates are provided below starting on page S16. The global minimum conformer (**1a**) is shown in Fig. 2 of the main text (but not here).

Table S1. Ab initio [MP2(full)/6-311++G(d,p)] equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of CH_3SOH in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for CH_3SOH in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the **CH_3SOH–toluene** conformers in Fig. S1

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	CH_3SOH charge	IPV[b]	CH_3SOH spin Density[c]
S1a	4.09	33	-6.53	-2.20	-2.82	0.003	8.71	0.6
S1b	4.07	36	-7.49	-2.86	-3.14	0.007	8.78	0.6
S1c	3.77	32	-6.91	-3.09	-2.53	-0.003	8.55	1.0
S1d	4.07	31	-8.21	-3.21	-2.93	0.007	8.98	0.6
S1e	3.76	32	-7.68	-3.47	-2.72	0.003	8.60	1.0
S1f	3.80	32	-7.87	-3.57	-2.85	0.002	8.61	1.0
S1g	3.97	21	-8.72	-4.27	-5.31	0.000	8.45	1.0
S1h	3.97	23	-8.96	-4.27	-5.45	0.004	8.48	1.0
S1i	3.95	28	-9.43	-4.71	-5.15	0.009	8.49	1.0
1a[a]	3.93	27	-9.77	-4.85	-5.00	0.009	8.48	1.0

[a]The structure of the global minimum conformer (**1a**) is shown in Fig. 2 of the main text.

[b]Calculated IPVs of the free ligands are: CH_3SOH (9.20; this work) and toluene (9.45).[15]

[c]Spin density on CH_3SOH ligand following loss of one electron from the complex; a value of 1.0 indicates CH_3SOH oxidation and 0.0 aromatic oxidation.

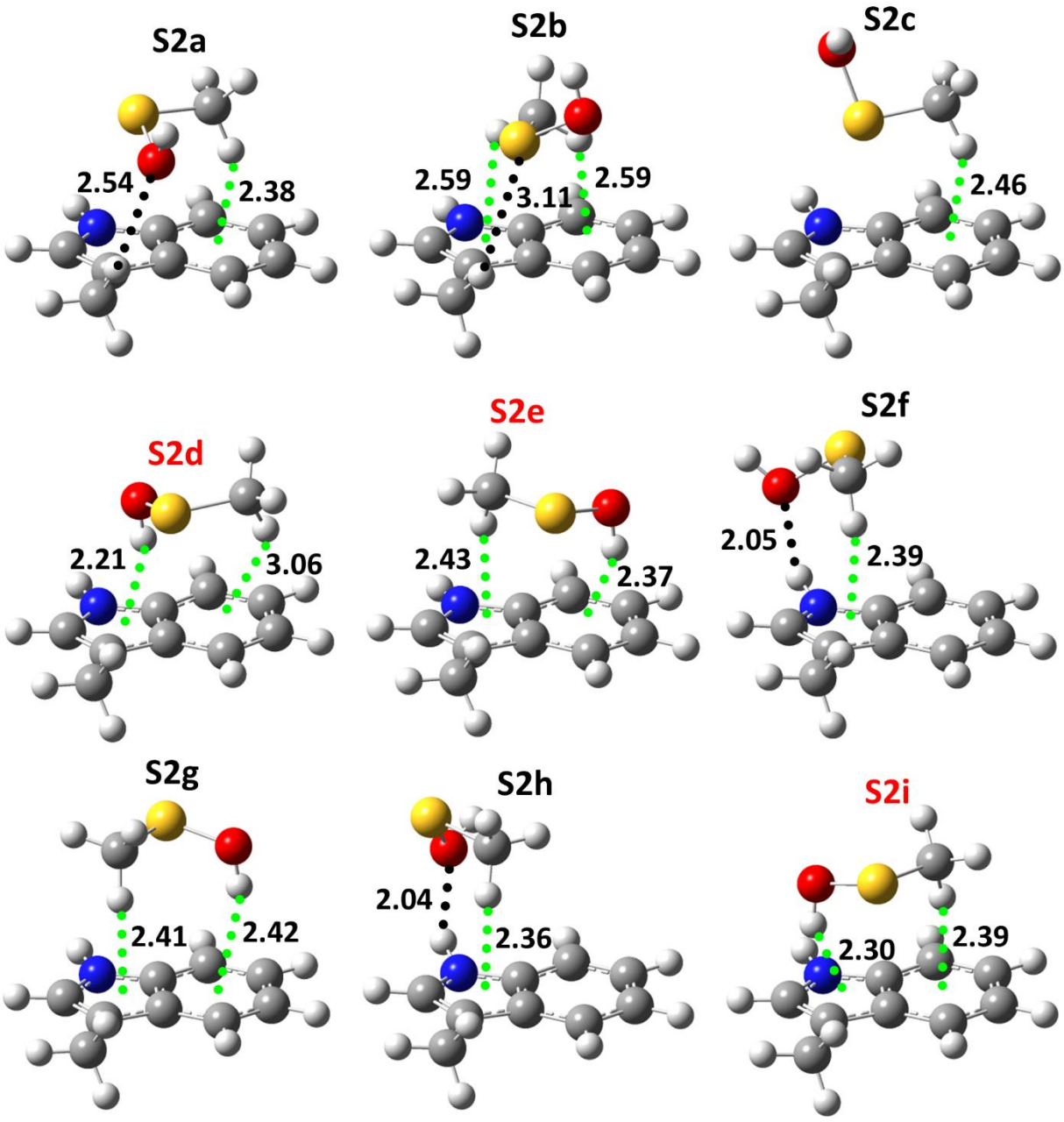

Fig. S2. Optimized geometries of the **CH_3SOH–3-methylindole** conformers (models for **CysOH–Trp** interactions) at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. Atom color code: hydrogen (white), carbon (gray), nitrogen (blue), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds and dotted green lines show intermolecular π-type H-bonds. Structures in which CH_3SOH is partially oxidized are indicated with red labels. The atomic coordinates are provided starting on page S22. The global minimum conformer (**1b**) is shown in Fig. 2 of the main text (but not here).

Table S2. Ab initio [MP2(full)/6-311++G(d,p)] equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of CH_3SOH in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for CH_3SOH in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the **CH_3SOH–3-methylindole** conformers in Fig. S2

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	CH_3SOH charge	IPV[b]	CH_3SOH spin density[c]
S2a	3.97	32	-9.58	-3.42	-3.87	0.009	7.65	0.0
S2b	4.16	36	-9.70	-4.00	-3.94	0.005	8.65	0.0
S2c	3.65	32	-10.22	-4.77	-3.68	0.004	8.65	0.0
S2d	4.07	29	-11.61	-5.88	-6.43	0.011	8.62	0.7
S2e	3.96	28	-12.49	-6.37	-6.82	0.005	8.50	0.7
S2f	4.43	47	-12.38	-6.44	-5.35	0.013	8.45	0.0
S2g	3.94	30	-12.34	-6.51	-6.18	0.004	8.90	0.0
S2h	5.01	49	-12.92	-6.78	-5.79	0.014	8.51	0.0
S2i	4.15	32	-13.24	-6.92	-6.08	-0.005	8.47	0.7
1b [a]	4.06	30	-13.05	-6.99	-6.40	-0.002	8.27	0.6

[a]Structure of the global minimum conformer (**1a**) is shown in Fig. 2 of the main text.

[b]Calculated IPVs of the free fragments are: CH_3SOH (9.20; this work) and 3-methylindole (7.88).[15]

[c]Spin density on CH_3SOH ligand following loss of one electron from the complex; a value of 1.0 indicates CH_3SOH oxidation and 0.0 aromatic oxidation.

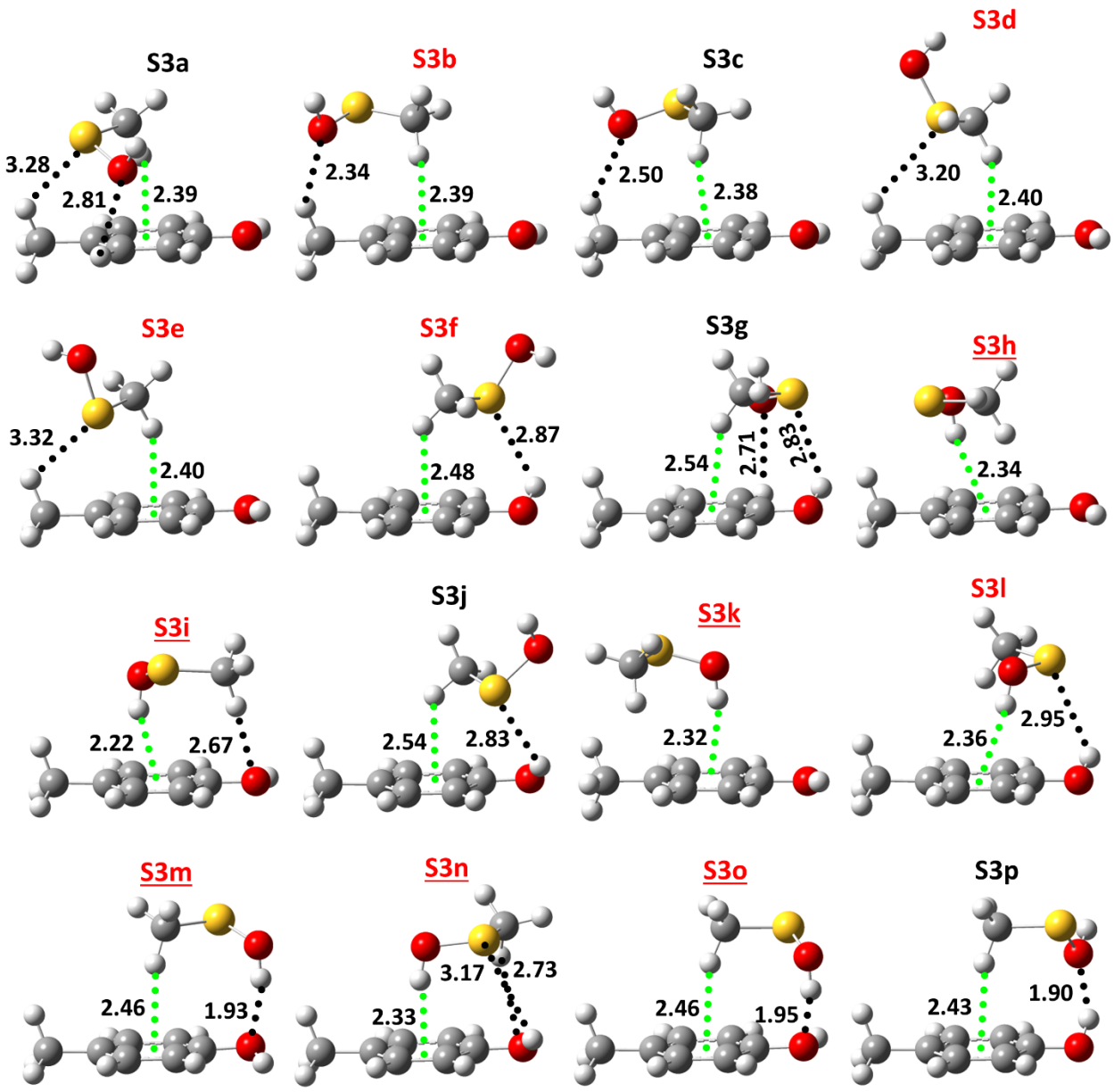

Fig. S3. Optimized geometries of the **CH_3SOH–4-methylphenol** conformers (models for **CysOH–Tyr** interactions) at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. Atom color code: hydrogen (white), carbon (gray), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds and dotted green lines show intermolecular π-type H-bonds. Structures in which CH_3SOH is partially or fully oxidized are indicated with red and underlined red labels, respectively. The atomic coordinates are provided starting on page S28. The global minimum conformer (**1c**) is shown in Fig. 2 of the main text (but not here).

Table S3. Ab initio [MP2(full)/6-311++G(d,p)] equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of CH_3SOH in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for CH_3SOH in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the **CH_3SOH–4-methylphenol** conformers in Fig. S3

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	CH_3SOH charge	IPV[b]	CH_3SOH spin density[c]
S3a	4.07	35	-7.57	-2.78	-3.18	0.007	8.63	0.0
S3b	4.14	30	-8.13	-3.33	-3.29	0.006	8.62	0.7
S3c	4.09	32	-8.14	-3.38	-3.56	0.005	8.56	0.0
S3d	3.77	32	-7.84	-3.50	-2.77	0.001	8.40	0.7
S3e	3.75	32	-7.93	-3.59	-3.06	0.000	8.47	0.6
S3f	3.77	39	-9.18	-4.54	-3.48	0.013	9.12	0.7
S3g	4.13	44	-9.37	-4.61	-4.56	0.014	8.69	0.0
S3h	3.95	28	-9.51	-4.67	-4.63	0.008	8.50	1.0
S3i	3.95	25	-9.89	-4.77	-5.46	0.003	8.39	1.0
S3j	3.86	40	-9.43	-4.80	-3.97	0.010	8.89	0.0
S3k	3.94	26	-9.90	-4.84	-4.63	0.006	8.47	1.0
S3l	3.95	36	-10.48	-5.50	-4.12	0.014	8.89	0.6
S3m	4.18	34	-10.85	-5.74	-5.63	-0.010	8.29	1.0
S3n	3.92	33	-11.09	-5.80	-4.56	0.009	8.62	1.0
S3o	4.15	37	-11.70	-6.08	-5.20	-0.006	8.47	1.0
S3p	4.19	34	-12.68	-6.61	-5.19	0.018	8.72	0.0
1c [a]	4.40	48	-12.41	-7.16	-5.95	0.024	8.60	0.0

[a]Structure of the global minimum conformer (**1c**) is shown in Fig. 2 of the main text.

[b]Calculated IPVs of the free ligands are: CH_3SOH (9.20; this work) and 4-methylphenol (8.77).[15]

[c]Spin density on CH_3SOH ligand following loss of one electron from the complex; a value of 1.0 indicates CH_3SOH oxidation and 0.0 aromatic oxidation.

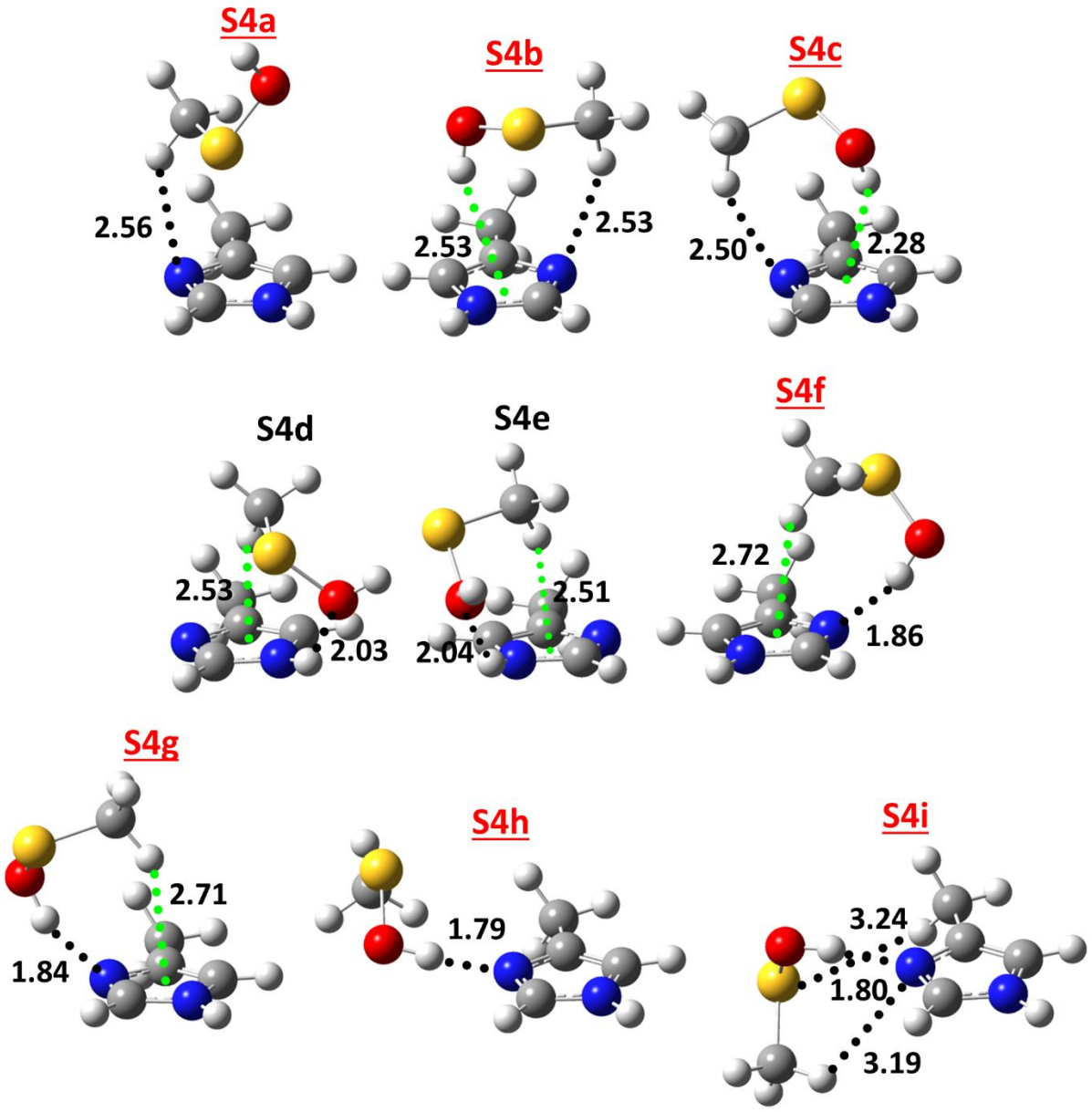

Fig. S4. Optimized geometries of the **CH_3SOH–4-methylimidazole** conformers (models for **CysOH–His** interactions) at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. Atom color code: hydrogen (white), carbon (gray), nitrogen (blue), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds and dotted green lines show intermolecular π-type H-bonds. Structures in which CH_3SOH is fully oxidized are indicated with underlined red labels. The atomic coordinates are provided starting on page S39. The global minimum conformer (**1d**) is shown in Fig. 2 of the main text (but not here).

Table S4. Ab initio [MP2(full)/6-311++G(d,p)] equilibrium distance ($r_{\mathrm{SX}}, \mathrm{\AA}$), angle ($\theta_{\mathrm{SXY}}$, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of CH_3SOH in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for CH_3SOH in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the **CH_3SOH–4-methylimidazole** conformers in Fig. S4

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	CH_3SOH charge	IPV[b]	CH_3SOH spin density[c]
S4a	3.43	11	-6.97	-3.35	-2.97	0.001	8.64	1.0
S4b	3.64	6	-9.36	-5.16	-4.66	-0.007	8.38	1.0
S4c	3.99	22	-9.64	-5.28	-5.18	-0.007	8.39	1.0
S4d	4.10	43	-10.49	-6.11	-4.85	0.011	8.52	0.0
S4e	4.09	42	-10.68	-6.21	-4.90	0.011	8.53	0.0
S4f	4.04	42	-13.58	-8.99	-8.51	-0.028	8.10	1.0
S4g	4.00	41	-13.76	-9.16	-8.52	-0.033	8.09	1.0
S4h	4.64	71	-12.99	-9.83	-9.05	-0.040	7.95	1.0
S4i	4.55	74	-13.56	-9.99	-9.12	-0.039	7.93	1.0
1d [a]	4.45	87	-13.67	-10.26	-9.06	-0.038	8.02	1.0

[a]Structure of the global minimum conformer (**1d**) is shown in Fig. 2 of the main text.

[b]Calculated IPVs of the free ligands are: CH_3SOH (9.20; this work) and 4-methylimidazole (8.78).[15]

[c]Spin density on CH_3SOH ligand following loss of one electron from the complex; a value of 1.0 indicates CH_3SOH oxidation and 0.0 aromatic oxidation.

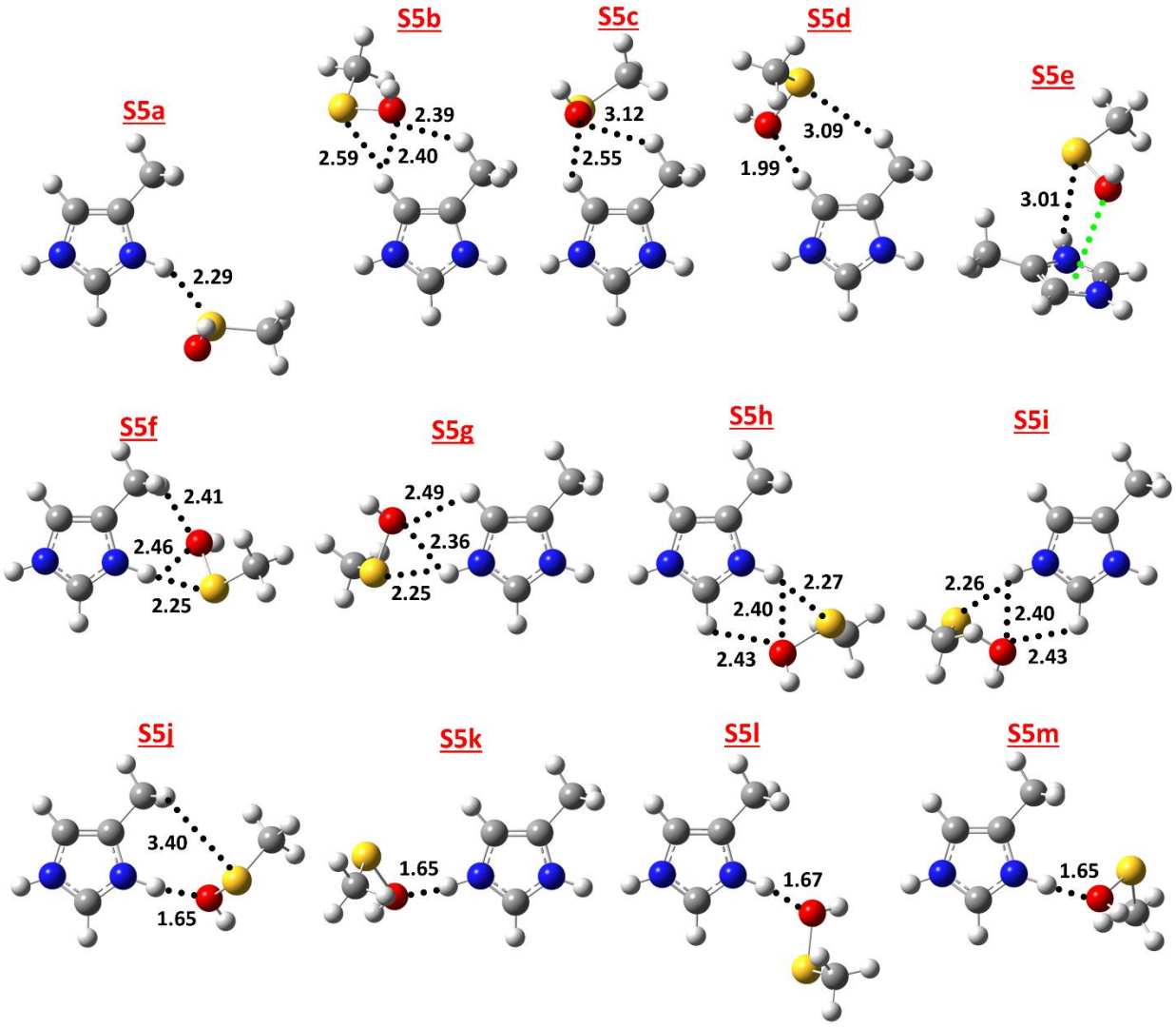

Fig. S5. Optimized geometries of the **CH_3SOH–4-methylimidazolium** conformers (models for **CysOH–His^+** interactions) at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. Atom color code: hydrogen (white), carbon (gray), nitrogen (blue), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds and dotted green line shows an intermolecular π-type H-bond. CH_3SOH is fully oxidized in all structures as indicated with underlined red labels. The atomic coordinates are provided starting on page S44. The global minimum conformer (**1e**) is shown in Fig. 2 of the main text (but not here).

Table S5. Ab initio [MP2(full)/6-311++G(d,p)] equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of CH_3SOH in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for CH_3SOH in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the **CH_3SOH–4-methylimidazolium** conformers in Fig.5

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	$E^{MM,opt}$	CH_3SOH charge	IPV[b]	CH_3SOH spin density[c]
S5a	4.29	90	-11.31	-8.92	-5.74	-6.42	0.075	12.47	1.0
S5b	4.82	90	-12.54	-9.55	-7.38	-7.68	0.030	11.99	1.0
S5c	4.70	61	-12.91	-9.62	-7.86	-8.26	0.018	11.94	1.0
S5d	4.98	85	-13.35	-9.94	-6.57	-7.00	0.029	11.93	1.0
S5e	3.78	35	-14.78	-10.47	-5.56	-10.76	0.020	12.38	1.0
S5f	4.38	83	-17.41	-13.87	-9.04	-10.99	0.084	12.72	1.0
S5g	4.36	90	-17.67	-14.29	-9.30	-12.23	0.074	12.69	1.0
S5h	4.35	90	-18.43	-14.92	-10.05	-13.01	0.076	12.78	1.0
S5i	4.35	90	-18.36	-14.97	-9.82	-12.77	0.074	12.76	1.0
S5j	4.74	70	-21.53	-16.61	-8.45	-14.80	0.062	12.50	1.0
S5k	4.66	81	-21.29	-16.70	-8.23	-14.65	0.059	12.49	1.0
S5l	4.62	84	-21.35	-16.74	-9.07	-15.29	0.061	12.59	1.0
S5m	4.76	74	-21.71	-16.78	-8.52	-14.89	0.062	12.50	1.0
1e [a]	4.64	82	-21.40	-16.86	-8.75	-15.14	0.059	12.56	1.0

[a]Structure of the global minimum conformer (**1e**) is shown in Fig. 2 of the main text.

[b]Calculated IPVs of the free ligands are: CH_3SOH (9.20; this work) and 4-methylimidazolium (14.64 eV).[24]

[c]Spin density on CH_3SOH ligand following loss of one electron from the complex; a value of 1.0 indicates CH_3SOH oxidation and 0.0 aromatic oxidation.

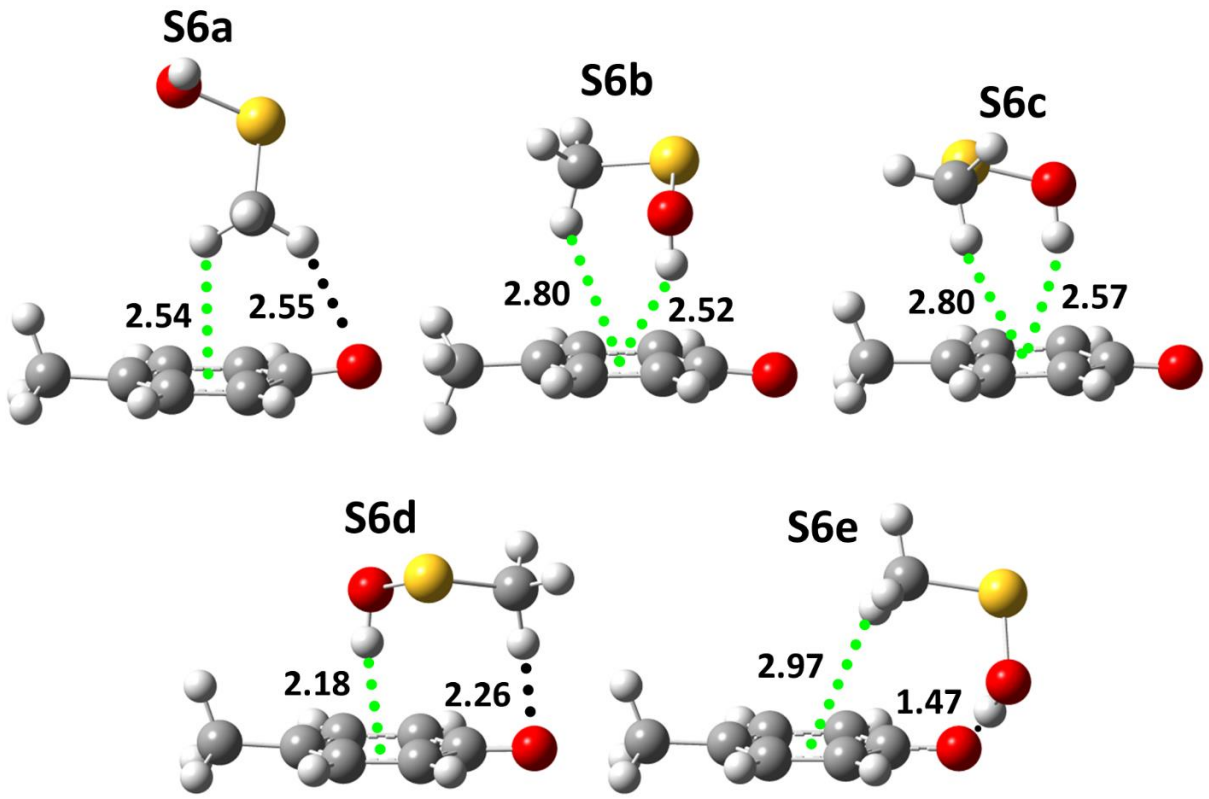

Fig. S6. Optimized geometries of the **CH_3SOH–4-methylphenolate** conformers (models for **CysOH–Tyr**$^-$ interactions) at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. Atom color code: hydrogen (white), carbon (gray), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds and dotted green lines show intermolecular π-type H-bonds. The atomic coordinates are provided starting on page S51. The global minimum conformer (**1f**) is shown in Fig. 2 of the main text (but not here). Note that CH_3SOH is not oxidized in any of the structures.

Table S6. Ab initio [MP2(full)/6-311++G(d,p)] equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of CH_3SOH in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for CH_3SOH in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the **CH_3SOH–4-methylphenolate** conformers in Fig. S6

Conformer	r_{SX}	θ_{SXY}	E	E^{CP}	E^{MM}	$E^{MM,opt}$	CH_3SOH charge	IPV[b]	CH_3SOH spin density[c]
S6a	4.81	18	-12.18	-8.29	-4.13	-5.80	-0.015	3.66	0.0
S6b	3.86	15	-18.15	-13.09	-12.29	-12.33	-0.030	3.89	0.0
S6c	3.93	28	-19.11	-13.78	-12.56	-12.58	-0.025	3.84	0.0
S6d	4.03	29	-20.09	-14.08	-13.40	-13.42	-0.020	3.85	0.0
S6e	4.80	51	-30.77	-24.71	-19.54	-25.10	-0.119	4.21	0.0
1f[a]	5.09	83	-31.05	-25.86	-18.84	-24.70	-0.122	4.15	0.0

[a]Structure of the global minimum conformer (**1f**) is shown in Fig. 2 of the main text.

[b]Calculated IPVs of the free fragments are: CH_3SOH (9.20; this work) and 4-methylphenolate (3.31 eV).[24]

[c]Spin density on CH_3SOH ligand following loss of one electron from the complex; a value of 1.0 indicates CH_3SOH oxidation and 0.0 aromatic oxidation.

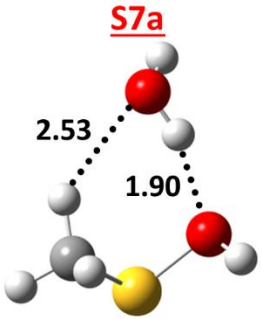

Fig. S7. Optimized geometry of the second **CH_3SOH–H_2O** conformer at the MP2(full)/6-311++G(d,p) level of theory in the gas phase. Atom color code: hydrogen (white), carbon (gray), oxygen (red) and sulfur (yellow). Dotted black lines show intermolecular σ-type H-bonds. Note that CH_3SOH is fully oxidized in this structure. The atomic coordinates are provided on page S55. The global minimum conformer (**1g**) is shown in Fig. 2 of the main text (but not here).

Table S7. Ab initio [MP2(full)/6-311++G(d,p)] equilibrium distance (r_{SX}, Å), angle (θ_{SXY}, degrees), binding energy (E and E^{CP}, kcal/mol), net charge of CH_3SOH in the neutral complexes (e), IPV (eV), sum of Mulliken atomic spin densities for CH_3SOH in the radical cation, and the MM binding energy (E^{MM}, kcal/mol) for the **CH_3SOH–H_2O** conformer in Fig. S7

Conformer	r_{SO}	E	E^{CP}	E^{MM}	CH_3SOH charge	IPV[b]	CH_3SOH spin density[c]
S7a	3.67	-7.56	-4.94	-3.80	0.013	9.38	1.0
1g [a]	3.27	-8.40	-5.87	-5.27	-0.013	8.64	1.0

[a] Structure of the global minimum conformer (**1g**) is shown in Fig. 2 of the main text.

[b]Calculated IPVs of the free ligands are: CH_3SOH (9.20; this work) and H_2O (12.60).[15]

[c]Spin density on CH_3SOH ligand following loss of one electron from the complex; a value of 1.0 indicates CH_3SOH oxidation.

We previously reported[8] PMFs for CH_3SH–imidazolium and CH_3SH–phenolate in bulk water and include in Fig. S8 the values for the corresponding methylated aromatic ions:

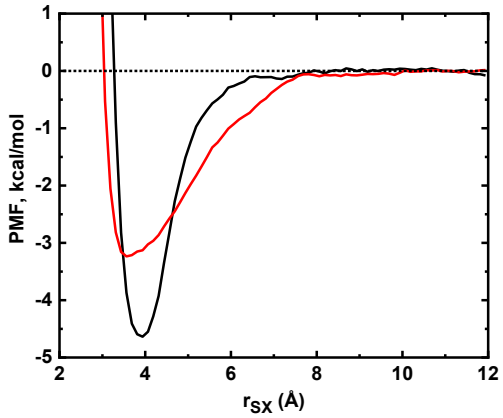

Fig. S8. Potential of mean force (PMF, kcal/mol) as a function of distance between the S atom of CH_3SH and the ring centroid X (r_{SX}, Å) of 4-methylimidazolium ion (black) and 4-methylphenolate ion (red) in bulk water at 298.15 K.

Force field (FF) for CH_3SOH and parameters for its interactions with imidazolium and phenolate

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* Topology and parameter for CH3SOH
* March 2019
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* Topology of sulfenic acid (CH3SOH)
* March 2019
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37

MASS   1 HGP    1.00800  ! polar H
MASS   2 HG3    1.00800  ! alphatic proton, CH3
MASS   3 CG3   12.01100  ! aliphatic C for methyl group (-CH3)
MASS   4 OGP   15.99940  ! hydroxyl oxygen
MASS   5 SG3   32.06000  ! sulfur

DEFA FIRS NONE LAST NONE
AUTOGENERATE ANGLES DIHEDRALS


RESI ENIC      0.000
GROUP
ATOM C1     CG3   -0.150
ATOM H2     HG3    0.090 !          H3         O6—H7
ATOM H3     HG3    0.090 !           |         /
ATOM H4     HG3    0.090 !    H2—C1—S5
ATOM S5     SG3   -0.120 !           |
GROUP                          !         H4
ATOM O6     OGP   -0.350
ATOM H7     HGP    0.350

BOND C1   H2
BOND C1   H3
BOND C1   H4
BOND C1   S5
BOND S5   O6
BOND O6   H7
PATCH FIRST NONE LAST NONE

END
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read param card !flex append
* Parameters for sulfenic acid
* March 2019
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BONDS
CG3  SG3   226.0     1.7800
CG3  HG3   338.0     1.1110
OGP  SG3   234.0     1.6660
OGP  HGP   515.0     0.9600

ANGLES
SG3  CG3  HG3     43.0    111.00
HG3  CG3  HG3     33.0    108.40    5.4   1.802
SG3  OGP  HGP     28.4    107.00   40.0   2.160
CG3  SG3  OGP     59.0    100.00

DIHEDRALS
HG3   CG3  SG3  OGP      0.32   3     0.00
HGP   OGP  SG3  CG3      3.06   2     0.00


IMPROPERS

NONBONDED nbxmod  5 atom cdiel fshift vatom vdistance vfswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5

HG3     0.0      -0.0240     1.3400                  ! alkane, yin and mackerell, 4/98
HGP     0.0      -0.0460     0.2245                  ! polar H
CG3     0.0      -0.0780     2.0500   0.0 -0.01 1.9 ! alkane (CT3), 4/98, yin, adm jr; Rmin/2 modified from 2.04 to 2.05
OGP     0.0       -0.1921     1.7650                ! og MeOH and EtOH 1/06 (was -0.1521 1.7682)
SG3     0.0      -0.4700     2.1000                  ! methylsulfate

NBFIX

NR3     OGP    -2.200    2.865    ! Sulfenic-imidazolium interaction
OC      OGP    -0.700    2.750    ! Sulfenic-phenolate interaction

END
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Atomic coordinates of the optimized structures of the 67 CH_3SOH–aromatic and 2 CH_3SOH–H_2O complexes shown in Fig. S1-S7 of the SI Information and Fig. 2A of the main text

Optimized conformers of the CH_3SOH–toluene complex

Conformer S1a

C	1.381371000	-1.410995000	-0.727317000
H	1.408525000	-1.646407000	-1.796448000
H	1.513018000	-2.335070000	-0.160883000
H	0.423361000	-0.947304000	-0.494500000
S	2.726569000	-0.262914000	-0.448970000
O	2.496475000	0.059800000	1.200237000
H	3.075067000	-0.539242000	1.684678000
C	-1.976002000	0.326379000	-1.095991000
C	-0.990945000	1.310974000	-1.232609000
C	-0.228592000	1.698949000	-0.125830000
C	-0.458170000	1.096978000	1.114963000
C	-1.445792000	0.115130000	1.244743000
C	-2.214918000	-0.288017000	0.142686000
H	-1.622594000	-0.345215000	2.214833000
H	0.140813000	1.383368000	1.973107000
H	0.542817000	2.455795000	-0.228675000
H	-0.824057000	1.778117000	-2.199698000
H	-2.567893000	0.031967000	-1.960410000
C	-3.253679000	-1.372391000	0.279976000
H	-4.067863000	-1.229215000	-0.435668000
H	-2.816811000	-2.360096000	0.095164000
H	-3.680928000	-1.380515000	1.286401000

Conformer S1b

C	-1.409563000	-0.448385000	1.536289000
H	-1.333183000	0.262450000	2.366028000
H	-1.882223000	-1.362355000	1.901320000
H	-0.408076000	-0.655186000	1.159907000
S	-2.406299000	0.365359000	0.291013000
O	-2.343495000	-0.791639000	-0.946693000
H	-3.126432000	-1.345040000	-0.850933000
C	1.248230000	1.015451000	-0.298558000
C	0.708985000	0.072326000	-1.186194000
C	1.023996000	-1.284620000	-1.070983000
C	1.888587000	-1.721814000	-0.061324000
C	2.432559000	-0.792152000	0.831678000

C	2.111082000	0.564715000	0.711687000
H	3.108635000	-1.120696000	1.616619000
H	2.542595000	1.283799000	1.405159000
H	2.139621000	-2.775276000	0.026380000
H	0.587392000	-1.996513000	-1.765362000
H	0.024534000	0.398251000	-1.965205000
C	0.875483000	2.470942000	-0.407172000
H	0.767551000	2.769448000	-1.453604000
H	-0.082208000	2.661776000	0.088945000
H	1.634388000	3.107933000	0.055546000

Conformer S1c

C	1.375067000	-1.019365000	-0.823436000
H	0.328561000	-0.723315000	-0.721727000
H	1.663038000	-0.947093000	-1.874208000
H	1.491894000	-2.044935000	-0.468884000
S	2.319607000	0.100697000	0.205910000
O	3.851818000	-0.620205000	0.060536000
H	4.288829000	-0.203495000	-0.689534000
C	-2.192590000	-0.490981000	0.118909000
C	-1.472561000	-0.080257000	1.250434000
C	-0.690184000	1.079196000	1.224535000
C	-0.621544000	1.853172000	0.060598000
C	-1.342114000	1.460130000	-1.072576000
C	-2.122733000	0.299828000	-1.038873000
H	-1.521817000	-0.674959000	2.160036000
H	-0.139197000	1.378692000	2.111419000
H	-0.013455000	2.752738000	0.037998000
H	-1.304408000	2.060529000	-1.977530000
H	-2.685205000	0.002955000	-1.921763000
C	-3.001730000	-1.762709000	0.137369000
H	-3.856799000	-1.693741000	-0.540409000
H	-2.392455000	-2.616835000	-0.178179000
H	-3.376900000	-1.974129000	1.142180000

Conformer S1d

C	1.265606000	-1.769110000	-0.249964000
H	1.279317000	-2.308515000	-1.202909000
H	1.612311000	-2.439815000	0.538683000
H	0.248795000	-1.432424000	-0.053232000
S	2.365312000	-0.373940000	-0.467514000

O	2.164735000	0.390287000	1.034744000
H	2.879984000	0.085812000	1.604088000
C	-2.461936000	-1.146267000	0.297767000
C	-2.235473000	-0.689720000	-1.005155000
C	-1.433974000	0.436957000	-1.224473000
C	-0.847569000	1.126870000	-0.153658000
C	-1.070832000	0.649008000	1.146855000
C	-1.875830000	-0.471340000	1.375137000
H	-3.087802000	-2.017134000	0.471782000
H	-2.683088000	-1.207746000	-1.849319000
H	-1.264587000	0.788768000	-2.240027000
H	-0.602456000	1.159600000	1.984529000
H	-2.041965000	-0.819926000	2.391132000
C	-0.019440000	2.364581000	-0.377359000
H	0.861668000	2.351355000	0.268536000
H	0.313406000	2.430545000	-1.416352000
H	-0.601766000	3.264355000	-0.149536000

Conformer S1e

C	1.355063000	-0.969347000	-1.053245000
H	0.308249000	-1.170963000	-0.814413000
H	1.399708000	-0.379896000	-1.971602000
H	1.878494000	-1.917554000	-1.187582000
S	2.036831000	-0.096226000	0.353684000
O	3.683786000	-0.138614000	-0.064116000
H	3.865228000	0.655152000	-0.578146000
C	-2.152545000	-1.578556000	0.248590000
C	-1.494163000	-0.973231000	1.324526000
C	-1.066625000	0.355279000	1.226563000
C	-1.266731000	1.094114000	0.049949000
C	-1.934867000	0.477501000	-1.017979000
C	-2.369471000	-0.849260000	-0.925985000
H	-2.494861000	-2.606663000	0.324984000
H	-1.325400000	-1.528098000	2.243312000
H	-2.113624000	1.040657000	-1.931623000
H	-2.889961000	-1.307247000	-1.762819000
H	-0.566851000	0.823705000	2.071386000
C	-0.771431000	2.511794000	-0.063427000
H	0.265333000	2.529756000	-0.416195000
H	-1.382482000	3.086388000	-0.764826000
H	-0.798796000	3.013536000	0.907555000

Conformer S1f

C	-1.316424000	-0.904580000	-1.091047000
H	-0.283052000	-1.149146000	-0.832566000
H	-1.824464000	-1.814583000	-1.416640000
H	-1.312781000	-0.165190000	-1.893864000
S	-2.056623000	-0.238064000	0.396156000
O	-3.620778000	0.084248000	-0.183084000
H	-4.154931000	-0.696607000	-0.002796000
C	1.903951000	0.540391000	-1.015439000
C	1.226219000	1.105836000	0.073916000
C	1.073960000	0.334736000	1.237213000
C	1.561433000	-0.974651000	1.302323000
C	2.229897000	-1.529447000	0.204684000
C	2.401151000	-0.766633000	-0.955526000
H	0.566199000	0.765421000	2.097231000
H	1.431881000	-1.554685000	2.212088000
H	2.618448000	-2.542643000	0.255576000
H	2.929760000	-1.184035000	-1.808363000
H	2.043062000	1.128657000	-1.920075000
C	0.649052000	2.493894000	-0.005331000
H	1.155271000	3.088709000	-0.770288000
H	-0.417549000	2.449917000	-0.251771000
H	0.744897000	3.011963000	0.952889000

Conformer S1g

C	2.477779000	-1.232389000	0.723268000
H	3.351443000	-1.200246000	1.381991000
H	1.572484000	-1.195751000	1.331490000
H	2.506011000	-2.157128000	0.144519000
S	2.600364000	0.189067000	-0.359130000
O	1.275835000	-0.113122000	-1.357864000
H	0.515646000	0.342131000	-0.970772000
C	-0.597509000	0.754066000	1.543731000
C	-1.210456000	-0.456396000	1.203956000
C	-1.897261000	-0.604187000	-0.010631000
C	-1.973516000	0.501403000	-0.871207000
C	-1.365016000	1.717963000	-0.536743000
C	-0.670946000	1.846884000	0.672754000
H	-0.067216000	0.847736000	2.487443000
H	-1.151265000	-1.301080000	1.887212000
H	-0.193199000	2.786624000	0.932679000
H	-1.433846000	2.561777000	-1.217675000

H	-2.506180000	0.408248000	-1.814904000
C	-2.502954000	-1.927256000	-0.399394000
H	-1.785997000	-2.524186000	-0.973269000
H	-2.788680000	-2.503240000	0.484719000
H	-3.392434000	-1.785511000	-1.018842000

Conformer S1h

C	-2.393334000	1.302940000	0.130816000
H	-3.176705000	1.629735000	0.822088000
H	-1.423897000	1.618290000	0.520338000
H	-2.572847000	1.755519000	-0.845972000
S	-2.512602000	-0.480960000	0.026732000
O	-1.354534000	-0.762507000	-1.164679000
H	-0.513358000	-0.923712000	-0.716060000
C	1.403417000	-1.850741000	0.418565000
C	0.906606000	-0.993821000	1.407495000
C	0.958468000	0.392731000	1.221949000
C	1.496076000	0.946543000	0.050904000
C	1.999886000	0.076344000	-0.928367000
C	1.954672000	-1.310186000	-0.750841000
H	0.577854000	1.051393000	1.999581000
H	0.479994000	-1.401958000	2.319033000
H	1.366242000	-2.927132000	0.558476000
H	2.346648000	-1.967666000	-1.521646000
H	2.423902000	0.488318000	-1.841333000
C	1.508092000	2.436757000	-0.169366000
H	2.422958000	2.749447000	-0.680160000
H	0.659208000	2.743133000	-0.790708000
H	1.444611000	2.976645000	0.779152000

Conformer S1i

C	2.610304000	-1.140316000	0.515560000
H	3.351299000	-1.015601000	1.311481000
H	1.697631000	-1.562265000	0.940760000
H	3.016564000	-1.808886000	-0.245133000
S	2.317684000	0.486703000	-0.172522000
O	1.281319000	0.075178000	-1.435135000
H	0.379954000	0.070974000	-1.081449000
C	-0.898897000	-0.001852000	1.303865000
C	-1.119584000	-1.366509000	1.089768000

C	-1.737511000	-1.803321000	-0.087399000
C	-2.131926000	-0.865973000	-1.047427000
C	-1.913213000	0.499422000	-0.825683000
C	-1.286044000	0.950755000	0.347710000
H	-1.909901000	-2.862461000	-0.254540000
H	-2.616887000	-1.192952000	-1.962786000
H	-2.227258000	1.224108000	-1.573686000
H	-0.822185000	-2.086769000	1.847306000
H	-0.416861000	0.331578000	2.219896000
C	-1.016369000	2.416337000	0.565609000
H	-1.075479000	2.669346000	1.627471000
H	-0.012406000	2.680656000	0.216609000
H	-1.738534000	3.032334000	0.023497000

Conformer 1a

C	2.364789000	0.525993000	1.064663000
H	3.079777000	1.332996000	0.875082000
H	1.390622000	0.959667000	1.298790000
H	2.719018000	-0.071616000	1.906213000
S	2.296226000	-0.464076000	-0.425999000
O	1.242211000	-1.670047000	0.095183000
H	0.345376000	-1.379702000	-0.124716000
C	-1.135571000	0.189467000	-1.273447000
C	-0.952393000	1.136306000	-0.252207000
C	-1.413341000	0.825070000	1.034580000
C	-2.040884000	-0.397909000	1.301141000
C	-2.221203000	-1.330642000	0.275876000
C	-1.767171000	-1.032671000	-1.016481000
H	-0.778265000	0.411986000	-2.276368000
H	-1.282493000	1.548151000	1.836888000
H	-2.387003000	-0.620514000	2.306462000
H	-2.707147000	-2.280550000	0.477837000
H	-1.903178000	-1.750339000	-1.820937000
C	-0.296035000	2.457760000	-0.553647000
H	-0.101827000	3.021232000	0.362886000
H	0.653846000	2.302308000	-1.074204000
H	-0.935168000	3.071728000	-1.196275000

Optimized conformers of the CH_3SOH–3-methylindole complex

Conformer S2a

C	0.675570000	-2.440115000	-0.229256000
H	0.323277000	-2.819896000	-1.194245000
H	1.031813000	-3.280306000	0.371106000
H	-0.152682000	-1.934304000	0.266454000
S	1.985200000	-1.278073000	-0.600774000
O	2.287094000	-0.681982000	0.958968000
H	2.985369000	-1.229077000	1.336413000
C	-0.637069000	0.804093000	0.408001000
C	-1.212500000	0.441269000	-0.844667000
C	-2.256507000	-0.488043000	-0.947486000
C	-2.745240000	-1.040031000	0.234708000
C	-2.196636000	-0.686052000	1.489869000
C	-1.158732000	0.237594000	1.587595000
C	0.364850000	1.796582000	0.155327000
C	0.381061000	1.983442000	-1.212000000
H	-2.690014000	-0.751257000	-1.909735000
H	-3.559632000	-1.758073000	0.189992000
H	-2.608211000	-1.131415000	2.391681000
H	-0.742917000	0.504969000	2.555973000
H	1.004519000	2.636564000	-1.809497000
H	-0.720022000	1.099132000	-2.804554000
N	-0.568355000	1.177469000	-1.810810000
C	1.231327000	2.462400000	1.175377000
H	0.628143000	2.956421000	1.945080000
H	1.873310000	1.722650000	1.662196000
H	1.868834000	3.220506000	0.710640000

Conformer S2b

C	1.343914000	-0.710048000	-1.394661000
H	0.655658000	0.050511000	-1.777654000
H	1.866620000	-1.170421000	-2.236361000
H	0.769975000	-1.453494000	-0.838787000
S	2.475773000	0.162838000	-0.318765000
O	3.431531000	-1.136116000	0.211930000
H	4.172026000	-1.206679000	-0.400067000
C	-0.970455000	0.321547000	0.599890000
C	-1.730046000	-0.025678000	-0.552136000
C	-2.229989000	-1.317894000	-0.761312000
C	-1.945447000	-2.276610000	0.208138000
C	-1.175643000	-1.957985000	1.352284000

C	-0.676599000	-0.674847000	1.551396000
C	-0.589390000	1.698726000	0.472400000
C	-1.119267000	2.132785000	-0.727569000
H	-2.808900000	-1.568797000	-1.646920000
H	-2.318691000	-3.289084000	0.081406000
H	-0.960480000	-2.737061000	2.078338000
H	-0.074984000	-0.442527000	2.426314000
H	-1.071820000	3.111596000	-1.188097000
H	-2.349995000	1.187286000	-2.182631000
N	-1.776690000	1.091050000	-1.357953000
C	0.162668000	2.510192000	1.479209000
H	-0.430431000	2.650279000	2.389338000
H	1.096977000	2.014578000	1.759178000
H	0.407780000	3.498857000	1.080572000

Conformer S2c

C	-1.705077000	-1.753805000	-0.603236000
H	-0.635026000	-1.812324000	-0.822225000
H	-1.930531000	-2.411585000	0.237910000
H	-2.265004000	-2.062954000	-1.488512000
S	-2.029504000	-0.043786000	-0.181934000
O	-3.693855000	-0.156693000	0.169439000
H	-4.164945000	0.049142000	-0.644994000
C	1.030520000	-0.134289000	1.014421000
C	1.172012000	0.435485000	-0.284859000
C	1.693605000	-0.358933000	-1.327027000
C	2.002742000	-1.690627000	-1.065560000
C	1.834565000	-2.241408000	0.227716000
C	1.350913000	-1.472103000	1.283317000
C	0.440746000	2.028743000	1.123275000
H	1.837252000	0.058337000	-2.321069000
H	2.401580000	-2.316766000	-1.859155000
H	2.093662000	-3.282118000	0.402041000
H	1.241682000	-1.892525000	2.280070000
H	0.082680000	2.931811000	1.600999000
C	0.783538000	2.810918000	-1.309180000
H	1.770247000	2.907026000	-1.774834000
H	0.074682000	2.507225000	-2.087362000
H	0.484772000	3.798924000	-0.947837000
C	0.804918000	1.818730000	-0.191149000
N	0.623701000	0.872561000	1.858073000
H	0.215061000	0.715732000	2.767584000

Conformer S2d

C	-3.007523000	0.844018000	0.022818000
H	-3.765972000	0.839090000	0.812286000
H	-2.172852000	1.474385000	0.335891000
H	-3.453504000	1.229453000	-0.895681000
S	-2.481312000	-0.854358000	-0.197016000
O	-1.412785000	-0.642401000	-1.483088000
H	-0.558880000	-0.408793000	-1.091453000
C	0.962908000	-0.028273000	0.579111000
C	1.476842000	0.550077000	-0.620669000
C	1.369524000	1.920862000	-0.897121000
C	0.799829000	2.726986000	0.084057000
C	0.317159000	2.180367000	1.297667000
C	0.411856000	0.818904000	1.563996000
C	1.225679000	-1.437597000	0.528665000
C	1.846613000	-1.668964000	-0.683822000
H	1.749552000	2.344171000	-1.823416000
H	0.708357000	3.794772000	-0.093757000
H	-0.106920000	2.847065000	2.043901000
H	0.040897000	0.406494000	2.498937000
H	2.188763000	-2.600681000	-1.115278000
H	2.370080000	-0.391702000	-2.304204000
N	2.000179000	-0.479223000	-1.369667000
C	0.873688000	-2.446818000	1.574506000
H	1.378711000	-2.226390000	2.520940000
H	-0.204874000	-2.450143000	1.760774000
H	1.169217000	-3.451584000	1.260447000

Conformer S2e

C	2.007959000	0.810969000	-1.386833000
H	2.357130000	1.847928000	-1.343125000
H	2.404976000	0.338809000	-2.287536000
H	0.917421000	0.810220000	-1.403177000
S	2.633449000	-0.004131000	0.080211000
O	2.040709000	-1.556449000	-0.199913000
H	1.166328000	-1.606532000	0.215487000
C	-0.917352000	0.217278000	0.557104000
C	-1.488565000	-0.193064000	-0.682164000
C	-1.697116000	-1.542096000	-1.002545000
C	-1.381558000	-2.487425000	-0.030330000
C	-0.834065000	-2.101993000	1.217934000
C	-0.617084000	-0.760521000	1.527717000
C	-0.846862000	1.648530000	0.551841000

C	-1.353562000	2.051934000	-0.668465000
H	-2.117580000	-1.841543000	-1.959220000
H	-1.534218000	-3.541723000	-0.241657000
H	-0.607008000	-2.867193000	1.955206000
H	-0.196619000	-0.474106000	2.488567000
H	-1.473874000	3.050841000	-1.068245000
H	-2.153956000	0.979598000	-2.325142000
N	-1.720453000	0.947843000	-1.414782000
C	-0.314325000	2.516592000	1.646674000
H	-0.862465000	2.352442000	2.580452000
H	0.741757000	2.298039000	1.836867000
H	-0.404393000	3.574789000	1.385317000

Conformer S2f

C	-1.770145000	-0.330344000	1.628039000
H	-1.677250000	0.329438000	2.497579000
H	-2.166263000	-1.292497000	1.957816000
H	-0.784675000	-0.447745000	1.176534000
S	-2.907615000	0.508678000	0.527876000
O	-2.977653000	-0.613197000	-0.753482000
H	-3.746011000	-1.177673000	-0.612908000
C	1.608306000	-0.144290000	-0.021673000
C	0.535735000	0.383682000	-0.797247000
C	0.315759000	1.762195000	-0.929591000
C	1.205409000	2.617058000	-0.284340000
C	2.290597000	2.114172000	0.472365000
C	2.506948000	0.745869000	0.601884000
C	1.503055000	-1.574787000	-0.064698000
C	0.393102000	-1.851724000	-0.840712000
H	-0.515431000	2.147782000	-1.513604000
H	1.064161000	3.691416000	-0.364517000
H	2.970332000	2.813583000	0.951532000
H	3.344462000	0.370355000	1.185445000
H	-0.032840000	-2.809947000	-1.110947000
H	-1.123792000	-0.624926000	-1.634515000
N	-0.161329000	-0.681459000	-1.320937000
C	2.430233000	-2.557573000	0.578172000
H	3.444952000	-2.467505000	0.175622000
H	2.489467000	-2.397586000	1.660179000
H	2.091259000	-3.583313000	0.406992000

Conformer S2g

C	1.321851000	-2.001677000	-0.819580000
H	1.323404000	-2.988082000	-0.343972000
H	0.342358000	-1.541777000	-0.678766000
H	1.533287000	-2.121189000	-1.883836000
S	2.613767000	-1.042745000	-0.030980000
O	2.502631000	0.364975000	-0.949025000
H	1.851862000	0.939216000	-0.517216000
C	-1.324814000	0.461372000	-0.112676000
C	-0.462230000	0.395635000	1.019730000
C	0.435964000	1.423247000	1.340973000
C	0.508491000	2.505907000	0.464182000
C	-0.326274000	2.583101000	-0.677767000
C	-1.230014000	1.569611000	-0.979538000
C	-2.136195000	-0.721699000	-0.106309000
C	-1.753642000	-1.442184000	1.009444000
H	1.073796000	1.366415000	2.219151000
H	1.193945000	3.320803000	0.680446000
H	-0.242196000	3.443616000	-1.335182000
H	-1.869317000	1.642390000	-1.855966000
H	-2.121551000	-2.392941000	1.373825000
H	-0.240183000	-1.129266000	2.473602000
N	-0.762231000	-0.764196000	1.691076000
C	-3.190872000	-1.086619000	-1.102843000
H	-3.976320000	-0.324762000	-1.143771000
H	-2.768448000	-1.181560000	-2.108917000
H	-3.659945000	-2.039541000	-0.842748000

Conformer S2h

C	1.671578000	-0.111035000	1.563577000
H	1.894696000	0.323689000	2.544141000
H	0.798483000	0.388725000	1.145409000
H	1.479329000	-1.178062000	1.691052000
S	3.145449000	0.172864000	0.581910000
O	2.779002000	-0.745878000	-0.805456000
H	3.154130000	-1.624593000	-0.678460000
C	-1.575254000	0.334583000	-0.037710000
C	-0.659673000	-0.471763000	-0.773265000
C	-0.722431000	-1.871975000	-0.765556000
C	-1.740340000	-2.464496000	-0.021878000
C	-2.672324000	-1.681706000	0.699908000
C	-2.609174000	-0.291512000	0.688245000
C	-1.177899000	1.701789000	-0.217285000

C	-0.059443000	1.670496000	-1.030588000
H	-0.015823000	-2.471785000	-1.333681000
H	-1.820416000	-3.547870000	0.004912000
H	-3.459333000	-2.179352000	1.259895000
H	-3.331516000	0.299674000	1.246554000
H	0.549965000	2.489710000	-1.391038000
H	1.138591000	0.061714000	-1.714513000
N	0.224578000	0.371607000	-1.403988000
C	-1.856806000	2.910814000	0.345463000
H	-2.879769000	3.004346000	-0.034832000
H	-1.914531000	2.860487000	1.438164000
H	-1.314465000	3.822087000	0.077927000

Conformer S2i

C	1.062730000	-2.330102000	-0.407592000
H	1.080450000	-3.200213000	0.256966000
H	0.081031000	-1.860896000	-0.339935000
H	1.262650000	-2.660176000	-1.428868000
S	2.359939000	-1.232769000	0.158819000
O	2.266429000	-0.045988000	-1.038885000
H	1.622151000	0.609102000	-0.726040000
C	-0.751694000	0.617917000	0.530785000
C	-1.343429000	0.484792000	-0.757178000
C	-2.288895000	-0.509040000	-1.049288000
C	-2.637078000	-1.380246000	-0.020564000
C	-2.068582000	-1.258643000	1.270193000
C	-1.127335000	-0.275084000	1.554336000
C	0.152400000	1.731861000	0.479979000
C	0.060547000	2.240720000	-0.805551000
H	-2.735419000	-0.597762000	-2.036449000
H	-3.367590000	-2.161782000	-0.209884000
H	-2.372832000	-1.952649000	2.048794000
H	-0.692518000	-0.191146000	2.547063000
H	0.570785000	3.087394000	-1.247636000
H	-0.982192000	1.588713000	-2.535591000
N	-0.846699000	1.503549000	-1.539173000
C	0.954926000	2.282661000	1.616944000
H	0.299930000	2.688251000	2.395353000
H	1.574714000	1.503052000	2.071204000
H	1.613747000	3.086465000	1.276839000

Conformer 1b

C	-1.639420000	-1.845441000	-0.926261000
H	-1.770711000	-2.852472000	-0.516737000
H	-2.067627000	-1.811603000	-1.929881000
H	-0.573609000	-1.616641000	-0.956686000
S	-2.525569000	-0.735607000	0.166086000
O	-2.312081000	0.716194000	-0.669623000
H	-1.469190000	1.089303000	-0.367347000
C	1.125265000	0.518228000	-0.204640000
C	0.898937000	-0.145206000	1.034002000
C	1.279172000	-1.476021000	1.251917000
C	1.922192000	-2.135940000	0.207688000
C	2.176202000	-1.488882000	-1.024918000
C	1.789832000	-0.169413000	-1.240046000
C	0.590668000	1.846626000	-0.087284000
C	0.077685000	1.939216000	1.195863000
H	1.094907000	-1.971099000	2.201990000
H	2.236975000	-3.166953000	0.342922000
H	2.688377000	-2.034175000	-1.812797000
H	1.988849000	0.319060000	-2.190873000
H	-0.407622000	2.776557000	1.681541000
H	-0.186256000	0.504207000	2.727912000
N	0.296240000	0.759546000	1.878540000
C	0.657527000	2.930772000	-1.117596000
H	1.696548000	3.207801000	-1.324696000
H	0.203333000	2.609959000	-2.060948000
H	0.129734000	3.825747000	-0.776938000

Optimized conformers of the CH_3SOH–4-methylphenol complex

Conformer S3a

C	-1.441685000	-0.719004000	1.524612000
H	-1.615267000	-0.074760000	2.393237000
H	-1.561773000	-1.760057000	1.831035000
H	-0.433828000	-0.540363000	1.151400000
S	-2.669772000	-0.237974000	0.313021000
O	-2.236197000	-1.250468000	-0.975191000
H	-2.776011000	-2.045179000	-0.900699000
C	1.568117000	1.384008000	0.714496000
C	0.600377000	1.574389000	-0.279928000
C	0.369261000	0.522503000	-1.180707000
C	1.081858000	-0.673558000	-1.102616000

C	2.043692000	-0.844898000	-0.102431000
C	2.292534000	0.188794000	0.805240000
H	1.774028000	2.181721000	1.425043000
H	3.044117000	0.064186000	1.583051000
H	0.888045000	-1.484927000	-1.796897000
H	-0.389503000	0.630424000	-1.951450000
C	-0.202386000	2.846560000	-0.360573000
H	-1.213838000	2.691601000	0.029761000
H	0.269584000	3.647260000	0.215522000
H	-0.297536000	3.183238000	-1.396978000
O	2.712895000	-2.042503000	-0.069332000
H	3.344137000	-2.014555000	0.656265000

Conformer S3b

C	-1.100956000	-1.811297000	-0.331259000
H	-0.713533000	-2.504301000	0.422418000
H	-1.385179000	-2.377401000	-1.220540000
H	-0.324438000	-1.084167000	-0.566570000
S	-2.506938000	-0.996844000	0.419054000
O	-2.839538000	0.149247000	-0.787433000
H	-3.497888000	-0.234759000	-1.377009000
C	1.948590000	0.303305000	-1.166624000
C	2.349219000	-0.431454000	-0.046865000
C	1.725012000	-0.213341000	1.184867000
C	0.717908000	0.752140000	1.294734000
C	0.293680000	1.493244000	0.184469000
C	0.931549000	1.252483000	-1.043152000
H	0.243825000	0.915456000	2.259653000
H	2.036849000	-0.778558000	2.061796000
H	2.446142000	0.129679000	-2.116215000
H	0.628554000	1.819921000	-1.920547000
C	-0.812124000	2.509797000	0.295339000
H	-0.564169000	3.415771000	-0.265878000
H	-1.744324000	2.101822000	-0.106273000
H	-0.980338000	2.790910000	1.338393000
O	3.342707000	-1.362200000	-0.223431000
H	3.622894000	-1.670514000	0.643770000

Conformer S3c

C	1.232268000	-1.381848000	1.131629000
H	0.801891000	-2.383590000	1.029497000
H	1.711118000	-1.301786000	2.109556000

H	0.433386000	-0.647613000	1.030132000
S	2.409420000	-1.211352000	-0.205471000
O	2.824473000	0.423389000	-0.007659000
H	3.620145000	0.444661000	0.535528000
C	-2.141693000	-0.679774000	-0.144739000
C	-1.242093000	-0.450338000	-1.191125000
C	-0.435148000	0.690344000	-1.178101000
C	-0.493568000	1.612966000	-0.124080000
C	-1.400066000	1.359901000	0.916397000
C	-2.222341000	0.229288000	0.912839000
H	-1.168228000	-1.159277000	-2.014118000
H	0.270372000	0.848798000	-1.990281000
H	-1.470562000	2.060747000	1.745460000
H	-2.927235000	0.041725000	1.717329000
C	0.402616000	2.823728000	-0.118735000
H	1.450081000	2.510059000	-0.109091000
H	0.238208000	3.436081000	-1.011004000
H	0.213614000	3.447873000	0.758814000
O	-2.952999000	-1.786012000	-0.092393000
H	-2.895158000	-2.240669000	-0.938375000

Conformer S3d

C	1.376957000	-1.070294000	1.071398000
H	0.310210000	-0.948476000	0.868769000
H	1.589970000	-2.130415000	1.223109000
H	1.634338000	-0.500327000	1.965833000
S	2.231571000	-0.424307000	-0.362759000
O	3.838398000	-0.630147000	0.149812000
H	4.125607000	-1.493996000	-0.164433000
C	-2.193837000	-0.006103000	1.010784000
C	-1.426829000	1.164820000	1.036222000
C	-0.668181000	1.563529000	-0.071331000
C	-0.706963000	0.751508000	-1.216932000
C	-1.457765000	-0.424942000	-1.254498000
C	-2.203478000	-0.807920000	-0.135054000
H	-2.785283000	-0.289419000	1.879772000
H	-1.430682000	1.779043000	1.933991000
H	-0.141281000	1.045555000	-2.098091000
H	-1.481815000	-1.049135000	-2.142797000
C	0.179681000	2.807213000	-0.032976000
H	1.221072000	2.556784000	0.195618000
H	0.165408000	3.317871000	-0.999880000
H	-0.181249000	3.505300000	0.727124000

O	-2.934992000	-1.962910000	-0.230963000
H	-3.356192000	-2.126273000	0.618663000

Conformer S3e

C	-1.394488000	-1.011142000	1.111074000
H	-0.323971000	-0.894154000	0.927689000
H	-1.654593000	-0.475710000	2.026646000
H	-1.624694000	-2.072699000	1.216583000
S	-2.230925000	-0.345425000	-0.325712000
O	-3.817925000	-0.844998000	0.021830000
H	-4.232921000	-0.136631000	0.525124000
C	2.163022000	-0.858681000	-0.116387000
C	1.407088000	-0.481326000	-1.230477000
C	0.694825000	0.723000000	-1.213536000
C	0.714987000	1.566806000	-0.094552000
C	1.494969000	1.176332000	1.005116000
C	2.207116000	-0.024694000	1.005857000
H	1.375553000	-1.119194000	-2.111834000
H	1.544432000	1.819762000	1.881013000
H	2.808339000	-0.323173000	1.859533000
H	0.117143000	1.006207000	-2.090170000
C	-0.077788000	2.847269000	-0.069209000
H	-1.066943000	2.684347000	0.371906000
H	0.435850000	3.613470000	0.518185000
H	-0.226266000	3.234654000	-1.080647000
O	2.891333000	-2.017991000	-0.067128000
H	2.697210000	-2.531541000	-0.857555000

Conformer S3f

C	1.322672000	-1.073977000	-1.074052000
H	0.268192000	-1.127682000	-0.790809000
H	1.429059000	-0.365427000	-1.897762000
H	1.663825000	-2.065288000	-1.377238000
S	2.222453000	-0.556671000	0.387188000
O	3.809646000	-0.822076000	-0.148573000
H	4.098435000	-0.020676000	-0.598364000
C	-2.370443000	-0.546897000	0.088956000
C	-1.551786000	-0.351318000	1.210181000
C	-0.590397000	0.664155000	1.239173000
C	-0.411311000	1.485015000	0.119767000
C	-1.233709000	1.322781000	-0.997487000
C	-2.204016000	0.318046000	-1.004464000

H	-1.673926000	-0.989761000	2.082473000
H	0.014590000	0.822600000	2.128378000
H	-1.095455000	1.981024000	-1.850189000
H	-2.838892000	0.200041000	-1.880081000
C	-3.385354000	-1.661184000	0.051505000
H	-4.254962000	-1.378616000	-0.547891000
H	-2.958241000	-2.569499000	-0.387320000
H	-3.731887000	-1.908829000	1.058333000
O	0.536305000	2.476781000	0.084325000
H	1.298470000	2.151485000	0.577964000

Conformer S3g

C	-1.528847000	-0.579867000	1.576175000
H	-1.622049000	0.244870000	2.290257000
H	-1.756933000	-1.517487000	2.086139000
H	-0.512383000	-0.586568000	1.181621000
S	-2.709095000	-0.234053000	0.273744000
O	-2.327910000	-1.474103000	-0.814887000
H	-2.926706000	-2.206528000	-0.630675000
C	1.380787000	1.603125000	0.546738000
C	0.358761000	1.434283000	-0.391520000
C	0.320600000	0.278448000	-1.177891000
C	1.281161000	-0.718872000	-0.990946000
C	2.305891000	-0.579195000	-0.044839000
C	2.347312000	0.606453000	0.705780000
H	1.228660000	-1.619902000	-1.598029000
H	-0.462436000	0.146841000	-1.919584000
H	1.404398000	2.512857000	1.139572000
H	3.138862000	0.748203000	1.438771000
C	3.323010000	-1.671649000	0.168611000
H	4.284513000	-1.256007000	0.482232000
H	2.994941000	-2.373547000	0.943206000
H	3.483335000	-2.241769000	-0.750467000
O	-0.578183000	2.429473000	-0.507339000
H	-1.392001000	2.014574000	-0.817777000

Conformer S3h

C	2.176113000	-1.912983000	0.395532000
H	2.861381000	-2.182390000	1.205436000
H	1.149309000	-1.967919000	0.763033000
H	2.316684000	-2.606866000	-0.434749000
S	2.596262000	-0.245439000	-0.103319000

O	1.535156000	-0.071323000	-1.399312000
H	0.695968000	0.258302000	-1.043997000
C	-0.580241000	1.574589000	0.323290000
C	-0.553329000	0.585196000	1.316729000
C	-1.246548000	-0.619527000	1.160626000
C	-2.006119000	-0.845161000	0.007281000
C	-2.053007000	0.130725000	-0.992613000
C	-1.358235000	1.330953000	-0.822145000
H	-1.220071000	-1.368376000	1.950418000
H	-2.649228000	-0.052585000	-1.881083000
H	-1.409688000	2.086833000	-1.602706000
H	0.033077000	0.747789000	2.217587000
C	0.199213000	2.854285000	0.478739000
H	1.214816000	2.745918000	0.082461000
H	-0.286318000	3.674613000	-0.056386000
H	0.282181000	3.133919000	1.532182000
O	-2.707615000	-1.999712000	-0.207160000
H	-2.615695000	-2.562391000	0.568060000

Conformer S3i

C	-2.919633000	0.383782000	-0.106368000
H	-3.785747000	0.485590000	0.555441000
H	-2.180751000	1.141114000	0.160141000
H	-3.247067000	0.523020000	-1.138234000
S	-2.289990000	-1.276615000	0.131740000
O	-1.070547000	-1.280919000	-1.033735000
H	-0.271060000	-0.939497000	-0.608980000
C	1.133586000	-0.336419000	1.242222000
C	0.441264000	0.876689000	1.235562000
C	0.543462000	1.727642000	0.131286000
C	1.333151000	1.356099000	-0.961600000
C	2.025084000	0.140812000	-0.938999000
C	1.927915000	-0.734193000	0.153488000
H	1.413619000	2.012238000	-1.826036000
H	2.634150000	-0.137036000	-1.795915000
H	-0.171037000	1.177059000	2.080403000
H	1.039662000	-0.992013000	2.104728000
C	2.630349000	-2.067652000	0.149967000
H	2.913453000	-2.361956000	1.163972000
H	1.982075000	-2.850430000	-0.258572000
H	3.536501000	-2.030524000	-0.460283000
O	-0.173403000	2.894439000	0.170850000
H	0.036578000	3.409563000	-0.614778000

Conformer S3j

C	1.370663000	-0.969820000	1.138690000
H	0.319447000	-1.096967000	0.864327000
H	1.722108000	-1.875359000	1.636819000
H	1.457670000	-0.108366000	1.802548000
S	2.260826000	-0.685155000	-0.389886000
O	3.828543000	-0.478921000	0.221523000
H	4.256882000	-1.341638000	0.202139000
C	-1.222713000	1.352990000	0.945687000
C	-0.385960000	1.428589000	-0.170615000
C	-0.601031000	0.572880000	-1.257236000
C	-1.609710000	-0.393815000	-1.192328000
C	-2.439791000	-0.506565000	-0.067940000
C	-2.238906000	0.395683000	0.988689000
H	-1.055663000	2.037386000	1.772318000
H	-2.882710000	0.344769000	1.864313000
H	0.014049000	0.667534000	-2.148307000
H	-1.760581000	-1.059456000	-2.039607000
C	-3.505777000	-1.570049000	0.009428000
H	-3.128256000	-2.474003000	0.499746000
H	-4.369266000	-1.217980000	0.580298000
H	-3.850519000	-1.851858000	-0.989057000
O	0.614142000	2.365394000	-0.162837000
H	1.361499000	1.987275000	-0.643107000

Conformer S3k

C	2.636927000	-0.195574000	1.153627000
H	3.589496000	0.337801000	1.072456000
H	1.842424000	0.521822000	1.367424000
H	2.707571000	-0.926467000	1.960959000
S	2.369720000	-1.015174000	-0.415852000
O	0.939449000	-1.831284000	-0.057800000
H	0.211512000	-1.252677000	-0.327817000
C	-0.650116000	0.786151000	-1.305417000
C	-0.221926000	1.544019000	-0.202867000
C	-0.818294000	1.286404000	1.037739000
C	-1.808363000	0.307618000	1.183616000
C	-2.216988000	-0.439149000	0.074974000
C	-1.633532000	-0.198297000	-1.175860000
H	-0.201808000	0.961085000	-2.280859000
H	-0.512809000	1.860753000	1.909607000
H	-2.258570000	0.128065000	2.157794000
H	-1.961281000	-0.783252000	-2.030170000

C	0.829254000	2.609328000	-0.370419000
H	1.114697000	3.036650000	0.594656000
H	1.724744000	2.193398000	-0.842748000
H	0.463494000	3.424388000	-1.002895000
O	-3.184067000	-1.403864000	0.137746000
H	-3.379819000	-1.580599000	1.063293000

Conformer S3l

C	2.295680000	-1.824844000	0.558707000
H	3.066133000	-1.907788000	1.331877000
H	1.310719000	-1.841103000	1.028615000
H	2.396971000	-2.661720000	-0.133849000
S	2.586376000	-0.277859000	-0.296191000
O	1.412682000	-0.397453000	-1.495310000
H	0.601964000	0.009346000	-1.154431000
C	-1.184788000	1.532625000	-0.683461000
C	-0.304542000	1.484000000	0.403608000
C	-0.393256000	0.428315000	1.318896000
C	-1.332974000	-0.587754000	1.120270000
C	-2.214807000	-0.564934000	0.030184000
C	-2.131029000	0.518035000	-0.857948000
H	0.268532000	0.407814000	2.181283000
H	-1.390423000	-1.403348000	1.838131000
H	-1.111027000	2.363336000	-1.379056000
H	-2.808904000	0.568157000	-1.707023000
C	-3.205930000	-1.678014000	-0.192401000
H	-2.794981000	-2.442458000	-0.860442000
H	-3.467348000	-2.163709000	0.751401000
H	-4.125343000	-1.298355000	-0.645854000
O	0.600320000	2.502841000	0.541254000
H	1.397565000	2.127886000	0.933737000

Conformer S3m

C	1.224264000	-1.746830000	-0.708406000
H	1.004673000	-2.746956000	-0.320169000
H	0.319979000	-1.139987000	-0.647381000
H	1.555068000	-1.836722000	-1.744871000
S	2.546234000	-1.096189000	0.311497000
O	2.883300000	0.330015000	-0.524056000
H	2.341053000	1.027181000	-0.125169000
C	-0.547380000	0.644873000	1.300453000
C	-1.623015000	-0.240377000	1.211024000

C	-2.388123000	-0.349044000	0.038937000
C	-2.042117000	0.462216000	-1.049966000
C	-0.955722000	1.341321000	-0.983827000
C	-0.213468000	1.427874000	0.194985000
H	-1.878697000	-0.849574000	2.075163000
H	0.042675000	0.729660000	2.207407000
H	-0.685754000	1.946804000	-1.846608000
H	-2.620010000	0.403660000	-1.969446000
C	-3.529046000	-1.329762000	-0.053502000
H	-3.175414000	-2.313566000	-0.380414000
H	-4.015825000	-1.456290000	0.917183000
H	-4.281512000	-0.990292000	-0.770081000
O	0.899890000	2.240396000	0.308168000
H	0.836157000	2.940207000	-0.350659000

Conformer S3n

C	2.659255000	-0.174322000	1.232548000
H	3.623046000	0.342050000	1.180109000
H	1.879858000	0.554120000	1.460658000
H	2.708226000	-0.938451000	2.009849000
S	2.400903000	-0.939265000	-0.366457000
O	0.992490000	-1.803536000	-0.039033000
H	0.246026000	-1.230022000	-0.267068000
C	-1.651032000	-0.200845000	-1.155616000
C	-0.575950000	0.675623000	-1.349300000
C	-0.111527000	1.452946000	-0.281840000
C	-0.751528000	1.378703000	0.958508000
C	-1.831352000	0.509862000	1.132856000
C	-2.292834000	-0.304931000	0.087946000
H	-1.998171000	-0.803652000	-1.991955000
H	-0.096243000	0.748704000	-2.322611000
H	-0.393188000	2.002109000	1.772495000
H	-2.317208000	0.458594000	2.104540000
C	-3.426301000	-1.275551000	0.297500000
H	-3.986403000	-1.429199000	-0.628589000
H	-3.052115000	-2.250104000	0.628772000
H	-4.119904000	-0.907563000	1.058014000
O	0.943104000	2.317175000	-0.404296000
H	1.494489000	2.003638000	-1.129880000

Conformer S3o

C	1.217785000	-1.885050000	-0.207150000
H	1.090092000	-2.675005000	0.540368000
H	0.292604000	-1.312121000	-0.276448000
H	1.457334000	-2.344117000	-1.167912000
S	2.593351000	-0.884413000	0.359182000
O	2.758299000	0.161271000	-0.951935000
H	2.242398000	0.953881000	-0.737687000
C	-0.138518000	1.328760000	0.208400000
C	-0.687338000	0.714874000	1.335582000
C	-1.833528000	-0.074448000	1.199888000
C	-2.447603000	-0.260942000	-0.046475000
C	-1.883673000	0.381094000	-1.159423000
C	-0.738229000	1.171074000	-1.042099000
H	-2.254956000	-0.549685000	2.082854000
H	-0.218164000	0.839242000	2.309168000
H	-0.302239000	1.662907000	-1.906693000
H	-2.345902000	0.263303000	-2.136906000
C	-3.660545000	-1.143978000	-0.192264000
H	-4.316608000	-0.779272000	-0.987095000
H	-3.371918000	-2.170519000	-0.442588000
H	-4.236501000	-1.175745000	0.736316000
O	1.011936000	2.085719000	0.263261000
H	1.338260000	2.073508000	1.170358000

Conformer S3p

C	1.192105000	-1.892297000	-0.127008000
H	1.180563000	-2.638375000	-0.929118000
H	1.277638000	-2.409834000	0.830125000
H	0.272065000	-1.310681000	-0.172796000
S	2.627194000	-0.876304000	-0.464587000
O	2.539372000	0.207624000	0.849265000
H	3.131978000	-0.110792000	1.539030000
C	-1.986965000	0.237358000	-1.152821000
C	-0.864507000	1.066302000	-1.236113000
C	-0.142574000	1.382937000	-0.081436000
C	-0.574573000	0.890996000	1.156511000
C	-1.693816000	0.056383000	1.225657000
C	-2.417914000	-0.288400000	0.074927000
H	-2.018356000	-0.318244000	2.194543000
H	-0.028485000	1.160184000	2.056457000
H	-0.524878000	1.463528000	-2.188133000
H	-2.538667000	-0.002313000	-2.059672000

C	-3.608772000	-1.210301000	0.151453000
H	-4.342028000	-0.968229000	-0.622716000
H	-3.311104000	-2.255622000	0.012774000
H	-4.103212000	-1.131480000	1.123565000
O	0.948788000	2.202769000	-0.194701000
H	1.646188000	1.801711000	0.345809000

Conformer 1c

C	1.710926000	-1.071760000	1.404918000
H	1.577625000	-2.113512000	1.715986000
H	2.244471000	-0.537597000	2.192701000
H	0.729093000	-0.631016000	1.226269000
S	2.671192000	-1.156499000	-0.103725000
O	2.838073000	0.506332000	-0.444517000
H	3.696436000	0.786943000	-0.106704000
C	-1.451551000	-0.623834000	-1.039513000
C	-0.401126000	0.297707000	-1.084751000
C	-0.361793000	1.355898000	-0.168564000
C	-1.405186000	1.511924000	0.749912000
C	-2.463122000	0.599841000	0.763841000
C	-2.499391000	-0.491617000	-0.117814000
H	-1.463644000	-1.446959000	-1.751130000
H	0.393285000	0.193950000	-1.819015000
H	-1.370424000	2.346441000	1.444257000
H	-3.270343000	0.734766000	1.480980000
C	-3.625409000	-1.493139000	-0.068748000
H	-3.761351000	-1.976244000	-1.040100000
H	-3.429213000	-2.278337000	0.669622000
H	-4.567593000	-1.009584000	0.203785000
O	0.662157000	2.262045000	-0.152534000
H	1.460658000	1.777996000	-0.416329000

Optimized conformers for the 4-methylimidazole-CH_3SOH complex

Conformer S4a

C	-1.414375000	1.385370000	-0.552952000
H	-0.562735000	1.338564000	-1.237380000
H	-2.218021000	1.962095000	-1.015232000
H	-1.092314000	1.855645000	0.377420000
S	-1.896799000	-0.313431000	-0.266115000
O	-3.147301000	-0.073362000	0.858021000
H	-3.964783000	0.008122000	0.355303000
C	1.610388000	-0.532546000	1.117368000
C	1.787751000	0.452411000	0.162314000
C	1.269394000	-1.345757000	-0.905480000
N	1.300891000	-1.672719000	0.416816000
H	1.021922000	-2.557349000	0.814558000
H	1.682599000	-0.518083000	2.194354000
H	1.036174000	-2.064724000	-1.678021000
N	1.570021000	-0.067691000	-1.095360000
C	2.188529000	1.877123000	0.362024000
H	1.477002000	2.550775000	-0.123202000
H	2.225988000	2.122733000	1.426624000
H	3.174860000	2.067288000	-0.070596000

Conformer S4b

C	-2.195415000	0.451123000	1.213918000
H	-2.782642000	-0.143346000	1.921443000
H	-1.192813000	0.594401000	1.620337000
H	-2.697008000	1.407959000	1.059040000
S	-2.155787000	-0.482223000	-0.315527000
O	-1.371294000	0.635720000	-1.312045000
H	-0.422900000	0.489518000	-1.185699000
C	1.729573000	-0.269564000	-0.970774000
C	1.521154000	0.604497000	0.085627000
C	1.253935000	-1.381064000	0.876983000
N	1.564052000	-1.528793000	-0.441670000
H	1.593878000	-2.399654000	-0.951638000
H	2.012641000	-0.106826000	-2.000500000
H	1.049924000	-2.222868000	1.523078000
N	1.221473000	-0.104569000	1.229021000
C	1.609003000	2.095600000	0.089032000
H	1.815094000	2.474522000	-0.915386000
H	0.670880000	2.536400000	0.437260000
H	2.407715000	2.429677000	0.756678000

Conformer S4c

C	2.267597000	-0.356939000	1.226487000
H	3.024859000	0.216781000	1.770945000
H	1.294049000	-0.198611000	1.692068000
H	2.542886000	-1.412896000	1.251274000
S	2.297946000	0.260413000	-0.455459000
O	1.172843000	-0.778675000	-1.171760000
H	0.310741000	-0.346819000	-1.084894000
C	-1.909101000	0.010592000	-0.921177000
C	-1.391831000	0.783759000	0.107647000
C	-1.527917000	-1.229766000	0.866325000
N	-1.994244000	-1.266384000	-0.413940000
H	-2.297644000	-2.089358000	-0.914491000
H	-2.238692000	0.260034000	-1.918953000
H	-1.466360000	-2.111862000	1.487541000
N	-1.156759000	-0.005961000	1.212801000
C	-1.122352000	2.252833000	0.121373000
H	-0.067627000	2.447794000	0.330751000
H	-1.372078000	2.700622000	-0.843963000
H	-1.721368000	2.740655000	0.895185000

Conformer S4d

C	1.466503000	1.578847000	-0.016010000
H	1.663869000	2.373273000	0.711332000
H	1.618799000	1.979668000	-1.019519000
H	0.440473000	1.233469000	0.112888000
S	2.653670000	0.292134000	0.364450000
O	2.276849000	-0.837234000	-0.854932000
H	2.884641000	-0.695937000	-1.589164000
C	-1.351934000	-0.528910000	-0.963024000
C	-2.248856000	0.088305000	-0.107120000
C	-0.812702000	-0.927232000	1.134938000
N	-0.459644000	-1.190691000	-0.154500000
H	0.425509000	-1.580806000	-0.459212000
H	-1.288040000	-0.564768000	-2.040319000
H	-0.253421000	-1.308849000	1.977278000
N	-1.898836000	-0.166580000	1.201064000
C	-3.448834000	0.909472000	-0.449769000
H	-3.377815000	1.903281000	0.001011000
H	-3.542708000	1.025205000	-1.532853000
H	-4.360512000	0.437199000	-0.073216000

Conformer S4e

C	1.486646000	-1.021784000	1.176573000
H	1.547338000	-2.103589000	1.335850000
H	1.896656000	-0.518832000	2.053798000
H	0.442599000	-0.748357000	1.022233000
S	2.478571000	-0.710038000	-0.282790000
O	2.381614000	0.989345000	-0.363097000
H	3.161357000	1.351089000	0.072568000
C	-1.125242000	0.068960000	-1.041509000
C	-2.149898000	-0.213086000	-0.153030000
C	-1.060413000	1.448465000	0.674137000
N	-0.457293000	1.145085000	-0.509296000
H	0.453458000	1.483752000	-0.799537000
H	-0.833018000	-0.383299000	-1.977274000
H	-0.715091000	2.250477000	1.311248000
N	-2.098030000	0.656299000	0.915101000
C	-3.206418000	-1.264332000	-0.255100000
H	-3.060206000	-1.874090000	-1.150629000
H	-3.183936000	-1.920221000	0.619655000
H	-4.199989000	-0.810108000	-0.305557000

Conformer S4f

C	1.693795000	-0.974602000	1.257676000
H	2.021584000	-0.762061000	2.280352000
H	0.602127000	-1.009672000	1.238961000
H	2.107588000	-1.935862000	0.946242000
S	2.333005000	0.346900000	0.225602000
O	1.917965000	-0.229421000	-1.294281000
H	0.963440000	-0.033708000	-1.404195000
C	-2.305117000	0.027784000	0.743239000
C	-1.426849000	0.780857000	-0.014079000
C	-1.349238000	-1.236127000	-0.797275000
N	-2.239691000	-1.248154000	0.231836000
H	-2.771141000	-2.046839000	0.546883000
H	-2.951173000	0.286303000	1.568396000
H	-1.097387000	-2.117138000	-1.369893000
N	-0.840012000	-0.022854000	-0.968891000
C	-1.101917000	2.233228000	0.098003000
H	-1.682745000	2.695912000	0.899924000
H	-0.038418000	2.368820000	0.310046000
H	-1.331792000	2.749428000	-0.838102000

Conformer S4g

C	-1.673233000	-0.297860000	1.499425000
H	-2.115590000	-1.100535000	2.098279000
H	-0.594714000	-0.458436000	1.433843000
H	-1.878964000	0.658642000	1.984202000
S	-2.452942000	-0.361050000	-0.115738000
O	-1.783678000	1.011744000	-0.810408000
H	-0.886822000	0.748639000	-1.109955000
C	2.320779000	-0.321566000	0.661429000
C	1.584165000	0.644549000	0.002694000
C	1.055923000	-1.253228000	-0.895541000
N	1.969039000	-1.518120000	0.078710000
H	2.334059000	-2.429082000	0.316253000
H	3.038365000	-0.259722000	1.465374000
H	0.599313000	-2.021736000	-1.501696000
N	0.804892000	0.047182000	-0.966034000
C	1.546248000	2.119079000	0.231726000
H	2.198525000	2.397707000	1.062949000
H	1.874856000	2.656377000	-0.662141000
H	0.526657000	2.441722000	0.460838000

Conformer S4h

C	3.145027000	0.824787000	0.504832000
H	3.807421000	1.478046000	-0.072107000
H	2.361285000	1.431303000	0.962869000
H	3.730714000	0.327742000	1.279960000
S	2.477429000	-0.380307000	-0.642740000
O	1.633506000	-1.353331000	0.428153000
H	0.703506000	-1.027977000	0.426327000
C	-2.864366000	0.679582000	-0.214121000
C	-1.507093000	0.779372000	0.024992000
C	-2.012345000	-1.319432000	0.189503000
N	-3.164086000	-0.659100000	-0.107413000
H	-4.074679000	-1.078725000	-0.223924000
H	-3.612350000	1.421889000	-0.446765000
H	-1.962355000	-2.390091000	0.324319000
N	-0.993803000	-0.475078000	0.276364000
C	-0.643796000	1.996659000	0.041932000
H	-1.219342000	2.881588000	-0.240487000
H	-0.228561000	2.161346000	1.040538000
H	0.188106000	1.879870000	-0.657599000

Conformer S4i

C	-2.663533000	-1.065630000	-1.002750000
H	-3.216844000	-0.831396000	-1.917590000
H	-1.679404000	-1.452462000	-1.274851000
H	-3.218232000	-1.815332000	-0.435443000
S	-2.527948000	0.457427000	-0.066161000
O	-1.779010000	-0.120916000	1.316247000
H	-0.821983000	-0.181319000	1.092401000
C	2.859960000	0.261871000	-0.383042000
C	1.595800000	0.725765000	-0.072659000
C	1.593481000	-1.402106000	0.333209000
N	2.838390000	-1.088280000	-0.117198000
H	3.605743000	-1.733031000	-0.236998000
H	3.741020000	0.762614000	-0.754097000
H	1.303141000	-2.403111000	0.617604000
N	0.819161000	-0.325944000	0.365628000
C	1.053253000	2.113112000	-0.165166000
H	0.774744000	2.486327000	0.824491000
H	1.797356000	2.789210000	-0.593353000
H	0.157092000	2.128496000	-0.790124000

Conformer 1d

C	-2.754480000	-0.005163000	1.356187000
H	-3.391903000	-0.777751000	1.797667000
H	-1.770104000	-0.044925000	1.826590000
H	-3.210613000	0.971382000	1.528316000
S	-2.653477000	-0.346573000	-0.401554000
O	-1.744042000	0.971858000	-0.894243000
H	-0.813925000	0.722274000	-0.692100000
C	2.937751000	-0.380849000	0.163040000
C	1.955239000	0.586424000	0.070684000
C	0.967164000	-1.325258000	-0.178074000
N	2.290783000	-1.584549000	0.000302000
H	2.717279000	-2.499303000	0.018781000
H	4.003159000	-0.314887000	0.321980000
H	0.222549000	-2.092976000	-0.329988000
N	0.734938000	-0.019730000	-0.136665000
C	2.083061000	2.070561000	0.168477000
H	1.465141000	2.456699000	0.983472000
H	3.120965000	2.356938000	0.354611000
H	1.752970000	2.548523000	-0.757872000

Optimized conformers of the CH_3SOH–4-methylimidazolium complex

Conformer S5a

C	3.692791000	0.900458000	-0.317192000
H	3.682542000	1.485973000	-1.240555000
H	3.692105000	1.576830000	0.538068000
H	4.579159000	0.265936000	-0.307619000
S	2.229502000	-0.128997000	-0.357782000
O	2.435634000	-1.094850000	1.003726000
H	2.301956000	-0.556993000	1.793919000
C	-3.171655000	-0.139140000	0.025987000
C	-2.110434000	0.737843000	0.076273000
C	-1.312757000	-1.321698000	-0.270911000
N	-2.647299000	-1.393264000	-0.187918000
H	-3.180240000	-2.251298000	-0.273098000
H	-4.231612000	0.034924000	0.124092000
H	-0.630398000	-2.141270000	-0.437225000
C	-2.061617000	2.212946000	0.276234000
H	-1.601290000	2.706409000	-0.583156000
H	-3.074381000	2.600538000	0.392104000
H	-1.492520000	2.465918000	1.174057000
H	-0.007952000	0.293785000	-0.140777000
N	-0.983050000	-0.035371000	-0.110288000

Conformer S5b

C	3.521806000	-0.037943000	1.073306000
H	4.053414000	-0.905491000	1.475737000
H	4.253244000	0.716000000	0.781716000
H	2.849999000	0.352692000	1.837980000
S	2.610285000	-0.639394000	-0.345076000
O	1.785896000	0.784022000	-0.788905000
H	2.308796000	1.220187000	-1.472998000
C	-1.032059000	-0.522212000	-0.070275000
C	-1.695745000	0.676663000	0.069506000
C	-3.205135000	-0.982631000	0.104733000
N	-1.985174000	-1.513207000	-0.041659000
H	-1.802277000	-2.506732000	-0.126210000
H	0.022663000	-0.726418000	-0.176779000
H	-4.140845000	-1.516687000	0.155576000
C	-1.180998000	2.071871000	0.117592000
H	-0.100439000	2.038518000	-0.024262000
H	-1.622381000	2.679062000	-0.676888000
H	-1.400460000	2.537157000	1.082037000

H	-3.791205000	1.009645000	0.287370000
N	-3.033319000	0.345450000	0.173088000

Conformer S5c

C	-3.273641000	0.857681000	-0.587098000
H	-3.785409000	0.827503000	-1.554052000
H	-4.020572000	1.013368000	0.192042000
H	-2.552850000	1.675575000	-0.598382000
S	-2.472266000	-0.733805000	-0.418523000
O	-1.723152000	-0.528275000	1.101730000
H	-2.350096000	-0.800991000	1.783582000
C	1.198833000	-0.643044000	0.416994000
C	1.465319000	0.689123000	0.192842000
C	3.225336000	-0.514647000	-0.499544000
N	2.295445000	-1.348612000	-0.018028000
H	2.395767000	-2.356882000	0.010611000
H	0.309636000	-1.094201000	0.831700000
H	4.187721000	-0.784132000	-0.905135000
C	0.638736000	1.897022000	0.461217000
H	0.406718000	2.424741000	-0.467805000
H	-0.293646000	1.574066000	0.925576000
H	1.151946000	2.583589000	1.139330000
H	3.216901000	1.564134000	-0.654989000
N	2.725677000	0.723397000	-0.371460000

Conformer S5d

C	-3.501508000	-0.107917000	1.150833000
H	-4.038953000	0.786902000	1.479522000
H	-4.226687000	-0.903914000	0.979912000
H	-2.788754000	-0.396052000	1.923798000
S	-2.668351000	0.354778000	-0.363574000
O	-1.837871000	-1.098030000	-0.689516000
H	-2.399585000	-1.645236000	-1.252124000
C	1.121834000	-0.549133000	-0.131744000
C	1.672673000	0.711189000	-0.044994000
C	3.301105000	-0.796669000	0.275875000
N	2.147935000	-1.443486000	0.070118000
H	2.054133000	-2.452728000	0.067290000
H	0.100646000	-0.861035000	-0.322910000
H	4.267087000	-1.238820000	0.462261000
C	1.056227000	2.059189000	-0.184411000
H	1.446670000	2.579661000	-1.062713000

H	-0.022465000	1.943696000	-0.297897000
H	1.245862000	2.669558000	0.702249000
H	3.704000000	1.248121000	0.324350000
N	3.016727000	0.511727000	0.206485000

Conformer S5e

C	-3.431425000	-0.189395000	0.421199000
H	-4.017181000	0.617105000	0.872530000
H	-4.028108000	-0.657141000	-0.362229000
H	-3.174345000	-0.916051000	1.192215000
S	-1.967824000	0.589500000	-0.256337000
O	-1.125634000	-0.780518000	-0.813333000
H	-1.422909000	-0.958727000	-1.714553000
C	2.343391000	-0.294841000	-0.686467000
C	1.732751000	0.674076000	0.076868000
C	1.093459000	-1.332725000	0.828815000
N	1.933368000	-1.512630000	-0.194832000
H	2.211850000	-2.419313000	-0.550448000
H	3.027776000	-0.206281000	-1.515222000
H	0.591561000	-2.103624000	1.390609000
C	1.780938000	2.160507000	0.014256000
H	2.459200000	2.472530000	-0.780764000
H	0.789441000	2.569865000	-0.196337000
H	2.142153000	2.579419000	0.956796000
H	0.341424000	0.416264000	1.664072000
N	0.988733000	-0.014173000	1.012455000

Conformer S5f

C	-3.199478000	0.286784000	-0.993875000
H	-3.531969000	-0.356434000	-1.813947000
H	-4.075178000	0.697695000	-0.491594000
H	-2.575738000	1.086159000	-1.394408000
S	-2.273090000	-0.769588000	0.117175000
O	-1.734394000	0.370709000	1.247713000
H	-2.338177000	0.364633000	2.001377000
C	2.905569000	0.523436000	0.003868000
C	1.552098000	0.765479000	-0.088723000
C	1.880442000	-1.443975000	-0.139844000
N	3.072746000	-0.841552000	-0.029726000
H	3.958698000	-1.330868000	0.020551000
H	3.736986000	1.205013000	0.090198000
H	1.700984000	-2.506757000	-0.181880000

C	0.773208000	2.033847000	-0.118703000
H	1.414261000	2.868342000	0.168028000
H	0.387634000	2.227332000	-1.123680000
H	-0.067296000	1.969608000	0.574976000
H	-0.057976000	-0.644626000	-0.236377000
N	0.958871000	-0.476418000	-0.176859000

Conformer S5g

C	-3.458107000	0.123279000	1.142315000
H	-3.990812000	1.070932000	1.265325000
H	-4.178439000	-0.693315000	1.189223000
H	-2.713521000	0.024659000	1.932402000
S	-2.687571000	0.198203000	-0.471934000
O	-1.802591000	-1.251463000	-0.448293000
H	-2.321438000	-1.931368000	-0.896789000
C	1.172687000	-0.597098000	-0.020711000
C	2.516114000	-0.318379000	0.102256000
C	1.396229000	1.606744000	-0.144869000
N	0.518504000	0.601563000	-0.170724000
H	-0.500342000	0.708555000	-0.278497000
H	0.634211000	-1.530329000	-0.016233000
H	1.175090000	2.658209000	-0.239428000
C	3.698342000	-1.205698000	0.283643000
H	4.218936000	-0.979672000	1.217637000
H	3.369632000	-2.244839000	0.319390000
H	4.400448000	-1.097814000	-0.546942000
H	3.472946000	1.588222000	0.070849000
N	2.610575000	1.057598000	0.019947000

Conformer S5h

C	-3.168428000	0.546237000	1.083215000
H	-3.450600000	1.601328000	1.149031000
H	-4.070675000	-0.062348000	1.142562000
H	-2.487845000	0.305889000	1.900242000
S	-2.371891000	0.351206000	-0.508042000
O	-1.881136000	-1.273080000	-0.399634000
H	-2.551842000	-1.820400000	-0.827639000
C	2.998902000	-0.208947000	0.197069000
C	1.993878000	0.705924000	-0.026441000
C	1.082724000	-1.332940000	0.077998000
N	2.405200000	-1.449441000	0.256626000
H	2.885832000	-2.328451000	0.407596000

H	4.062058000	-0.070189000	0.313743000
H	0.347177000	-2.120479000	0.069738000
C	2.027662000	2.187238000	-0.178426000
H	1.441926000	2.672515000	0.606106000
H	3.057051000	2.540042000	-0.105467000
H	1.629471000	2.487749000	-1.150597000
H	-0.116905000	0.341301000	-0.248773000
N	0.829838000	-0.031514000	-0.092526000

Conformer S5i

C	3.449057000	-0.739063000	1.017689000
H	3.793614000	-1.772608000	0.916775000
H	4.310405000	-0.099489000	1.209867000
H	2.733771000	-0.678476000	1.838081000
S	2.684432000	-0.324092000	-0.546718000
O	2.093643000	1.229464000	-0.188614000
H	2.740788000	1.876877000	-0.496102000
C	-1.653847000	-1.009474000	-0.292368000
C	-2.741526000	-0.225908000	0.024015000
C	-0.884049000	1.023813000	0.148357000
N	-0.536237000	-0.214326000	-0.207612000
H	0.438086000	-0.499985000	-0.379660000
H	-1.602225000	-2.051029000	-0.567605000
H	-0.204442000	1.848123000	0.289728000
C	-4.196404000	-0.535540000	0.096228000
H	-4.762272000	0.074325000	-0.612517000
H	-4.357694000	-1.584950000	-0.152758000
H	-4.584996000	-0.359516000	1.102422000
H	-2.760982000	1.839637000	0.555382000
N	-2.218549000	1.024880000	0.291792000

Conformer S5j

C	-3.372021000	0.842055000	0.158945000
H	-4.033134000	1.232439000	-0.621593000
H	-3.986774000	0.514286000	0.997515000
H	-2.686677000	1.632311000	0.465714000
S	-2.508379000	-0.526962000	-0.601635000
O	-1.488641000	-0.976807000	0.703853000
H	-1.955435000	-1.595924000	1.280114000
C	2.900052000	0.715303000	-0.227374000
C	1.555345000	0.809315000	0.056926000
C	2.122736000	-1.345267000	0.069193000

N	3.217171000	-0.623007000	-0.211648000
H	4.134731000	-1.016119000	-0.385090000
H	3.631704000	1.480149000	-0.434598000
H	2.070808000	-2.419975000	0.144684000
C	0.651055000	1.987359000	0.167193000
H	0.208036000	2.044078000	1.164672000
H	1.213913000	2.904118000	-0.012558000
H	-0.150831000	1.921720000	-0.572635000
H	0.131833000	-0.748696000	0.459042000
N	1.114545000	-0.484868000	0.234616000

Conformer S5k

C	3.612668000	-0.297769000	1.141156000
H	4.117401000	-1.234523000	1.397970000
H	4.365775000	0.481949000	1.027818000
H	2.909165000	-0.048832000	1.935455000
S	2.770079000	-0.624355000	-0.401522000
O	1.987262000	0.887844000	-0.615141000
H	2.539391000	1.460593000	-1.162668000
C	-1.263107000	-0.594610000	-0.286233000
C	-2.594924000	-0.426305000	0.023921000
C	-1.547068000	1.545313000	0.195961000
N	-0.649730000	0.629460000	-0.171182000
H	0.358626000	0.818369000	-0.354594000
H	-0.719135000	-1.481741000	-0.569974000
H	-1.362301000	2.594424000	0.365036000
C	-3.730716000	-1.388552000	0.069387000
H	-3.375710000	-2.382546000	-0.204783000
H	-4.158540000	-1.443415000	1.073577000
H	-4.516381000	-1.100703000	-0.633691000
H	-3.592313000	1.372496000	0.587327000
N	-2.728334000	0.916597000	0.316731000

Conformer S5l

C	3.432665000	0.068301000	1.121776000
H	4.136857000	-0.735984000	1.357274000
H	3.991240000	0.998780000	1.020960000
H	2.698182000	0.139464000	1.923818000
S	2.671539000	-0.407349000	-0.424607000
O	1.563177000	0.889179000	-0.600283000
H	1.965984000	1.586698000	-1.133297000
C	-3.062049000	-0.381631000	0.252752000

C	-2.114880000	0.603993000	0.080917000
C	-1.117452000	-1.375227000	-0.158876000
N	-2.416225000	-1.586359000	0.098803000
H	-2.845350000	-2.501395000	0.169241000
H	-4.116985000	-0.314399000	0.466768000
H	-0.363312000	-2.129569000	-0.319944000
C	-2.224464000	2.088832000	0.127711000
H	-1.982449000	2.527885000	-0.843323000
H	-3.244415000	2.374547000	0.387605000
H	-1.548690000	2.504106000	0.879191000
H	-0.009328000	0.399640000	-0.352616000
N	-0.928731000	-0.052389000	-0.170999000

Conformer S5m

C	3.361310000	-0.862195000	-0.853890000
H	4.014741000	-0.410292000	-1.606963000
H	3.976595000	-1.437559000	-0.162141000
H	2.636919000	-1.501778000	-1.358010000
S	2.564271000	0.514012000	-0.036746000
O	1.551969000	-0.352637000	1.045347000
H	2.010155000	-0.471210000	1.887327000
C	-2.985827000	0.321443000	-0.402863000
C	-1.722136000	0.738926000	-0.046186000
C	-1.819890000	-1.475714000	0.186654000
N	-3.012972000	-1.045058000	-0.248454000
H	-3.808213000	-1.645792000	-0.430729000
H	-3.841982000	0.881467000	-0.744399000
H	-1.549370000	-2.498290000	0.397607000
C	-1.107437000	2.095236000	-0.016878000
H	-0.264022000	2.151834000	-0.709118000
H	-1.847877000	2.841184000	-0.308251000
H	-0.751070000	2.336930000	0.987453000
H	-0.045842000	-0.424530000	0.639543000
N	-1.034206000	-0.402261000	0.310143000

Conformer 1e

C	-3.634887000	-0.102372000	1.225673000
H	-4.269540000	0.728137000	1.550695000
H	-4.258580000	-0.987873000	1.103952000
H	-2.862289000	-0.269913000	1.975853000
S	-2.932923000	0.421127000	-0.333227000
O	-1.927047000	-0.930036000	-0.653066000

H	-2.404323000	-1.566130000	-1.201151000
C	1.766585000	-0.995812000	-0.037624000
C	2.826902000	-0.131257000	0.125419000
C	0.967877000	1.053858000	-0.268548000
N	0.644550000	-0.240377000	-0.276541000
H	-0.318867000	-0.598172000	-0.444620000
H	1.737224000	-2.073260000	0.001027000
H	0.292951000	1.881452000	-0.421188000
C	4.270299000	-0.375061000	0.399500000
H	4.448426000	-1.447772000	0.481957000
H	4.893742000	0.013407000	-0.409742000
H	4.576371000	0.094957000	1.337502000
H	2.805725000	1.999297000	0.036445000
N	2.287114000	1.130661000	-0.026472000

Optimized conformers of the CH_3SOH–4-methylphenolate complex

Conformer S6a

C	-1.505207000	-0.355833000	-0.462048000
H	-1.153131000	-1.368468000	-0.231254000
H	-1.551022000	-0.247268000	-1.547962000
H	-0.797119000	0.354781000	-0.033880000
S	-3.124481000	-0.204308000	0.277218000
O	-3.504224000	1.412386000	-0.120517000
H	-3.822755000	1.397894000	-1.028486000
C	1.667661000	-0.907201000	-1.163408000
C	1.312626000	-1.646399000	0.021637000
C	1.472217000	-0.887956000	1.236862000
C	1.731057000	0.483706000	1.239379000
C	1.969305000	1.200082000	0.052282000
C	1.924245000	0.465556000	-1.145509000
H	1.783674000	1.011368000	2.194597000
H	1.275240000	-1.407550000	2.174362000
H	1.629472000	-1.443423000	-2.111769000
H	2.138143000	0.977389000	-2.087095000
C	2.188415000	2.692555000	0.059398000
H	2.783603000	3.005612000	-0.806664000
H	1.245180000	3.255435000	0.027760000
H	2.724787000	3.008965000	0.962051000
O	0.900937000	-2.855245000	-0.001819000

Conformer S6b

C	-1.665981000	-1.830884000	-0.585830000
H	-2.023106000	-2.177436000	-1.562038000
H	-0.599331000	-1.605535000	-0.658277000
H	-1.841971000	-2.609550000	0.160671000
S	-2.584712000	-0.341665000	-0.198760000
O	-1.908436000	0.028525000	1.289662000
H	-1.042189000	0.461297000	1.123277000
C	0.894395000	0.953998000	-1.321410000
C	1.508998000	-0.286746000	-1.175380000
C	1.778227000	-0.848875000	0.090357000
C	1.483457000	-0.050008000	1.202307000
C	0.858159000	1.199797000	1.080119000
C	0.624610000	1.832616000	-0.200998000
H	0.697782000	1.351859000	-2.316426000
H	1.730062000	-0.873639000	-2.070947000
H	0.684611000	1.806744000	1.969171000
H	1.680814000	-0.442840000	2.202324000
C	2.491100000	-2.170353000	0.225748000
H	2.075398000	-2.924145000	-0.455358000
H	3.563915000	-2.089175000	0.002234000
H	2.396445000	-2.559343000	1.245779000
O	0.182833000	3.012866000	-0.333378000

Conformer S6c

C	2.116947000	0.028292000	1.374966000
H	2.857920000	0.820389000	1.530684000
H	1.117898000	0.471036000	1.347025000
H	2.186805000	-0.697484000	2.188382000
S	2.495389000	-0.741968000	-0.197452000
O	1.295118000	-1.909721000	-0.236408000
H	0.456939000	-1.462076000	-0.490138000
C	-1.215535000	1.385970000	0.856611000
C	-1.970360000	0.234264000	1.071131000
C	-2.127769000	-0.798618000	0.069897000
C	-1.295648000	-0.587705000	-1.097197000
C	-0.555297000	0.586043000	-1.296919000
C	-0.445821000	1.574569000	-0.308631000
H	-1.176561000	2.145435000	1.642100000
H	-2.560729000	0.132047000	1.981247000
H	-1.399376000	-1.307442000	-1.909882000
H	0.008848000	0.703121000	-2.224567000
C	0.405706000	2.801327000	-0.507083000

H	-0.011347000	3.662948000	0.027645000
H	1.435425000	2.658019000	-0.146926000
H	0.472004000	3.067907000	-1.568088000
O	-2.893540000	-1.798686000	0.212045000

Conformer S6d

C	-2.875278000	0.329463000	-0.347401000
H	-3.829180000	0.498672000	0.165793000
H	-2.164309000	1.101700000	-0.041742000
H	-3.041993000	0.374237000	-1.426156000
S	-2.340591000	-1.313626000	0.135190000
O	-0.939443000	-1.459320000	-0.781083000
H	-0.241827000	-0.966282000	-0.310775000
C	1.259272000	-0.315995000	1.186422000
C	0.351931000	0.748189000	1.237222000
C	0.251744000	1.744112000	0.198754000
C	1.164685000	1.523698000	-0.895453000
C	2.058857000	0.453438000	-0.934892000
C	2.125324000	-0.504100000	0.094299000
H	1.278240000	-1.034082000	2.009009000
H	-0.305697000	0.859933000	2.098235000
H	1.139125000	2.243805000	-1.712548000
H	2.714176000	0.342426000	-1.801314000
C	3.041161000	-1.698587000	0.008125000
H	3.330863000	-2.044655000	1.006988000
H	2.568762000	-2.545309000	-0.508543000
H	3.959472000	-1.452640000	-0.537817000
O	-0.588602000	2.704182000	0.232757000

Conformer S6e

C	-1.810990000	-1.689461000	-0.529019000
H	-2.039344000	-2.391530000	-1.339463000
H	-0.867650000	-1.184400000	-0.745215000
H	-1.716657000	-2.242402000	0.409292000
S	-3.178570000	-0.526554000	-0.439744000
O	-2.749253000	0.356800000	0.898566000
H	-1.990797000	1.005354000	0.622866000
C	1.835899000	-0.467009000	1.097935000
C	0.626313000	0.229992000	1.142119000
C	0.250375000	1.167834000	0.130346000
C	1.177889000	1.290698000	-0.948471000
C	2.387809000	0.593065000	-0.975994000

C	2.731315000	-0.330918000	0.024706000
H	2.072517000	-1.167581000	1.901035000
H	-0.051970000	0.098164000	1.983158000
H	0.931408000	1.997884000	-1.738695000
H	3.063488000	0.735416000	-1.821611000
C	4.013891000	-1.122755000	-0.038604000
H	4.383354000	-1.354374000	0.966715000
H	3.887737000	-2.076795000	-0.568105000
H	4.798126000	-0.561915000	-0.559617000
O	-0.861760000	1.835496000	0.164865000

Conformer 1f

C	-3.610798000	0.350107000	1.220084000
H	-3.929516000	-0.163777000	2.133660000
H	-2.732082000	0.963241000	1.431026000
H	-4.426137000	0.981038000	0.856233000
S	-3.182548000	-0.906713000	0.009299000
O	-2.678509000	0.060523000	-1.242394000
H	-1.817286000	0.531725000	-0.900213000
C	2.887709000	1.037859000	0.110274000
C	1.608591000	1.582130000	-0.024681000
C	0.443474000	0.767849000	-0.151467000
C	0.689919000	-0.638498000	-0.191408000
C	1.975795000	-1.168227000	-0.062404000
C	3.107973000	-0.348525000	0.072372000
H	3.742861000	1.709176000	0.208934000
H	1.463451000	2.660863000	-0.003498000
H	-0.168628000	-1.299912000	-0.285619000
H	2.105791000	-2.251427000	-0.096970000
C	4.484820000	-0.933361000	0.266292000
H	5.256959000	-0.260525000	-0.124055000
H	4.714735000	-1.114733000	1.324899000
H	4.582538000	-1.891386000	-0.256805000
O	-0.746092000	1.282868000	-0.241451000

Optimized conformers for the CH_3SOH–H_2O complex

Conformer S7a

C	-0.743850000	1.351754000	0.289131000
H	-1.430320000	2.045484000	-0.206136000
H	-0.890270000	1.422821000	1.367846000
H	0.280664000	1.610314000	0.020189000
S	-1.162844000	-0.272212000	-0.340492000
O	0.101422000	-1.174417000	0.355492000
H	-0.212426000	-1.534085000	1.192366000
O	2.455858000	0.318179000	-0.103945000
H	1.784616000	-0.362581000	0.036387000
H	3.078099000	-0.087172000	-0.709940000

Conformer 1g

C	1.322956000	1.103441000	0.371079000
H	1.992282000	1.663827000	-0.288804000
H	0.466866000	1.730954000	0.624203000
H	1.867063000	0.828330000	1.275688000
S	0.822406000	-0.365329000	-0.525771000
O	-0.088275000	-1.125467000	0.664617000
H	-0.970740000	-0.724567000	0.616599000
O	-2.301347000	0.468887000	-0.044158000
H	-3.257432000	0.384404000	-0.034937000
H	-2.077289000	0.594312000	-0.970556000