Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Oxidative ability of organic iodine (III) reagents: a theoretical assessment

Maxim R. Radzhabov*[a], Aleksei B. Sheremetev and Tatyana S. Pivina

N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 119991, Moscow, Russian Federation

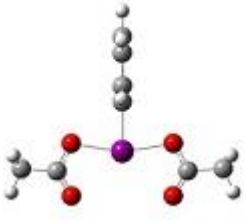
All quantum chemical calculations were performed using the Gaussian 09 software package. Widely used for organic systems, B3LYP (spin-unrestricted for radical species) has been shown to be the most successful at reproducing the experimental geometric parameters, so this functional with the split-valence basis 6-31+G(d,p) for nitrogen, oxygen, hydrogen, sulfur, chlorine and fluorine atoms was used to calculate oxidative potentials, unless stated otherwise. To take relativistic effects of the iodine atom into account, the Stuttgart-Dresden fully relativistic multielectron pseudopotential SDD ECP46MDF with its adapted basis set was applied. The UltraFine integration grid was used for all DFT calculations.

The localization of the stable states of molecules on the potential energy surface (PES) was estimated by the absence of negative frequencies of the corresponding fully converged local minima (reactants and intermediates). Solvent (acetonitrile, water, dichloromethane (DCM) and acetone) effects were taken into account by performing SCRF (IEF-PCM) calculations. All Gibbs Free Energies are calculated at 298.15 K.

*Corresponding Author. E-mail: mradzh2@uic.edu

[a]*Author's present affiliation: Department of Chemistry, University of Illinois at Chicago, 845 West Taylor Street, Chicago, Illinois 60607-7061, United States*

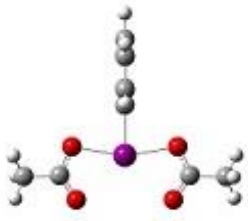
[Bis(acetoxy)iodo]benzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) Gas Phase = -699.848512

I	0.00014700	-0.62657800	0.00000000
C	-0.00033500	1.48175800	0.00000000
C	-0.00049100	2.15908200	-1.21786600
C	-0.00082100	3.55692700	-1.21095300
C	-0.00098700	4.25423200	0.00000000
C	-0.00082400	3.55692800	1.21095200
C	-0.00049500	2.15908300	1.21786600
O	2.16892900	-0.28356500	0.00000300
O	-2.16878400	-0.28454900	-0.00000300
C	2.77988200	-1.45238500	0.00000200
C	-2.77921800	-1.45364100	-0.00000300
O	2.16341100	-2.51831400	0.00000200
O	-2.16227500	-2.51929600	-0.00000300
C	4.29208900	-1.35955200	-0.00000200
C	-4.29146600	-1.36147700	0.00000100
H	-0.00124400	5.34020200	-0.00000100
H	-0.00094600	4.09594800	-2.15366800
H	-0.00036200	1.61711700	-2.15734100
H	-0.00036900	1.61711900	2.15734100
H	-0.00095100	4.09594800	2.15366700
H	-4.72012500	-2.36401400	-0.00001200
H	-4.62831900	-0.80898300	0.88223000
H	-4.62832700	-0.80895200	-0.88220600
H	4.72119200	-2.36190000	-0.00000600
H	4.62869900	-0.80689200	-0.88222000
H	4.62870500	-0.80689600	0.88221600

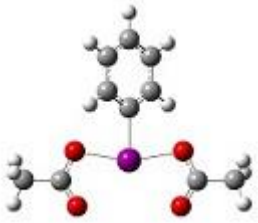
[Bis(acetoxy)iodo]benzene



Gibbs Free Energy (hartrees):
BP86/6-31+G(d,p) Gas Phase = -699.906843

I	-0.61825000	0.00000000	0.00000000
C	1.51673100	-0.00000100	0.00000000
C	2.19705100	0.01323300	-1.22497600
C	3.60313600	0.01316800	-1.21766500
C	4.30450800	-0.00000200	0.00000000
C	3.60313500	-0.01317100	1.21766600
C	2.19705000	-0.01323500	1.22497600
O	-0.25088200	-2.23637800	-0.01784900
O	-0.25088000	2.23637900	0.01784800
C	-1.46433400	-2.75609800	-0.02004300
C	-1.46433100	2.75610000	0.02004300
O	-2.49629600	-2.05341200	-0.02066300
O	-2.49629400	2.05341400	0.02066400
C	-1.50724600	-4.27654800	0.00940000
C	-1.50724300	4.27655000	-0.00940000
H	5.39934500	-0.00000300	0.00000100
H	4.14648800	0.02343000	-2.16822000
H	1.64918600	0.02342500	-2.17149300
H	1.64918500	-0.02342600	2.17149200
H	4.14648700	-0.02343500	2.16822100
H	-2.43547700	4.62643400	0.46481100
H	-0.62615000	4.70945700	0.48643600
H	-1.50803500	4.60677200	-1.06259400
H	-2.43546800	-4.62643200	-0.46483600
H	-0.62614100	-4.70945800	-0.48641100
H	-1.50807100	-4.60676800	1.06259500

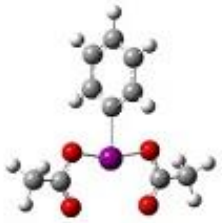
[Bis(acetoxy)iodo]benzene



Gibbs Free Energy (hartrees):
M06L/6-31+G(d,p) Gas Phase = -699.770787

I	-0.00001300	-0.62842900	-0.00000200
C	0.00002900	1.49387700	-0.00000200
C	-0.87801000	2.16857300	0.83980100
C	-0.87372200	3.56239900	0.83187200
C	0.00008700	4.25851100	0.00000300
C	0.87386700	3.56236500	-0.83186900
C	0.87809600	2.16853900	-0.83980300
O	-2.18430700	-0.26110900	-0.09971400
O	2.18429400	-0.26119500	0.09971000
C	-2.74406000	-1.44692900	-0.14104900
C	2.74400200	-1.44703600	0.14105200
O	-2.09089300	-2.49120700	-0.12808200
O	2.09079600	-2.49129000	0.12808800
C	-4.24651900	-1.41436000	-0.18505300
C	4.24646200	-1.41452300	0.18505800
H	0.00011000	5.34452000	0.00000500
H	-1.55678500	4.10025400	1.48284900
H	-1.56724300	1.62182900	1.47332500
H	1.56730700	1.62176800	-1.47332900
H	1.55695200	4.10019400	-1.48284400
H	4.63310600	-2.39713300	0.45146600
H	4.62921800	-1.13846900	-0.80105900
H	4.59796800	-0.66062400	0.89122000
H	-4.63320000	-2.39695900	-0.45145000
H	-4.62926200	-1.13828200	0.80106100
H	-4.59799800	-0.66045700	-0.89122300

[Bis(acetoxy)iodo]benzene in MeCN



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -699.866857

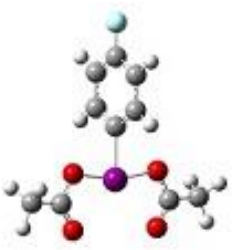
I	-0.04854300	-0.59963800	-0.00000200
C	0.11881200	1.49925200	-0.00000100
C	0.17298100	2.16855700	1.22252400
C	0.28603900	3.56245000	1.21275600
C	0.34249100	4.25620400	0.00000100
C	0.28603900	3.56245100	-1.21275600
C	0.17298200	2.16855900	-1.22252600
O	-2.19988700	-0.14505200	-0.00000400
O	2.14682900	-0.48905900	-0.00000300
C	-2.90058400	-1.25848500	-0.00000100
C	2.66460600	-1.69848500	0.00000400
O	-2.36759600	-2.37466200	0.00000100
O	1.96358100	-2.71751000	0.00001100
C	-4.39909000	-1.04901400	0.00000400
C	4.17743900	-1.72573400	0.00000400
H	0.43044800	5.33825200	0.00000100
H	0.32964600	4.09956100	2.15506900
H	0.12914100	1.62935200	2.16217000
H	0.12914100	1.62935500	-2.16217300
H	0.32964600	4.09956500	-2.15506800
H	4.53211300	-2.75672200	0.00001500
H	4.55619200	-1.20238700	-0.88280600
H	4.55619300	-1.20236900	0.88280400
H	-4.91029100	-2.01200800	-0.00001800
H	-4.69158000	-0.47304800	0.88284900
H	-4.69158300	-0.47300400	-0.88281200

[Bis(acetoxy)iodo]-4-cyanobenzene

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -792.112950

I	-1.07582200	0.00000000	-0.00000400
C	1.03332000	0.00000000	-0.00000100
C	1.70552600	-0.00000100	-1.22173000
C	3.09997400	-0.00000100	-1.22117600
C	3.79542900	0.00000000	0.00000100
C	3.09997200	0.00000100	1.22117700
C	1.70552300	0.00000100	1.22172800
O	-0.75415500	-2.17044500	0.00000300
O	-0.75415500	2.17044500	0.00000000
C	-1.91628200	-2.78851700	0.00000100
C	-1.91628100	2.78851700	0.00000100
O	-2.98743800	-2.17007700	-0.00000200
O	-2.98743800	2.17007800	0.00000300
C	-1.81944900	-4.29744000	0.00000400
C	-1.81944800	4.29744000	0.00000600
H	3.64209400	-0.00000200	-2.16017800
H	1.16793400	-0.00000200	-2.16272600
H	1.16792900	0.00000200	2.16272400
H	3.64209000	0.00000200	2.16018100
H	-2.81779100	4.73537100	-0.00000500
H	-1.26672400	4.63151500	0.88290500
H	-1.26670100	4.63152100	-0.88287600
H	-2.81779100	-4.73537100	0.00000100
H	-1.26671000	-4.63151900	-0.88288400
H	-1.26671600	-4.63151700	0.88289600
C	5.23158700	0.00000000	0.00000300
N	6.39531600	0.00000000	0.00000500

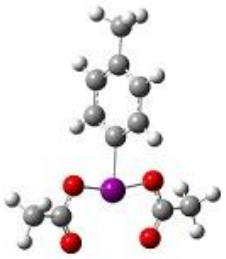
[Bis(acetoxy)iodo]-4-fluorobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -799.115206

I	-0.87485000	0.00000000	-0.00000200
C	1.22434700	0.00000000	-0.00000100
C	1.90032100	-0.00000100	1.22138000
C	3.29673200	-0.00000100	1.22270400
C	3.95863600	0.00000000	0.00000200
C	3.29673300	0.00000100	-1.22270200
C	1.90032200	0.00000100	-1.22138000
O	-0.58681800	2.17922100	0.00000000
O	-0.58681900	-2.17922100	-0.00000300
C	-1.75345900	2.78744400	0.00000300
C	-1.75345900	-2.78744400	0.00000100
O	-2.82172900	2.16376500	0.00000200
O	-2.82172900	-2.16376500	0.00000700
C	-1.66693100	4.29773000	0.00000100
C	-1.66693100	-4.29773000	0.00000000
H	3.85786300	-0.00000100	2.15043800
H	1.36356500	-0.00000100	2.16311400
H	1.36356800	0.00000100	-2.16311500
H	3.85786600	0.00000100	-2.15043500
H	-2.66813200	-4.72924600	0.00001700
H	-1.11651800	-4.63585600	-0.88284100
H	-1.11648500	-4.63585700	0.88281900
H	-2.66813200	4.72924600	0.00000100
H	-1.11650000	4.63585800	0.88283000
H	-1.11650200	4.63585600	-0.88283000
F	5.31614800	0.00000000	0.00000300

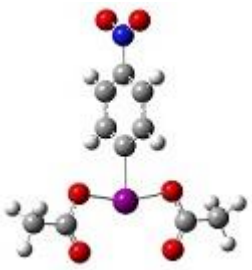
[Bis(acetoxy)iodo]-4-methylbenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -739.164602

I	-0.89048000	0.00201600	-0.00000100
C	1.20992200	-0.00328500	0.00000100
C	1.88821100	-0.00742100	-1.21859500
C	3.28470600	-0.01528700	-1.20595500
C	4.00390000	-0.01601000	0.00000300
C	3.28470500	-0.01523300	1.20595900
C	1.88821000	-0.00736700	1.21859800
O	-0.62375100	-2.18261100	0.00005800
O	-0.61280600	2.18518300	-0.00005900
C	-1.79154800	-2.78786600	0.00007400
C	-1.77768700	2.79606500	-0.00007600
O	-2.86023400	-2.16500500	0.00005700
O	-2.84933500	2.17832200	-0.00006000
C	-1.70614900	-4.29886500	0.00011200
C	-1.68511100	4.30662700	-0.00011400
H	3.81874600	-0.02251500	-2.15208700
H	1.35283200	-0.00825100	-2.16165900
H	1.35283000	-0.00815500	2.16166000
H	3.81874400	-0.02242000	2.15209300
H	-2.68454700	4.74233000	-0.00014500
H	-1.13339900	4.64280600	0.88268600
H	-1.13336100	4.64276200	-0.88290500
H	-2.70761900	-4.72987100	0.00014600
H	-1.15601700	-4.63764400	-0.88268000
H	-1.15597400	-4.63760100	0.88289400
C	5.51298200	0.00555500	0.00000300
H	5.88275900	1.03844800	-0.00002600
H	5.91829100	-0.48763500	0.88798300
H	5.91829200	-0.48768400	-0.88794900

[Bis(acetoxy)iodo]-4-nitrobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -904.373771

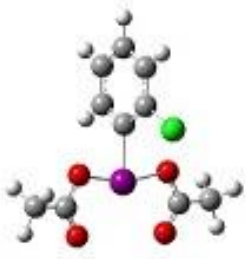
I	-1.38152900	0.00000000	-0.00000600
C	0.72842100	0.00000000	-0.00000300
C	1.40042100	0.00000200	-1.22230500
C	2.79530200	0.00000200	-1.22357200
C	3.46422100	0.00000000	0.00000000
C	2.79529900	-0.00000300	1.22357000
C	1.40041800	-0.00000300	1.22230000
O	-1.04814600	-2.16725700	0.00000100
O	-1.04814600	2.16725700	0.00000700
C	-2.20906400	-2.78802200	0.00000900
C	-2.20906300	2.78802200	-0.00000100
O	-3.28067600	-2.17038600	0.00001400
O	-3.28067500	2.17038600	-0.00001000
C	-2.10994800	-4.29648800	0.00001000
C	-2.10994700	4.29648800	0.00000700
H	3.34946000	0.00000400	-2.15351200
H	0.86303100	0.00000500	-2.16319900
H	0.86302600	-0.00000500	2.16319300
H	3.34945400	-0.00000500	2.15351200
H	-3.10765300	4.73580600	-0.00001100
H	-1.55670600	4.62959200	0.88293400
H	-1.55666900	4.62960100	-0.88289400
H	-3.10765400	-4.73580600	0.00001500
H	-1.55669200	-4.62959800	-0.88290600
H	-1.55668500	-4.62959500	0.88292200
N	4.93699000	-0.00000100	0.00000200
O	5.51649900	-0.00000200	1.08812100
O	5.51650100	0.00000200	-1.08811500

[Bis(acetoxy)iodo]-4-methoxybenzene

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -814.369276

I	-1.15804500	0.00000000	-0.01094900
C	0.92840400	0.00000000	0.10727100
C	1.67779700	0.00000200	-1.06753900
C	3.07297300	0.00000100	-0.99539100
C	3.70409200	-0.00000100	0.25906900
C	2.93173600	-0.00000300	1.43587000
C	1.54457500	-0.00000300	1.36434200
O	-0.90263800	-2.18984900	0.00475100
O	-0.90263800	2.18984900	0.00475600
C	-2.07189700	-2.78867200	-0.05143600
C	-2.07189600	2.78867300	-0.05143600
O	-3.13643500	-2.16066200	-0.10649600
O	-3.13643400	2.16066300	-0.10650200
C	-1.99525500	-4.30035900	-0.04397100
C	-1.99525400	4.30036000	-0.04396800
H	3.64521000	0.00000300	-1.91459400
H	1.19679800	0.00000300	-2.03946300
H	0.95970100	-0.00000400	2.27744900
H	3.43521600	-0.00000500	2.39695700
H	-2.99853600	4.72587600	-0.07751300
H	-1.47691500	4.64028900	0.85733400
H	-1.41776800	4.64423600	-0.90722300
H	-2.99853800	-4.72587500	-0.07751300
H	-1.41777400	-4.64423400	-0.90722900
H	-1.47691300	-4.64029100	0.85732700
O	5.04760200	-0.00000200	0.43825300
C	5.90269900	0.00000100	-0.71307600
H	5.74143600	0.89699600	-1.31993700
H	6.91951500	0.00000100	-0.32187800
H	5.74143600	-0.89699200	-1.31994000

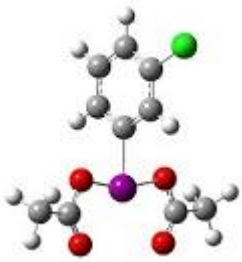
[Bis(acetoxy)iodo]-2-chlorobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1159.463253

I	-0.77371400	0.01379800	-0.15398400
C	1.31187000	-0.03578800	-0.40618900
C	1.80490200	-0.07336700	-1.71271900
C	3.18311100	-0.10828200	-1.93232800
C	4.05972200	-0.10490800	-0.84520400
C	3.56818700	-0.06726900	0.46091400
C	2.18921500	-0.03259900	0.68529600
O	-0.51123600	-2.16603200	-0.15651400
O	-0.41327900	2.17938900	-0.18399300
C	-1.68528700	-2.74970500	-0.04715400
C	-1.55983700	2.81593700	-0.07788400
O	-2.73536900	-2.10034000	0.03251500
O	-2.63745200	2.21474700	0.01204700
C	-1.63119500	-4.26066200	-0.02193900
C	-1.43893100	4.32317500	-0.07098100
H	3.56333300	-0.13759700	-2.94792200
H	1.12105300	-0.07644100	-2.55423900
H	-2.42974700	4.77678900	-0.03831100
H	-0.85940500	4.63884400	0.80185600
H	-0.90295500	4.65813700	-0.96339900
H	-2.64144300	-4.66994300	-0.00031100
H	-1.09575800	-4.62986300	-0.90098300
H	-1.08077000	-4.59060800	0.86443500
H	5.13241000	-0.13163600	-1.00763700
H	4.24545600	-0.06472400	1.30766900
Cl	1.61898800	0.01379100	2.33980600

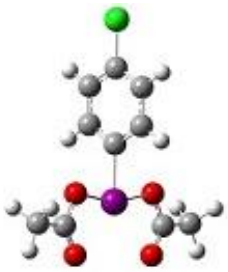
[Bis(acetoxy)iodo]-3-chlorobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1159.467265

I	1.05567800	0.00000000	0.01498900
C	-0.99332600	0.00000000	0.50237800
C	-1.36721400	0.00000000	1.84489000
C	-2.73081600	0.00000000	2.15318600
C	-3.69181400	0.00000000	1.13977600
C	-3.27639400	0.00000000	-0.19298300
C	-1.92293100	0.00000000	-0.53678400
O	0.76057300	-2.17506600	0.08395800
O	0.76057300	2.17506600	0.08396000
C	1.89260600	-2.78785200	-0.18887700
C	1.89260500	2.78785200	-0.18887600
O	2.93293900	-2.16694400	-0.43851000
O	2.93293900	2.16694400	-0.43850900
C	1.80447800	-4.29753500	-0.16394500
C	1.80447700	4.29753500	-0.16394600
H	-3.04557300	0.00000000	3.19169400
H	-0.62677800	0.00000000	2.63622300
H	-1.62070200	0.00000000	-1.57707600
H	2.76393200	4.73219900	-0.44521200
H	1.02453100	4.63618400	-0.85172400
H	1.52798400	4.63121800	0.84077900
H	2.76392400	-4.73219800	-0.44524200
H	1.52802200	-4.63121600	0.84079100
H	1.02450800	-4.63618600	-0.85169300
Cl	-4.47695500	-0.00000100	-1.47473800
H	-4.74876800	0.00000000	1.38151100

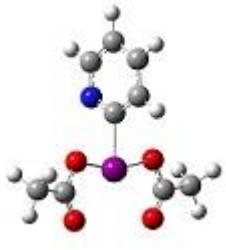
[Bis(acetoxy)iodo]-4-chlorobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1159.468012

I	1.16775100	0.00000000	0.00000100
C	-0.93398000	0.00000000	0.00000000
C	-1.61070400	-0.00000300	-1.21936200
C	-3.00736600	-0.00000300	-1.21910300
C	-3.68795300	0.00000000	0.00000000
C	-3.00736700	0.00000300	1.21910300
C	-1.61070500	0.00000300	1.21936200
O	0.87300800	2.17767300	-0.00000100
O	0.87300800	-2.17767300	0.00000200
C	2.03861400	2.78809000	-0.00000100
C	2.03861500	-2.78809000	-0.00000100
O	3.10769700	2.16587500	0.00000300
O	3.10769700	-2.16587400	-0.00000500
C	1.94953800	4.29811700	0.00000000
C	1.94953800	-4.29811700	0.00000000
H	-3.55192700	-0.00000600	-2.15653000
H	-1.07635000	-0.00000600	-2.16260000
H	-1.07635100	0.00000600	2.16260100
H	-3.55192700	0.00000500	2.15653000
H	2.95003100	-4.73124600	-0.00001700
H	1.39855000	-4.63526400	0.88284800
H	1.39852000	-4.63526500	-0.88283000
H	2.95003000	4.73124600	0.00000300
H	1.39853700	4.63526500	-0.88284000
H	1.39853200	4.63526400	0.88283700
Cl	-5.44288800	0.00000000	-0.00000100

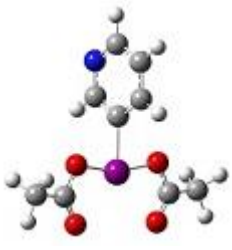
2-[Bis(acetoxy)iodo]pyridine



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -715.914418

I	-0.00000200	-0.62559700	0.00499100
C	0.00000400	1.51672700	0.00302900
C	0.00000500	2.18298300	1.22489200
C	0.00000800	3.57974000	1.16523300
C	0.00001100	4.20807500	-0.08126300
C	0.00001000	3.41849700	-1.23295000
O	-2.16877300	-0.29329500	0.01156900
O	2.16877100	-0.29330600	0.01156900
C	-2.81062600	-1.44222900	-0.00403400
C	2.81061900	-1.44224200	-0.00403300
O	-2.21962600	-2.52812600	-0.01573600
O	2.21961400	-2.52813700	-0.01573600
C	-4.31768600	-1.30996800	-0.00849200
C	4.31767900	-1.30998900	-0.00849100
H	0.00000900	4.16061300	2.08197400
H	0.00000200	1.65332000	2.16956600
H	4.77888600	-2.29780900	0.00206900
H	4.63590900	-0.76197500	-0.90033800
H	4.64243600	-0.73766700	0.86520800
H	-4.77889800	-2.29778600	0.00206700
H	-4.64244000	-0.73764500	0.86520800
H	-4.63591300	-0.76195100	-0.90033700
H	0.00001400	5.28944500	-0.16431800
H	0.00001200	3.86503200	-2.22280700
N	0.00000600	2.07377000	-1.18849900

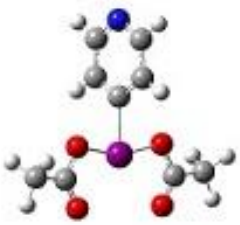
3-[Bis(acetoxy)iodo]pyridine



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -715.911609

I	0.00000200	-0.60685100	0.00278400
C	-0.00000600	1.49633200	0.01461200
C	-0.00000700	2.18958800	1.22247000
C	-0.00001300	3.58373100	1.16147000
C	-0.00001700	4.19889500	-0.09253800
C	-0.00001000	2.18418300	-1.19972600
O	-2.17285300	-0.29758800	0.00511200
O	2.17285500	-0.29757100	0.00511100
C	-2.78800800	-1.46118400	0.00213500
C	2.78801900	-1.46116300	0.00213400
O	-2.16813600	-2.53149500	0.00008000
O	2.16815600	-2.53147900	0.00007900
C	-4.29732100	-1.36726300	-0.00208600
C	4.29733200	-1.36723100	-0.00208600
H	-0.00001500	4.17911800	2.06810300
H	-0.00000400	1.67508300	2.17699700
H	-0.00000800	1.65528900	-2.14858600
H	4.73347300	-2.36590100	0.02907100
H	4.62971500	-0.84597000	-0.90479100
H	4.63543100	-0.78512200	0.85991600
H	-4.73345500	-2.36593600	0.02908300
H	-4.63542500	-0.78514500	0.85990800
H	-4.62970700	-0.84601600	-0.90479800
H	-0.00002100	5.28293100	-0.17150600
N	-0.00001500	3.52206900	-1.25176200

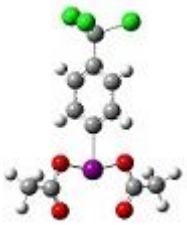
4-[Bis(acetoxy)iodo]pyridine



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -715.910461

I	0.00004300	-0.62406000	0.00000000
C	-0.00009800	1.49118300	0.00000000
C	-0.00014500	2.17677200	-1.20904900
C	-0.00024500	3.57540000	-1.14702900
C	-0.00024400	3.57539900	1.14703200
C	-0.00014500	2.17677100	1.20905000
O	2.16689000	-0.29118900	-0.00000100
O	-2.16684600	-0.29147400	0.00000000
C	2.79176900	-1.44989500	-0.00000100
C	-2.79157400	-1.45026100	0.00000000
O	2.17936500	-2.52436800	-0.00000100
O	-2.17903100	-2.52465400	0.00000000
C	4.29998600	-1.34411300	-0.00000100
C	-4.29980500	-1.34467300	0.00000100
H	-0.00028600	4.15400300	-2.06719200
H	-0.00010800	1.67217800	-2.16792400
H	-0.00010800	1.67217600	2.16792500
H	-0.00028500	4.15400200	2.06719500
H	-4.74341300	-2.34049600	0.00000000
H	-4.63065800	-0.79001700	0.88289300
H	-4.63065900	-0.79001500	-0.88289000
H	4.74372100	-2.33987900	-0.00000100
H	4.63076800	-0.78941400	-0.88289400
H	4.63076900	-0.78941300	0.88289000
N	-0.00029400	4.26800800	0.00000200

[Bis(acetoxy)iodo]-4-trichloromethylbenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -2117.941413

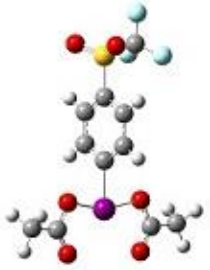
I	2.30348100	-0.00028200	0.00404800
C	0.19749400	0.00004600	0.02755700
C	-0.49428100	0.00902200	-1.18429400
C	-1.88610600	0.00746100	-1.16142400
C	-2.58143800	-0.00406000	0.05927600
C	-1.86550700	-0.01165600	1.25968200
C	-0.46648400	-0.00954000	1.24852400
O	1.99371900	2.17303400	0.00899200
O	1.99180200	-2.17339700	0.00327400
C	3.15693800	2.78851400	-0.00239600
C	3.15431400	-2.79019400	-0.00752100
O	4.22764700	2.16938600	-0.01309500
O	4.22577400	-2.17234800	-0.01654300
C	3.06221400	4.29787500	-0.00234500
C	3.05775300	-4.29945800	-0.00687600
H	-2.42469200	0.01459000	-2.10256300
H	0.02752000	0.01672800	-2.13417400
H	0.07397100	-0.01593300	2.18800400
H	-2.37733700	-0.01935300	2.21310900
H	4.05600600	-4.73735900	-0.02293200
H	2.51966700	-4.63380000	0.88498700
H	2.49063100	-4.63369700	-0.88049500
H	4.06114300	4.73452700	0.00010200
H	2.51299200	4.63225200	-0.88741400
H	2.50694200	4.63343700	0.87831100
C	-4.10551600	-0.00094800	0.01731500
Cl	-4.87053200	-0.05535700	1.64354500
Cl	-4.69902200	-1.43829500	-0.92153200
Cl	-4.69039600	1.50116600	-0.82186400

[Bis(acetoxy)iodo]-4-trifluoromethylbenzene

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1036.922908

I	-1.67228600	0.00667600	-0.00077200
C	0.43583900	-0.01750800	0.00045600
C	1.10968900	-0.02452800	-1.21963000
C	2.50561500	-0.04008700	-1.21391000
C	3.19561700	-0.05115900	0.00263500
C	2.50403800	-0.04198600	1.21779300
C	1.10776400	-0.02644300	1.22123900
O	-1.38279400	-2.16879900	-0.00075700
O	-1.33140000	2.17470400	-0.00013700
C	-2.55230600	-2.77255300	-0.00008900
C	-2.48619100	2.80611800	0.00045500
O	-3.61646100	-2.14217700	-0.00003300
O	-3.56504600	2.20124700	0.00029300
C	-2.47311800	-4.28270500	0.00054300
C	-2.37113700	4.31396700	0.00115400
H	3.04413200	-0.04848800	-2.15502300
H	0.57391800	-0.01933400	-2.16168500
H	0.57067600	-0.02268800	2.16255200
H	3.04105700	-0.05169400	2.15957100
H	-3.36412200	4.76394500	0.00399900
H	-1.81198000	4.64100400	0.88263200
H	-1.81685800	4.64190500	-0.88309800
H	-3.47648900	-4.70903300	0.00237800
H	-1.92584600	-4.62369000	-0.88312800
H	-1.92282600	-4.62292500	0.88261600
C	4.70300000	-0.01776300	0.00080500
F	5.23214000	-0.66329900	-1.06759700
F	5.17842600	1.25880400	-0.04716200
F	5.23523500	-0.58380900	1.11103400

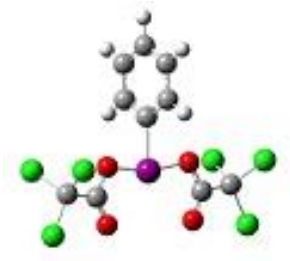
[Bis(acetoxy)iodo]-4-trifluoro(methylsulfonyl)benzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1585.469521

I	-2.51300400	0.12034300	0.00065300
C	-0.42970300	-0.21902100	-0.00028100
C	0.23123900	-0.33103100	1.22227000
C	1.60905300	-0.55638800	1.22359100
C	2.27178100	-0.66037800	-0.00189400
C	1.60803200	-0.55364900	-1.22658300
C	0.23021400	-0.32851100	-1.22361300
O	-1.82910200	2.20322800	0.00001600
O	-2.52563500	-2.07152100	0.00069700
C	-2.87401000	3.00414500	-0.00060200
C	-3.77069100	-2.49933900	0.00066100
O	-4.03130400	2.56766100	-0.00033700
O	-4.72956800	-1.71807200	0.00080100
C	-2.53229000	4.47654500	-0.00185600
C	-3.91377400	-4.00411100	0.00049400
H	2.14571400	-0.65974900	2.15972500
H	-0.30029800	-0.25143800	2.16324800
H	-0.30214200	-0.24697800	-2.16396100
H	-4.96886000	-4.27827500	-0.00038100
H	-3.41999500	-4.42129000	-0.88195900
H	-3.42155200	-4.42123900	0.88385300
H	-3.44591800	5.07127600	-0.00082600
H	-1.93107400	4.71631000	0.87996700
H	-1.93393700	4.71523200	-0.88594000
H	2.14406300	-0.65474300	-2.16333000
S	4.03770800	-0.96518300	-0.00316200
O	4.43787100	-1.56363200	1.27685000
O	4.43738800	-1.55276500	-1.28836200
C	4.79674800	0.77734300	0.00357100
F	6.12645400	0.65029000	-0.01049100
F	4.42432500	1.44071000	1.10312100
F	4.40289700	1.45820200	-1.07777400

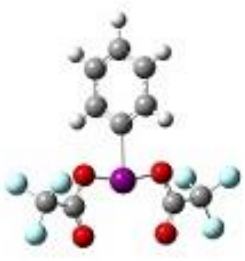
[Bis(trichloroacetoxy)iodo]benzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -3457.407121

I	0.00000000	-0.13273500	-0.00000200
C	0.00000000	1.96784100	0.00000000
C	0.00000000	2.63254700	1.22661200
C	0.00000000	4.03026200	1.21398400
C	0.00000000	4.72449700	0.00000200
C	0.00000000	4.03026400	-1.21398100
C	0.00000000	2.63254900	-1.22661200
O	-2.18466000	0.10950000	-0.00000200
O	2.18466000	0.10950000	-0.00000200
C	-2.80789400	-1.03035100	0.00000000
C	2.80789400	-1.03035100	-0.00000100
O	-2.29540900	-2.13792700	-0.00000100
O	2.29540900	-2.13792700	-0.00000100
C	-4.36834400	-0.84322200	0.00000100
C	4.36834400	-0.84322200	0.00000100
H	0.00000000	5.80994800	0.00000300
H	0.00000000	4.56965300	2.15569500
H	0.00000000	2.09079600	2.16538500
H	0.00000000	2.09080000	-2.16538500
H	0.00000000	4.56965700	-2.15569200
Cl	-4.83852000	0.07712400	1.47443400
Cl	-5.19212700	-2.42676900	0.00000500
Cl	-4.83852300	0.07711700	-1.47443500
Cl	4.83852100	0.07712400	1.47443400
Cl	5.19212700	-2.42676900	0.00000500
Cl	4.83852300	0.07711800	-1.47443500

[Bis(trifluoroacetoxy)iodo]benzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1295.361142

I	0.00000000	0.31238800	0.00000100
C	0.00000000	-1.78875900	-0.00000100
C	0.00000000	-2.45229300	1.22717100
C	0.00000000	-3.84997600	1.21408300
C	0.00000000	-4.54402800	-0.00000400
C	0.00000000	-3.84997400	-1.21408900
C	0.00000000	-2.45229100	-1.22717400
O	2.18973600	0.07295200	0.00000100
O	-2.18973600	0.07295200	0.00000200
C	2.81785300	1.20891800	-0.00000200
C	-2.81785300	1.20891800	0.00000100
O	2.33190200	2.32877200	-0.00000700
O	-2.33190200	2.32877200	-0.00000100
C	4.36232300	1.00262500	0.00000100
C	-4.36232300	1.00262500	0.00000100
H	0.00000000	-5.62945800	-0.00000500
H	0.00000000	-4.38940700	2.15574500
H	0.00000000	-1.91052500	2.16585900
H	0.00000000	-1.91052100	-2.16586200
H	0.00000000	-4.38940300	-2.15575200
F	-4.75304100	0.30949300	-1.09167900
F	-4.75304100	0.30949000	1.09167900
F	-5.01125100	2.17716300	0.00000200
F	5.01125100	2.17716300	-0.00002300
F	4.75304100	0.30946900	-1.09166400
F	4.75304000	0.30951300	1.09169400

[Bis(benzoyloxy)iodo]benzene

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1083.259833

I	0.00000000	0.19194200	-0.00000100
C	0.00000100	-1.91403000	0.00000300
C	-0.00001200	-2.58530400	-1.22272000
C	-0.00001100	-3.98376800	-1.21287300
C	0.00000200	-4.67969300	0.00000600
C	0.00001400	-3.98376400	1.21288400
C	0.00001300	-2.58530100	1.22272700
O	-2.17232700	-0.09173600	0.00002700
O	2.17232600	-0.09173500	-0.00002700
C	-2.78075600	1.07521900	0.00003300
C	2.78075500	1.07522100	-0.00003500
O	-2.15298900	2.14413900	0.00002200
O	2.15298900	2.14414100	-0.00002900
H	0.00000200	-5.76530900	0.00000800
H	-0.00002100	-4.52279200	-2.15509100
H	-0.00002100	-2.04423600	-2.16233000
H	0.00002300	-2.04423000	2.16233600
H	0.00002300	-4.52278600	2.15510400
C	4.27595000	1.01746000	-0.00005500
C	5.00141300	2.21917800	-0.00006400
C	4.95921900	-0.20909700	-0.00006500
C	6.39678600	2.19418300	-0.00008300
H	4.46348200	3.16117500	-0.00005700
C	6.35530200	-0.23043800	-0.00008300
H	4.39546400	-1.13526700	-0.00005800
C	7.07540100	0.96970800	-0.00009200
H	6.95412800	3.12619700	-0.00009000
H	6.88069700	-1.18081800	-0.00009100
H	8.16144100	0.95101200	-0.00010700
C	-4.27595100	1.01745900	0.00005300
C	-5.00141400	2.21917700	0.00005800
C	-4.95922000	-0.20909700	0.00006700
C	-6.39678600	2.19418200	0.00007600
H	-4.46348200	3.16117400	0.00004700
C	-6.35530400	-0.23043800	0.00008500
H	-4.39546500	-1.13526800	0.00006400
C	-7.07540200	0.96970800	0.00009000
H	-6.95412800	3.12619700	0.00007900
H	-6.88069800	-1.18081800	0.00009600
H	-8.16144100	0.95101300	0.00010400

[Bis(isonicotinoyloxy)iodo]benzene

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1115.351161

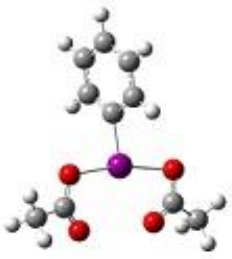
I	0.00000000	0.20348800	-0.00000100	C	-5.03999300	2.19059500	0.00000100
C	-0.00000100	-1.90156800	0.00000000	C	-4.96645000	-0.21276000	-0.00000200
C	-0.00000600	-2.57098600	1.22372800	C	-6.43230800	2.09421300	0.00000000
C	-0.00000600	-3.96931100	1.21313500	H	-4.54833200	3.15674900	0.00000300
C	-0.00000100	-4.66481100	0.00000200	C	-6.36273800	-0.19972300	0.00000000
C	0.00000400	-3.96931200	-1.21313200	H	-4.42328400	-1.15035600	-0.00000400
C	0.00000400	-2.57098800	-1.22372600	N	-7.09479900	0.92581800	0.00000000
O	2.17461400	-0.07119800	-0.00000100	H	-7.04208000	2.99438200	0.00000300
O	-2.17461300	-0.07119600	-0.00000100	H	-6.91670300	-1.13529900	-0.00000300
C	2.78688000	1.08940900	0.00000000				
C	-2.78688000	1.08941000	-0.00000100				
O	2.18480900	2.16866400	0.00000200				
O	-2.18480900	2.16866500	-0.00000100				
H	-0.00000200	-5.75037900	0.00000200				
H	-0.00001000	-4.50840500	2.15523400				
H	-0.00001000	-2.02978700	2.16314200				
H	0.00000900	-2.02978900	-2.16314100				
H	0.00000700	-4.50840700	-2.15523000				
C	4.28844900	1.01092400	0.00000000				
C	5.03999300	2.19059400	0.00000100				
C	4.96645100	-0.21276100	-0.00000100				
C	6.43230900	2.09421300	0.00000300				
H	4.54833200	3.15674800	0.00000200				
C	6.36273900	-0.19972300	-0.00000200				
H	4.42328600	-1.15035700	-0.00000100				
N	7.09480000	0.92581800	0.00000100				
H	7.04208000	2.99438200	0.00000300				
H	6.91670500	-1.13529900	0.00000000				
C	-4.28844800	1.01092500	0.00000000				

[Bis(((trifluoromethyl)sulfonyl)oxy)iodo]benzene

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -2165.804209

I	-0.18323200	-0.54004600	-0.07365400
C	0.32396800	1.48600000	-0.17437700
C	0.21240600	2.25195200	0.98871700
C	0.56088500	3.60159900	0.91084000
C	1.00215000	4.14715900	-0.29994800
C	1.10075500	3.35282900	-1.44737800
C	0.76259400	1.99882200	-1.39749600
O	-2.18293300	0.14570400	-0.76261900
O	1.78358000	-1.04156900	0.70436000
H	1.27042500	5.19764200	-0.34924800
H	0.48499400	4.22163700	1.79799300
H	-0.13265900	1.82173500	1.92156700
H	0.84026600	1.37549600	-2.28041000
H	1.44318000	3.78011900	-2.38410000
S	-3.44489000	-0.76677100	-0.67323900
S	3.02839700	-1.45973700	-0.16291700
O	-4.32254400	-0.53677000	-1.81863700
O	-3.08431000	-2.13252900	-0.27657400
O	2.81162500	-1.19525700	-1.58669000
O	3.54715600	-2.75326300	0.27565900
C	-4.32684300	-0.00859800	0.80634200
C	4.26359900	-0.17421700	0.44778500
F	3.80777100	1.05697900	0.20063100
F	4.46539200	-0.31662300	1.76078300
F	5.42140000	-0.35382400	-0.19846500
F	-4.62733500	1.27075300	0.56200900
F	-5.45494500	-0.68880400	1.04122200
F	-3.53991600	-0.07668600	1.88776200

[Bis(acetoxy)iodo]benzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -700.032899

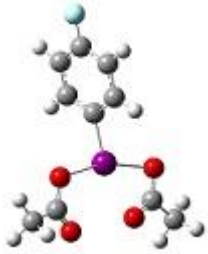
I	0.35421900	0.03298200	-0.00073900
C	-1.50696200	-0.94033200	0.00080100
C	-2.11643100	-1.26933000	1.21845600
C	-3.34947900	-1.92800400	1.21334100
C	-3.96664700	-2.26042000	0.00254400
C	-3.34853200	-1.93297400	-1.20912800
C	-2.11547200	-1.27435800	-1.21597300
O	2.37611300	-2.11248700	-0.00461200
O	-1.16550100	2.33316000	-0.01467700
C	3.36569000	-1.31219800	-0.00965200
C	-0.35632000	3.32746000	-0.01219400
O	3.28652600	-0.05146600	-0.00632900
O	0.89430400	3.26034800	-0.00898300
C	4.76602900	-1.94188800	0.01141100
C	-1.02056000	4.71293900	0.01507100
H	-4.92378900	-2.77324100	0.00321800
H	-3.82445100	-2.18043100	2.15683600
H	-1.64061700	-1.01441200	2.15966000
H	-1.63891400	-1.02332300	-2.15784100
H	-3.82276800	-2.18925700	-2.15195500
H	-0.48706800	5.39145200	-0.65605300
H	-2.07528100	4.66452000	-0.26204900
H	-0.94229100	5.11521400	1.03135800
H	5.14622900	-1.91588600	1.03936500
H	4.74343300	-2.98160100	-0.32225200
H	5.45248100	-1.36291000	-0.61236900

[Bis(acetoxy)iodo]-4-cyanobenzene radical anion

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -792.280576

I	-0.80349100	-0.08402900	-0.00370200
C	1.28712300	-0.32451400	-0.00145100
C	1.97686300	-0.42588100	-1.21683200
C	3.35927800	-0.59830200	-1.21865400
C	4.05390000	-0.67519500	0.00215600
C	3.35840100	-0.58015200	1.22119200
C	1.97599400	-0.40788200	1.21580200
O	-2.23721200	-2.71205600	0.00566000
O	-0.08099100	2.52732900	-0.01323700
C	-3.36425400	-2.12653500	0.00462400
C	-1.15783300	3.22849600	-0.00708100
O	-3.53258600	-0.87146900	-0.00106200
O	-2.32525000	2.78489700	-0.00418300
C	-4.62206000	-3.00535900	0.01065800
C	-0.93867000	4.74895400	0.01092700
H	3.89763900	-0.67301200	-2.15737100
H	1.44528200	-0.36750200	-2.16030200
H	1.44368100	-0.33548200	2.15788000
H	3.89608500	-0.64081300	2.16130700
H	-1.30147300	5.14170700	0.96649900
H	0.11248300	5.01438300	-0.11101900
H	-1.53230300	5.20597300	-0.78607900
H	-5.22837100	-2.77866600	-0.87268000
H	-4.37333100	-4.06844400	0.01658100
H	-5.22713600	-2.76842400	0.89213800
C	5.47681800	-0.85338300	0.00405500
N	6.63248500	-0.99817900	0.00563900

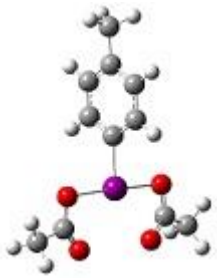
[Bis(acetoxy)iodo]-4-fluorobenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -799.277787

I	-0.60457700	-0.08554100	-0.00673200
C	1.46349200	-0.45310400	-0.00147800
C	2.14549900	-0.58401600	1.21589800
C	3.51837100	-0.84107800	1.22482300
C	4.17380500	-0.96692300	0.00542400
C	3.52314700	-0.84870100	-1.21728600
C	2.15025700	-0.59158300	-1.21534100
O	0.23169000	2.50586400	-0.00817000
O	-2.24664000	-2.61164800	0.00178400
C	-0.79156300	3.28241500	-0.00435800
C	-3.32840100	-1.94593500	-0.00656000
O	-1.98879100	2.92511200	-0.00977600
O	-3.40642100	-0.68228400	-0.01480000
C	-0.46615200	4.78395500	0.02076600
C	-4.64352000	-2.73698800	0.02338800
H	4.06759000	-0.94231300	2.15462200
H	1.61792500	-0.48356700	2.15830100
H	1.62642100	-0.49705500	-2.16044100
H	4.07600000	-0.95576800	-2.14427500
H	-5.04415300	-2.71533600	1.04371100
H	-5.38338600	-2.26957600	-0.63254500
H	-4.49257200	-3.77890000	-0.26746300
H	-1.01091700	5.28233900	-0.78652200
H	-0.81850000	5.20187900	0.96961000
H	0.60317100	4.97541900	-0.08160200
F	5.51252300	-1.21867200	0.00882400

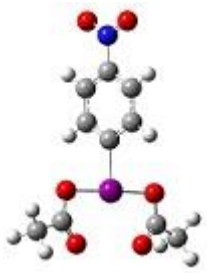
[Bis(acetoxy)iodo]-4-methylbenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -739.328657

I	0.68388600	0.01093300	-0.03928700
C	-1.40580700	-0.07491200	-0.01516500
C	-2.08921900	-0.11757100	1.20665100
C	-3.48345100	-0.18671000	1.21311100
C	-4.21949600	-0.21238000	0.01697900
C	-3.51195100	-0.17251800	-1.19523000
C	-2.11742100	-0.10361500	-1.22068000
O	0.97181900	-2.83682600	0.02148000
O	0.57782900	2.82906800	0.01118600
C	2.24500100	-2.92030500	0.00742600
C	1.81408500	3.15342400	0.00637400
O	3.04412900	-1.94899600	-0.05410600
O	2.78356400	2.35541900	-0.05260400
C	2.83663700	-4.33512800	0.10347300
C	2.11453900	4.65658200	0.11404200
H	-4.00520200	-0.22328300	2.16602100
H	-1.54474700	-0.10127900	2.14502400
H	-1.59528700	-0.07646200	-2.17141300
H	-4.05588100	-0.19778400	-2.13595800
H	2.98001000	4.91224000	-0.50294800
H	1.25420600	5.26292700	-0.17696900
H	2.36491600	4.88715300	1.15605400
H	3.70568300	-4.42457100	-0.55406000
H	3.17752900	-4.50160800	1.13189100
H	2.09846600	-5.10013300	-0.14601100
C	-5.72846000	-0.25756300	0.03584000
H	-6.14628200	0.75473400	0.10606300
H	-6.12529000	-0.71333600	-0.87586200
H	-6.09956500	-0.82319700	0.89578700

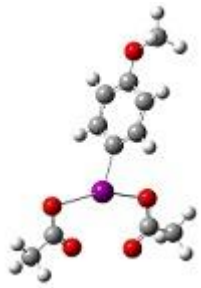
[Bis(acetoxy)iodo]-4-nitrobenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -904.541809

I	1.18257500	0.00161300	-0.03607500
C	-0.90788700	-0.04363900	-0.01807700
C	-1.61328700	-0.04098400	-1.23032200
C	-3.00528700	-0.07601900	-1.22241600
C	-3.66965400	-0.11584200	0.00592100
C	-2.98281500	-0.12148200	1.22248500
C	-1.59093700	-0.08519300	1.20617600
O	1.02817000	2.78028900	0.01024400
O	1.41672400	-2.81619400	0.00329800
C	2.26777200	3.09542000	0.01295300
C	2.69139600	-2.88501400	0.00104000
O	3.22897100	2.28755700	-0.03201300
O	3.47638200	-1.90138600	-0.04606500
C	2.57762600	4.59612000	0.11048500
C	3.29861900	-4.29181800	0.09259900
H	-3.56665900	-0.07288900	-2.14821200
H	-1.08601000	-0.01074800	-2.17698600
H	-1.04633900	-0.08853900	2.14347100
H	-3.52703100	-0.15288700	2.15793900
H	3.63815300	-4.45801000	1.12134000
H	2.56975600	-5.06341800	-0.16293700
H	4.17032900	-4.36683400	-0.56294500
H	3.44253300	4.84078200	-0.51145600
H	1.72006000	5.20530200	-0.18177800
H	2.83339300	4.83036300	1.15016400
N	-5.13286200	-0.15242100	0.01876500
O	-5.70775000	-0.19565300	1.11189400
O	-5.72848700	-0.13848600	-1.06398900

[Bis(acetoxy)iodo]-4-methoxybenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -814.532649

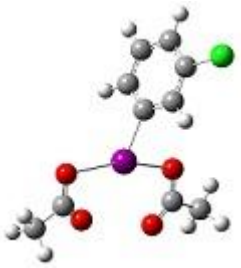
I	-0.87781100	-0.11474100	0.00278500
C	1.20283300	-0.27852100	0.10976500
C	1.96212100	-0.38187700	-1.06137700
C	3.35231500	-0.50699600	-0.99921500
C	3.99122100	-0.53546500	0.25061800
C	3.22756800	-0.43844400	1.42887900
C	1.84587800	-0.31461600	1.35926700
O	-2.33557200	-2.79110900	0.01533400
O	-0.37001100	2.58313300	-0.05857400
C	-3.46469900	-2.21645200	-0.06771800
C	-1.46481000	3.25324700	-0.04585000
O	-3.64468300	-0.96536500	-0.14566700
O	-2.62078800	2.77933900	0.00278000
C	-4.71672900	-3.10614100	-0.06378200
C	-1.29055400	4.78023500	-0.07422100
H	3.91630500	-0.58035800	-1.92103500
H	1.47932100	-0.36196400	-2.03301600
H	1.27074500	-0.24197000	2.27654500
H	3.73499300	-0.46242700	2.38806400
H	-1.99127700	5.21301200	-0.79381000
H	-1.53929300	5.17692700	0.91621800
H	-0.26948900	5.07215200	-0.32607500
H	-5.33869300	-2.87277300	-0.93408100
H	-4.46021300	-4.16757700	-0.07203000
H	-5.31127700	-2.88760100	0.83024500
O	5.33379300	-0.65430500	0.42444600
C	6.17484300	-0.76265800	-0.73038000
H	6.09238500	0.12887000	-1.36111700
H	7.19122600	-0.84636600	-0.34641800
H	5.92739800	-1.65607900	-1.31358400

[Bis(acetoxy)iodo]-2-chlorobenzene radical anion

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1159.629696

I	-0.53401100	-0.05660200	-0.19280400
C	1.46333800	-0.68747800	-0.40614100
C	1.95449000	-0.90479300	-1.70304700
C	3.26324300	-1.34188700	-1.90970100
C	4.10029400	-1.57223700	-0.81436700
C	3.62773100	-1.36545200	0.48297700
C	2.31545100	-0.92799500	0.68260500
O	-2.60397300	-2.28934200	-0.11565600
O	0.70120100	2.34052300	-0.19909000
C	-3.52203900	-1.41821400	-0.02972400
C	-0.16488600	3.28513300	-0.08401700
O	-3.33591500	-0.16399500	-0.00931100
O	-1.40129300	3.14577100	-0.00000900
C	-4.96822000	-1.91751200	0.08594800
C	0.43902200	4.69645600	-0.02462200
H	3.62402200	-1.50061900	-2.92101000
H	1.30542400	-0.72718500	-2.55420700
H	-0.17631700	5.38008700	-0.61517200
H	0.41839900	5.03512000	1.01701500
H	1.47054100	4.71630600	-0.38014700
H	-5.63769900	-1.28480600	-0.50356900
H	-5.05996900	-2.95788400	-0.23392900
H	-5.28285800	-1.84686800	1.13384700
H	5.11990000	-1.91383400	-0.96275800
H	4.26967100	-1.54098100	1.33936300
Cl	1.78357500	-0.68819000	2.34189800

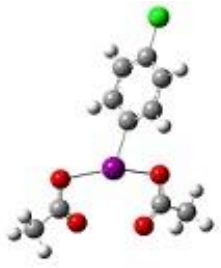
[Bis(acetoxy)iodo]-3-chlorobenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1159.633442

I	-0.79288500	-0.07721300	0.12116200
C	1.25573600	-0.36186800	0.52077200
C	1.70507600	-0.42569600	1.84497600
C	3.06328600	-0.63154000	2.10043600
C	3.97311000	-0.77916400	1.04971900
C	3.49931400	-0.71671200	-0.26179200
C	2.14887100	-0.51310800	-0.54674800
O	-0.00801200	2.51244900	0.10032100
O	-2.39619200	-2.64499600	-0.03321000
C	-1.02201900	3.26351500	-0.14831900
C	-3.45814200	-1.98232800	-0.24383200
O	-2.19663900	2.88124400	-0.32579600
O	-3.52414100	-0.71999400	-0.32983800
C	-0.69687800	4.76132400	-0.25279000
C	-4.76986100	-2.76720700	-0.38187900
H	3.41788800	-0.67844700	3.12549400
H	1.00916600	-0.31373900	2.66927300
H	1.80879800	-0.47053700	-1.57500300
H	-5.35635200	-2.37728400	-1.21900600
H	-4.58816000	-3.83502500	-0.52138300
H	-5.36323100	-2.62786300	0.52924800
H	-1.48769900	5.34108000	0.23011900
H	0.27052100	5.00186900	0.19130500
H	-0.67522900	5.03507700	-1.31341200
Cl	4.63346100	-0.90323700	-1.59757800
H	5.02727100	-0.94069600	1.24551700

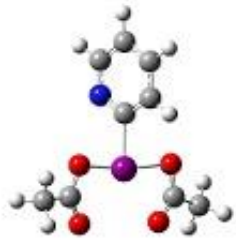
[Bis(acetoxy)iodo]-4-chlorobenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1159.633715

I	-0.89866900	-0.08123600	-0.00222700
C	1.19245400	-0.28204900	-0.00084300
C	1.88517300	-0.36844100	1.21315900
C	3.27432900	-0.51191500	1.21788600
C	3.95493900	-0.57275400	0.00045000
C	3.27727400	-0.49483700	-1.21765600
C	1.88812200	-0.35134800	-1.21426000
O	-0.28085200	2.57112800	0.02273000
O	-2.28598400	-2.74831700	-0.01679700
C	-1.38120400	3.23319800	0.01413700
C	-3.43150800	-2.19896500	-0.01323800
O	-2.53246800	2.74737800	0.00111300
O	-3.64206700	-0.95084100	-0.01073300
C	-1.21797300	4.76081800	-0.00304000
C	-4.65576700	-3.12466400	0.01569200
H	3.81496100	-0.57481200	2.15590700
H	1.35433000	-0.32110500	2.15803300
H	1.35954800	-0.29068700	-2.15964100
H	-5.42729200	-2.75311500	-0.66491500
H	-4.39016400	-4.15091900	-0.24707100
H	-5.07748400	-3.12066900	1.02758700
H	-1.91501900	5.20907900	0.71028600
H	-0.19647000	5.06619800	0.22967400
H	-1.47878900	5.12552300	-1.00255000
Cl	5.70480000	-0.75461400	0.00127300
H	3.82016800	-0.54459900	-2.15515600

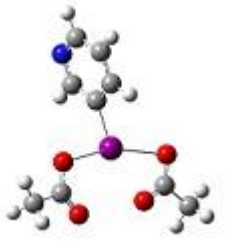
2-[Bis(acetoxy)iodo]pyridine radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -716.080639

I	0.21861400	-0.45286200	-0.01189300
C	-0.49642200	1.53809000	-0.00614500
C	-0.70393800	2.18315200	1.21739500
C	-1.17378000	3.49691700	1.17779600
C	-1.40866100	4.09746000	-0.06124500
C	-1.16163700	3.35524800	-1.21742400
O	-2.50327700	-1.03161600	0.03851600
O	2.90086200	0.45254700	-0.01620800
C	-2.61537200	-2.30717500	0.02715600
C	3.51508900	-0.66758700	-0.01647700
O	-1.66913800	-3.13062100	0.00892400
O	2.97210600	-1.80220900	-0.02715600
C	-4.05641500	-2.84072100	0.00105300
C	5.04864300	-0.59639100	0.03162000
H	-1.35190200	4.03861800	2.10166100
H	-0.50951100	1.68107500	2.15763900
H	5.48175900	-1.39764700	-0.57275700
H	5.41795300	0.37310100	-0.30916300
H	5.37119800	-0.74525000	1.06862900
H	-4.11507300	-3.79832000	0.52438300
H	-4.75695000	-2.12752800	0.44102800
H	-4.34625600	-3.00586500	-1.04321100
H	-1.77331300	5.11644700	-0.13445200
H	-1.32892900	3.78347300	-2.20216500
N	-0.70928200	2.08926100	-1.19375100

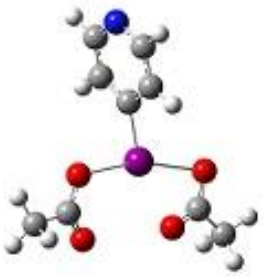
3-[Bis(acetoxy)iodo]pyridine radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -716.078415

I	-0.34851300	-0.11846000	-0.01404300
C	1.61420900	-0.87581500	0.01726600
C	2.27523000	-1.12207500	1.22411400
C	3.57000000	-1.64004200	1.17725600
C	4.14500100	-1.89524000	-0.06998300
O	1.02351400	2.19963300	-0.02934300
O	-2.59606200	-2.18779000	0.03449000
C	0.22145300	3.20535000	0.02635500
C	-3.44819800	-1.24897100	-0.00950800
O	-1.02201000	3.15436800	0.09667200
O	-3.16850300	-0.01377400	-0.06863000
C	0.91920000	4.57268500	-0.02945600
C	-4.93358700	-1.63165600	0.03601500
H	4.12254500	-1.84335300	2.08884900
H	1.79809600	-0.91413100	2.17639000
H	-5.49521700	-1.05376900	-0.70398700
H	-5.07947800	-2.69991100	-0.13838100
H	-5.33461600	-1.37873100	1.02441300
H	0.42856200	5.26020800	0.66417300
H	1.98301600	4.49933900	0.20238400
H	0.80659000	4.97398300	-1.04261800
H	5.15099600	-2.30165300	-0.14007800
N	3.51460900	-1.66680900	-1.23370900
C	2.27177500	-1.16805000	-1.18486300
H	1.78239200	-0.99255600	-2.13959000

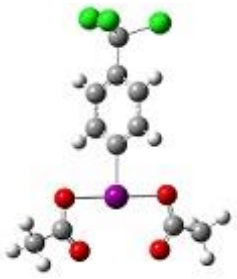
4-[Bis(acetoxy)iodo]pyridine radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -716.078117

I	0.36284000	-0.10537100	-0.01139400
C	-1.60077100	-0.87991300	0.00219200
C	-2.26275600	-1.11750500	1.20885100
C	-3.55511100	-1.64807500	1.16002700
C	-3.54165900	-1.71787800	-1.12979300
C	-2.24886000	-1.19005700	-1.19546700
O	2.58545800	-2.16285100	0.02629300
O	-1.05147800	2.18438000	-0.04336300
C	3.44754300	-1.23208300	-0.00925400
C	-0.25452100	3.19393600	0.01916700
O	3.17967600	0.00585100	-0.05468800
O	0.98835600	3.14916100	0.09873000
C	4.92824200	-1.63188400	0.02849700
C	-0.95914000	4.55763500	-0.04017900
H	-4.09562000	-1.83980000	2.08415800
H	-1.80254700	-0.89887600	2.16624900
H	-1.77750000	-1.02945600	-2.15891700
H	-4.07113400	-1.96590100	-2.04689400
H	-0.48206900	5.24372100	0.66423200
H	-0.83339300	4.96462000	-1.04945300
H	-2.02567400	4.47739200	0.17597600
H	5.33622700	-1.38722600	1.01604600
H	5.06116700	-2.70089600	-0.15112500
H	5.49256700	-1.05716500	-0.71190100
N	-4.19520200	-1.94844400	0.01935500

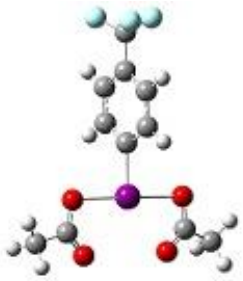
[Bis(acetoxy)iodo]-4-trichloromethylbenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -2118.109406

I	-2.16622800	-0.00623600	-0.00659400
C	-0.07395600	-0.02397400	0.02218300
C	0.64121500	0.00576700	-1.18290100
C	2.03182200	-0.01586800	-1.16024300
C	2.72813000	-0.07036000	0.05997700
C	2.00482500	-0.10088100	1.25678600
C	0.60713400	-0.07831200	1.23959000
O	-2.37875200	-2.84120600	-0.02827300
O	-1.95489000	2.77170000	0.01897000
C	-3.65201800	-2.92954100	-0.02338800
C	-3.17195800	3.16901100	0.00541700
O	-4.45356900	-1.95820300	-0.04071100
O	-4.18563400	2.42937500	-0.02303700
C	-4.23636700	-4.34807300	0.03896100
C	-3.35721500	4.69377000	0.04151000
H	2.57249100	0.00906700	-2.10031200
H	0.12336700	0.04631800	-2.13471700
H	0.06574500	-0.10314900	2.17879800
H	2.51334800	-0.14244500	2.21141200
H	-4.40734500	4.95995000	-0.09296300
H	-3.00927600	5.07740300	1.00662200
H	-2.75207500	5.16683600	-0.73756200
H	-5.12462200	-4.41708600	-0.59461800
H	-3.50317400	-5.09995600	-0.25986400
H	-4.54442000	-4.55245700	1.07085700
C	4.24769600	-0.09218900	0.02089700
Cl	5.01153300	-0.17988500	1.64746300
Cl	4.87047500	1.40897500	-0.80029100
Cl	4.82639900	-1.52811400	-0.93696500

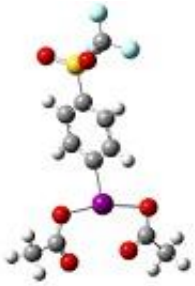
[Bis(acetoxy)iodo]-4-trifluoromethylbenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1037.088246

I	1.48813600	-0.00596900	-0.03790600
C	-0.60720100	-0.01629500	-0.01855700
C	-1.29016100	-0.02230800	1.20335600
C	-2.68542200	-0.03786300	1.21472700
C	-3.39160100	-0.04533700	0.00689200
C	-2.70701700	-0.04319300	-1.21409000
C	-1.31236500	-0.02777800	-1.22834400
O	1.72386800	-2.84581000	0.01951200
O	1.36839200	2.78333600	0.00088400
C	2.99787800	-2.91647600	0.01060400
C	2.60613100	3.10610500	0.00507500
O	3.78559000	-1.93500300	-0.04538000
O	3.57367500	2.30638400	-0.04139900
C	3.60457500	-4.32395600	0.10511600
C	2.90476600	4.60936500	0.10752100
H	-3.21406800	-0.03921600	2.16161800
H	-0.74690100	-0.01300600	2.14169300
H	-0.78604000	-0.02264100	-2.17631200
H	-3.25277000	-0.04845700	-2.15152200
H	3.77487000	4.86110000	-0.50430300
H	2.04642800	5.21346700	-0.19327200
H	3.14694000	4.84436900	1.15035800
H	4.47070000	-4.40417400	-0.55733600
H	3.95302800	-4.48511900	1.13172900
H	2.87294100	-5.09648000	-0.13984600
C	-4.89429700	-0.11354800	0.01543800
F	-5.43504700	0.41427100	1.14191200
F	-5.45006700	0.54316500	-1.03497300
F	-5.34825000	-1.39932800	-0.05906600

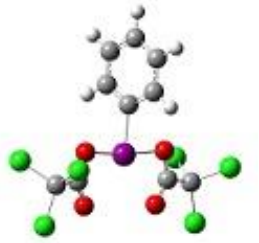
[Bis(acetoxy)iodo]-4-trifluoro(methylsulfonyl)benzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1585.637591

I	-2.27804100	-0.13843000	-0.00125700
C	-0.18982100	0.14948300	0.00303300
C	0.49919200	0.24684000	-1.21308700
C	1.88369200	0.41286300	-1.21704400
C	2.55609800	0.47204800	0.00842400
C	1.88319900	0.37670600	1.23132400
C	0.49869000	0.21089900	1.22178100
O	-3.07007400	-3.02985100	-0.02754800
O	-2.18226400	2.55652200	0.02799100
C	-4.29548400	-2.69861500	-0.01435100
C	-3.38951900	3.00110300	0.01353200
O	-4.72555300	-1.50662200	-0.00882600
O	-4.42845900	2.31069300	-0.00041700
C	-5.33658400	-3.82440600	0.01881000
C	-3.50236000	4.53271300	-0.01659000
H	2.42417500	0.50304300	-2.15265000
H	-0.03360100	0.20154500	-2.15646500
H	-0.03465100	0.13764000	2.16308200
H	-4.34134800	4.84946200	0.60789800
H	-2.58165700	5.01563100	0.31495800
H	-3.70923100	4.84122500	-1.04726100
H	-6.13332300	-3.61971100	-0.70244100
H	-4.88585000	-4.79641400	-0.19198300
H	-5.79349700	-3.85535000	1.01456500
H	2.42317300	0.43922700	2.16948600
S	4.32611200	0.68436900	0.01174600
O	4.76598300	1.27211000	-1.26167200
O	4.76578900	1.23536500	1.30155300
C	4.99925600	-1.09196500	-0.01349000
F	6.33526600	-1.03458400	-0.01237400
F	4.58499700	-1.73176100	-1.11322800
F	4.58447600	-1.76267400	1.06746800

[Bis(trichloroacetoxy)iodo]benzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -3457.603042

I	-0.00000800	0.15853500	-0.06742600
C	0.00002800	2.24409200	-0.01605600
C	0.00005100	2.89873600	1.22190800
C	0.00007600	4.29553000	1.24727600
C	0.00007600	5.02334600	0.05224700
C	0.00005200	4.35515200	-1.17707600
C	0.00002700	2.95878700	-1.22032200
O	-2.80267000	0.28523400	-0.02913100
O	2.80264300	0.28519600	-0.02915700
C	-3.18668200	-0.91496200	-0.04153900
C	3.18666000	-0.91499900	-0.04154200
O	-2.53292100	-1.96341600	-0.09011800
O	2.53290400	-1.96345800	-0.09009000
C	-4.78371700	-1.04472900	0.02136700
C	4.78369600	-1.04475700	0.02136300
H	0.00009500	6.10868600	0.07892100
H	0.00009400	4.81111500	2.20271900
H	0.00005100	2.33511300	2.14828600
H	0.00000900	2.44125800	-2.17321200
H	0.00005200	4.91711600	-2.10600000
Cl	-5.37399200	-0.28280500	1.55172700
Cl	-5.33256800	-2.75401500	-0.01509600
Cl	-5.50510800	-0.17788600	-1.39177700
Cl	5.37395100	-0.28287900	1.55175400
Cl	5.33255700	-2.75403900	-0.01515200
Cl	5.50509400	-0.17786400	-1.39174500

[Bis(trifluoroacetoxy)iodo]benzene radical anion

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1295.553503

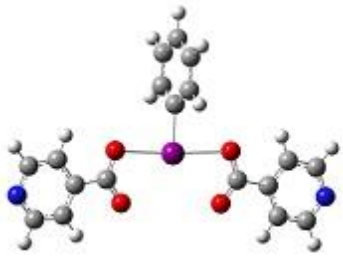
I	0.00000200	-0.07421100	-0.00000100
C	-0.00000400	2.01258200	-0.00000100
C	0.00001200	2.69760200	1.22141500
C	0.00000900	4.09460600	1.21252100
C	-0.00001000	4.79284300	0.00000000
C	-0.00002600	4.09460700	-1.21252000
C	-0.00002300	2.69760300	-1.22141600
O	-2.81980200	0.04620100	0.00000800
O	2.81980500	0.04620700	-0.00000500
C	-3.17935500	-1.16373400	0.00000400
C	3.17935900	-1.16372800	-0.00000700
O	-2.50591200	-2.20547600	0.00000100
O	2.50591500	-2.20547000	-0.00001100
C	-4.74313800	-1.32319700	0.00000200
C	4.74314100	-1.32319200	0.00000000
H	-0.00001200	5.87851000	0.00000100
H	0.00002200	4.63350300	2.15501700
H	0.00002600	2.15699800	2.16142200
H	-0.00003500	2.15700000	-2.16142300
H	-0.00004100	4.63350400	-2.15501700
F	5.29813600	-0.73505400	-1.09204900
F	5.29812000	-0.73509200	1.09207700
F	5.14690500	-2.61173300	-0.00001900
F	-5.14690200	-2.61173800	-0.00000600
F	-5.29812400	-0.73507200	-1.09205700
F	-5.29812500	-0.73508500	1.09206800

[Bis(benzoyloxy)iodo]benzene radical anion

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1083.425905

I	-0.03059900	0.46032400	-0.00001800
C	0.12177200	2.54915100	0.00000000
C	0.17027500	3.23964400	1.21819100
C	0.27081500	4.63366600	1.21154300
C	0.32138800	5.33170800	0.00002600
C	0.27084900	4.63368600	-1.21150300
C	0.17030900	3.23966400	-1.21817800
O	-2.87779600	0.42659800	-0.00003100
O	2.76669700	0.26241700	0.00001900
C	-3.05431400	-0.83690700	-0.00002300
C	2.93437900	-1.00436400	0.00001100
O	-2.14086900	-1.70353600	-0.00002900
O	2.01797700	-1.86475900	0.00000000
H	0.39929800	6.41473000	0.00003600
H	0.30942700	5.17080500	2.15458200
H	0.13112400	2.70123200	2.15918200
H	0.13118400	2.70126800	-2.15917900
H	0.30948700	5.17084000	-2.15453300
C	4.38074100	-1.48844500	0.00001000
C	4.65766600	-2.86397100	0.00000900
C	5.44809900	-0.57731100	0.00000800
C	5.97823400	-3.32161400	0.00000600
H	3.82855400	-3.56369100	0.00001200
C	6.76946500	-1.03328800	0.00000500
H	5.23201100	0.48570500	0.00001000
C	7.03791100	-2.40698300	0.00000400
H	6.18093300	-4.38916900	0.00000600
H	7.58820900	-0.31887000	0.00000300
H	8.06480800	-2.76200200	0.00000100
C	-4.50146000	-1.31828700	-0.00000500
C	-4.78304300	-2.69292000	0.00001700
C	-5.56601300	-0.40394700	-0.00001000
C	-6.10508700	-3.14638700	0.00003300
H	-3.95617500	-3.39529900	0.00002200
C	-6.88890400	-0.85553600	0.00000600
H	-5.34609600	0.65832200	-0.00002700
C	-7.16184700	-2.22837600	0.00002700
H	-6.31125300	-4.21329800	0.00005000
H	-7.70536400	-0.13848300	0.00000100
H	-8.18989400	-2.58008800	0.00003900

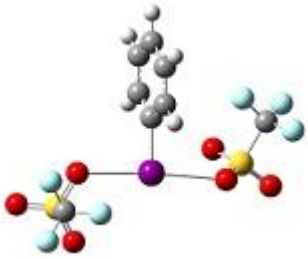
[Bis(isonicotinoyloxy)iodo]benzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1115.521900

I	-0.00000400	0.13411700	0.00006500
C	0.00000000	2.22571100	0.00003500
C	0.00004600	2.91374700	-1.21920900
C	0.00004900	4.31152000	-1.21154600
C	0.00000500	5.01098100	-0.00000500
C	-0.00004100	4.31155500	1.21155500
C	-0.00004400	2.91378200	1.21925800
O	2.79448300	0.24825000	0.00004700
O	-2.79449000	0.24826500	0.00000900
C	3.16035200	-0.97318700	0.00003700
C	-3.16035200	-0.97317400	0.00002600
O	2.41112300	-1.97828900	0.00007300
O	-2.41111800	-1.97827200	0.00007600
H	0.00000700	6.09674500	-0.00002100
H	0.00008500	4.84982700	-2.15461500
H	0.00007900	2.37363400	-2.15976400
H	-0.00007900	2.37369600	2.15982900
H	-0.00007500	4.84988900	2.15460900
C	4.67277300	-1.20717200	-0.00002500
C	5.19131500	-2.50653600	-0.00005200
C	5.58148200	-0.14296300	-0.00005900
C	6.57622100	-2.68297300	-0.00011000
H	4.52170100	-3.35911000	-0.00002800
C	6.94975300	-0.42187200	-0.00011600
H	5.22549600	0.88104800	-0.00004000
N	7.45556400	-1.66671800	-0.00014200
H	7.00006000	-3.68495000	-0.00013200
H	7.67329200	0.39058500	-0.00014200
C	-4.67277200	-1.20716800	-0.00001900
C	-5.19130700	-2.50653400	0.00001600
C	-5.58148700	-0.14296300	-0.00009700
C	-6.57621200	-2.68297900	-0.00002600
H	-4.52168800	-3.35910400	0.00007600
C	-6.94975600	-0.42187900	-0.00013600
H	-5.22550600	0.88105000	-0.00012700
N	-7.45556000	-1.66672800	-0.00010200
H	-7.00004500	-3.68495800	0.00000100
H	-7.67330000	0.39057400	-0.00019700

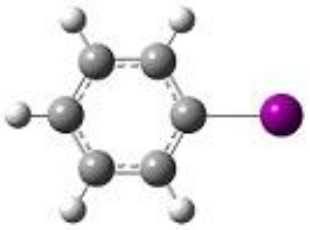
[Bis(trifluoromethylsulfonyloxy)iodo]benzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -2166.030872

I	-0.16221400	-0.52653000	-0.15540900
C	0.31334700	1.47655900	-0.20275200
C	0.24007000	2.22604900	0.98545400
C	0.56630300	3.57902600	0.94374800
C	0.96046500	4.17263300	-0.26378200
C	1.02993900	3.41395300	-1.44047900
C	0.70872500	2.05901800	-1.42067100
O	-2.85796600	0.28181800	-0.81805500
O	2.44537600	-1.55433000	0.62634300
H	1.21384000	5.22779900	-0.28747900
H	0.51365200	4.17038000	1.85205800
H	-0.06500900	1.76070200	1.91570300
H	0.76187200	1.46647100	-2.32677100
H	1.33541700	3.87764100	-2.37277400
S	-4.03756900	-0.63796600	-0.73505000
S	3.70067400	-1.52456400	-0.19043000
O	-5.11543700	-0.31454400	-1.69519300
O	-3.68815700	-2.06880500	-0.60195900
O	3.50732800	-1.14618700	-1.60692700
O	4.60346100	-2.67035200	0.05916700
C	-4.78630300	-0.20378600	0.93315700
C	4.63142100	-0.06244600	0.53694000
F	3.91843700	1.07235800	0.40868900
F	4.88086800	-0.25350900	1.84632400
F	5.80975900	0.11096100	-0.09193300
F	-5.14763700	1.09243700	0.97536300
F	-5.88051700	-0.95141200	1.17127200
F	-3.90454900	-0.42453200	1.92661100

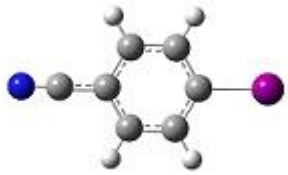
Iodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -243.020904

I	-1.55653000	0.00000000	-0.00000100
C	0.56258700	0.00000000	-0.00001000
C	1.24940400	-1.21662000	0.00000900
C	2.64925100	-1.20909800	0.00000700
C	3.35118800	0.00000000	-0.00002100
C	2.64925100	1.20909800	0.00000700
C	1.24940400	1.21662000	0.00000900
H	4.43697500	0.00000000	-0.00003800
H	3.18512300	-2.15388500	0.00001500
H	0.71119000	-2.15828000	0.00003400
H	0.71118900	2.15828000	0.00003400
H	3.18512300	2.15388500	0.00001500

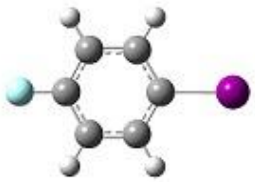
4-Cyanoiodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -335.270777

I	0.00000000	-2.17168900	0.00000000
C	0.00000000	-0.06470000	0.00000000
C	-1.21713800	0.62452800	0.00000000
C	-1.21840100	2.01844600	0.00000000
C	0.00000000	2.72018300	0.00000000
C	1.21840200	2.01844600	0.00000000
C	1.21713800	0.62452800	0.00000000
H	-2.15910700	2.55847900	0.00000000
H	-2.15944300	0.08878500	0.00000000
H	2.15944300	0.08878500	0.00000000
H	2.15910700	2.55847900	0.00000000
C	0.00000000	4.15410800	0.00000000
N	-0.00000100	5.31882500	0.00000000

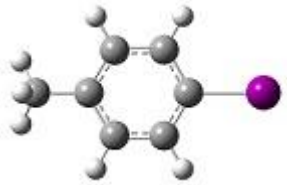
4-Fluoroiodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -342.269046

I	0.00000000	0.00000000	1.92288400
C	0.00000000	0.00000000	-0.19116200
C	0.00000000	1.21551400	-0.88119000
C	0.00000000	1.21886500	-2.27993100
C	0.00000000	0.00000000	-2.94567600
C	0.00000000	-1.21886500	-2.27993100
C	0.00000000	-1.21551400	-0.88119000
H	0.00000000	2.14899800	-2.83791900
H	0.00000000	2.15905000	-0.34710800
H	0.00000000	-2.15905000	-0.34710800
H	0.00000000	-2.14899800	-2.83791900
F	0.00000000	0.00000000	-4.30981400

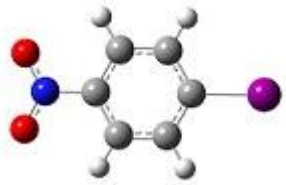
4-Methyliodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -282.317780

I	1.95868500	0.00000000	0.00221000
C	-0.15989800	0.00000000	-0.00157800
C	-0.85223400	-1.21235300	-0.00528100
C	-2.25100500	-1.20184900	-0.01071400
C	-2.97485600	0.00000200	-0.01024400
C	-2.25100500	1.20185300	-0.01028600
C	-0.85223300	1.21235500	-0.00485000
H	-2.78237800	-2.15031600	-0.01721900
H	-0.31972900	-2.15745400	-0.00754200
H	-0.31972900	2.15745700	-0.00677600
H	-2.78237900	2.15032200	-0.01645400
C	-4.48567600	-0.00000300	0.01611400
H	-4.85854800	-0.00021900	1.04811800
H	-4.89305600	0.88713600	-0.47792300
H	-4.89305700	-0.88693500	-0.47829300

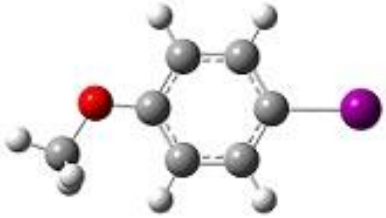
4-Nitroiodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -447.532541

I	0.00000000	2.53771100	0.00000000
C	0.00000000	0.43529200	0.00000000
C	1.21835100	-0.25457300	0.00000000
C	1.22137300	-1.64789200	0.00000000
C	0.00000000	-2.32478200	0.00000000
C	-1.22137300	-1.64789200	0.00000000
C	-1.21835100	-0.25457300	0.00000000
H	2.15309900	-2.19947400	0.00000000
H	2.16038900	0.28117600	0.00000000
H	-2.16038900	0.28117600	0.00000000
H	-2.15309900	-2.19947400	0.00000000
N	0.00000000	-3.78814200	0.00000000
O	-1.08815800	-4.37366200	0.00000000
O	1.08815800	-4.37366200	0.00000000

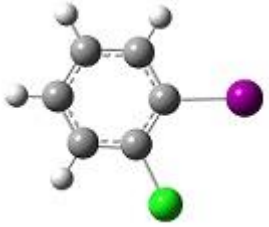
4-Methoxyiodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -357.521094

I	2.31715100	-0.07872200	0.00000000
C	0.20615100	0.07444900	0.00000000
C	-0.57496000	-1.07920100	0.00000000
C	-1.97305800	-0.98314300	0.00000000
C	-2.58469800	0.27758400	0.00000000
C	-1.78908200	1.43520700	0.00000000
C	-0.39983500	1.33643900	0.00000000
H	-2.55898300	-1.89425100	0.00000000
H	-0.11520900	-2.06167900	0.00000000
H	0.19879200	2.24097300	0.00000000
H	-2.27147300	2.40768200	0.00000000
O	-3.93387500	0.48187000	0.00000000
C	-4.79889500	-0.65768500	0.00000000
H	-4.64582600	-1.26932800	0.89614900
H	-5.81319800	-0.25864300	0.00000000
H	-4.64582600	-1.26932800	-0.89614900

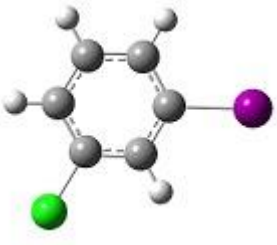
2-Chloroiodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -702.619298

I	1.66510000	-0.23970200	0.00000000
C	-0.43408500	-0.42687300	-0.00000400
C	-0.98407400	-1.71518700	0.00000000
C	-2.36839700	-1.89557600	0.00000100
C	-3.21782300	-0.78621600	0.00000100
C	-2.68096800	0.50095900	0.00000000
C	-1.29291900	0.68053200	-0.00000400
H	-2.77585400	-2.90159700	0.00000400
H	-0.32719900	-2.57802600	0.00000200
H	-4.29532200	-0.91650200	0.00000300
H	-3.32851800	1.37101700	0.00000200
Cl	-0.68551700	2.32843900	0.00000100

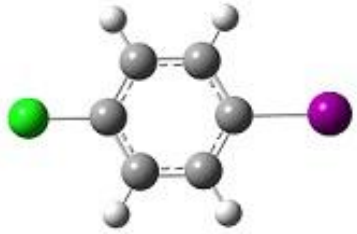
3-Chloroiodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -702.622968

I	-2.09918700	0.16267900	0.00000000
C	0.00000000	0.40702300	0.00000000
C	0.54656800	1.69250200	0.00000000
C	1.93728600	1.83926600	0.00000000
C	2.77780200	0.72331100	0.00000000
C	2.19996100	-0.54613200	0.00000000
C	0.81499600	-0.72767800	0.00000000
H	2.36980800	2.83506500	0.00000000
H	-0.09233500	2.56826900	0.00000000
H	0.39506400	-1.72628200	0.00000000
Cl	3.23934000	-1.96861800	0.00000000
H	3.85588100	0.83771000	0.00000000

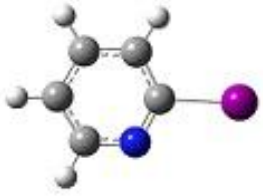
4-Chloroiodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -702.622529

I	0.00000000	0.00000000	2.30091000
C	0.00000000	0.00000000	0.18839800
C	0.00000000	1.21381400	-0.50299200
C	0.00000000	1.21576100	-1.90129500
C	0.00000000	0.00000000	-2.58513700
C	0.00000000	-1.21576100	-1.90129500
C	0.00000000	-1.21381400	-0.50299200
H	0.00000000	2.15501600	-2.44351800
H	0.00000000	2.15874700	0.02887000
H	0.00000000	-2.15874700	0.02887000
H	0.00000000	-2.15501600	-2.44351800
Cl	0.00000000	0.00000000	-4.34629600

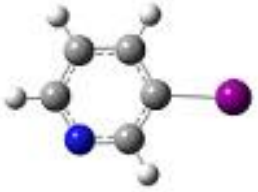
2-Iodopyridine



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -259.071152

I	-0.01759200	-1.54182700	0.00000000
C	0.00000000	0.59171200	0.00000000
C	1.22959600	1.25766400	0.00000000
C	1.19809300	2.65284000	0.00000000
C	-0.03620500	3.30871500	0.00000000
C	-1.19589200	2.53553700	0.00000000
H	2.12681700	3.21534600	0.00000000
H	2.16602500	0.71309100	0.00000000
H	-0.10045800	4.39148300	0.00000000
H	-2.17870000	2.99918400	0.00000000
N	-1.17926500	1.18841400	0.00000000

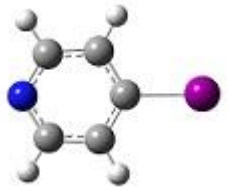
3-Iodopyridine



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -259.068477

I	-0.04705400	-1.54229900	0.00000000
C	0.00000000	0.56576400	0.00000000
C	-1.18138900	1.30768900	0.00000000
C	-1.08236200	2.70079200	0.00000000
C	0.18560800	3.28475400	0.00000000
C	1.22883300	1.23378700	0.00000000
H	-1.97398700	3.31937100	0.00000000
H	-2.15139000	0.82240600	0.00000000
H	2.16356100	0.67976500	0.00000000
H	0.29578400	4.36626700	0.00000000
N	1.32225000	2.57104600	0.00000000

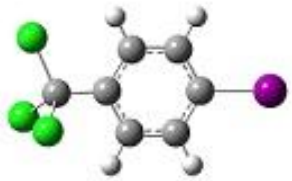
4-Iodopyridine



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -259.068840

I	0.00000000	1.54746100	0.00000000
C	0.00000000	-0.56038500	0.00000000
C	0.00000000	-1.26459900	1.20388400
C	0.00000000	-2.66183400	1.14393500
C	0.00000000	-2.66183400	-1.14393500
C	0.00000000	-1.26459900	-1.20388400
H	0.00000000	-3.23775200	2.06651900
H	0.00000000	-0.76243100	2.16442300
H	0.00000000	-0.76243100	-2.16442300
H	0.00000000	-3.23775200	-2.06651900
N	0.00000000	-3.36221900	0.00000000

4-trichloromethyliodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1661.098115

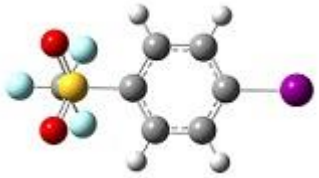
I	-3.60014600	-0.00364700	0.00002300
C	-1.49165600	0.02491900	-0.00138600
C	-0.78206800	-1.18098500	-0.00194300
C	0.60992300	-1.15853300	-0.00329700
C	1.30918400	0.06033700	-0.00460700
C	0.58594200	1.25689200	-0.00320500
C	-0.81312700	1.24192400	-0.00172300
H	1.14765900	-2.10069800	-0.00361100
H	-1.30057200	-2.13303400	-0.00153800
H	-1.35261600	2.18227000	-0.00107300
H	1.09426100	2.21264100	-0.00324000
C	2.82805800	0.02039000	-0.00102900
Cl	3.59362400	1.64871200	-0.03442700
Cl	3.43550500	-0.90162700	-1.44917500
Cl	3.42625200	-0.83870500	1.49015300

4-trifluoromethyliodobenzene

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -580.079886

I	2.89664700	-0.00070200	0.00586900
C	0.78690600	0.00125600	-0.01010200
C	0.09624200	-1.21380600	-0.01635800
C	-1.29964100	-1.20998600	-0.02857600
C	-1.99557500	0.00376000	-0.03778800
C	-1.29793600	1.21586200	-0.02846800
C	0.09843800	1.21707200	-0.01629300
H	-1.83594800	-2.15289600	-0.03630900
H	0.62974800	-2.15744400	-0.01373700
H	0.63336200	2.15991000	-0.01356600
H	-1.83258100	2.15947100	-0.03597100
C	-3.49841200	0.00076900	-0.00029600
F	-4.03324900	-1.05933900	-0.65933400
F	-3.98010800	-0.06633100	1.27632000
F	-4.03742300	1.11884700	-0.54856100

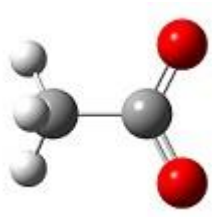
4-(trifluoromethylsulfonyl)iodobenzene



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1128.628190

I	3.80458200	0.16640600	-0.00027000
C	1.72477300	-0.14572300	-0.00009000
C	1.04505400	-0.24991700	-1.21897100
C	-0.33398400	-0.45800300	-1.22290100
C	-1.00544800	-0.55600100	0.00014500
C	-0.33382600	-0.45765100	1.22307600
C	1.04521200	-0.24956600	1.21890800
H	-0.86969200	-0.55199600	-2.16084300
H	1.57625300	-0.17638700	-2.16079300
H	1.57653200	-0.17576500	2.16064000
H	-0.86941200	-0.55137400	2.16111500
S	-2.76567400	-0.83228600	0.00029900
O	-3.18323700	-1.41802700	-1.28149400
O	-3.18307100	-1.41765600	1.28231600
C	-3.50706700	0.91662000	0.00009400
F	-4.83964700	0.80725800	0.00019700
F	-3.11822400	1.58729500	-1.09051600
F	-3.11808200	1.58761000	1.09045900

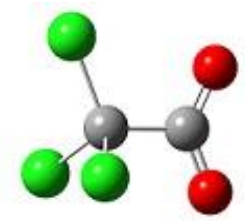
Acetate anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -228.625438

O	0.76363300	1.12864000	0.00201700
C	0.18592600	0.00000000	-0.01066200
O	0.76363500	-1.12863800	0.00201700
C	-1.35371600	-0.00000100	-0.00437000
H	-1.70279100	0.00000700	1.03597100
H	-1.75430900	0.89468300	-0.48903200
H	-1.75430800	-0.89469200	-0.48901900

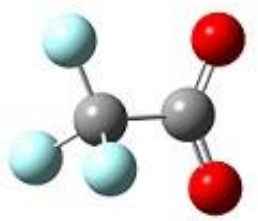
Trichloroacetate anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -1607.427958

O	-2.10555600	-0.81799300	-0.00023700
C	-1.45229200	0.24401100	-0.00023800
O	-1.81735900	1.43336900	-0.00030700
C	0.14325800	0.00063300	-0.00001800
Cl	0.60184200	-0.95101900	1.47513100
Cl	1.10402900	1.52732600	-0.00053900
Cl	0.60221900	-0.95224100	-1.47424600

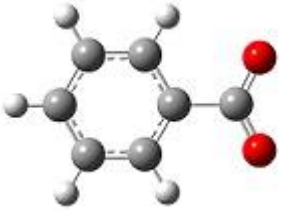
Trifluoroacetate anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -526.394013

O	1.53940600	-1.13858800	-0.00001800
C	1.04846200	0.01246600	-0.00000100
O	1.59272400	1.13655700	0.00002000
C	-0.52518600	0.01312800	-0.00000100
F	-1.02542000	-0.63227900	-1.09231500
F	-1.02541600	-0.63226000	1.09232600
F	-1.08213000	1.24928200	-0.00001100

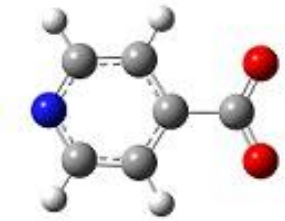
Benzoate anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -420.327325

O	-2.38542000	1.12855800	-0.00002200
C	-1.81133300	-0.00000700	-0.00002400
O	-2.38540700	-1.12855900	-0.00004400
C	-0.27825200	0.00000800	-0.00000300
C	0.43873000	-1.20651400	0.00000300
C	0.43872900	1.20651800	0.00001100
C	1.83683800	-1.20943100	0.00002100
H	-0.11508500	-2.13946400	-0.00000700
C	1.83684700	1.20942700	0.00002800
H	-0.11506100	2.13948200	0.00000700
C	2.54104600	0.00000100	0.00003300
H	2.37676200	-2.15268500	0.00002500
H	2.37675600	2.15268800	0.00003800
H	3.62762700	-0.00001400	0.00004700

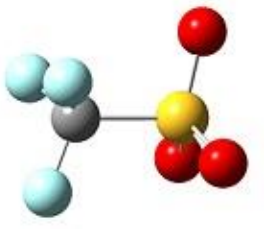
Isonicotinate anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -436.378014

O	-2.37084100	1.13052800	-0.00000400
C	-1.80733700	-0.00000500	0.00000200
O	-2.37083400	-1.13052900	0.00000000
C	-0.27029700	0.00000900	0.00000100
C	0.45866400	-1.19498300	0.00000200
C	0.45865700	1.19498800	-0.00000100
C	1.85363800	-1.14488200	0.00000100
H	-0.06209600	-2.14602700	0.00000400
C	1.85365200	1.14486700	-0.00000100
H	-0.06206800	2.14605000	-0.00000200
N	2.55807800	0.00000400	0.00000000
H	2.43458100	-2.06492500	0.00000200
H	2.43457400	2.06492600	-0.00000300

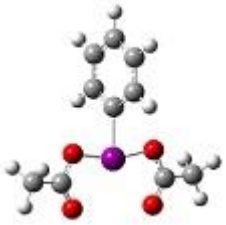
Triflate anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -961.642985

O	-1.25501800	-0.33472300	1.40622300
S	-0.91972500	0.00001800	-0.00003800
O	-1.25519500	-1.05050300	-0.99290300
O	-1.25531400	1.38515100	-0.41322900
C	0.96163500	0.00001900	-0.00001300
F	1.44695600	-1.20629900	0.35894400
F	1.44715600	0.29228500	-1.22414500
F	1.44699900	0.91403700	0.86519600

[Bis(acetoxy)iodo]benzene in water



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) water = -699.867341

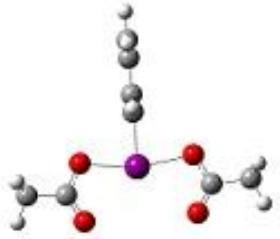
I	0.04830500	-0.59862700	0.00000000
C	-0.11856900	1.50017100	0.00000100
C	-0.17249400	2.16934300	-1.22265900
C	-0.28513700	3.56328800	-1.21281400
C	-0.34137700	4.25701900	0.00000200
C	-0.28513900	3.56328700	1.21281800
C	-0.17249600	2.16934100	1.22266100
O	2.20022000	-0.14643300	0.00000100
O	-2.14725100	-0.48968200	-0.00000100
C	2.90006000	-1.26024500	0.00000100
C	-2.66466200	-1.69912200	-0.00000200
O	2.36609800	-2.37617300	0.00000200
O	-1.96320800	-2.71808300	-0.00000100
C	4.39867100	-1.05208700	-0.00000200
C	-4.17741000	-1.72699500	-0.00000200
H	-0.42899300	5.33908600	0.00000300
H	-0.32856500	4.10042300	-2.15511200
H	-0.12877100	1.63008900	-2.16227000
H	-0.12877500	1.63008700	2.16227200
H	-0.32856900	4.10042100	2.15511600
H	-4.53185300	-2.75806600	-0.00000500
H	-4.55636100	-1.20382800	0.88282600
H	-4.55636100	-1.20382300	-0.88282700
H	4.90922000	-2.01542900	0.00002000
H	4.69164000	-0.47640200	-0.88286700
H	4.69164100	-0.47635800	0.88283400

[Bis(acetoxy)iodo]benzene in acetone

Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) acetone = -699.866258

I	0.04866000	-0.60094200	0.00000000
C	-0.11866900	1.49811500	0.00000000
C	-0.17293200	2.16761900	-1.22234700
C	-0.28607800	3.56147900	-1.21267700
C	-0.34258200	4.25527800	0.00000100
C	-0.28607800	3.56147800	1.21267900
C	-0.17293200	2.16761800	1.22234800
O	2.19940400	-0.14391200	0.00000000
O	-2.14643300	-0.48758200	0.00000000
C	2.90078800	-1.25711700	0.00000000
C	-2.66499100	-1.69686000	-0.00000100
O	2.36863000	-2.37340800	-0.00000100
O	-1.96477800	-2.71614000	-0.00000100
C	4.39923700	-1.04653200	0.00000000
C	-4.17793900	-1.72292400	-0.00000100
H	-0.43062900	5.33733100	0.00000200
H	-0.32974000	4.09857900	-2.15500700
H	-0.12910300	1.62845300	-2.16203300
H	-0.12910300	1.62845200	2.16203400
H	-0.32973900	4.09857800	2.15501000
H	-4.53316300	-2.75371900	-0.00000100
H	-4.55630900	-1.19923300	0.88277700
H	-4.55630800	-1.19923300	-0.88277800
H	4.91090300	-2.00927700	0.00000000
H	4.69133600	-0.47029500	-0.88280500
H	4.69133600	-0.47029400	0.88280400

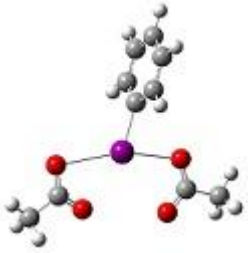
[Bis(acetoxy)iodo]benzene in DCM



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) DCM = -699.865021

I	0.04818400	-0.60440400	0.00000000
C	-0.11639700	1.49529400	0.00000100
C	-0.16997300	2.16543600	-1.22184700
C	-0.28150300	3.55935300	-1.21246400
C	-0.33723900	4.25335300	0.00000200
C	-0.28151800	3.55935100	1.21246800
C	-0.16998800	2.16543400	1.22184900
O	2.19786200	-0.14344600	-0.00000200
O	-2.14599200	-0.48081800	0.00000200
C	2.89923500	-1.25720800	0.00000200
C	-2.66777300	-1.68921500	-0.00000200
O	2.36740000	-2.37288500	0.00000600
O	-1.97070600	-2.70982200	-0.00000600
C	4.39789700	-1.04622100	-0.00000500
C	-4.18105200	-1.71071400	0.00000100
H	-0.42408200	5.33553700	0.00000300
H	-0.32457000	4.09649100	-2.15484100
H	-0.12682000	1.62626000	-2.16160400
H	-0.12684700	1.62625600	2.16160600
H	-0.32459700	4.09648600	2.15484500
H	-4.53867200	-2.74067100	-0.00000500
H	-4.55790400	-1.18577800	0.88270700
H	-4.55790700	-1.18576700	-0.88269800
H	4.90912400	-2.00919600	0.00001700
H	4.68992600	-0.46983200	-0.88275400
H	4.68993000	-0.46978600	0.88271200

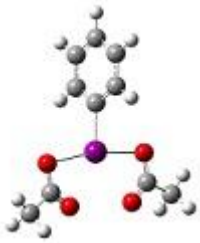
[Bis(acetoxy)iodo]benzene radical anion in water



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) water = -700.033776

I	-0.33622600	-0.08921900	-0.00340200
C	1.62234900	-0.85577400	0.00008900
C	2.25922600	-1.12748500	1.21801800
C	3.55514800	-1.65178500	1.21468200
C	4.20832900	-1.90948700	0.00446300
C	3.56343100	-1.64153700	-1.20796300
C	2.26757400	-1.11711500	-1.21570700
O	0.97171200	2.29014900	0.01287100
O	-2.48848900	-2.23338000	-0.01755800
C	0.13353200	3.26472300	0.01585200
C	-3.40732300	-1.35691700	-0.01278000
O	-1.11167200	3.16717300	0.02026000
O	-3.22036700	-0.10436800	-0.01449400
C	0.77322100	4.66110600	-0.01089800
C	-4.86049500	-1.85180200	0.01736000
H	5.21413000	-2.31871700	0.00617300
H	4.05084400	-1.85884400	2.15856900
H	1.75590600	-0.93082500	2.15903000
H	1.77072600	-0.91241200	-2.15844200
H	4.06555100	-1.84064500	-2.15016200
H	-5.45678300	-1.30891100	-0.72230700
H	-4.92679900	-2.92554300	-0.17066100
H	-5.28817200	-1.63916600	1.00391500
H	0.26009100	5.30981300	0.70421000
H	1.84061000	4.62775200	0.21371400
H	0.63443800	5.08593600	-1.01107000

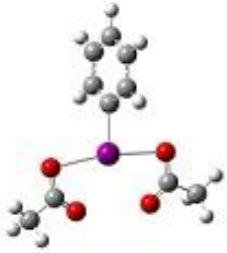
[Bis(acetoxy)iodo]benzene radical anion in acetone



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) acetone = -700.018444
Optimized geometry for BP86/6-31+G(d,p):

I	-0.31082000	-0.00380400	0.00275900
C	1.73444400	-0.57222800	0.00084500
C	2.40608800	-0.76828000	1.22400700
C	3.75817400	-1.15413800	1.21634800
C	4.43537400	-1.34613500	-0.00211000
C	3.75644500	-1.15089600	-1.21909100
C	2.40436500	-0.76500200	-1.22378900
O	0.53733100	2.78823000	0.00080600
O	-1.68785800	-2.65504800	-0.00946800
C	-0.63404300	3.31278300	0.00018800
C	-2.83835200	-2.09167600	-0.00974900
O	-1.74356800	2.69627000	0.00310300
O	-3.06370600	-0.83799500	-0.00132300
C	-0.68524000	4.85939200	-0.00530100
C	-4.06707600	-3.02742000	0.00028100
H	5.48779200	-1.64772700	-0.00326300
H	4.28040000	-1.30458400	2.16713800
H	1.88292300	-0.62053500	2.17364300
H	1.87983600	-0.61472100	-2.17227400
H	4.27730700	-1.29881600	-2.17102600
H	-4.54523100	-2.97461700	0.99390800
H	-4.80460100	-2.68390300	-0.74322500
H	-3.78543300	-4.07080200	-0.20506300
H	0.32081900	5.30366000	-0.00336200
H	-1.23613100	5.19849200	-0.89865000
H	-1.24289900	5.20511600	0.88122900

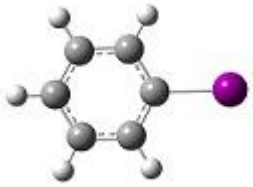
[Bis(acetoxy)iodo]benzene radical anion in DCM



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) DCM = -700.010684
Optimized geometry for BP86/6-31+G(d,p):

I	-0.31648000	0.00643700	0.00798400
C	1.72719500	-0.56952100	0.00213800
C	2.39358200	-0.76899400	-1.22328200
C	3.74472400	-1.15789400	-1.22237100
C	4.42813400	-1.34931200	-0.00739900
C	3.75539600	-1.15054900	1.21234300
C	2.40424600	-0.76171400	1.22284100
O	-1.66549000	-2.66144500	-0.00825900
O	0.54185900	2.80070700	-0.00409000
C	-2.81846000	-2.10414600	-0.00979100
C	-0.63598700	3.30902500	-0.01622200
O	-3.05485500	-0.85306900	0.00449300
O	-1.73844400	2.68040200	-0.00872800
C	-4.04152400	-3.04924100	-0.00666300
C	-0.69826900	4.85626200	-0.00759400
H	5.48010500	-1.65291400	-0.01111000
H	4.26167600	-1.31086000	-2.17579800
H	1.86568700	-0.62116700	-2.17030800
H	1.88476000	-0.60820600	2.17360100
H	4.28075900	-1.29773600	2.16207300
H	-0.84895000	5.19293500	1.03321300
H	0.23561600	5.29874200	-0.38591500
H	-1.55472200	5.20536700	-0.60534300
H	-4.79745600	-2.68678400	-0.72201100
H	-3.75518800	-4.08293600	-0.25158500
H	-4.49766100	-3.03385300	0.99868800

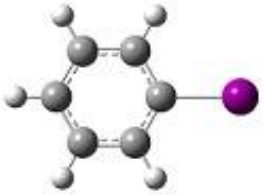
Iodobenzene in water



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) water = -243.020998

I	-1.55656900	0.00000000	-0.00000100
C	0.56265700	0.00000000	-0.00001000
C	1.24942900	-1.21666600	0.00000900
C	2.64930700	-1.20913000	0.00000700
C	3.35124000	0.00000000	-0.00002100
C	2.64930700	1.20913000	0.00000700
C	1.24943000	1.21666600	0.00000900
H	4.43702300	0.00000000	-0.00003800
H	3.18516300	-2.15392100	0.00001500
H	0.71128700	-2.15836600	0.00003400
H	0.71128600	2.15836600	0.00003400
H	3.18516300	2.15392100	0.00001500

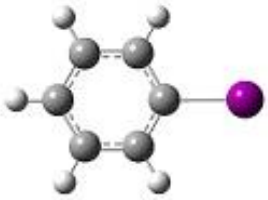
Iodobenzene in acetone



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) acetone = -243.020779

I	1.55646000	0.00000000	0.00000000
C	-0.56246800	0.00000000	-0.00000200
C	-1.24935000	1.21655800	0.00000000
C	-2.64915100	1.20906200	0.00000000
C	-3.35108100	0.00000000	0.00000000
C	-2.64915100	-1.20906200	0.00000000
C	-1.24935000	-1.21655800	0.00000000
H	-4.43687700	0.00000000	0.00000100
H	-3.18507000	2.15382800	0.00000100
H	-0.71102000	2.15815700	0.00000000
H	-0.71102000	-2.15815700	0.00000000
H	-3.18507000	-2.15382800	0.00000100

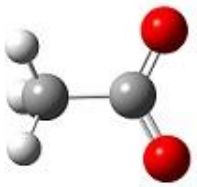
Iodobenzene in DCM



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) DCM = -243.020423

I	-1.55633300	0.00000000	-0.00000100
C	0.56220800	0.00000000	-0.00001100
C	1.24927400	-1.21638400	0.00000900
C	2.64896700	-1.20893500	0.00000700
C	3.35092200	0.00000000	-0.00002100
C	2.64896700	1.20893600	0.00000700
C	1.24927400	1.21638400	0.00000900
H	4.43673100	0.00000000	-0.00003800
H	3.18491700	-2.15370800	0.00001600
H	0.71070600	-2.15784800	0.00003500
H	0.71070500	2.15784700	0.00003400
H	3.18491700	2.15370700	0.00001600

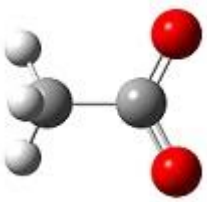
Acetate anion in water



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) water = -228.627241

O	-0.76389500	-1.12843300	0.00200800
C	-0.18539900	0.00000000	-0.01063500
O	-0.76387700	1.12844200	0.00200800
C	1.35378600	-0.00000800	-0.00435800
H	1.70295500	0.00001600	1.03592200
H	1.75444500	-0.89460900	-0.48902800
H	1.75444700	0.89457100	-0.48906600

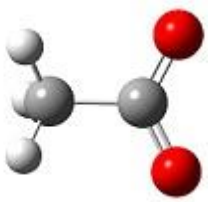
Acetate anion in acetone



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) acetone = -228.623003

O	0.76329300	1.12891300	0.00202800
C	0.18663100	0.00000000	-0.01069800
O	0.76330800	-1.12890500	0.00202800
C	-1.35362600	-0.00000700	-0.00438500
H	-1.70257200	0.00004500	1.03603900
H	-1.75413400	0.89478900	-0.48903900
H	-1.75413000	-0.89485100	-0.48895200

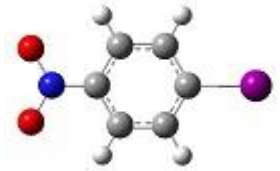
Acetate anion in DCM



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) DCM = -228.615714

O	-0.76234400	-1.12971200	0.00206100
C	-0.18870100	0.00000100	-0.01080100
O	-0.76233500	1.12971600	0.00206000
C	1.35339300	-0.00000500	-0.00443100
H	1.70196400	0.00003500	1.03624500
H	1.75365200	-0.89523400	-0.48888100
H	1.75366100	0.89519000	-0.48894100

4-Nitroiodobenzene radical anion



Gibbs Free Energy (hartrees):
B3LYP/6-31+G(d,p) MeCN = -447.665168

I	0.00000000	0.00000000	2.55329500
C	0.00000000	0.00000000	0.43627600
C	0.00000000	1.21535100	-0.26147500
C	0.00000000	1.22038100	-1.65363900
C	0.00000000	0.00000000	-2.37075700
C	0.00000000	-1.22038100	-1.65363900
C	0.00000000	-1.21535100	-0.26147500
H	0.00000000	2.15514100	-2.19970700
H	0.00000000	2.15973700	0.27303200
H	0.00000000	-2.15973700	0.27303200
H	0.00000000	-2.15514100	-2.19970700
N	0.00000000	0.00000000	-3.76597000
O	0.00000000	-1.13103000	-4.40757600
O	0.00000000	1.13103000	-4.40757600