Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Concerning the Mechanism of Iodine(III)-Mediated Oxidative Dearomatization of Phenols

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SUPPORTING INFORMATION

General computational details and references

Calculations were performed using the *Gaussian 09* suite[1] of electronic structure programs. All geometries were fully optimized at the M06-2X level[2] of density functional theory.[3] The 6–31+G(d) basis set[4] was used for C, H, and O. For iodine, the LANL2DZdp basis set[5] was used. An ultrafine grid density was used for numerical integration.[6] Unless otherwise noted, optimizations were performed with no frozen coordinates. Energy minima and transition states were identified though frequency analysis. The Gibbs energies for all relevant species can be found in Table S1. In order to account for solvation effects, the SMD solvation model[7] for CH_2Cl_2 and CH_3CN was employed during geometry optimizations. Graphics were generated using CYLview, 1.0b.[8]

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

(2) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

(3) Cramer, C. J. Essentials of Computational Chemistry: Theories and Models, 2nd ed.; Wiley: West Sussex, 2004.

(4) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.

(5) Check, C. E.; Faust, T.O.; Bailey, J.M.; Wright, B.J.; Gilbert, T.M.; Sunderlin, L.S. *J. Phys. Chem. A* **2001**, *105*, 8111.

(6) Wheeler, S. E.; Houk, K. N. *J. Chem. Theory Comput.* **2010**, *6*, 395.

(7) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

(8) Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

Table S1: Tabulated free energies for all fully optimized[a] structures. All energies are in Hartrees (kcal) and calculated for T = 298.15 K and 1 atm.

compound	G_{calc} in CH_2Cl_2	G_{calc} in CH_3CN
water	-76.389817 (-47935.2977)	-76.389988 (-47935.4050)
acetic acid	-228.968230 (-143679.6250)	-228.969988 (-143680.7282)
acetate	-228.500600 (-143386.1830)	-228.508137 (-143390.9125)
iodobenzene	-242.833334 (-152380.1026)	-242.832376 (-152379.5014)
Ph–I•OAc anion	n.d.	-471.329517 (-295763.5139)
Compound **3**	-817.070019 (-512718.7906)	-817.071023 (-512719.4206)
Compound **3H+**	-817.479867 (-512975.9739)	-817.485208 (-512979.3254)
4-methylphenoxenium (**4**)	-345.702753 (-216931.5888)	-345.709859 (-216936.0479)
protonated quinol (**5**)	-422.089333 (-264864.8553)	-422.097769 (-264870.1489)
quinol (**6**)	-421.715108 (-264630.0257)	-421.715341 (-264630.1719)
TS1	-817.021848 (-512688.5628)	-817.025820 (-512691.0553)
TS1H+	-817.465050 (-512966.6761)	-817.469584 (-512969.5212)
TS2	-422.081526 (-264859.9563)	-422.089015 (-264864.6557)
Structure **7*f***	-817.023962 (-512689.8894)	-817.031657 (-512694.7181)
Structure **9*f***	n.d.	-893.383608 (-560606.2545)
Structure **10**	n.d.	-893.405699 (-560620.1168)
Iodonium **S1**	-588.518692 (-369300.7759)	-588.526512 (-369305.6830)

[a] Obtained from calculations using M06-2X/6–31+G(d) for CHO, and LANL2DZdp for I

Method used to generate structure 7*f*

Structure **7*f*** was generated as follows. **TS1** was opened in GaussView and the vibrations visualized. The single negative frequency (-109.1 in CH_3CN; -62.97 in CH_2Cl_2) was selected. Using the manual displacement slider, the displacement along this mode was set such that the oxygen atom of the phenolic group and the iodine atom were at a maximum displacement. This new structure was then saved and used as a starting point for a new optimization. Before optimizing this new structure, the I–O13 and I–O30 (one of the acetate oxygen atoms) distances were frozen. Freezing these distances ensures that the starting structure will be optimized to a structure on the reaction coordinate that is close to the transition state and will not fall to a local minimum.

Comparison of partial charges

Table S2. Mulliken charges with hydrogens summed into heavy atoms. Atom numbering as shown in Figure 2.

Compound **3** (CH_2Cl_2)		Compound **3** (CH_3CN)		**TS1** (CH_2Cl_2)		**TS1** (CH_3CN)		***7f*** (CH_2Cl_2)		***7f*** (CH_3CN)		Iodobenzene (CH_2Cl_2)	
atom	charge	atom	charge	atom	charge	atom	charge	atom	charge	atom	charge	atom	charge
I1	0.900811	I1	0.902663	I1	0.362816	I1	0.413641	I1	0.259003	I1	0.190768	I1	-0.001204
C2	0.962014	C2	1.048084	C2	0.978119	C2	1.008238	C2	0.892963	C2	0.848751	C2	0.741310
C3	0.016334	C3	0.014404	C3	0.042986	C3	0.056370	C3	0.074688	C3	0.067012	C3	-0.036417
C4	-0.442980	C4	-0.441791	C4	-0.345745	C4	-0.365070	C4	-0.279822	C4	-0.274349	C4	-0.378443
C5	-0.518582	C5	-0.594850	C5	-0.626525	C5	-0.585245	C5	-0.701180	C5	-0.674281	C5	-0.378443
C6	0.078058	C6	0.084127	C6	0.035334	C6	0.023759	C6	0.038696	C6	0.048459	C6	0.026599
C7	0.049033	C7	0.049156	C7	0.050926	C7	0.035295	C7	0.067235	C7	0.080448	C7	0.026599
sum	*1.044688*	*sum*	*1.061793*	*sum*	*0.497911*	*sum*	*0.586988*	*sum*	*0.351583*	*sum*	*0.286808*	*sum*	*0.000001*
O13	-0.579274	O13	-0.578849	O13	-0.355292	O13	-0.392426	O13	-0.320578	O13	-0.327251	Iodobenzene (CH_3CN)	
C14	0.133746	C14	0.170171	C14	-0.043479	C14	0.081486	C14	-0.115226	C14	-0.078496	atom	charge
C15	0.210489	C15	0.192209	C15	0.477349	C15	0.442823	C15	0.481787	C15	0.531710	I1	0.003016
C16	0.182663	C16	0.166857	C16	0.548439	C16	0.506311	C16	0.589671	C16	0.587047	C2	0.723419
C17	0.209891	C17	0.154542	C17	0.320439	C17	0.285597	C17	0.408705	C17	0.426640	C3	-0.036221
C18	0.120512	C18	0.134586	C18	-0.532302	C18	-0.606069	C18	-0.539213	C18	-0.545640	C4	-0.370189
C19	-0.627874	C19	-0.606402	C19	-0.037694	C19	0.002770	C19	0.003447	C19	-0.004109	C5	-0.370189
C24	-0.104808	C24	-0.100617	C24	0.051009	C24	0.015212	C24	0.092778	C24	0.094482	C6	0.025081
sum	*-0.454655*	*sum*	*-0.467503*	*sum*	*0.428469*	*sum*	*0.335704*	*sum*	*0.601371*	*sum*	*0.684383*	C7	0.025081
O28	-0.495653	O28	-0.497660	O28	-0.654452	O28	-0.655632	O28	-0.666913	O28	-0.678739	*sum*	*-0.000002*
C29	0.639848	C29	0.644693	C29	0.713194	C29	0.714712	C29	0.717754	C29	0.715076		
O30	-0.546102	O30	-0.550861	O30	-0.646395	O30	-0.647082	O30	-0.659622	O30	-0.668609	Acetate (CH_2Cl_2)	
C31	-0.188126	C31	-0.190462	C31	-0.338727	C31	-0.334690	C31	-0.344171	C31	-0.338919	atom	charge
sum	*-0.590033*	*sum*	*-0.59429*	*sum*	*-0.92638*	*sum*	*-0.922692*	*sum*	*-0.952952*	*sum*	*-0.971191*	O28	-0.709148
												C29	0.588798
Phenoxenium **4** (CH_2Cl_2)		Phenoxenium **4** (CH_3CN)		4-Methyl-phenoxide (CH_2Cl_2)		4-Methyl-phenoxide (CH_3CN)		4-Methylphenol (CH_2Cl_2)		4-Methylphenol (CH_3CN)		O30	-0.721190
atom	charge	atom	charge	atom	charge	atom	charge	atom	charge	atom	charge	C31	-0.158460
O13	-0.373210	O13	-0.387193	O13	-0.835834	O13	-0.838269	O13	-0.203459	O13	-0.202351	*sum*	*-1.000000*
C14	-0.071075	C14	-0.059201	C14	0.082087	C14	0.111320	C14	0.082202	C14	0.087995		
C15	0.734113	C15	0.763141	C15	0.256768	C15	0.244239	C15	0.359223	C15	0.349376	Acetate (CH_3CN)	
C16	0.603725	C16	0.605862	C16	0.053257	C16	0.040183	C16	0.296850	C16	0.285174	atom	charge
C17	0.603725	C17	0.605862	C17	0.206642	C17	0.176716	C17	0.323213	C17	0.322954	O28	-0.711824
C18	-0.262090	C18	-0.273436	C18	-0.017183	C18	-0.036154	C18	-0.638494	C18	-0.633682	C29	0.587196
C19	-0.262090	C19	-0.273436	C19	-0.545546	C19	-0.518661	C19	-0.085819	C19	-0.081666	O30	-0.724050
C24	0.026901	C24	0.018400	C24	-0.200192	C24	-0.179374	C24	-0.133715	C24	-0.127801	C31	-0.151322
sum	*0.999999*	*sum*	*0.999999*	*sum*	*-1.000001*	*sum*	*-1.000000*	*sum*	*0.000001*	*sum*	*-0.000001*	*sum*	*-1.000000*

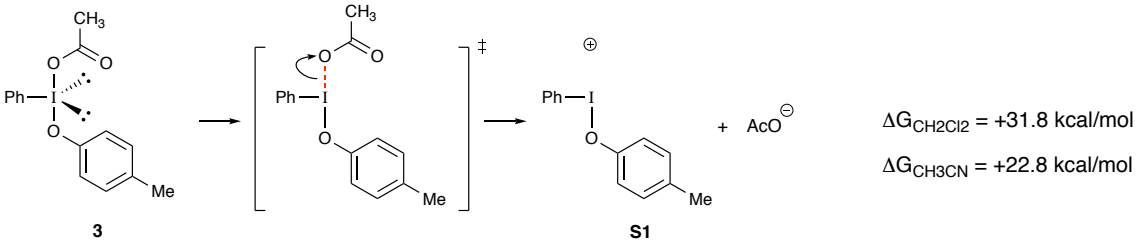
Comparison of partial charges for protonated pathway

Table S3. Mulliken charges with hydrogens summed into heavy atoms. Atom numbering as shown in Figure 2.

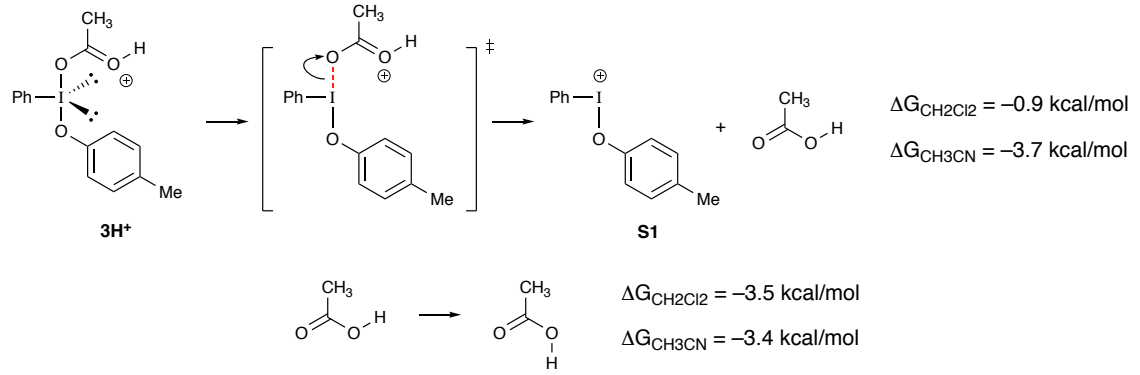
Compound **3H$^+$** **(CH_2Cl_2)**		Compound **3H$^+$** **(CH_3CN)**		**TS1H$^+$** **(CH_2Cl_2)**		**TS1H$^+$** **(CH_3CN)**	
atom	charge	atom	charge	atom	charge	atom	charge
I1	0.903306	I1	0.916655	I1	0.441373	I1	0.460952
C2	0.919047	C2	0.994977	C2	1.338982	C2	1.342367
C3	0.053714	C3	0.043483	C3	0.012056	C3	0.018893
C4	-0.297471	C4	-0.325236	C4	-0.584996	C4	-0.582522
C5	-0.434152	C5	-0.479322	C5	-0.792231	C5	-0.791836
C6	-0.021332	C6	-0.014749	C6	0.109897	C6	0.104163
C7	0.031873	C7	0.031570	C7	0.154867	C7	0.150103
sum	*1.154985*	*sum*	*1.167378*	*sum*	0.679948	*sum*	0.70212
O13	-0.490687	O13	-0.498012	O13	-0.379157	O13	-0.384669
C14	-0.184782	C14	-0.148137	C14	0.141667	C14	0.158954
C15	0.288374	C15	0.271111	C15	0.368242	C15	0.383331
C16	0.392096	C16	0.380321	C16	0.459606	C16	0.457338
C17	0.540996	C17	0.494612	C17	0.194032	C17	0.188954
C18	-0.028705	C18	-0.002196	C18	-0.591415	C18	-0.608782
C19	-0.694122	C19	-0.691620	C19	0.076005	C19	0.063492
C24	-0.090872	C24	-0.091945	C24	0.038646	C24	0.025874
sum	*-0.267702*	*sum*	*-0.285866*	*sum*	0.307626	*sum*	0.284492
O28	-0.481560	O28	-0.483737	O28	-0.485987	O28	-0.493508
C29	0.828146	C29	0.834482	C29	0.852798	C29	0.851785
O30	-0.031051	O30	-0.028282	O30	-0.076523	O30	-0.074624
C31	-0.202818	C31	-0.203973	C31	-0.277862	C31	-0.270267
sum	*0.112717*	*sum*	*0.11849*	*sum*	0.012426	*sum*	0.013386

Examining a pathway proceeding through an iodonium intermediate

Pathways proceeding through iodonium intermediate **S1** were examined. The overall energetics of the formation of iodonium **S1** from iodane **3** are shown below. The formation of iodonium **S1** + acetate is about 10 kcal/mol higher in energy than the formation of phenoxenium **4** + PhI + acetate (compare to Figure 2). The formation of **S1** from iodane **3** represents an energy change comparable to **TS1**. We were unable to locate a transition structure for this transformation. This may not be surprising considering that the addition of strong Brønsted or Lewis acids are usually needed in order to form iodonium species (see reference 26 in Main Text).



The overall energetics of the formation of iodonium **S1** from iodane **3H$^+$** are shown below. The formation of iodonium **S1** + AcOH from is about 10 kcal/mol higher in energy than the formation of phenoxenium **4** + PhI + acetate (compare to Figure 5). We were unable to locate a transition structure for this transformation. Several attempts were made to scan the I–HOAc coordinate. All either led to an imaginary frequency representing rocking of iodine between the oxygen atoms of HOAc (~4.4 kcal/mol higher in energy than **3H$^+$**) for led to structures of increasing energy. Part of this difficulty may be due to the formation of the acetic acid moiety in iodane **3H$^+$**. The microscopic reverse of the necessary I–O bond cleavage requires an acetic acid molecule with an energetically disfavored conformation (shown below). This conformation was used to calculate the overall energetics for the conversion of iodane **3H$^+$** into iodonium **S1**.



Also, attempts were made to force water to add to the 4-position of the phenolate moiety of iodonium **S1**. All attempts failed to locate a transition structure and were met with similar difficulties to those described in the Main Text. Once again, analysis of the partial charges in iodonium **S1** reveals that the phenolate portion of iodonium **S1** has an overall partial negative charge (Table S4), albeit not as negative as that found with iodanes **3** and **3H$^+$**. At this time we cannot rule out the formation of iodonium **S1**. But, given the choice between the redox decomposition of iodanes **3** and **3H$^+$** to give phenoxenium ion **4** directly, or a more protracted mechanism proceeding through an additional intermediate, we favor the simpler option.[9]

(9) Hoffmann, R.; Minkin, V. I.; Carpenter, B. K. Ockham's Razor and Chemistry. *HYLE—International Journal for Philosophy of Chemistry* **1997**, *3*, 3–28.

Table S4. Mulliken charges with hydrogens summed into heavy atoms. Atom numbering as shown in Figure 2.

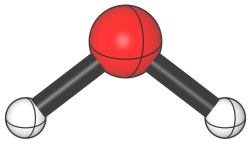
Compound **S1** (CH_2Cl_2)		Compound **S1** (CH_3CN)	
atom	charge	atom	charge
I1	0.857110	I1	0.864424
C2	0.892576	C2	1.310972
C3	0.027894	C3	-0.031220
C4	-0.344486	C4	-0.526204
C5	-0.275332	C5	-0.611131
C6	-0.038134	C6	0.099681
C7	0.004928	C7	0.061338
sum	*1.124556*	*sum*	*1.16786*
O13	-0.421404	O13	-0.418063
C14	-0.074665	C14	0.238651
C15	0.309952	C15	0.219733
C16	0.321204	C16	0.123569
C17	0.488055	C17	0.141957
C18	0.017749	C18	0.152882
C19	-0.653044	C19	-0.545253
C24	-0.112405	C24	-0.081337
sum	*-0.124558*	*sum*	*-0.167861*

Final coordinates and energies for fully optimized structures

The final optimized geometry of each species is given below, along with the following:
(i) Number of imaginary frequencies (frequency if present)
(ii) Returned energies (in Hartrees) at 298.15 K and 1 atm using SMD solvation as appropriate.

H_2O in CH_2Cl_2

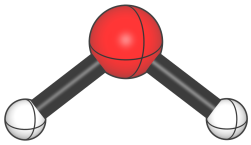
O	0.0000000	0.3929553	0.0000000
H	0.7700900	-0.1964777	0.0000000
H	-0.7700900	-0.1964777	0.0000000



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -76.371498
Sum of electronic and thermal Energies= -76.368663
Sum of electronic and thermal Enthalpies= -76.367719
Sum of electronic and thermal Free Energies= -76.389817

H_2O in CH_3CN

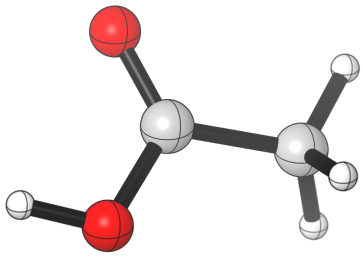
O	0.0000000	0.0000000	0.3938680
H	0.0000000	0.7694180	-0.1969340
H	0.0000000	-0.7694180	-0.1969340



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -76.372322
Sum of electronic and thermal Energies= -76.369486
Sum of electronic and thermal Enthalpies= -76.368542
Sum of electronic and thermal Free Energies= -76.389988

CH_3CO_2H in CH_2Cl_2

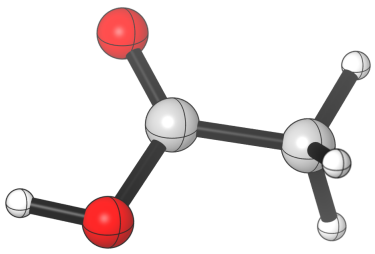
C	-0.5133269	0.2709740	0.0000148
O	-1.0572379	1.3536180	-0.0001012
C	0.9658041	0.0310630	-0.0000202
H	1.2434971	-0.5512560	-0.8835553
H	1.2436411	-0.5501130	0.8842307
H	1.4939331	0.9840120	-0.0006522
O	-1.2116999	-0.8786200	0.0000408
H	-2.1646109	-0.6596780	0.0000428



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -228.940503
Sum of electronic and thermal Energies= -228.935907
Sum of electronic and thermal Enthalpies= -228.934963
Sum of electronic and thermal Free Energies= -228.968230

CH_3CO_2H in CH_3CN

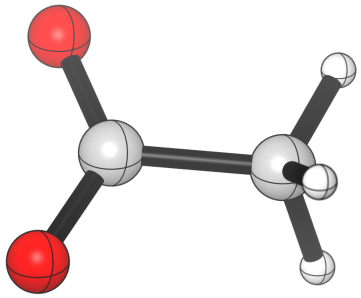
C	-0.5128689	0.2705440	0.0000798
O	-1.0561469	1.3541070	-0.0000862
C	0.9658571	0.0301770	-0.0000142
H	1.2437161	-0.5517530	-0.8837543
H	1.2439241	-0.5505650	0.8844497
H	1.4947221	0.9827590	-0.0006892
O	-1.2130289	-0.8776530	0.0000208
H	-2.1661749	-0.6576160	-0.0000062



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -228.941470
Sum of electronic and thermal Energies= -228.936819
Sum of electronic and thermal Enthalpies= -228.935875
Sum of electronic and thermal Free Energies= -228.969988

$CH_3CO_2^-$ (acetate anion) in CH_2Cl_2

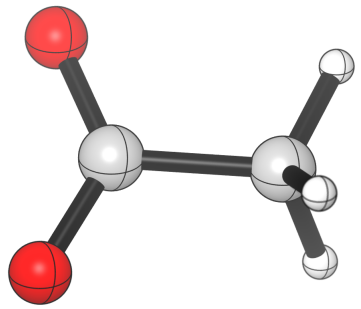
C	-0.6565501	-0.0337386	-0.0000251
H	-1.0319531	-1.0602636	-0.0000311
H	-1.0422601	0.4908524	-0.8815341
H	-1.0422861	0.4908524	0.8814729
C	0.8819779	0.0186484	-0.0000071
O	1.3907269	1.1708544	0.0000649
O	1.5003449	-1.0772056	0.0000599



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -228.473733
Sum of electronic and thermal Energies= -228.469464
Sum of electronic and thermal Enthalpies= -228.468520
Sum of electronic and thermal Free Energies= -228.500600

$CH_3CO_2^-$ (acetate anion) in CH_3CN

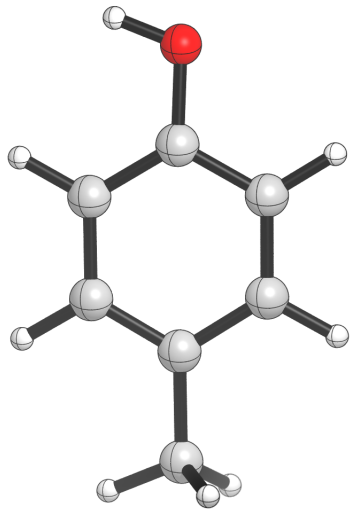
C	0.8804786	0.0189257	-0.0002057
O	1.3901296	1.1712317	-0.0000397
C	-0.6563114	-0.0340383	-0.0000937
H	-1.0416134	0.4879797	0.8830343
H	-1.0317404	-1.0604053	-0.0024087
H	-1.0423194	0.4924067	-0.8802487
O	1.5013766	-1.0761003	-0.0000377



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -228.481198
Sum of electronic and thermal Energies= -228.476912
Sum of electronic and thermal Enthalpies= -228.475968
Sum of electronic and thermal Free Energies= -228.508137

4-methylphenol in CH_2Cl_2

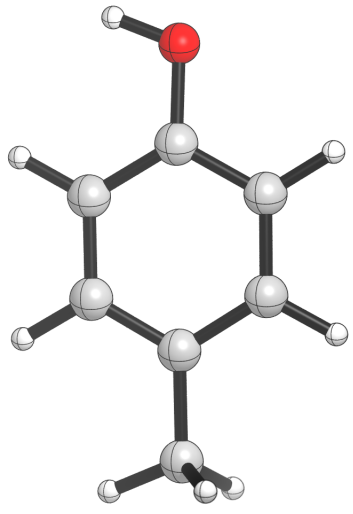
C	1.8330202	-0.0650516	0.0004067
C	-0.9831018	-0.0333516	-0.0066923
C	1.1200462	-1.2662806	-0.0016793
C	1.1486192	1.1488994	-0.0016663
C	-0.2479078	1.1540744	-0.0054333
C	-0.2705208	-1.2408456	-0.0053763
H	1.6645172	-2.2064396	-0.0019093
H	1.7025452	2.0854474	-0.0020283
H	-0.7709368	2.1078774	-0.0079863
H	-0.8163538	-2.1824216	-0.0076373
C	-2.4913818	-0.0277446	0.0047437
H	-2.8816578	-0.4074496	0.9562437
H	-2.8981938	-0.6619316	-0.7903283
H	-2.8820568	0.9843284	-0.1363423
O	3.1963482	-0.1419546	0.0024917
H	3.5770152	0.7528444	0.0031937



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -346.519800
Sum of electronic and thermal Energies= -346.512524
Sum of electronic and thermal Enthalpies= -346.511580
Sum of electronic and thermal Free Energies= -346.551452

4-methylphenol in CH_3CN

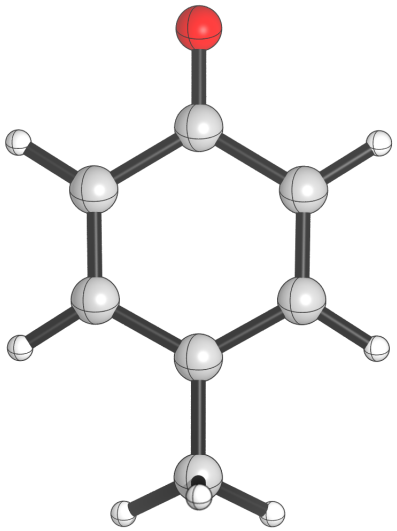
C	1.8332289	-0.0655879	0.0004606
C	-0.9832041	-0.0332639	-0.0056604
C	1.1198279	-1.2668789	-0.0013714
C	1.1492799	1.1489511	-0.0013354
C	-0.2475071	1.1542201	-0.0046184
C	-0.2711231	-1.2411689	-0.0045594
H	1.6629269	-2.2079619	-0.0017524
H	1.7037759	2.0850301	-0.0017514
H	-0.7704801	2.1080931	-0.0071154
H	-0.8172271	-2.1825939	-0.0067354
C	-2.4914111	-0.0271029	0.0040406
H	-2.8830301	-0.4205839	0.9493176
H	-2.8969101	-0.6505229	-0.8002184
H	-2.8806671	0.9873141	-0.1233634
O	3.1964429	-0.1420339	0.0021806
H	3.5760769	0.7540911	0.0024826



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -346.519366
Sum of electronic and thermal Energies= -346.512089
Sum of electronic and thermal Enthalpies= -346.511145
Sum of electronic and thermal Free Energies= -346.551118

4-methylphenoxenium (4) in CH_2Cl_2

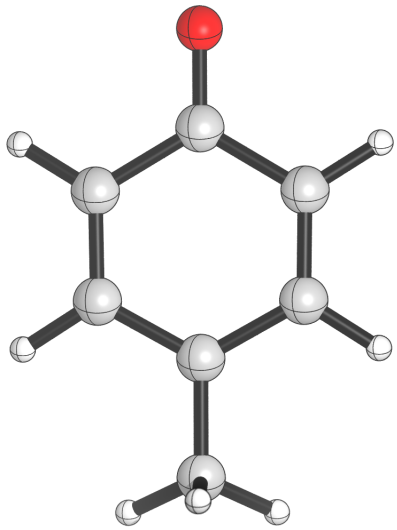
C	-0.0256807	-2.0928293	0.0000000
C	-0.0287017	0.7250607	0.0000000
C	-0.0241837	-1.3265663	1.2801340
C	-0.0241837	-1.3265663	-1.2801340
C	-0.0241837	0.0219257	-1.2590160
C	-0.0241837	0.0219257	1.2590160
H	-0.0236297	-1.9037573	2.2003080
H	-0.0236297	-1.9037573	-2.2003080
H	-0.0245787	0.6076617	-2.1729040
H	-0.0245787	0.6076617	2.1729040
O	-0.0233487	-3.3061033	0.0000000
C	0.0125803	2.1879737	0.0000000
H	1.0896123	2.4503467	0.0000000
H	-0.4156547	2.6185117	0.9077380
H	-0.4156547	2.6185117	-0.9077380



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -345.670297
Sum of electronic and thermal Energies= -345.662840
Sum of electronic and thermal Enthalpies= -345.661896
Sum of electronic and thermal Free Energies= -345.702753

4-methylphenoxenium (4) in CH_3CN

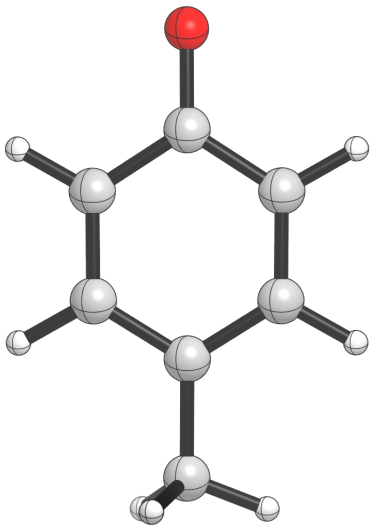
C	-0.0238696	-2.0921223	0.0000000
C	-0.0286156	0.7257217	0.0000000
C	-0.0215636	-1.3259333	1.2798120
C	-0.0215636	-1.3259333	-1.2798120
C	-0.0215636	0.0219947	-1.2590940
C	-0.0215636	0.0219947	1.2590940
H	-0.0208046	-1.9016663	2.2008280
H	-0.0208046	-1.9016663	-2.2008280
H	-0.0216086	0.6080667	-2.1727050
H	-0.0216086	0.6080667	2.1727050
O	-0.0228566	-3.3062053	0.0000000
C	0.0061244	2.1873277	0.0000000
H	1.0835594	2.4495447	0.0000000
H	-0.4216306	2.6154047	0.9090590
H	-0.4216306	2.6154047	-0.9090590



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -345.677841
Sum of electronic and thermal Energies= -345.670432
Sum of electronic and thermal Enthalpies= -345.669488
Sum of electronic and thermal Free Energies= -345.709859

4-methylphenoxide anion in CH_2Cl_2

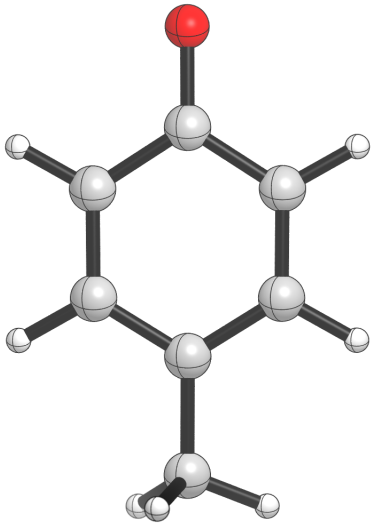
C	-2.1558786	0.0006211	0.0007830
C	0.7554834	0.0038131	-0.0041040
C	-1.3778796	1.2047461	-0.0008360
C	-1.3731156	-1.2042549	-0.0008750
C	0.0168154	-1.1908379	-0.0032090
C	0.0153794	1.1935921	-0.0031910
H	-1.9137446	2.1531871	-0.0014220
H	-1.9085456	-2.1530099	-0.0013990
H	0.5524844	-2.1419229	-0.0046380
H	0.5486954	2.1454491	-0.0047290
O	-3.4382366	-0.0045179	0.0023720
C	2.2659194	-0.0026969	0.0037700
H	2.6723944	-0.4490519	0.9207540
H	2.6609454	1.0169281	-0.0648850
H	2.6792834	-0.5720449	-0.8383910



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -346.041228
Sum of electronic and thermal Energies= -346.034209
Sum of electronic and thermal Enthalpies= -346.033265
Sum of electronic and thermal Free Energies= -346.072873

4-methylphenoxide anion in CH_3CN

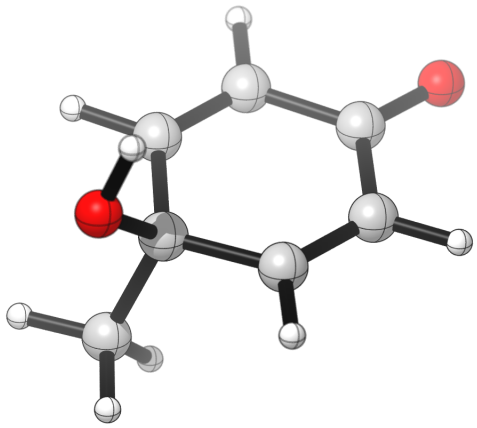
C	-2.1560548	0.0006313	0.0014820
C	0.7556312	0.0035353	-0.0076200
C	-1.3779528	1.2047473	-0.0014420
C	-1.3735618	-1.2041997	-0.0014960
C	0.0171142	-1.1911817	-0.0059260
C	0.0158672	1.1937803	-0.0058740
H	-1.9127578	2.1538883	-0.0026300
H	-1.9080028	-2.1536047	-0.0025340
H	0.5528142	-2.1419787	-0.0086230
H	0.5495422	2.1452233	-0.0087730
O	-3.4391598	-0.0041227	0.0042040
C	2.2659672	-0.0023467	0.0068050
H	2.6681482	-0.3834487	0.9545800
H	2.6616922	1.0097573	-0.1312270
H	2.6807132	-0.6306797	-0.7909260



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -346.047552
Sum of electronic and thermal Energies= -346.040519
Sum of electronic and thermal Enthalpies= -346.039575
Sum of electronic and thermal Free Energies= -346.079343

***p*-quinol (6) in CH_2Cl_2**

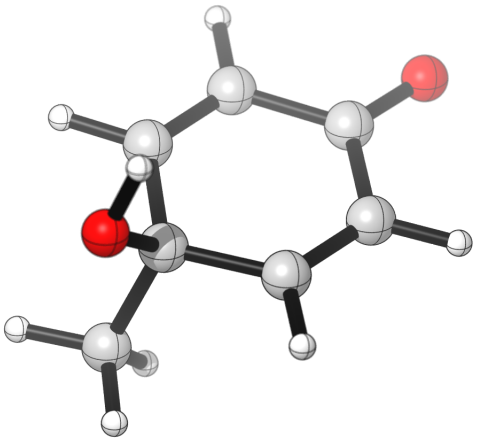
C	-0.1809739	2.1277816	0.0000000
C	-0.2122059	0.0188356	1.2559220
C	-0.2122059	0.0188356	-1.2559220
C	-0.1429329	-0.8111264	0.0000000
C	-0.2122059	1.3564806	-1.2621360
C	-0.2122059	1.3564806	1.2621360
H	-0.2445669	1.9318706	-2.1835830
H	-0.2445669	1.9318706	2.1835830
H	-0.2474849	-0.5480194	2.1854660
H	-0.2474849	-0.5480194	-2.1854660
O	-0.1489399	3.3528756	0.0000000
C	1.1544041	-1.6244534	0.0000000
H	2.0247241	-0.9623194	0.0000000
H	1.1878731	-2.2601774	-0.8903570
H	1.1878731	-2.2601774	0.8903570
O	-1.1987579	-1.7759904	0.0000000
H	-2.0503429	-1.3047474	0.0000000



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -421.682431
Sum of electronic and thermal Energies= -421.674205
Sum of electronic and thermal Enthalpies= -421.673261
Sum of electronic and thermal Free Energies= -421.715108

***p*-quinol (6) in CH_3CN**

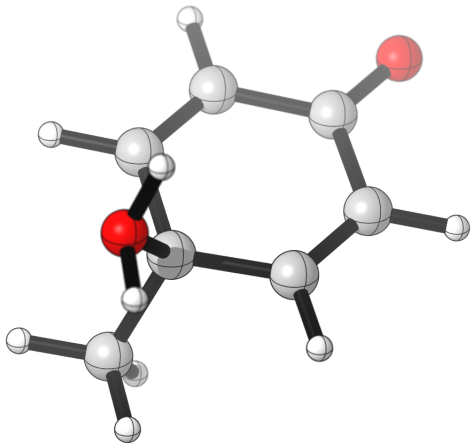
C	0.1832252	-2.1248379	0.0000000
C	0.2174692	-0.0164029	1.2558250
C	0.2174692	-0.0164029	-1.2558250
C	0.1432272	0.8127781	0.0000000
C	0.2174692	-1.3542179	-1.2619190
C	0.2174692	-1.3542179	1.2619190
H	0.2511282	-1.9284399	-2.1841360
H	0.2511282	-1.9284399	2.1841360
H	0.2533312	0.5500051	2.1855790
H	0.2533312	0.5500051	-2.1855790
O	0.1459732	-3.3506179	0.0000000
C	-1.1615008	1.6140741	0.0000000
H	-2.0249828	0.9430601	0.0000000
H	-1.2012098	2.2486471	-0.8909370
H	-1.2012098	2.2486471	0.8909370
O	1.1913812	1.7862011	0.0000000
H	2.0463002	1.3201601	0.0000000



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -421.682671
Sum of electronic and thermal Energies= -421.674463
Sum of electronic and thermal Enthalpies= -421.673519
Sum of electronic and thermal Free Energies= -421.715341

protonated quinol (5) in CH_2Cl_2

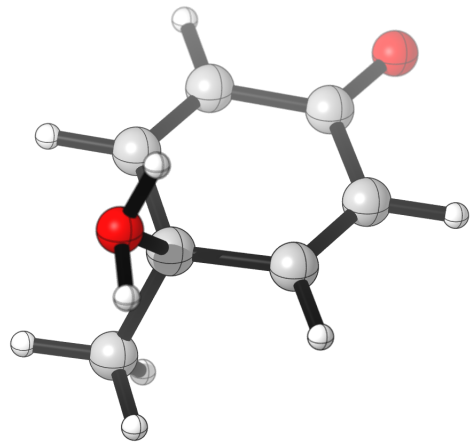
C	-2.2749491	-0.0203927	0.0642875
C	-0.1743331	-1.3016447	0.0845545
C	-0.1621051	1.2380243	0.0631105
C	0.6228879	-0.0364117	-0.0051485
C	-1.4968311	1.2441253	0.0669235
C	-1.5090011	-1.2922437	0.0868275
H	0.3961849	-2.2277627	0.1008715
H	0.4132929	2.1624593	0.0551705
H	-2.0662131	2.1689913	0.0688825
H	-2.0882061	-2.2108247	0.1054315
O	-3.4934621	-0.0139927	0.0591745
C	1.6267779	-0.0535877	-1.1401235
H	2.2427969	-0.9555837	-1.0969785
H	2.2607149	0.8390243	-1.1156245
H	1.0684819	-0.0516617	-2.0806895
O	1.5109589	-0.0884777	1.2722525
H	0.9694949	-0.0647957	2.1020375
H	2.1535089	0.6647543	1.3090405



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -422.056185
Sum of electronic and thermal Energies= -422.047605
Sum of electronic and thermal Enthalpies= -422.046661
Sum of electronic and thermal Free Energies= -422.089333

protonated quinol (5) in CH_3CN

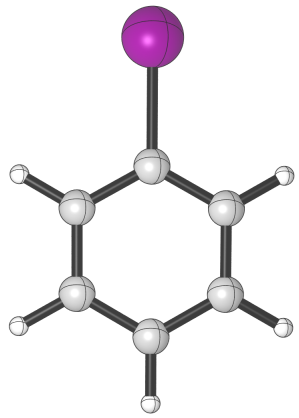
C	-2.2732077	0.0204767	-0.0701310
C	-0.1749577	1.3027777	-0.1098040
C	-0.1603177	-1.2365003	-0.0761780
C	0.6221413	0.0390387	-0.0016770
C	-1.4951547	-1.2428693	-0.0782820
C	-1.5095857	1.2921137	-0.1081510
H	0.3947853	2.2290397	-0.1372780
H	0.4179023	-2.1590983	-0.0755320
H	-2.0626627	-2.1689183	-0.0837240
H	-2.0881027	2.2109727	-0.1349690
O	-3.4931697	0.0135207	-0.0490990
C	1.5983213	0.0623087	1.1579700
H	2.2212193	0.9597337	1.1189250
H	2.2250713	-0.8354283	1.1582390
H	1.0159323	0.0754657	2.0835830
O	1.5335383	0.0836217	-1.2570160
H	1.0123003	-0.0106283	-2.0958460
H	2.2159463	-0.6356273	-1.2410300



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -422.064526
Sum of electronic and thermal Energies= -422.055911
Sum of electronic and thermal Enthalpies= -422.054966
Sum of electronic and thermal Free Energies= -422.097769

iodobenzene in CH_2Cl_2

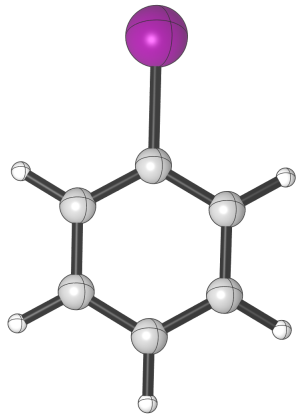
C	0.0000000	0.0000000	1.3003498
C	0.0000000	0.0000000	-1.4807282
C	0.0000000	1.2149870	0.6148288
C	0.0000000	-1.2149870	0.6148288
C	0.0000000	-1.2068840	-0.7813502
C	0.0000000	1.2068840	-0.7813502
H	0.0000000	2.1550530	1.1570588
H	0.0000000	-2.1550530	1.1570588
H	0.0000000	-2.1507630	-1.3191102
H	0.0000000	2.1507630	-1.3191102
H	0.0000000	0.0000000	-2.5667772
I	0.0000000	0.0000000	3.4043008



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -242.802297
Sum of electronic and thermal Energies= -242.796458
Sum of electronic and thermal Enthalpies= -242.795514
Sum of electronic and thermal Free Energies= -242.833334

iodobenzene in CH_3CN

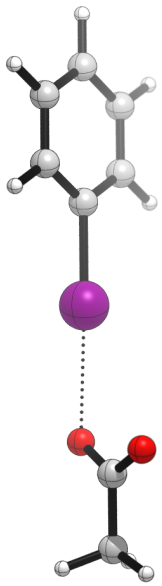
C	0.0000000	0.0000000	1.3005743
C	0.0000000	0.0000000	-1.4809367
C	0.0000000	1.2151920	0.6150063
C	0.0000000	-1.2151920	0.6150063
C	0.0000000	-1.2070920	-0.7814317
C	0.0000000	1.2070920	-0.7814317
H	0.0000000	2.1554250	1.1570833
H	0.0000000	-2.1554250	1.1570833
H	0.0000000	-2.1509940	-1.3192217
H	0.0000000	2.1509940	-1.3192217
H	0.0000000	0.0000000	-2.5670187
I	0.0000000	0.0000000	3.4045083



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -242.801341
Sum of electronic and thermal Energies= -242.795501
Sum of electronic and thermal Enthalpies= -242.794557
Sum of electronic and thermal Free Energies= -242.832376

Ph–I•OAc anion in CH_3CN

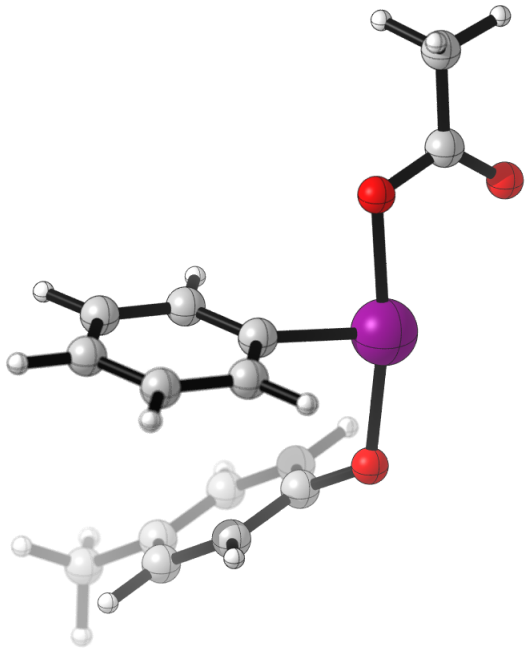
I	-0.243000	-0.085000	-0.210000
C	1.862000	-0.008000	-0.014000
C	4.645000	0.091000	0.246000
C	2.539000	1.200000	-0.203000
C	2.576000	-1.166000	0.305000
C	3.965000	-1.113000	0.434000
C	3.929000	1.245000	-0.072000
H	1.989000	2.103000	-0.451000
H	2.054000	-2.107000	0.453000
H	4.514000	-2.018000	0.682000
H	4.449000	2.188000	-0.220000
H	5.726000	0.129000	0.347000
O	-3.475000	0.773000	1.266000
C	-3.787000	0.124000	0.240000
O	-2.985000	-0.320000	-0.635000
C	-5.272000	-0.162000	-0.013000
H	-5.599000	0.387000	-0.904000
H	-5.893000	0.139000	0.835000
H	-5.423000	-1.227000	-0.216000



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -471.287220
Sum of electronic and thermal Energies= -471.275188
Sum of electronic and thermal Enthalpies= -471.274243
Sum of electronic and thermal Free Energies= -471.329517

Compound 3 in CH_2Cl_2

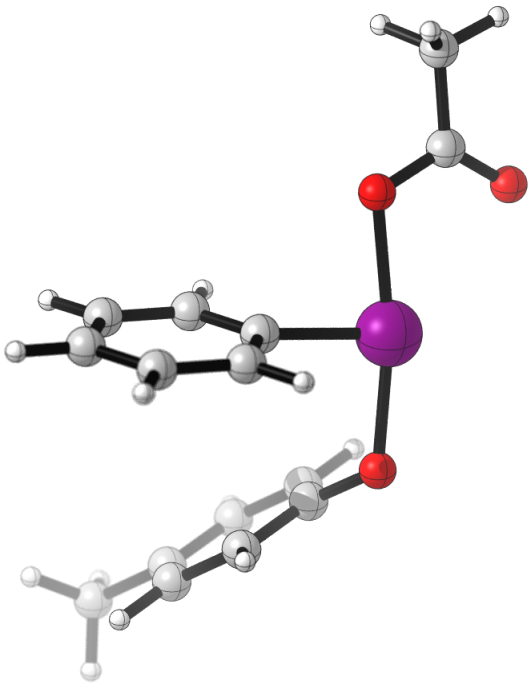
I	-1.9130351	-0.9897823	-0.8843055
C	-1.0679691	0.8809877	-0.4953455
C	0.2023169	3.2881787	-0.0332975
C	-0.9966121	1.8118267	-1.5286295
C	-0.5184791	1.1202937	0.7621125
C	0.1180579	2.3412907	0.9878185
C	-0.3540771	3.0261567	-1.2858395
H	-1.4239361	1.5974587	-2.5035975
H	-0.5765201	0.3732577	1.5480355
H	0.5557359	2.5439617	1.9607185
H	-0.2897901	3.7648607	-2.0792545
H	0.7050979	4.2338037	0.1470605
O	-0.1598951	-1.4625943	-1.8923055
C	1.0027089	-1.4127383	-1.1827765
C	3.4378489	-1.2759813	0.2411015
C	1.2798139	-2.3328173	-0.1671845
C	1.9450219	-0.4204983	-1.4830205
C	3.1456299	-0.3624473	-0.7807925
C	2.4856509	-2.2581543	0.5319445
H	0.5509389	-3.1049293	0.0682565
H	1.7208359	0.2969137	-2.2681835
H	3.8697779	0.4120937	-1.0265685
H	2.6889539	-2.9827183	1.3176495
C	4.7461589	-1.2004173	0.9875435
H	5.5933889	-1.3972913	0.3205985
H	4.7809189	-1.9332723	1.7989105
H	4.8987759	-0.2061933	1.4218855
O	-3.5814971	-0.1113603	0.1700555
C	-4.5606681	-0.9653003	0.3570145
O	-4.5146471	-2.1218603	-0.0538005
C	-5.7322631	-0.4001313	1.1189375
H	-6.1172061	0.4833687	0.6015795
H	-5.4024011	-0.0857713	2.1138205
H	-6.5186361	-1.1501943	1.2098585



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -817.018254
Sum of electronic and thermal Energies= -816.998725
Sum of electronic and thermal Enthalpies= -816.997781
Sum of electronic and thermal Free Energies= -817.070019

Compound 3 in CH_3CN

I	-1.9751921	-0.9697931	-0.8419341
C	-1.0234881	0.8615709	-0.5189681
C	0.3923519	3.2021409	-0.1412641
C	-0.8993961	1.7505829	-1.5836321
C	-0.4549181	1.1095779	0.7288459
C	0.2556649	2.2965749	0.9116979
C	-0.1839121	2.9318289	-1.3831571
H	-1.3429881	1.5296599	-2.5498891
H	-0.5561321	0.3943459	1.5397589
H	0.7082169	2.5053279	1.8765499
H	-0.0783061	3.6379369	-2.2014421
H	0.9514979	4.1214919	0.0060309
O	-0.2461991	-1.5777951	-1.8272511
C	0.9217329	-1.5162571	-1.1291241
C	3.3696209	-1.3517771	0.2722509
C	1.1614629	-2.3412461	-0.0256331
C	1.9085499	-0.6049641	-1.5286291
C	3.1148319	-0.5331511	-0.8368731
C	2.3736679	-2.2534861	0.6616599
H	0.3971209	-3.0471771	0.2912909
H	1.7143029	0.0400939	-2.3818051
H	3.8729409	0.1774359	-1.1611091
H	2.5470669	-2.9032501	1.5169129
C	4.6813429	-1.2581481	1.0104839
H	5.5228899	-1.5092791	0.3548689
H	4.7032679	-1.9417161	1.8641849
H	4.8535419	-0.2427361	1.3846709
O	-3.5934771	0.0354159	0.1778009
C	-4.6200141	-0.7531901	0.3936139
O	-4.6428641	-1.9239831	0.0218359
C	-5.7547981	-0.0953761	1.1363429
H	-6.0939651	0.7865499	0.5851459
H	-5.4034921	0.2392759	2.1171359
H	-6.5809281	-0.7964861	1.2596289



*** 0 imaginary frequencies ***

Sum of electronic and zero-point Energies= -817.018261

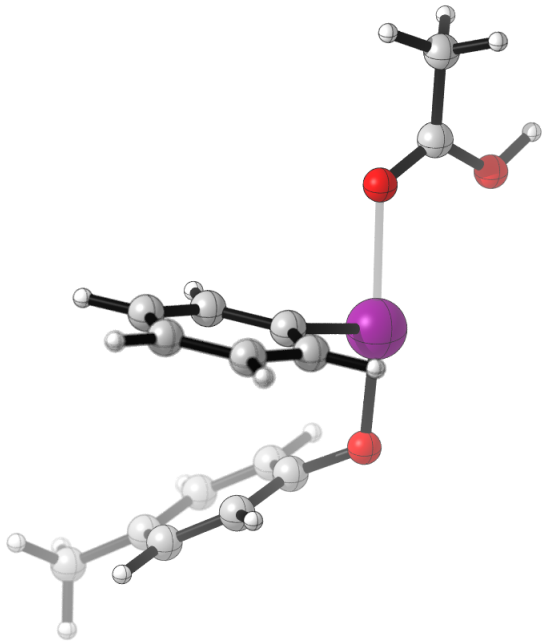
Sum of electronic and thermal Energies= -816.998597

Sum of electronic and thermal Enthalpies= -816.997653

Sum of electronic and thermal Free Energies= -817.071023

Compound $3H^+$ in CH_2Cl_2

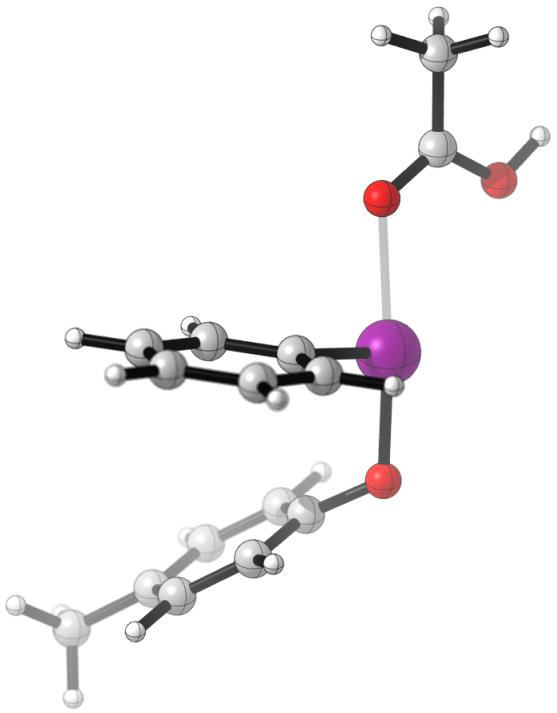
I	-1.4578720	-1.0741480	-0.8121527
C	-0.9517830	0.9181070	-0.4842607
C	-0.1315230	3.5159410	-0.0995207
C	-1.1716400	1.8435450	-1.5043417
C	-0.3365730	1.2511370	0.7214623
C	0.0726030	2.5714130	0.9065283
C	-0.7508070	3.1561840	-1.2981467
H	-1.6521940	1.5518450	-2.4330307
H	-0.1757670	0.5046610	1.4931173
H	0.5567600	2.8549530	1.8358303
H	-0.9082640	3.8958370	-2.0769287
H	0.1935940	4.5410560	0.0505423
O	0.2374360	-1.4463010	-1.7964777
C	1.4177910	-1.3381890	-1.0830787
C	3.8651270	-1.1259100	0.2619423
C	1.8182170	-2.3536650	-0.2180327
C	2.2144060	-0.2088570	-1.2746747
C	3.4323300	-0.1148790	-0.6061977
C	3.0394760	-2.2410430	0.4456963
H	1.1825680	-3.2241370	-0.0767967
H	1.8768380	0.5766560	-1.9455617
H	4.0579450	0.7615880	-0.7602557
H	3.3570500	-3.0376420	1.1140443
C	5.1921760	-1.0092910	0.9667383
H	6.0186760	-1.0236440	0.2474903
H	5.3421150	-1.8339220	1.6689623
H	5.2621230	-0.0687380	1.5235983
O	-3.4478100	-0.3128400	0.3775523
C	-4.4809990	-0.9800220	0.4061953
O	-4.4711590	-2.1565710	-0.2002737
C	-5.7320290	-0.5232580	1.0781133
H	-6.5152290	-0.3949960	0.3228333
H	-5.5537540	0.4220100	1.5885153
H	-6.0674820	-1.2806500	1.7932333
H	-5.3323470	-2.6162290	-0.1326637



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -817.426888
Sum of electronic and thermal Energies= -817.406769
Sum of electronic and thermal Enthalpies= -817.405824
Sum of electronic and thermal Free Energies= -817.479867

Compound $3H^+$ in CH_3CN

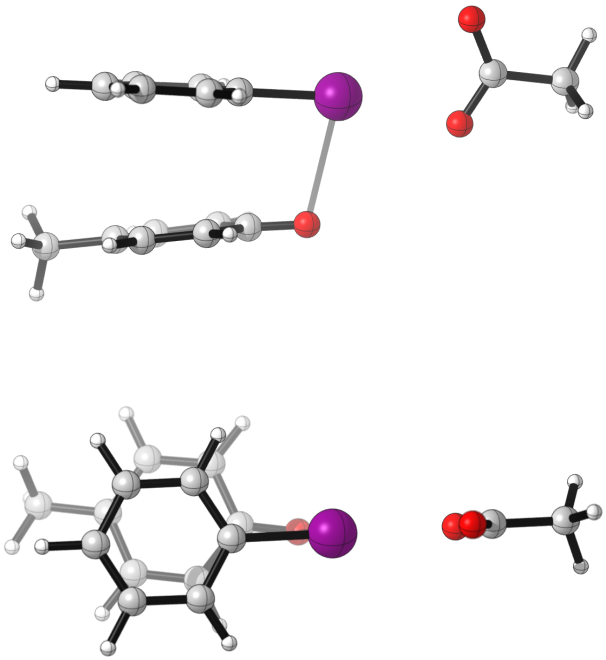
I	-1.5607246	-0.9872450	-0.7693718
C	-0.8638346	0.9573400	-0.5124328
C	0.2118974	3.4750440	-0.2270328
C	-1.0059626	1.8652780	-1.5613208
C	-0.2005656	1.2692890	0.6735942
C	0.3379384	2.5487850	0.8086602
C	-0.4567496	3.1372170	-1.4054568
H	-1.5263516	1.5905960	-2.4736488
H	-0.1020106	0.5360520	1.4683382
H	0.8606654	2.8142430	1.7224132
H	-0.5531036	3.8622810	-2.2076698
H	0.6371334	4.4680690	-0.1159528
O	0.0945044	-1.5287080	-1.7505458
C	1.2792844	-1.4914330	-1.0397058
C	3.7347714	-1.4243670	0.3092142
C	1.5851864	-2.4875320	-0.1149248
C	2.1764824	-0.4516840	-1.2888818
C	3.3972174	-0.4300080	-0.6185748
C	2.8106634	-2.4478370	0.5499452
H	0.8707484	-3.2844610	0.0764932
H	1.9123124	0.3234840	-2.0035738
H	4.0993614	0.3769420	-0.8169028
H	3.0525534	-3.2292850	1.2662732
C	5.0628594	-1.3852090	1.0206792
H	5.8911444	-1.4620760	0.3076022
H	5.1531654	-2.2082920	1.7348912
H	5.1902484	-0.4437280	1.5660312
O	-3.4488346	-0.0105620	0.3985472
C	-4.5454636	-0.5700680	0.4303062
O	-4.6504226	-1.7496120	-0.1583268
C	-5.7460206	0.0188810	1.0891312
H	-6.5221556	0.1845590	0.3341752
H	-5.4829586	0.9628410	1.5638892
H	-6.1371686	-0.6819400	1.8332362
H	-5.5558116	-2.1168550	-0.0890988



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -817.431897
Sum of electronic and thermal Energies= -817.411758
Sum of electronic and thermal Enthalpies= -817.410814
Sum of electronic and thermal Free Energies= -817.485208

TS1 in CH_2Cl_2

I	2.3652104	0.5363197	-0.0048216
C	0.4366314	1.3004637	-0.1084576
C	-2.1673976	2.3113537	-0.2589146
C	-0.0957656	2.0615117	0.9579884
C	-0.3508416	1.0605867	-1.2485756
C	-1.6490156	1.5594487	-1.3157966
C	-1.3809976	2.5780587	0.8693354
H	0.5118864	2.2495627	1.8391044
H	0.0630754	0.4972867	-2.0808586
H	-2.2558696	1.3652527	-2.1962496
H	-1.7819436	3.1728847	1.6848424
H	-3.1781986	2.7054807	-0.3195826
O	0.9034584	-1.7981013	0.6417044
C	-0.2953496	-1.5473393	0.4359014
C	-3.0520076	-1.0755033	0.0386044
C	-0.9648446	-1.9852343	-0.7921426
C	-1.0884276	-0.8227263	1.4256744
C	-2.4259246	-0.6178773	1.2236794
C	-2.3012966	-1.7860403	-0.9498286
H	-0.3598206	-2.4917093	-1.5392626
H	-0.5812176	-0.4962113	2.3291394
H	-3.0225236	-0.0866003	1.9593794
H	-2.8148046	-2.1292713	-1.8436826
C	-4.5048686	-0.8479843	-0.1832086
H	-5.0352046	-1.8043763	-0.0659566
H	-4.6921796	-0.5129073	-1.2092586
H	-4.9207236	-0.1300363	0.5259474
O	5.5137954	1.1147227	-0.3722676
C	5.5964544	-0.0896303	-0.0420176
O	4.6085284	-0.8409083	0.2339674
C	6.9779294	-0.7344363	0.0624444
H	7.1855354	-0.9750333	1.1111814
H	7.7579304	-0.0665613	-0.3102206
H	6.9987874	-1.6744453	-0.4977926

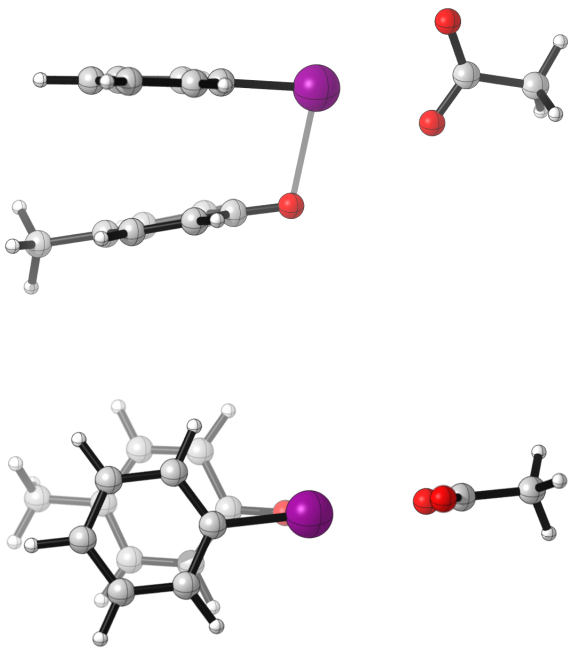


top view

*** 1 imaginary frequency (-48.0842) ***
Sum of electronic and zero-point Energies= -816.970287
Sum of electronic and thermal Energies= -816.950607
Sum of electronic and thermal Enthalpies= -816.949663
Sum of electronic and thermal Free Energies= -817.021848

TS1 in CH_3CN

I	2.3294204	0.6304366	-0.0537395
C	0.4184984	1.4172516	-0.1508995
C	-2.2048656	2.3673406	-0.2485325
C	-0.1040176	2.1650946	0.9271615
C	-0.3829166	1.1573206	-1.2764375
C	-1.6936686	1.6261756	-1.3158675
C	-1.4023996	2.6526626	0.8634225
H	0.5143634	2.3593726	1.7992495
H	0.0253144	0.5985956	-2.1144225
H	-2.3165456	1.4124616	-2.1801665
H	-1.8016716	3.2351306	1.6884835
H	-3.2270736	2.7337306	-0.2853435
O	1.0315864	-1.5818324	0.5983895
C	-0.2018946	-1.4216684	0.4135455
C	-2.9865076	-1.1431344	0.0558015
C	-0.8490926	-1.9036154	-0.7965845
C	-1.0195326	-0.7597004	1.4102995
C	-2.3740336	-0.6411354	1.2266225
C	-2.2026136	-1.7994974	-0.9370905
H	-0.2234516	-2.3650964	-1.5558875
H	-0.5262036	-0.3922164	2.3057655
H	-2.9900806	-0.1471804	1.9723405
H	-2.6989906	-2.1801294	-1.8256285
C	-4.4536936	-0.9966654	-0.1581375
H	-4.9215656	-1.9892014	-0.1999485
H	-4.6471876	-0.5205404	-1.1270815
H	-4.9257066	-0.4133794	0.6344455
O	5.4591984	1.0174796	-0.3907155
C	5.4970244	-0.1825404	-0.0339045
O	4.4790264	-0.8891244	0.2502815
C	6.8523424	-0.8748504	0.0933065
H	7.0436714	-1.1055394	1.1473285
H	7.6591714	-0.2423154	-0.2838815
H	6.8440964	-1.8236894	-0.4521735



top view

*** 1 imaginary frequency (-100.8214) ***

Sum of electronic and zero-point Energies= -816.974175

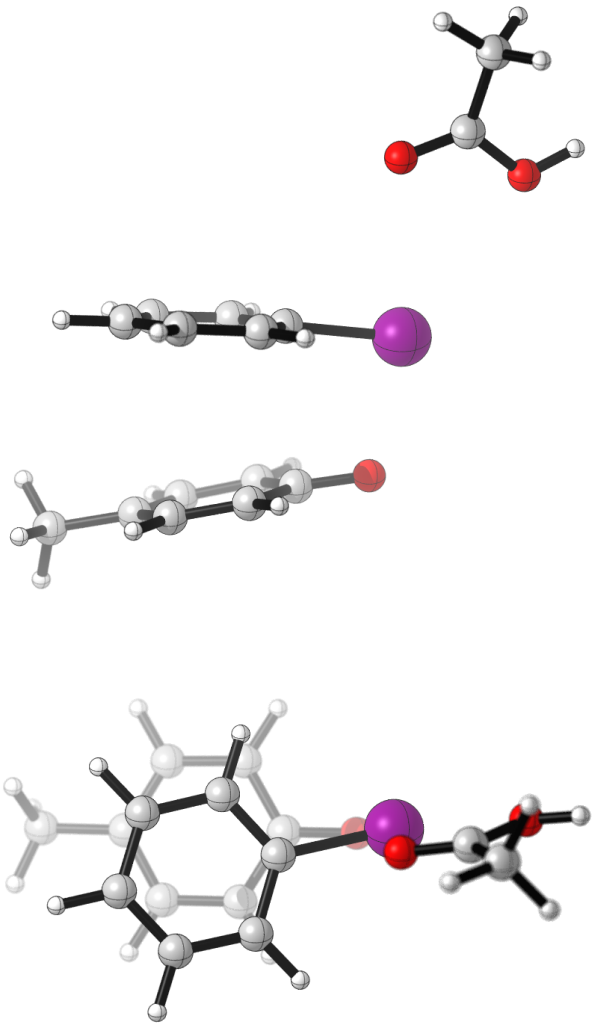
Sum of electronic and thermal Energies= -816.954458

Sum of electronic and thermal Enthalpies= -816.953514

Sum of electronic and thermal Free Energies= -817.025820

TS1H$^+$ in CH_2Cl_2

I	-1.8008029	-1.6347043	-0.1642383
C	-0.6441349	0.0498867	-0.0879263
C	1.0654711	2.2304287	-0.0347443
C	-0.5622869	0.8888067	-1.2149263
C	0.1126201	0.3018047	1.0661637
C	0.9776061	1.3934487	1.0781867
C	0.2873461	1.9862787	-1.1726243
H	-1.1577689	0.6780617	-2.0979453
H	0.0184251	-0.3401853	1.9366657
H	1.5760931	1.5933577	1.9622097
H	0.3542501	2.6461957	-2.0320253
H	1.7356791	3.0850937	-0.0148223
O	0.3314171	-2.8378023	-0.6786003
C	1.3483951	-2.1119123	-0.4308893
C	3.6455791	-0.5654313	0.0791487
C	2.0332851	-2.2089383	0.8361297
C	1.8391981	-1.1801083	-1.4108863
C	2.9676961	-0.4376123	-1.1525643
C	3.1697041	-1.4784483	1.0579477
H	1.6309001	-2.8891583	1.5819977
H	1.3072581	-1.1043033	-2.3550493
H	3.3457351	0.2629097	-1.8917843
H	3.7057851	-1.5663793	1.9990897
C	4.8612261	0.2500347	0.3709487
H	5.7287871	-0.4085053	0.5052947
H	4.7335591	0.7965077	1.3130457
H	5.0771821	0.9593617	-0.4300863
O	-4.0977749	0.6172347	0.2170987
C	-5.1850779	0.0871387	0.1891487
O	-5.2457379	-1.2596013	0.1779117
C	-6.5013279	0.8127387	0.1647367
H	-7.0632849	0.5382127	-0.7342803
H	-6.3270559	1.8882517	0.1732657
H	-7.0987499	0.5302427	1.0380387
H	-6.1691969	-1.5729053	0.1563637

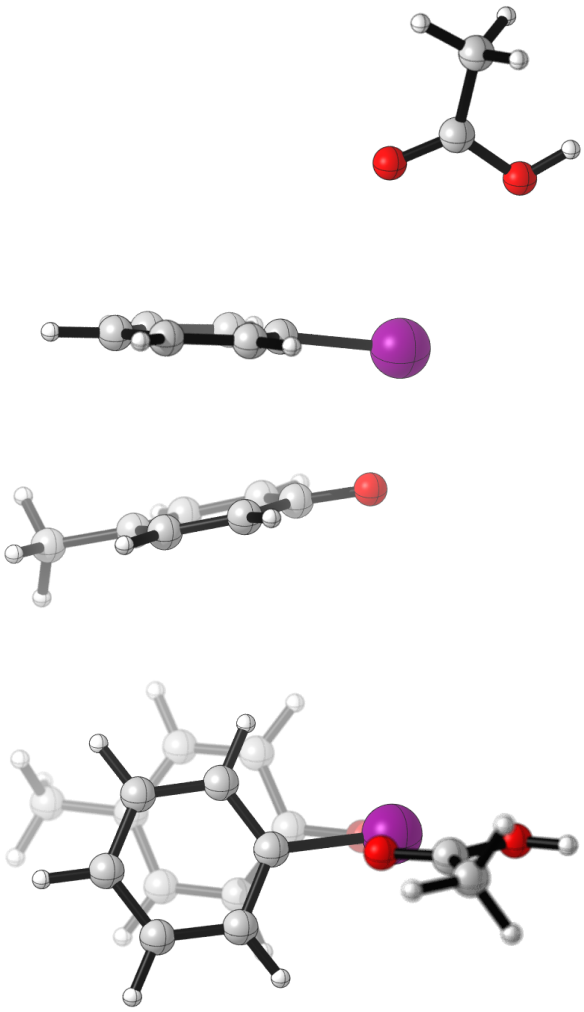


top view

*** 1 imaginary frequency (-117.5894) ***
Sum of electronic and zero-point Energies= -817.411204
Sum of electronic and thermal Energies= -817.391175
Sum of electronic and thermal Enthalpies= -817.390231
Sum of electronic and thermal Free Energies= -817.465050

TS1H$^+$ in CH_3CN

I	-1.7780082	-1.6919473	-0.1401227
C	-0.6533152	0.0140257	-0.0780257
C	1.0362068	2.2098407	-0.0480077
C	-0.5769282	0.8392567	-1.2153087
C	0.0978098	0.2866977	1.0749613
C	0.9533678	1.3860637	1.0752603
C	0.2617368	1.9456477	-1.1840967
H	-1.1648102	0.6093417	-2.0986207
H	0.0096468	-0.3480163	1.9515113
H	1.5518328	1.5990037	1.9562553
H	0.3272438	2.5937527	-2.0525877
H	1.7015598	3.0684907	-0.0383227
O	0.3467758	-2.8656113	-0.6326327
C	1.3604878	-2.1242953	-0.3962977
C	3.6405718	-0.5461203	0.0868093
C	2.0455828	-2.1948503	0.8698543
C	1.8391548	-1.2049683	-1.3906407
C	2.9604898	-0.4457603	-1.1456847
C	3.1754558	-1.4486433	1.0790293
H	1.6500928	-2.8640253	1.6293653
H	1.3040708	-1.1469553	-2.3343937
H	3.3283538	0.2479077	-1.8964847
H	3.7116878	-1.5142623	2.0218953
C	4.8455908	0.2896637	0.3666033
H	5.0617978	0.9776807	-0.4528337
H	5.7179408	-0.3554763	0.5303613
H	4.7006878	0.8625247	1.2904553
O	-4.0587212	0.5735067	0.2825453
C	-5.1615612	0.0824347	0.1913373
O	-5.2672272	-1.2594773	0.1349633
C	-6.4500542	0.8529527	0.1344063
H	-6.9863752	0.6173117	-0.7906837
H	-6.2419452	1.9217277	0.1756173
H	-7.0886232	0.5694327	0.9777343
H	-6.2005752	-1.5368553	0.0657803

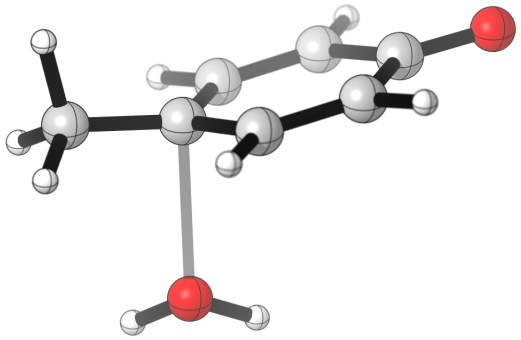


top view

*** 1 imaginary frequency (-135.9751) ***
Sum of electronic and zero-point Energies= -817.416355
Sum of electronic and thermal Energies= -817.396258
Sum of electronic and thermal Enthalpies= -817.395314
Sum of electronic and thermal Free Energies= -817.469584

TS2 in CH_2Cl_2

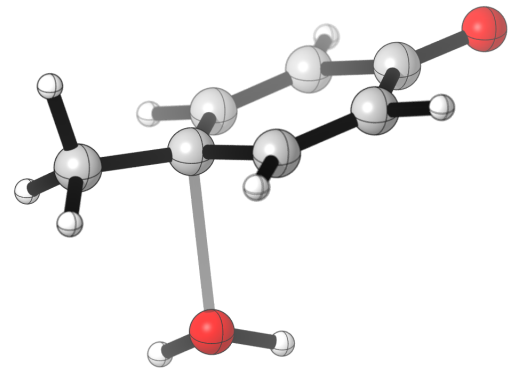
O	-3.0021807	-1.8123639	-0.0381967
C	-2.0216487	-1.0971139	0.0177183
C	0.2762033	0.5509581	0.1389063
C	-1.1018747	-1.1474559	1.1891733
C	-1.6935527	-0.1552149	-1.0886977
C	-0.5892347	0.6061201	-1.0295667
C	-0.0023467	-0.3769549	1.2245533
H	-1.3673757	-1.8269069	1.9940183
H	-2.3838697	-0.1211179	-1.9265527
H	-0.3242487	1.3002031	-1.8210257
H	0.6825053	-0.3890499	2.0672223
C	1.2247033	1.6492871	0.3689073
H	1.6140743	2.0614401	-0.5640077
H	2.0218303	1.3722151	1.0621143
H	0.6284223	2.4425651	0.8556863
O	1.8209793	-0.6956169	-0.9331247
H	1.5354163	-1.6217719	-1.0392247
H	2.6821983	-0.7392219	-0.4779027



*** 1 imaginary frequency (-134.4585) ***
Sum of electronic and zero-point Energies= -422.047200
Sum of electronic and thermal Energies= -422.037640
Sum of electronic and thermal Enthalpies= -422.036696
Sum of electronic and thermal Free Energies= -422.081526

TS2 in CH_3CN

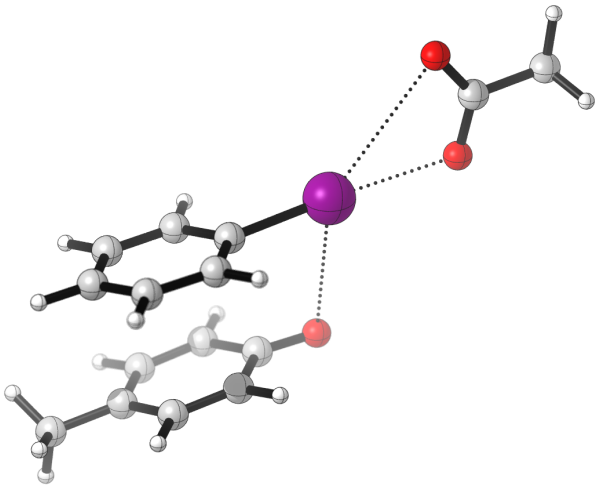
O	-2.9991447	-1.8100649	-0.0283037
C	-2.0141727	-1.0991109	0.0203993
C	0.2698973	0.5652631	0.1393343
C	-1.0881747	-1.1498919	1.1861603
C	-1.6907067	-0.1591089	-1.0894777
C	-0.5920657	0.6108201	-1.0309237
C	0.0052143	-0.3708029	1.2202953
H	-1.3434707	-1.8345099	1.9897863
H	-2.3806907	-0.1301539	-1.9278317
H	-0.3331647	1.3082581	-1.8215517
H	0.6946013	-0.3817209	2.0592033
C	1.2171343	1.6626511	0.3643983
H	1.5956813	2.0805201	-0.5701147
H	2.0196013	1.3852711	1.0510283
H	0.6200553	2.4503051	0.8607973
O	1.8684933	-0.6942389	-0.9312997
H	1.5119793	-1.5779219	-1.1359107
H	2.6389333	-0.8555639	-0.3559897



*** 1 imaginary frequency (-96.7234) ***
Sum of electronic and zero-point Energies= -422.054743
Sum of electronic and thermal Energies= -422.045169
Sum of electronic and thermal Enthalpies= -422.044224
Sum of electronic and thermal Free Energies= -422.089015

Structure 7*f* in CH_2Cl_2

I	2.4243684	0.3266562	0.0828235
C	0.4834584	1.0877372	-0.0697695
C	-2.0628246	2.2212372	-0.3409305
C	-0.0435036	1.9146762	0.9498445
C	-0.2778336	0.8495962	-1.2263365
C	-1.5451496	1.4123992	-1.3556305
C	-1.2987526	2.4867102	0.8041435
H	0.5478014	2.1101052	1.8402895
H	0.1327254	0.2385132	-2.0261295
H	-2.1290726	1.2218632	-2.2524475
H	-1.6943776	3.1284442	1.5861235
H	-3.0489436	2.6645112	-0.4502415
O	0.5773544	-2.2581388	0.5907175
C	-0.5399856	-1.7933568	0.4037595
C	-3.1872916	-0.8578968	0.0795505
C	-1.3201216	-2.1250108	-0.8100425
C	-1.1769316	-0.9224308	1.4143735
C	-2.4653236	-0.5112498	1.2537795
C	-2.5973906	-1.6964678	-0.9315015
H	-0.8324806	-2.7412778	-1.5601595
H	-0.5909566	-0.6822098	2.2972225
H	-2.9513866	0.1090052	1.9999855
H	-3.1949976	-1.9476978	-1.8031265
C	-4.5841376	-0.4022798	-0.1049525
H	-5.2461076	-1.2728888	0.0258125
H	-4.7441786	-0.0501628	-1.1300435
H	-4.8694696	0.3669892	0.6137525
O	5.6874874	1.1142422	-0.4708575
C	5.8092254	-0.0572698	-0.0479305
O	4.8584794	-0.8142098	0.3217425
C	7.2138214	-0.6582438	0.0527135
H	7.4390674	-0.8856468	1.1005845
H	7.9712514	0.0260982	-0.3366445
H	7.2561774	-1.6023448	-0.5004735

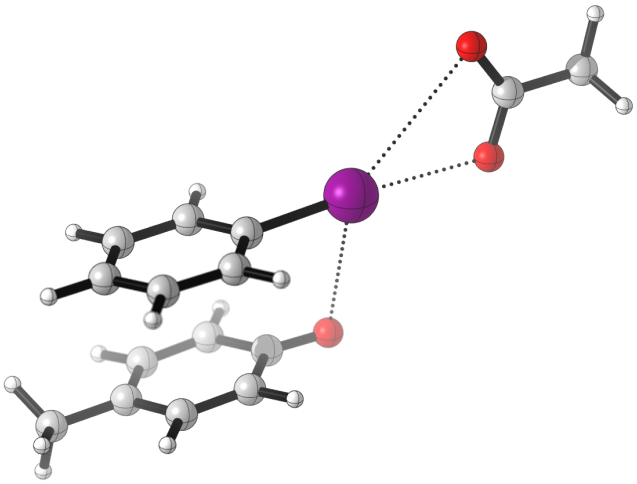


This structure was only partially optimized as the I–O13 and I–O30 bonds were frozen.

*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -816.970754
Sum of electronic and thermal Energies= -816.950063
Sum of electronic and thermal Enthalpies= -816.949119
Sum of electronic and thermal Free Energies= -817.023962

Structure 7*f* in CH_3CN

I	2.4077255	0.4283436	0.1162981
C	0.4514515	1.1554106	-0.0617469
C	-2.1243545	2.2092386	-0.3410709
C	-0.0996975	1.9630806	0.9563911
C	-0.2923615	0.8960886	-1.2222679
C	-1.5771695	1.4200476	-1.3553559
C	-1.3735185	2.4941146	0.8073851
H	0.4788355	2.1708846	1.8522071
H	0.1353875	0.2917096	-2.0181769
H	-2.1536835	1.2076756	-2.2520599
H	-1.7936405	3.1163046	1.5923881
H	-3.1261315	2.6156746	-0.4499449
O	0.5989795	-2.2363964	0.5786641
C	-0.5248375	-1.7919624	0.3958111
C	-3.1778865	-0.8817844	0.0666241
C	-1.2992215	-2.1297134	-0.8236949
C	-1.1775275	-0.9369854	1.4158021
C	-2.4653775	-0.5367934	1.2524691
C	-2.5767905	-1.7104984	-0.9497099
H	-0.8029695	-2.7370654	-1.5753189
H	-0.5964735	-0.6941524	2.3012831
H	-2.9642825	0.0736986	1.9983051
H	-3.1704785	-1.9585534	-1.8246329
C	-4.5717255	-0.4351784	-0.1226039
H	-5.2211155	-1.3170164	0.0060891
H	-4.7312065	-0.0923434	-1.1511069
H	-4.8667225	0.3295126	0.5964011
O	5.7873685	1.0896316	-0.5873539
C	5.8751765	-0.0337014	-0.0394569
O	4.9112695	-0.7036064	0.4408351
C	7.2581795	-0.6838744	0.0733011
H	7.4829375	-0.8982934	1.1237101
H	8.0405865	-0.0425744	-0.3395789
H	7.2592745	-1.6409234	-0.4598859

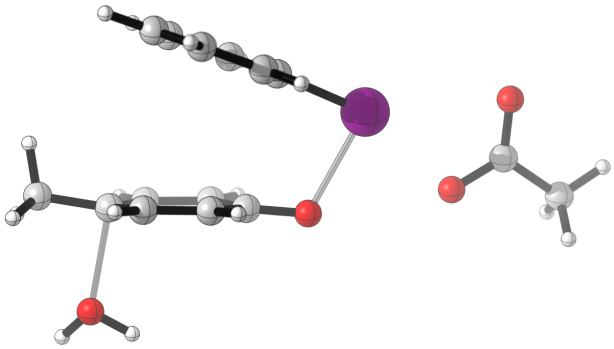


This structure was only partially optimized as the I–O13 and I–O30 bonds were frozen.

*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -816.977763
Sum of electronic and thermal Energies= -816.956955
Sum of electronic and thermal Enthalpies= -816.956011
Sum of electronic and thermal Free Energies= -817.031657

Structure 9*f* in CH_3CN

I	-2.6779843	0.7240903	-0.0844560
C	-0.9209973	1.8306753	-0.1488460
C	1.5303727	3.1541643	-0.2806490
C	-0.4903693	2.3909233	-1.3637870
C	-0.1180883	1.9328503	0.9975800
C	1.1089347	2.5910833	0.9252260
C	0.7249077	3.0650683	-1.4209690
H	-1.1073223	2.2971673	-2.2535830
H	-0.4539973	1.5049983	1.9386300
H	1.7346037	2.6639223	1.8105700
H	1.0531307	3.5077693	-2.3570360
H	2.4855507	3.6695233	-0.3325100
O	-1.2737493	-1.2197127	-0.3601380
C	-0.0270683	-1.0052837	-0.1414770
C	2.7533347	-0.7421967	0.2882790
C	0.5387987	-1.2282517	1.1615890
C	0.8378727	-0.5462487	-1.1907180
C	2.1862157	-0.4134407	-0.9711990
C	1.8884897	-1.1150577	1.3569660
H	-0.1344193	-1.5005597	1.9708810
H	0.3951797	-0.3238377	-2.1581860
H	2.8450127	-0.0756917	-1.7669260
H	2.3234007	-1.3095967	2.3340250
C	4.1742567	-0.3831627	0.5844080
H	4.7983727	-0.4526047	-0.3094520
H	4.5883397	-1.0160267	1.3735490
H	4.2048587	0.6557303	0.9397210
O	-5.7799883	0.4728073	0.1817110
C	-5.5179113	-0.7389297	0.0228940
O	-4.3457593	-1.2107797	-0.1510600
C	-6.6480963	-1.7616067	0.0465870
H	-7.6235073	-1.2733897	0.1036180
H	-6.5243283	-2.4189397	0.9142790
H	-6.6039373	-2.3907517	-0.8480480
O	3.4192677	-2.7250577	-0.3258810
H	4.0241977	-3.3672167	0.0892100
H	2.6324267	-3.2424287	-0.5748010

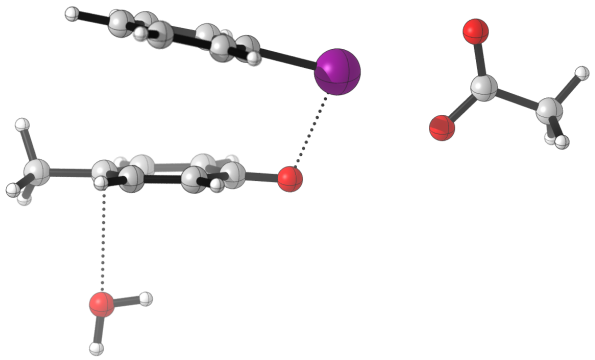


This structure was only partially optimized as the C15–O35 distance was frozen.

*** 3 imaginary frequencies (-258.2488, -57.8255, -44.8615) ***
Sum of electronic and zero-point Energies= -893.331649
Sum of electronic and thermal Energies= -893.310534
Sum of electronic and thermal Enthalpies= -893.309590
Sum of electronic and thermal Free Energies= -893.383608

Structure 10 in CH_3CN

I	-2.7047534	0.5817203	0.0130751
C	-0.9412394	1.6650373	0.0065701
C	1.5038086	3.0114833	-0.0397179
C	-0.5145744	2.3162883	-1.1702069
C	-0.1332814	1.6966003	1.1566971
C	1.0894496	2.3630473	1.1248201
C	0.6929536	3.0013063	-1.1814319
H	-1.1357664	2.2829153	-2.0611149
H	-0.4686744	1.2102743	2.0691791
H	1.7178096	2.3779393	2.0111851
H	1.0157626	3.5116723	-2.0842419
H	2.4560466	3.5346923	-0.0578529
O	-1.0797864	-1.4495097	-0.3119349
C	0.1122476	-1.0880577	-0.1245909
C	2.8262846	-0.4106317	0.2409351
C	0.7633476	-1.2915317	1.1585371
C	0.8753576	-0.4707997	-1.1896059
C	2.1960466	-0.1536787	-0.9992079
C	2.0878956	-0.9949747	1.3090861
H	0.1714376	-1.7150297	1.9658621
H	0.3759576	-0.3060567	-2.1404419
H	2.7767396	0.2944523	-1.8006219
H	2.5952396	-1.1829737	2.2514501
C	4.2580876	-0.0594317	0.4489091
H	4.7767106	0.0963933	-0.4996329
H	4.7638896	-0.8401037	1.0251741
H	4.3208676	0.8695593	1.0336151
O	-5.8406964	0.5025743	0.3518221
C	-5.7030274	-0.7012467	0.0334511
O	-4.5873014	-1.2756717	-0.1708179
C	-6.9485714	-1.5661057	-0.1440479
H	-7.0288604	-1.8758617	-1.1920819
H	-7.8540354	-1.0240257	0.1381441
H	-6.8642984	-2.4761337	0.4586061
O	3.6754086	-3.1690877	-0.3968029
H	4.0414316	-3.9760247	-0.7944949
H	2.7120856	-3.2890197	-0.4382689

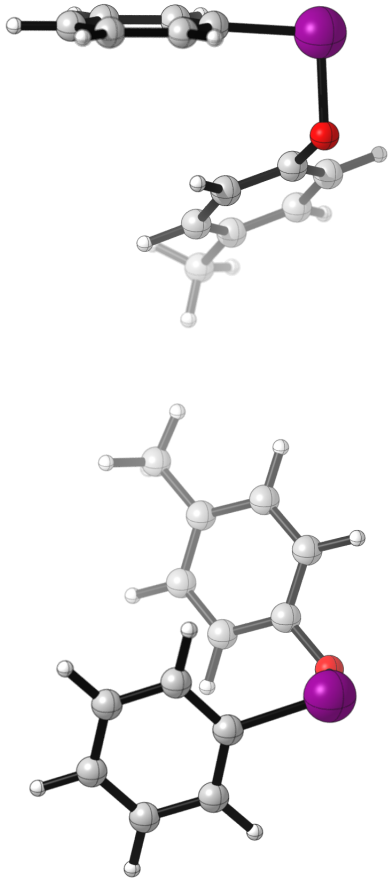


This structure was only partially optimized.

*** 2 imaginary frequencies (-124.6351, -9.8505) ***
Sum of electronic and zero-point Energies= -893.347670
Sum of electronic and thermal Energies= -893.324312
Sum of electronic and thermal Enthalpies= -893.323368
Sum of electronic and thermal Free Energies= -893.405699

Iodonium S1 in CH_2Cl_2

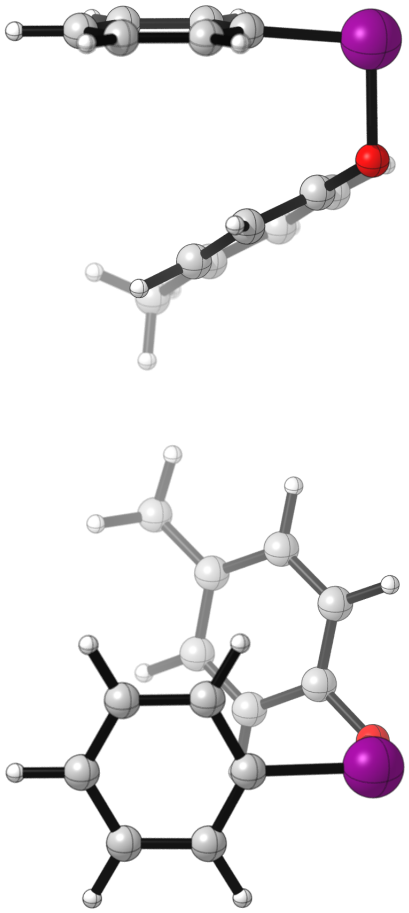
I	1.361000	-1.453000	-0.219000
C	1.668000	0.588000	-0.202000
C	1.938000	3.323000	-0.103000
C	2.445000	1.146000	0.818000
C	1.023000	1.360000	-1.174000
C	1.170000	2.744000	-1.114000
C	2.573000	2.531000	0.858000
H	2.932000	0.518000	1.558000
H	0.423000	0.894000	-1.949000
H	0.680000	3.366000	-1.856000
H	3.169000	2.991000	1.639000
H	2.046000	4.402000	-0.063000
O	-0.162000	-1.443000	1.066000
C	-1.311000	-0.784000	0.662000
C	-3.681000	0.523000	-0.018000
C	-2.270000	-1.458000	-0.091000
C	-1.503000	0.538000	1.066000
C	-2.692000	1.178000	0.728000
C	-3.452000	-0.800000	-0.418000
H	-2.091000	-2.485000	-0.401000
H	-0.735000	1.042000	1.647000
H	-2.854000	2.205000	1.047000
H	-4.212000	-1.323000	-0.994000
C	-4.962000	1.231000	-0.372000
H	-5.526000	1.490000	0.530000
H	-5.599000	0.604000	-1.003000
H	-4.760000	2.164000	-0.909000



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -588.475079
Sum of electronic and thermal Energies= -588.461149
Sum of electronic and thermal Enthalpies= -588.460205
Sum of electronic and thermal Free Energies= -588.518692

Iodonium S1 in CH_3CN

I	1.906000	-0.954000	-0.171000
C	1.213000	0.989000	-0.219000
C	0.112000	3.511000	-0.192000
C	1.561000	1.859000	0.818000
C	0.335000	1.348000	-1.247000
C	-0.217000	2.627000	-1.221000
C	0.998000	3.132000	0.821000
H	2.244000	1.547000	1.601000
H	0.087000	0.648000	-2.038000
H	-0.904000	2.929000	-2.005000
H	1.250000	3.826000	1.616000
H	-0.323000	4.505000	-0.179000
O	0.403000	-1.648000	0.967000
C	-0.862000	-1.218000	0.620000
C	-3.454000	-0.368000	0.016000
C	-1.549000	-1.815000	-0.436000
C	-1.439000	-0.189000	1.367000
C	-2.735000	0.219000	1.066000
C	-2.843000	-1.389000	-0.725000
H	-1.071000	-2.598000	-1.019000
H	-0.874000	0.271000	2.173000
H	-3.194000	1.014000	1.650000
H	-3.387000	-1.854000	-1.543000
C	-4.853000	0.094000	-0.298000
H	-5.526000	-0.104000	0.543000
H	-5.249000	-0.417000	-1.180000
H	-4.874000	1.173000	-0.486000



*** 0 imaginary frequencies ***
Sum of electronic and zero-point Energies= -588.481850
Sum of electronic and thermal Energies= -588.467706
Sum of electronic and thermal Enthalpies= -588.466762
Sum of electronic and thermal Free Energies= -588.526512