Supporting Information

Why does Togni's Reagent I Exist in the High-Energy Hypervalent Iodine Form? Re-evaluation of the Existing Forms of Benziodoxole-based Hypervalent Iodine Reagents

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Computational details

All the theoretical studies were carried out with the Gaussian 09 package.[1] Structures and energies optimizations were performed with four popular DFT functionals (B3LYP[2], BP86,[3] M06-2X,[4] ωB97X-D[5]) and one ab initio method (MP2[6]). The triple-ζ augmented correlation-consistent basis set, designated aug-cc-pVTZ, was employed for H, C, N, O, F,[7] and d sets were added (aug-cc-pV(T+d)Z) for the second row elements, S and Cl.[8] For I and Br, aug-cc-pVTZ-PP basis set was used,[9] in which the PP notation stands for pseudopotential, i.e., the relativistic effective core potentials are used for the core electrons. Frequencies were computed to obtain the thermodynamic energy corrections and to verify the stationary points to be minima or saddle points. For the MP2 method, geometry structures were obtained from the B3LYP level, and then single-point energies were conducted. Solvent effects were evaluated with the SMD solvation model in solvents used in the experiment (Acetonitrile for **X** = **-CF_3**, **-OAc**, **-F**, **-Cl**; Dichloromethane for **X** = **-NCO**; Tetrahydrofuran for **X** = **-SCF_3**; Chloroform for **X** = **-Br**).[10] The relative free energies (at 298.15K) are in kcal/mol.

Triplet and singlet

The open-shell triplet states of Togni's Reagent I and Shen's Reagent were explored at the B3LYP level, and their energies are much higher than corresponding closed-shell singlet states (see **Fig. S1**). Thus only singlet state isomers are discussed in this paper.

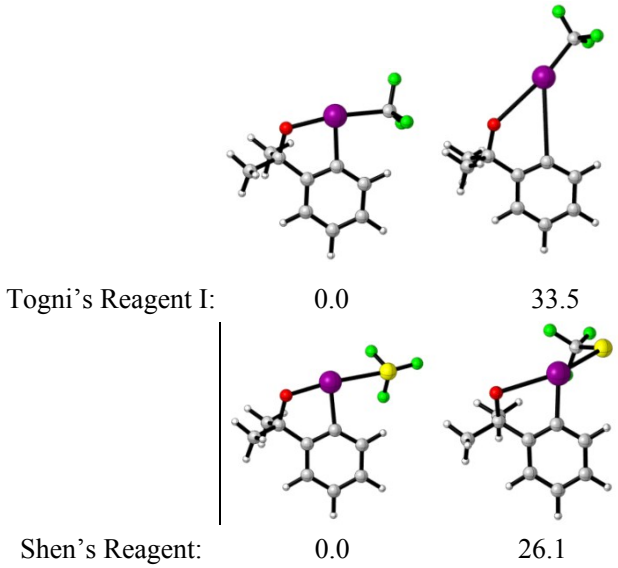

Fig. S1 Structures and energies of the open-shell triplet and closed-shell singlet states of Togni's Reagent I and Shen's Reagent (in kcal/mol).

Enthalpy of isomerization predicted by our DFT methods (in kcal/mol):

B3LYP: -51.1 BP86: -43.2 M06-2X: -64.0 ωB97X-D: -58.3 MP2: -77.3

Correlation between the free energy of isomerization and the *trans* influence

The correlation between the energy of isomerization and *trans* influence was establish. As shown in **Fig. S2**, the deviation of **X** = **-CN** is large. NBO analysis indicated that the lone pair on iodine interacts with the antibonding orbital of **-C≡N** (see **Fig. S3**). However, there is no such interaction in **X** = **-N_3, NCO** or other groups. We think that is the reason why **X** = **-CN** is deviated.

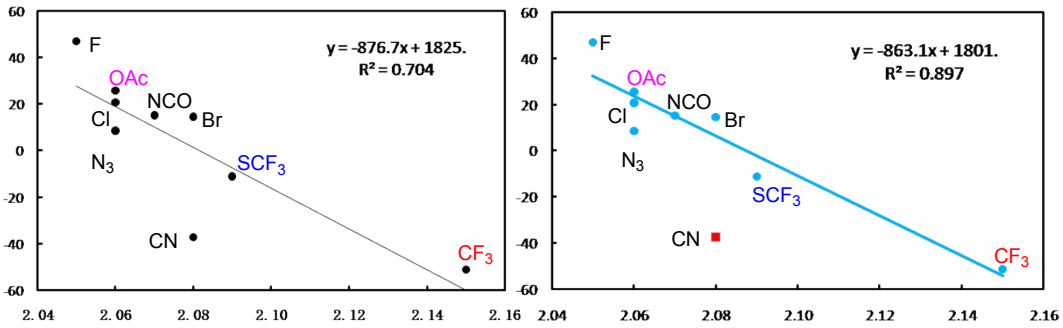

Fig. S2 Correlation between the free energy of isomerization and the *trans* influence.

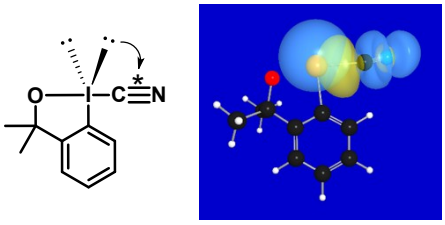

Fig. S3 Interaction between the lone pair on iodine and the antibonding orbital of -C≡N.

Bimolecular decomposition pathway

The bimolecular decomposition pathways were explored. As shown in **Fig. S4**, the energy barriers are inaccessibly high. For such a formal redox process involving CF_3^+ transfer between two molecules, charge separation is inevitable, which leads to the failure of locating the unstable transition states.

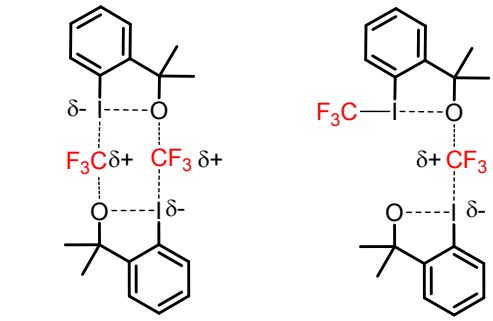

Fig. S4 The bimolecular decomposition pathway (in kcal/mol at B3LYP/BS2//B3LYP/BS1, BS2: aug-cc-pVTZ for C, H, O, F and aug-cc-pVTZ-PP for I; BS1: 6-31(d) for C, H, O, F and SDD for I).

Reference

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Cartesian Coordinates

Hypervalent iodine form **3**, B3LYP, **X** = **-CF_3**

C	-0.06897800	2.12184300	-0.15540900
C	-0.53898500	0.82091400	-0.09968200
C	-1.87830700	0.48756100	0.00357500
C	-2.78774600	1.54646500	0.06862900
C	-2.35436700	2.86523800	0.01565400
C	-0.99942100	3.15530500	-0.10024800
H	0.97972500	2.35295100	-0.24916500
H	-3.84415700	1.33629300	0.16176900
H	-3.07756200	3.66854500	0.06098500
H	-0.65832200	4.18029800	-0.15216800
C	-2.29097500	-0.99027900	0.07547500
C	-3.52958500	-1.26842300	-0.78403500
H	-3.74444300	-2.33735000	-0.75760200
H	-4.40894300	-0.73872000	-0.41728900
H	-3.35096200	-0.97770500	-1.81953000
C	-2.56520600	-1.36361600	1.54431100
H	-2.83552000	-2.41889200	1.60488900
H	-1.67641300	-1.19926300	2.15562800
H	-3.38083700	-0.77116000	1.96153900
O	-1.23558600	-1.77179000	-0.44466900
I	0.71468300	-0.92442300	-0.15269000
C	2.65160600	0.30326800	0.12055100
F	2.98385900	1.12789100	-0.90230900
F	3.64905900	-0.61609800	0.20339700
F	2.71993600	1.04421800	1.25090300

Triplet, Hypervalent iodine form **3**, B3LYP, **X** = **-CF_3**

C	-2.10059600	2.38821300	-0.19001600
C	-1.90460800	1.03150100	-0.19212800
C	-2.85911500	0.05690700	-0.02730600
C	-4.16663800	0.53291400	0.16287600
C	-4.43429700	1.89790600	0.17633400
C	-3.41409000	2.82966100	0.00168200
H	-1.29008800	3.09254100	-0.32763400
H	-4.97787200	-0.17037200	0.30284900
H	-5.45064900	2.23734400	0.32590800
H	-3.63040700	3.89028600	0.01394500
C	-2.51873200	-1.43454500	-0.05460800
C	-3.32755500	-2.20064600	-1.12197000
H	-3.06526700	-3.25722500	-1.09274400
H	-4.39560100	-2.09614800	-0.93742700
H	-3.10436100	-1.80546100	-2.11277100

C	-2.79666300	-2.07407900	1.35504800
H	-2.55659700	-3.13448500	1.33177400
H	-2.20795900	-1.57585200	2.12187400
H	-3.85672400	-1.94390900	1.56808200
O	-1.18142600	-1.66372900	-0.23281300
I	1.49898400	-0.31468600	-0.03680300
C	3.54868300	0.37467500	0.04427400
F	3.85370100	1.13572100	-1.01870400
F	4.41240200	-0.65297900	0.06348800
F	3.77638900	1.11019300	1.14344700

TS_1, B3LYP, **X = -CF_3**

C	1.78150000	-2.24949500	-0.00828300
C	1.41720100	-0.91887800	-0.03847600
C	2.31422900	0.14087000	0.01743700
C	3.66832200	-0.18086400	0.10106900
C	4.07414200	-1.51178000	0.12908800
C	3.14139400	-2.54233700	0.07573800
H	1.04468200	-3.03867500	-0.05125400
H	4.40688200	0.60838300	0.14657800
H	5.12865100	-1.74380900	0.19191600
H	3.46518400	-3.57408700	0.09641500
C	1.76212400	1.55796700	0.04379900
C	2.53924700	2.53283100	-0.83509300
H	2.03322200	3.49739200	-0.85447800
H	3.53748000	2.68227700	-0.42326300
H	2.63024600	2.15477900	-1.85195600
C	1.62847900	2.06567500	1.47788600
H	1.18180700	3.05990300	1.48012600
H	1.01035700	1.39627800	2.07763000
H	2.61256000	2.12342700	1.94281400
O	0.43503200	1.52694400	-0.59808600
I	-0.59014500	-0.12606800	-0.14460300
C	-3.52181700	-0.14945000	0.06936400
F	-4.05580400	-1.43964900	0.28429500
F	-4.29193000	0.29201200	-1.02670500
F	-4.10588200	0.57351800	1.13118400

5, B3LYP, **X = -CF_3**

C	2.32620100	-1.87705100	-0.03471600
C	1.50248000	-0.76182300	-0.03072800
C	1.98459900	0.52725400	-0.03598300
C	3.36718000	0.72020400	-0.04425500
C	4.21799900	-0.38091100	-0.05554400

C	3.70427400	-1.67632300	-0.05194000
H	1.91633800	-2.87925800	-0.02956100
H	3.78273200	1.71891800	-0.04192400
H	5.28899100	-0.22778500	-0.06837900
H	4.37323900	-2.52678200	-0.06492500
C	0.94678800	1.65183900	0.01828700
C	1.24140900	2.74212100	-1.01734500
H	0.45268800	3.49432900	-0.99252500
H	2.18836700	3.23643400	-0.80012000
H	1.29018600	2.31859200	-2.02019200
C	0.88741500	2.23813000	1.43603300
H	0.13700100	3.02856800	1.47804800
H	0.62026300	1.46594300	2.15903800
H	1.85136500	2.65792000	1.72610000
O	-0.33375100	1.12514600	-0.32984200
I	-0.66646600	-0.90538100	0.04082900
C	-2.77902500	0.10319300	-0.05333600
F	-3.10401700	0.70035500	-1.22210800
F	-3.04363400	0.99575100	0.92680500
F	-3.66394900	-0.92084300	0.11157100

TS_2, B3LYP, **X = -CF_3**

C	-1.75663900	-1.95348400	-0.46103800
C	-1.05756700	-0.83392700	-0.02339800
C	-1.59833200	0.44352600	0.01736000
C	-2.92679800	0.55129500	-0.41899900
C	-3.65667600	-0.54732600	-0.85190000
C	-3.07443500	-1.80932100	-0.87233100
H	-1.27812600	-2.92236300	-0.48807100
H	-3.40450100	1.52075000	-0.40858800
H	-4.68091100	-0.41521300	-1.17475400
H	-3.62983700	-2.67254800	-1.21296400
C	-0.84029900	1.69315500	0.54342600
C	-1.40533500	2.02421300	1.95047300
H	-0.89853600	2.90758800	2.34097100
H	-2.47746600	2.22421500	1.90978000
H	-1.22955400	1.19242300	2.63275900
C	-1.08083300	2.91123000	-0.37686200
H	-0.46174600	3.73405900	-0.01753400
H	-0.80277600	2.69659400	-1.40730800
H	-2.11888500	3.24290700	-0.36510900
O	0.50339500	1.43051700	0.71127200
I	0.96095300	-1.24713300	0.56659100
C	1.87782400	0.71189500	-0.76720700

F	2.72762800	1.50642500	-0.14833700
F	1.16785400	1.31752900	-1.70768500
F	2.67554300	-0.15751300	-1.47351100

The acyclic isomer form **4**, B3LYP, **X** = **-CF_3**

C	2.89291700	0.17114200	-0.41168000
C	1.54005900	0.13703100	-0.07947800
C	0.79965900	1.32195600	0.08473800
C	1.50108900	2.52129000	-0.09477700
C	2.85065400	2.56241300	-0.41539300
C	3.55375400	1.38004500	-0.57898900
H	3.43564800	-0.75399700	-0.53816200
H	0.98180600	3.45883900	0.01822700
H	3.34077100	3.51843000	-0.54033900
H	4.60478700	1.38636600	-0.83467200
C	-0.68575400	1.39515700	0.47870900
C	-1.29391600	2.78540600	0.31979200
H	-2.35026300	2.75072100	0.56979500
H	-0.82289100	3.48331100	1.00879600
H	-1.18510400	3.16073900	-0.69628200
C	-0.90465000	0.90423200	1.90985800
H	-1.95097500	0.98870200	2.19879100
H	-0.57306700	-0.11874600	2.05935300
H	-0.32343900	1.55087400	2.56727800
O	-1.33510200	0.51127300	-0.54867600
I	0.78670400	-1.85728100	0.13347600
C	-2.56713800	0.03762300	-0.47574400
F	-2.80046600	-0.79117500	0.57235600
F	-3.54081700	0.98470500	-0.41422300
F	-2.80225000	-0.67989800	-1.59366700

Hypervalent iodine form of model without the five-memberd ring constrain, B3LYP, **X** = **-CF_3**

C	-0.29581700	1.71254700	1.22527300
C	-0.25073300	1.16401600	-0.04852800
C	-0.33461300	1.94043500	-1.19585100
C	-0.47075100	3.31802800	-1.05445500
C	-0.51966300	3.89246000	0.21208600
C	-0.43328600	3.09339900	1.34658100
H	-0.22833300	1.08911800	2.10430900
H	-0.53972900	3.93791500	-1.93820000
H	-0.62446000	4.96416600	0.31426600
H	-0.46860000	3.53798200	2.33201000
C	2.97813800	-0.34583200	0.30760300
O	2.05686300	-0.57666900	-0.75289400

I	-0.00566200	-0.94157000	-0.26555600
C	-2.29801100	-1.07301400	0.13819100
F	-2.68513800	-0.67392300	1.37726900
F	-2.69018900	-2.37185800	0.02225300
F	-3.06259000	-0.36970700	-0.73715100
H	-0.29528700	1.49102000	-2.17712800
H	2.53723500	0.34703000	1.03892900
C	4.21491200	0.32619300	-0.28167200
H	4.94620500	0.54847500	0.49900400
H	4.68875700	-0.32676100	-1.01838000
H	3.94647500	1.26141700	-0.77503700
C	3.33466900	-1.64159500	1.03448700
H	4.02446700	-1.45178400	1.86021300
H	2.44264300	-2.11610500	1.44743200
H	3.80799700	-2.34637300	0.34656200

TS_3 of model without the five-memberd ring constrain, B3LYP, **X** = **-CF_3**

C	-2.46765000	-0.13411200	1.21470400
C	-1.85512500	-0.42053100	0.00030800
C	-2.46869000	-0.13496000	-1.21376300
C	-3.73382800	0.44543900	-1.20435700
C	-4.36584900	0.73407200	0.00098600
C	-3.73279800	0.44627500	1.20598800
H	-1.97619300	-0.35947900	2.15017000
H	-4.22298000	0.66841300	-2.14327300
H	-5.34956200	1.18375700	0.00125100
H	-4.22114600	0.66989000	2.14517000
C	0.68445800	2.40968900	0.00076100
O	0.83601000	1.02233200	0.00061900
I	0.03847700	-1.37732800	-0.00023900
C	2.43318300	-0.41228500	-0.00011400
F	2.96180000	0.12348200	1.09684300
F	2.96235800	0.12547100	-1.09584700
F	2.87617800	-1.71716400	-0.00125500
H	-1.97804500	-0.36096000	-2.14950200
H	-0.40866000	2.57956200	0.00472800
C	1.24033100	3.05958400	-1.27148200
H	1.01281000	4.12750000	-1.29827400
H	2.32551200	2.94412900	-1.31785900
H	0.80846400	2.59508400	-2.15920200
C	1.24919200	3.05984500	1.26899800
H	1.02228600	4.12785500	1.29683900
H	0.82319000	2.59588200	2.15982000
H	2.33460600	2.94389700	1.30799600

Hypervalent iodine form, B3LYP, **X** = **-NCO**

C	-0.08319100	2.20177300	-0.23375500
C	-0.44520800	0.87286900	-0.14036300
C	-1.73821800	0.42222200	0.06587000
C	-2.72856900	1.39881300	0.18587300
C	-2.40860400	2.74865600	0.09184100
C	-1.09404400	3.15201900	-0.11786800
H	0.94470100	2.48999900	-0.39094400
H	-3.75465900	1.10305600	0.35656600
H	-3.19122100	3.48982800	0.18296700
H	-0.84789500	4.20240200	-0.19390600
C	-1.98938400	-1.08105100	0.20346800
C	-3.23315900	-1.52926500	-0.56455500
H	-3.32439900	-2.61355200	-0.50007600
H	-4.13725900	-1.08830000	-0.14483800
H	-3.16091900	-1.24808800	-1.61484100
C	-2.10175500	-1.45389800	1.68898400
H	-2.25816400	-2.52903700	1.78449200
H	-1.19165500	-1.18599000	2.22747700
H	-2.93934100	-0.93729600	2.15935300
O	-0.88490700	-1.77355100	-0.39361900
I	0.91129300	-0.76021400	-0.28215700
N	2.60070300	0.72915800	-0.25098700
C	3.64182800	0.57723700	0.32571000
O	4.68980700	0.47954500	0.87033900

The acyclic isomer form, B3LYP, **X** = **-NCO**

C	2.64211400	-0.61358700	-0.46952300
C	1.35069000	-0.22395000	-0.12018800
C	1.01114900	1.13469000	0.01134900
C	2.03888300	2.05928500	-0.21573600
C	3.32981900	1.67763500	-0.55140700
C	3.63511900	0.33228400	-0.68366800
H	2.87535600	-1.66334800	-0.57075500
H	1.82697700	3.11292900	-0.12613400
H	4.08653000	2.43359700	-0.71185200
H	4.63305300	0.01147400	-0.95084700
C	-0.36918100	1.66309900	0.43136800
C	-0.57272100	3.15489300	0.18151300
H	-1.61664700	3.39846100	0.37512200
H	0.03302700	3.76045100	0.85349600
H	-0.34125500	3.42377000	-0.84820900
C	-0.65914400	1.33569100	1.89743900

H	-1.64216600	1.70668300	2.18426500
H	-0.61727500	0.26727400	2.09344300
H	0.08533100	1.83085500	2.52060300
O	-1.26687100	0.93981600	-0.47951200
I	0.02658300	-1.88185400	0.18194400
N	-2.61072700	1.12210800	-0.11692400
O	-4.46977400	-0.00130300	-1.08933100
C	-3.50065900	0.49550500	-0.66330300

Hypervalent iodine form, B3LYP, **X** = **-OAc**

C	-0.32596400	2.22048200	-0.14926900
C	-0.68987900	0.88727600	-0.09319500
C	-1.99823300	0.44189500	0.01728900
C	-2.99446800	1.41732000	0.07854000
C	-2.66879000	2.76787400	0.02057400
C	-1.34251100	3.17031500	-0.09424800
H	0.70692100	2.51627200	-0.23421000
H	-4.02986200	1.12054900	0.17407100
H	-3.45560500	3.50901300	0.06401300
H	-1.09103900	4.22111400	-0.14420000
C	-2.26125800	-1.06211200	0.11667700
C	-3.47082000	-1.49572700	-0.71118900
H	-3.56388700	-2.58109100	-0.66970600
H	-4.39188500	-1.06310000	-0.32102300
H	-3.35522400	-1.19494900	-1.75228600
C	-2.43973200	-1.45858800	1.58942300
H	-2.60140300	-2.53488300	1.66169700
H	-1.55471300	-1.19945000	2.17242500
H	-3.29771800	-0.94748500	2.02777000
O	-1.13122700	-1.74390800	-0.44614200
I	0.65933800	-0.75766400	-0.16027200
O	2.26605100	0.77100200	0.09795600
C	3.44756000	0.21377200	0.12168100
O	3.62386400	-0.99883100	0.01114500
C	4.58546500	1.19072500	0.29979900
H	4.56858400	1.92888400	-0.50286600
H	4.46507800	1.72808100	1.24139300
H	5.53813100	0.66772300	0.29717300

The acyclic isomer form, B3LYP, **X** = **-OAc**

C	2.83643800	0.55675000	-0.65852900
C	1.56772300	0.28520100	-0.15052500
C	0.67840300	1.32465400	0.17940700
C	1.14154500	2.63113200	-0.02627900

C	2.40847900	2.90762200	-0.51977800
C	3.26255800	1.86479400	-0.84243500
H	3.49773600	-0.25946000	-0.90918100
H	0.49699600	3.46244500	0.21087100
H	2.71754200	3.93546300	-0.65323800
H	4.25285200	2.05605500	-1.23348500
C	-0.72353300	1.13058900	0.78443700
C	-1.57817300	2.39591700	0.80497100
H	-2.58577200	2.13311900	1.12356500
H	-1.19190000	3.11902600	1.52139800
H	-1.63561500	2.86477000	-0.17579900
C	-0.63795600	0.55121300	2.20006500
H	-1.63393300	0.40164600	2.61322200
H	-0.09953700	-0.39207100	2.22999200
H	-0.11389200	1.26680200	2.83344800
O	-1.31937300	0.19072700	-0.16935000
I	1.18074400	-1.81263300	0.05253600
O	-2.58714700	-0.28997200	0.36660200
C	-3.60657900	-0.23784100	-0.54087100
O	-4.66444000	-0.66190300	-0.14231400
C	-3.33542000	0.30146500	-1.90619400
H	-2.97948400	1.32902800	-1.84908800
H	-2.56146800	-0.28470500	-2.40078200
H	-4.25618700	0.25765600	-2.48042100

Hypervalent iodine form, B3LYP, **X** = **-F**

C	-0.38042400	2.24769200	-0.04615100
C	-0.31444200	0.86799400	-0.04593100
C	-1.41638700	0.02911400	-0.02034200
C	-2.67077500	0.63972900	0.00445600
C	-2.78165600	2.02644200	-0.00321300
C	-1.64561300	2.82926400	-0.02891500
H	0.51471800	2.84982700	-0.06272400
H	-3.56422700	0.03107500	0.03288200
H	-3.76253200	2.48219900	0.01108700
H	-1.73696700	3.90689500	-0.03829400
C	-1.18398900	-1.48215400	0.03330300
C	-2.14112600	-2.24872000	-0.87795500
H	-1.88168800	-3.30749500	-0.86490300
H	-3.17120000	-2.14968700	-0.53556400
H	-2.07505600	-1.88481000	-1.90300700
C	-1.29636800	-1.97190600	1.48372000
H	-1.10059400	-3.04413600	1.52450900
H	-0.57464300	-1.46160200	2.12322300

H	-2.29487300	-1.78448200	1.87978400
O	0.13750000	-1.74374500	-0.47247400
I	1.48431000	-0.24962000	-0.07067300
F	2.54036600	1.54636700	0.26274000

The acyclic isomer form, B3LYP, **X** = **-F**

C	0.61744900	2.31596600	-0.11775800
C	0.23128700	0.98123400	-0.01246300
C	-1.13003200	0.62473000	0.04340900
C	-2.05835000	1.67272600	-0.02734500
C	-1.67686300	3.00250000	-0.12092300
C	-0.33027300	3.32854900	-0.16709600
H	1.66702900	2.56676000	-0.16159000
H	-3.11187000	1.44727200	0.00439000
H	-2.43372800	3.77403300	-0.16079000
H	-0.00980500	4.35885300	-0.24389100
C	-1.67022500	-0.81037700	0.21893300
C	-3.17747800	-0.94709600	0.02451700
H	-3.43588500	-2.00413800	0.04888700
H	-3.72168800	-0.45810800	0.83039500
H	-3.50075300	-0.53279900	-0.92887100
C	-1.26137400	-1.42188500	1.55951300
H	-1.61661100	-2.44899900	1.62807000
H	-0.18651700	-1.41088300	1.71292500
H	-1.73105600	-0.84808000	2.35814700
O	-1.00534100	-1.44467100	-0.90990200
I	1.89513800	-0.36690700	0.02929800
F	-1.28705900	-2.87983900	-0.86288600

Hypervalent iodine form **1**, B3LYP, **X** = **-SCF_3**

C	-0.35179400	2.05059100	-0.62473700
C	-0.89568600	0.81759200	-0.33094900
C	-2.18802300	0.61512400	0.12168100
C	-2.97453900	1.75730200	0.28724100
C	-2.46850500	3.01851500	-0.00298400
C	-1.16363400	3.16898400	-0.45939800
H	0.66612000	2.14879900	-0.97121900
H	-3.98972000	1.65891200	0.64658200
H	-3.09727200	3.88873600	0.12838800
H	-0.77115400	4.15009000	-0.68909300
C	-2.65592900	-0.80238900	0.45377100
C	-4.06735100	-1.07668200	-0.07116100
H	-4.32354600	-2.11916000	0.11786200
H	-4.80729600	-0.45167100	0.42921700

H	-4.12158100	-0.89397000	-1.14394100
C	-2.58856400	-1.02431100	1.97220800
H	-2.89334800	-2.04511200	2.20552400
H	-1.57440500	-0.87341000	2.34461000
H	-3.24847900	-0.33481200	2.50007000
O	-1.79764900	-1.72529700	-0.21870700
I	0.16082700	-1.04553900	-0.50511200
S	2.49164000	0.07199100	-1.06657000
C	3.16773800	0.29828100	0.58349300
F	2.47089100	1.17475100	1.34653000
F	4.43031400	0.77990600	0.50443800
F	3.23985100	-0.84380400	1.30933700

The acyclic isomer form **2**, B3LYP, **X** = **-SCF_3**

C	3.13246800	0.72559500	-0.85070600
C	1.94232500	0.37085400	-0.21982500
C	1.02552300	1.34835900	0.20800000
C	1.38495800	2.68213300	-0.02558100
C	2.57377300	3.04249700	-0.64359100
C	3.45379000	2.05874700	-1.06411600
H	3.81559900	-0.04499100	-1.17612100
H	0.71810200	3.46994500	0.28570100
H	2.80114500	4.08878600	-0.79648900
H	4.38348500	2.31464000	-1.55432400
C	-0.29469800	1.06195200	0.93926200
C	-1.22845200	2.26053400	1.03225400
H	-2.17486800	1.94005300	1.46480300
H	-0.82002900	3.02171100	1.69488700
H	-1.42280100	2.70432900	0.05771900
C	-0.03991300	0.50181400	2.33871900
H	-0.98142100	0.28572000	2.84473100
H	0.56523800	-0.40061100	2.31853400
H	0.48542700	1.25359800	2.92768000
O	-0.93299100	0.03722100	0.05755700
I	1.71646500	-1.74831700	0.00502300
S	-2.28323300	-0.75561900	0.54847900
C	-3.52646300	-0.07631500	-0.59801700
F	-4.64345900	-0.80400000	-0.39999400
F	-3.84025100	1.21684000	-0.40848700
F	-3.17037000	-0.19475900	-1.88794800

Hypervalent iodine form, B3LYP, **X** = **-Cl**

C	0.07500900	2.20574400	-0.10039500
C	-0.26758100	0.86987600	-0.07307800

C	-1.56579400	0.38999800	-0.00901100
C	-2.58274700	1.34507400	0.03060100
C	-2.28236000	2.70257500	-0.00177900
C	-0.96210400	3.13459000	-0.06782600
H	1.10651100	2.52038600	-0.14639100
H	-3.61407600	1.02545600	0.08954900
H	-3.08536400	3.42683500	0.02468000
H	-0.73074100	4.19066500	-0.09666200
C	-1.79583000	-1.11824800	0.07163700
C	-2.96070500	-1.57677500	-0.80503600
H	-3.03086200	-2.66398400	-0.77205700
H	-3.90443900	-1.16665600	-0.44575200
H	-2.81330900	-1.26602700	-1.83889300
C	-2.01140700	-1.53408700	1.53268200
H	-2.14746100	-2.61465500	1.58964500
H	-1.15407800	-1.25697300	2.14788700
H	-2.89681600	-1.04914400	1.94507200
O	-0.62975800	-1.77210600	-0.46266600
I	1.12231900	-0.75096500	-0.11483300
Cl	3.17334900	0.84233000	0.22492000

The acyclic isomer form, B3LYP, **X** = **-Cl**

C	2.49819600	0.69691000	-0.25562200
C	1.16301100	0.35752600	-0.04828800
C	0.16948100	1.34791700	0.06036900
C	0.59828300	2.67753300	-0.05137400
C	1.92788500	3.02150900	-0.24775300
C	2.88636500	2.02595300	-0.35362200
H	3.24114600	-0.08241100	-0.33927900
H	-0.12608600	3.47240500	0.02434800
H	2.20477800	4.06449500	-0.32080300
H	3.92826200	2.27006300	-0.51183000
C	-1.32249700	1.08054100	0.33392800
C	-2.21970900	2.29654300	0.12932900
H	-3.25906600	1.98620500	0.22731600
H	-2.03711300	3.05436000	0.88913600
H	-2.08312200	2.73844900	-0.85657600
C	-1.53818200	0.51243000	1.73674900
H	-2.59580900	0.32047400	1.91349000
H	-0.98230300	-0.40583300	1.90398800
H	-1.20871600	1.25342200	2.46491200
O	-1.62514400	0.10540800	-0.73123700
I	0.84628200	-1.75700600	0.07146900
Cl	-3.17122000	-0.61733700	-0.65617400

Hypervalent iodine form, B3LYP, **X** = **-Br**

C	-0.05300300	2.12951400	-0.15273300
C	-0.55964400	0.84848100	-0.09914100
C	-1.90533800	0.53648300	0.00735800
C	-2.79138900	1.61303000	0.05957300
C	-2.32445800	2.92136900	0.00034900
C	-0.96323800	3.18253700	-0.10582300
H	1.00875800	2.31171300	-0.22860900
H	-3.85316200	1.42740200	0.14653400
H	-3.02971100	3.74072900	0.03591600
H	-0.60151100	4.20037500	-0.15579500
C	-2.32075400	-0.93121100	0.10855600
C	-3.57650000	-1.23945200	-0.70718000
H	-3.77179400	-2.31121800	-0.67344000
H	-4.44784200	-0.72547100	-0.30100600
H	-3.44508500	-0.94261300	-1.74712800
C	-2.51718300	-1.31600900	1.58244300
H	-2.77202800	-2.37395900	1.65214100
H	-1.60647800	-1.14116600	2.15710000
H	-3.31928500	-0.73316900	2.03646300
O	-1.27722000	-1.72175300	-0.47478600
I	0.62362300	-0.93833300	-0.16702800
Br	3.00208300	0.38813100	0.15909100

The acyclic isomer form, B3LYP, **X** = **-Br**

C	2.96043700	0.24998400	-0.36438500
C	1.60108100	0.16015000	-0.07329900
C	0.81140400	1.31475400	0.07459900
C	1.46490200	2.54308900	-0.09147100
C	2.82013700	2.63865400	-0.37171700
C	3.57526300	1.48527900	-0.51130200
H	3.54291600	-0.65241500	-0.47714400
H	0.90202500	3.45720100	0.00753100
H	3.27592200	3.61325600	-0.48247300
H	4.63242600	1.53535600	-0.73500800
C	-0.68608800	1.31957300	0.44664800
C	-1.35628000	2.68049100	0.27684000
H	-2.42597900	2.56962800	0.45023200
H	-0.98782300	3.40394900	1.00250700
H	-1.21355600	3.07486000	-0.72794000
C	-0.88992800	0.82255500	1.88028300
H	-1.94858200	0.81695600	2.13864100
H	-0.49080400	-0.17642600	2.03288700

H	-0.38370800	1.50252200	2.56559700
O	-1.22345400	0.40895100	-0.56362300
I	0.91031700	-1.85804900	0.10060900
Br	-3.00478800	-0.09220200	-0.40558000

Hypervalent iodine form, B3LYP, **X** = **-CN**

C	0.20029300	2.20013000	-0.09309400
C	-0.17180000	0.87066300	-0.06495400
C	-1.47950500	0.42293100	-0.00876600
C	-2.47385000	1.40370900	0.02313800
C	-2.14357400	2.75323900	-0.00958800
C	-0.81290100	3.15396500	-0.06824100
H	1.23618400	2.50116100	-0.13838900
H	-3.51285300	1.10932800	0.07612700
H	-2.92979000	3.49595800	0.00987300
H	-0.55540600	4.20385100	-0.09876600
C	-1.75997700	-1.08189400	0.06645800
C	-2.91974800	-1.49115000	-0.84405600
H	-3.03562400	-2.57470700	-0.80874400
H	-3.85847600	-1.04115200	-0.52157600
H	-2.72379700	-1.19569600	-1.87466200
C	-2.05080600	-1.47364000	1.52390300
H	-2.22818300	-2.54827800	1.58315400
H	-1.20633400	-1.22471700	2.16834400
H	-2.93242300	-0.95394000	1.90095100
O	-0.60585200	-1.77502600	-0.40666200
I	1.19535800	-0.77600500	-0.10203700
C	2.93106200	0.67259300	0.16852100
N	3.90348500	1.28191700	0.31500400

The acyclic isomer form, B3LYP, **X** = **- CN**

C	2.53231300	0.00915700	-0.23604500
C	1.15266300	0.05288800	-0.04946800
C	0.47418800	1.28151700	0.04495200
C	1.25623600	2.44066600	-0.03994000
C	2.63247500	2.40155400	-0.21065500
C	3.27593600	1.17876100	-0.31492900
H	3.03121000	-0.94527700	-0.31710500
H	0.77963400	3.40517600	0.03385900
H	3.19045500	3.32617500	-0.26689700
H	4.34685300	1.12371700	-0.45686400
C	-1.02312100	1.44879600	0.28853700
C	-1.57743800	2.83277300	-0.00404000
H	-2.66509000	2.80004800	0.05854500

H	-1.23180600	3.54655700	0.74154600
H	-1.29152600	3.18422600	-0.99347100
C	-1.45785700	0.97125100	1.66462400
H	-2.53971800	1.04528300	1.77619000
H	-1.14442300	-0.04786400	1.87195100
H	-0.99985000	1.62925700	2.40306300
O	-1.65785400	0.54725900	-0.79745200
I	0.25402100	-1.88728000	0.06812400
C	-2.88229100	0.24041500	-0.70217700
N	-3.99638000	-0.08088800	-0.67527500

Hypervalent iodine form, B3LYP, **X** = -$\mathbf{N_3}$

C	0.26097400	2.07985200	-0.49340800
C	-0.24713300	0.81310500	-0.26778300
C	-1.57049000	0.54232800	0.03815700
C	-2.43214200	1.63437100	0.13870600
C	-1.96224100	2.92515100	-0.08266400
C	-0.62569900	3.15000400	-0.40152500
H	1.30931300	2.22369700	-0.74642100
H	-3.48022600	1.47321100	0.39126300
H	-2.64862000	3.76654300	-0.00722900
H	-0.26659300	4.16122300	-0.58205700
C	-1.96626800	-0.90611600	0.29988300
C	-3.29505400	-1.25447800	-0.35619500
H	-3.49013300	-2.32471200	-0.21739200
H	-4.12885800	-0.69431900	0.08717000
H	-3.25573800	-1.04579000	-1.43165500
C	-2.02610900	-1.14191000	1.80928400
H	-2.27238800	-2.19334800	2.00451700
H	-1.05756900	-0.92139800	2.27881300
H	-2.78443300	-0.50568900	2.28567900
O	-1.00401300	-1.75159400	-0.29259400
I	0.89831400	-0.96895500	-0.33303700
N	2.73326400	0.24618900	-0.48041700
N	3.11810400	0.68229500	0.59719300
N	3.53173200	1.12495700	1.57212600

The acyclic isomer form, B3LYP, **X** = - $\mathbf{N_3}$

C	2.52773700	-0.90163900	-0.39456700
C	1.28415700	-0.35333300	-0.08827300
C	1.10468300	1.03873300	0.00945600
C	2.23884700	1.82882800	-0.21995800
C	3.48211400	1.28924200	-0.51804100
C	3.63030900	-0.08584500	-0.60734500

H	2.63647000	-1.97376200	-0.46495400
H	2.15217200	2.90190100	-0.16002000
H	4.32498200	1.94683200	-0.68198200
H	4.58870600	-0.52991200	-0.84069400
C	-0.21199400	1.73623700	0.39191400
C	-0.20467300	3.24738900	0.16938800
H	-1.20538100	3.63175700	0.36071000
H	0.47371500	3.74665900	0.85923200
H	0.07357500	3.50242000	-0.85225900
C	-0.59158000	1.43489300	1.84409100
H	-1.52339600	1.93436600	2.10581600
H	-0.70183500	0.36922600	2.02570400
H	0.19227200	1.81777100	2.49749400
O	-1.16020200	1.15124300	-0.56213800
I	-0.23303700	-1.84152100	0.19258400
N	-2.50605400	1.55923600	-0.25909800
N	-3.26902500	0.68691100	-0.68621500
N	-4.07296800	-0.01237600	-1.06595900

Hypervalent iodine form **3**, BP86, **X** = **-CF_3**

C	-0.07049800	2.13388000	-0.16871000
C	-0.54361300	0.82773600	-0.10780700
C	-1.88854700	0.48783000	0.00598200
C	-2.80414900	1.55128900	0.07443100
C	-2.37008800	2.87835100	0.01378200
C	-1.00922200	3.17184600	-0.11121200
H	0.98712100	2.36602500	-0.27107100
H	-3.86866800	1.33652300	0.17625600
H	-3.10045400	3.68745800	0.06004900
H	-0.66658500	4.20563700	-0.17054700
C	-2.29132700	-0.99759000	0.08628800
C	-3.58054100	-1.27835800	-0.70158200
H	-3.78465000	-2.35826200	-0.67609700
H	-4.44706500	-0.76029900	-0.26691700
H	-3.47208800	-0.96760100	-1.75005500
C	-2.47361700	-1.38435800	1.57143000
H	-2.73823100	-2.44969300	1.64071500
H	-1.54152100	-1.22000400	2.13235700
H	-3.26974700	-0.79296600	2.04704800
O	-1.26070400	-1.77183800	-0.51606900
I	0.71135400	-0.92783400	-0.17233600
C	2.66259700	0.30956000	0.13559300
F	3.01214100	1.14162400	-0.89107000
F	3.65969400	-0.62632300	0.22852800

F	2.71702800	1.05158300	1.27936800

TS_1, BP86, **X = -CF_3**

C	1.87360400	-2.24361900	0.01159100
C	1.43909300	-0.92665900	-0.01927800
C	2.29701300	0.17873200	0.00862400
C	3.67452600	-0.08111200	0.05938700
C	4.14648600	-1.39865700	0.08594000
C	3.25625500	-2.47668200	0.06384600
H	1.16992500	-3.07619200	-0.00904900
H	4.38191600	0.75062000	0.07536300
H	5.22109800	-1.58232500	0.12163500
H	3.63019000	-3.50146100	0.08267200
C	1.68064500	1.57298400	0.03819400
C	2.43393100	2.60057200	-0.81316500
H	1.88188300	3.54967800	-0.83124500
H	3.41918400	2.79031900	-0.36350800
H	2.57362600	2.23973000	-1.83973300
C	1.49853000	2.05854300	1.47933600
H	1.00766800	3.04158100	1.48746000
H	0.89059800	1.34993100	2.06111800
H	2.47701500	2.14745300	1.97125800
O	0.37868100	1.50001100	-0.65375500
I	-0.65448600	-0.17791700	-0.11385700
C	-3.40231300	-0.15531700	0.05827600
F	-3.94073100	-1.44674000	0.27164000
F	-4.11490400	0.28970100	-1.07683000
F	-3.98674500	0.59564900	1.10207600

TS_2, BP86, **X = -CF_3**

C	-1.71661300	-1.97842600	-0.48757600
C	-1.04506800	-0.84463500	-0.02468300
C	-1.60577700	0.43079500	0.01457000
C	-2.93327200	0.52399600	-0.45030400
C	-3.64105700	-0.58935000	-0.90955500
C	-3.03600100	-1.84878700	-0.92831900
H	-1.21484800	-2.94635000	-0.51241800
H	-3.42920200	1.49526300	-0.44043700
H	-4.66906600	-0.46935800	-1.25520500
H	-3.57454800	-2.72478100	-1.29195800
C	-0.86556900	1.68648600	0.57058200
C	-1.42409000	1.95479800	2.00024100
H	-0.92747800	2.83981700	2.42334700
H	-2.50888500	2.13638200	1.97006100

H	-1.22642300	1.09364100	2.65350700
C	-1.14193900	2.93157100	-0.30909500
H	-0.54977800	3.76803200	0.08865500
H	-0.84390800	2.75955800	-1.35141500
H	-2.19926100	3.23050500	-0.29574500
O	0.48929000	1.44514800	0.71408500
I	0.97750500	-1.21666200	0.61323800
C	1.87311900	0.70787000	-0.83456100
F	2.73343100	1.53561100	-0.24602200
F	1.12343100	1.30173300	-1.77133500
F	2.65857400	-0.18253600	-1.54380900

The acyclic isomer form **4**, BP86, **X** = **-CF_3**

C	2.90719700	0.17520600	-0.42014100
C	1.54912100	0.13709800	-0.07809900
C	0.79916300	1.32364600	0.09172500
C	1.49686600	2.53299100	-0.09599500
C	2.85153300	2.58105500	-0.42637700
C	3.56385200	1.39480000	-0.59305100
H	3.45562500	-0.75729300	-0.55010000
H	0.96384200	3.47410600	0.02043000
H	3.34006400	3.54739500	-0.55713400
H	4.62224700	1.40572000	-0.85698700
C	-0.68596400	1.38720600	0.49715300
C	-1.29978300	2.78048100	0.36694200
H	-2.36182100	2.73867200	0.63108500
H	-0.81838500	3.47177200	1.07028600
H	-1.20127000	3.17986500	-0.65052600
C	-0.89564900	0.86104400	1.91982900
H	-1.94806100	0.93921600	2.22129400
H	-0.55712900	-0.17359700	2.04278800
H	-0.30486200	1.49785000	2.59333200
O	-1.33594500	0.51133900	-0.55999200
I	0.79418200	-1.85850800	0.13393300
C	-2.57902300	0.04330900	-0.48553000
F	-2.82610400	-0.79738900	0.56952200
F	-3.56084100	1.00471700	-0.42227600
F	-2.81729900	-0.67560600	-1.61854600

Hypervalent iodine form **3**, M06-2X, **X** = **-CF_3**

C	-0.01841600	2.09711900	-0.22257000
C	-0.49943600	0.80422900	-0.13096800
C	-1.83655300	0.49256300	0.01586900
C	-2.73374400	1.55374700	0.10644600

C	-2.28694000	2.86484700	0.02697200
C	-0.93626900	3.13728000	-0.14541100
H	1.02804800	2.31799600	-0.36537200
H	-3.78878900	1.35259900	0.23880000
H	-2.99762600	3.67791700	0.09230900
H	-0.58787900	4.15799600	-0.22509500
C	-2.24136500	-0.98082500	0.09543600
C	-3.53363400	-1.24032000	-0.67104400
H	-3.73329200	-2.31215000	-0.66323200
H	-4.38251200	-0.73260900	-0.21305900
H	-3.43745100	-0.90864900	-1.70510800
C	-2.40909900	-1.36510800	1.56897100
H	-2.67832400	-2.42006200	1.63648700
H	-1.47472000	-1.20778200	2.11132800
H	-3.18965700	-0.76946100	2.04412800
O	-1.22220200	-1.73756700	-0.50063700
I	0.70585200	-0.93850200	-0.19918600
C	2.55887400	0.30212800	0.15754500
F	2.96099400	1.07798400	-0.86618400
F	3.56313900	-0.56802100	0.38365500
F	2.50132900	1.10019000	1.23844900

TS_1, M06-2X, **X = -CF_3**

C	-1.54670400	2.27778500	-0.04136500
C	-1.31488500	0.91925600	-0.06207300
C	-2.29576100	-0.05042500	0.06500900
C	-3.60382400	0.39048800	0.22623400
C	-3.88122700	1.75154400	0.25030300
C	-2.86498000	2.68951700	0.11715200
H	-0.74311100	2.99181200	-0.15063900
H	-4.40417400	-0.33043200	0.33384700
H	-4.90337800	2.08359200	0.37100800
H	-3.09324100	3.74649200	0.13077100
C	-1.86902000	-1.50570500	0.07436500
C	-2.79803600	-2.40245100	-0.72241500
H	-2.37672600	-3.40553600	-0.77698600
H	-3.76296500	-2.46493500	-0.21993100
H	-2.94247100	-2.01375800	-1.72900700
C	-1.69026500	-2.00183900	1.50062700
H	-1.34783200	-3.03615800	1.48990200
H	-0.96938600	-1.38880300	2.04350000
H	-2.64509400	-1.94749900	2.02334700
O	-0.59714700	-1.58608400	-0.64083700
I	0.54630700	-0.03734700	-0.28893900

C	3.62919100	0.08039400	0.00905300
F	3.69529200	1.43377800	0.39490800
F	4.84120800	-0.04927800	-0.68234400
F	3.95509500	-0.54651200	1.22335800

TS_2, M06-2X, **X** = **$-CF_3$**

C	1.51397900	-2.06584500	0.40624200
C	0.92033300	-0.88785800	-0.02554200
C	1.55626200	0.34106700	-0.03889600
C	2.87944000	0.33890300	0.41551200
C	3.51005300	-0.82003300	0.83989500
C	2.83007400	-2.03034900	0.83686500
H	0.95407000	-2.99094300	0.41272900
H	3.43291800	1.26771500	0.42491600
H	4.53732600	-0.77625900	1.17683700
H	3.31037200	-2.93835700	1.17509800
C	0.90426600	1.64044700	-0.56372200
C	1.41644400	1.83212400	-2.00435200
H	0.99262000	2.74986900	-2.41469000
H	2.50559800	1.90126600	-2.03198300
H	1.10032200	0.99199400	-2.62448900
C	1.34457300	2.84746700	0.28037800
H	0.77062800	3.71059000	-0.05807200
H	1.14057900	2.68950200	1.33897600
H	2.40228900	3.08117700	0.16200900
O	-0.46667700	1.53459800	-0.61723000
I	-1.09814700	-1.08330900	-0.62933100
C	-1.62726800	0.72531500	0.86800200
F	-2.50278500	1.61230200	0.46430700
F	-0.74195200	1.16957900	1.73835700
F	-2.38864600	-0.12359200	1.64675200

The acyclic isomer form **4**, M06-2X, **X** = **$-CF_3$**

C	2.89623400	-0.07177300	-0.33107900
C	1.53276000	0.02192900	-0.07144000
C	0.90048000	1.26764000	0.04515500
C	1.71204400	2.39586000	-0.09885300
C	3.07294400	2.30991300	-0.34701800
C	3.67116300	1.06849300	-0.46838900
H	3.35568200	-1.04541500	-0.42574300
H	1.27534000	3.37885400	-0.01686000
H	3.65428800	3.21625400	-0.44911600
H	4.73021700	0.97707900	-0.66891400
C	-0.58479200	1.46863600	0.36506400

C	-1.06179800	2.89234000	0.11374300
H	-2.13404700	2.94701100	0.27953400
H	-0.58932100	3.57965400	0.81225900
H	-0.84233200	3.20692900	-0.90549100
C	-0.88049800	1.08048000	1.80937100
H	-1.93113900	1.24507100	2.04866900
H	-0.61666100	0.04960400	2.02870900
H	-0.28394300	1.73387100	2.44540000
O	-1.27420000	0.61268800	-0.61736200
I	0.58799600	-1.86019000	0.12058100
C	-2.49908400	0.14757500	-0.42394000
F	-2.60249800	-0.75035200	0.56851500
F	-3.41404700	1.09503400	-0.15329100
F	-2.88845600	-0.46545000	-1.54367300

Hypervalent iodine form **3**, ωB97X-D, **X** = **-CF_3**

C	-0.05656100	2.10808100	-0.18892200
C	-0.51897500	0.80741400	-0.11700100
C	-1.85457900	0.48178300	0.00664800
C	-2.76344800	1.53221400	0.09064600
C	-2.33311600	2.84749900	0.02790300
C	-0.98447000	3.13642400	-0.11959400
H	0.98878300	2.34309600	-0.30917500
H	-3.81731300	1.31992300	0.20852200
H	-3.05553600	3.65021600	0.08743800
H	-0.64643500	4.16144800	-0.18477700
C	-2.25706800	-0.99312600	0.07763100
C	-3.49965000	-1.26944800	-0.76671000
H	-3.70589700	-2.34009000	-0.74584600
H	-4.37755100	-0.74881500	-0.38411300
H	-3.33265700	-0.96803800	-1.80110800
C	-2.51833300	-1.35845200	1.54510700
H	-2.77637200	-2.41592600	1.61594800
H	-1.62620700	-1.17854200	2.14801800
H	-3.33725300	-0.76871900	1.95944000
O	-1.20741800	-1.75625800	-0.44607400
I	0.71617700	-0.91920000	-0.16493900
C	2.59857200	0.30560700	0.13302500
F	2.95691700	1.10002700	-0.89234700
F	3.59011900	-0.60040500	0.27403400
F	2.62120600	1.06983700	1.23871300

TS_1, ωB97X-D, **X** = **-CF_3**

C	1.72309100	-2.24979900	-0.02480400

C	1.38709600	-0.91369500	-0.05047200
C	2.30378300	0.12086600	0.03333300
C	3.64411800	-0.22281400	0.14924800
C	4.01980000	-1.55847700	0.17570500
C	3.07005200	-2.56665800	0.08853400
H	0.97110500	-3.02239100	-0.09178100
H	4.39530400	0.55224800	0.22119400
H	5.06697200	-1.81271600	0.26524500
H	3.37350600	-3.60425100	0.10722200
C	1.77665700	1.54378400	0.04861200
C	2.59412400	2.48976000	-0.81407000
H	2.10083800	3.45951500	-0.86649800
H	3.57861300	2.63316500	-0.36983400
H	2.71412900	2.09091200	-1.82000100
C	1.63883900	2.05258100	1.47704100
H	1.20672600	3.05280400	1.47294600
H	1.00672500	1.39306100	2.07360800
H	2.62153600	2.09514500	1.94586700
O	0.46710700	1.52856800	-0.60022900
I	-0.55679600	-0.09349500	-0.18698400
C	-3.55499000	-0.14539500	0.06364000
F	-4.06764700	-1.44882300	0.21238100
F	-4.43163000	0.37961300	-0.90097400
F	-4.04267000	0.46790700	1.23230600

TS_2, ωB97X-D, **X** = **-CF_3**

C	-1.63483300	-2.00226400	-0.43907200
C	-0.97799000	-0.86206700	0.00294000
C	-1.56541900	0.39163100	0.03033400
C	-2.88756300	0.45563400	-0.41665900
C	-3.57225800	-0.66572400	-0.85166400
C	-2.94787000	-1.90365600	-0.86353600
H	-1.12481100	-2.95542100	-0.45913100
H	-3.39871200	1.40807400	-0.41188600
H	-4.59705200	-0.57003400	-1.18477300
H	-3.46947500	-2.78552700	-1.20882400
C	-0.85686100	1.65591500	0.56589600
C	-1.38073100	1.88912000	1.99701100
H	-0.90953100	2.78085300	2.41301500
H	-2.46311200	2.02977000	2.00432800
H	-1.13298000	1.03675500	2.63097600
C	-1.20383400	2.88648500	-0.29128600
H	-0.57748100	3.71333500	0.04480300
H	-1.00713600	2.71196600	-1.34783000

H	-2.24480200	3.19071900	-0.18271100
O	0.50303900	1.46488400	0.66113800
I	1.02906400	-1.16886100	0.59506200
C	1.72458200	0.73149400	-0.82239000
F	2.60108900	1.56615700	-0.32208300
F	0.92184300	1.25351300	-1.72777700
F	2.49674400	-0.12959800	-1.57178700

The acyclic isomer form **4**, ωB97X-D, **X** = **-CF_3**

C	2.88920800	0.04469300	-0.37051500
C	1.53024000	0.07458600	-0.07606700
C	0.84939700	1.29329300	0.06054100
C	1.60728800	2.45368300	-0.10281100
C	2.96192400	2.42835600	-0.38696300
C	3.60948900	1.21606300	-0.52559300
H	3.39154300	-0.90591600	-0.47844800
H	1.13244000	3.41678400	-0.00698300
H	3.49887300	3.35959900	-0.50430200
H	4.66612200	1.17026300	-0.75128600
C	-0.63631300	1.43445400	0.42014000
C	-1.17889900	2.84189800	0.21092200
H	-2.24382100	2.85376500	0.42520600
H	-0.70627000	3.53832700	0.90016600
H	-1.02051600	3.18383200	-0.81052100
C	-0.87891700	1.01096200	1.86559500
H	-1.92207800	1.15260600	2.14406300
H	-0.59308900	-0.01998200	2.05488100
H	-0.27093300	1.65714800	2.49781000
O	-1.30232700	0.56331100	-0.56759700
I	0.68330700	-1.85691300	0.12937500
C	-2.53122400	0.09026600	-0.44740600
F	-2.71810100	-0.73389000	0.59789900
F	-3.48673300	1.03527400	-0.34434100
F	-2.80206600	-0.61538900	-1.55063900

Hypervalent iodine form, BP86, **X** = **-OAc**

C	-0.36462000	2.24057100	-0.15726100
C	-0.70665600	0.89440500	-0.09942400
C	-2.01318500	0.42063600	0.01940600
C	-3.03207000	1.38344600	0.08634700
C	-2.73017000	2.74771800	0.02552000
C	-1.40519700	3.17667200	-0.09702000
H	0.67119400	2.55854800	-0.24877900
H	-4.06969600	1.06267700	0.18880100

H	-3.53706200	3.48037200	0.07285800
H	-1.17016400	4.24057000	-0.14986400
C	-2.24519200	-1.09289000	0.12483500
C	-3.48687200	-1.54837400	-0.64983200
H	-3.56076000	-2.64382700	-0.60512200
H	-4.40292100	-1.12926900	-0.21073700
H	-3.42662700	-1.24123600	-1.70275200
C	-2.34930300	-1.49180800	1.60936900
H	-2.49842900	-2.57829300	1.68982200
H	-1.43162600	-1.22147700	2.15244200
H	-3.19610100	-0.98425900	2.09360200
O	-1.12849100	-1.75835000	-0.50254200
I	0.67776300	-0.73598900	-0.17414300
O	2.27156300	0.83621900	0.11168300
C	3.43850500	0.22569000	0.13156100
O	3.56447500	-1.00432900	0.00745100
C	4.61723300	1.15722900	0.32304000
H	4.63110800	1.91379600	-0.47413000
H	4.51931900	1.69018600	1.27957800
H	5.55510300	0.59155200	0.31188700

The acyclic isomer form, BP86, **X** = **-OAc**

C	2.84596800	0.57972500	-0.66909000
C	1.57670200	0.29216100	-0.15071500
C	0.67180800	1.32445800	0.19064200
C	1.11849100	2.64452100	-0.01954100
C	2.38578500	2.93918900	-0.52227800
C	3.25605900	1.90124700	-0.85341900
H	3.51896900	-0.23705100	-0.92791300
H	0.45562800	3.47163500	0.22706300
H	2.68389000	3.97966200	-0.65675800
H	4.24996500	2.10690100	-1.25338700
C	-0.72595300	1.10999500	0.80903400
C	-1.58396800	2.37575500	0.87351000
H	-2.59368400	2.09902100	1.20433300
H	-1.18537200	3.08895400	1.60704900
H	-1.66010900	2.87198100	-0.10258400
C	-0.62282100	0.48711100	2.20930300
H	-1.62377600	0.30665600	2.62220300
H	-0.06448200	-0.45638600	2.20591600
H	-0.10535800	1.19621500	2.87012400
O	-1.31480900	0.19276800	-0.17882000
I	1.20410500	-1.81010300	0.04452400
O	-2.62113400	-0.30731800	0.36109900

C	-3.63933400	-0.23758700	-0.55663000
O	-4.70463800	-0.67749000	-0.15433500
C	-3.36509100	0.32539500	-1.91414200
H	-2.97362300	1.34830200	-1.83819900
H	-2.60428900	-0.27503900	-2.43174300
H	-4.29654800	0.31910200	-2.48946500

Hypervalent iodine form, M06-2X, **X** = **-OAc**

C	-0.28901800	2.20292100	-0.15559100
C	-0.66258800	0.87375200	-0.09961600
C	-1.97270400	0.44460700	0.01124900
C	-2.96282800	1.41962400	0.07653500
C	-2.62643900	2.76537700	0.01948200
C	-1.29885600	3.15602100	-0.09825800
H	0.74655700	2.49130700	-0.24178700
H	-3.99972700	1.12556400	0.17608900
H	-3.40605200	3.51394900	0.06770200
H	-1.04123600	4.20542100	-0.14713800
C	-2.23431300	-1.05410700	0.11457500
C	-3.45585700	-1.47715300	-0.68678100
H	-3.54745100	-2.56253400	-0.64587400
H	-4.36553300	-1.04219500	-0.27366500
H	-3.35584800	-1.16978800	-1.72758600
C	-2.39129100	-1.43298900	1.58665600
H	-2.55563400	-2.50794000	1.66909900
H	-1.49320700	-1.16898600	2.14827300
H	-3.24043400	-0.91038500	2.02839200
O	-1.11567900	-1.72599100	-0.44890900
I	0.64923200	-0.76399600	-0.16183500
O	2.20480100	0.73861100	0.09997000
C	3.39777400	0.21231800	0.12231000
O	3.59612500	-0.98976700	0.00901100
C	4.50721100	1.21201800	0.30587700
H	4.43946700	1.97776000	-0.46622800
H	4.38790700	1.70391800	1.27141000
H	5.47338200	0.71855100	0.25936800

The acyclic isomer form, M06-2X, **X** = **-OAc**

C	2.85987100	-0.26828800	-0.58214900
C	1.55972900	-0.07171100	-0.12865600
C	1.04240000	1.22031500	0.04409000
C	1.89183700	2.28585500	-0.26196400
C	3.19057100	2.09658500	-0.70701500
C	3.67917200	0.81195300	-0.86975300

H	3.23524600	-1.27375100	-0.70861700
H	1.53277900	3.29716100	-0.14609200
H	3.81044800	2.95450400	-0.92963800
H	4.68863600	0.64092500	-1.21901900
C	-0.35443800	1.52711000	0.59053700
C	-0.78587700	2.97461100	0.41081600
H	-1.83018000	3.06143900	0.70654700
H	-0.20382000	3.63831200	1.04794200
H	-0.68573300	3.29192900	-0.62642100
C	-0.44869200	1.14112100	2.06433200
H	-1.42529400	1.40610100	2.46506500
H	-0.27516600	0.07946700	2.22035400
H	0.30993300	1.70179600	2.61011100
O	-1.19207300	0.70354100	-0.25131400
I	0.51580600	-1.87638300	0.24715600
O	-2.49633000	0.67409500	0.32318800
C	-3.40943800	0.16863100	-0.54726800
O	-4.53513500	0.09189700	-0.13587700
C	-2.93555700	-0.23751700	-1.90049200
H	-2.52490800	0.62575500	-2.42251300
H	-2.14078000	-0.97734500	-1.81135400
H	-3.77804900	-0.64625700	-2.44847100

Hypervalent iodine form, ωB97X-D, **X** = **-OAc**

C	-0.30067700	2.20522500	-0.18110300
C	-0.66648000	0.87545600	-0.10897900
C	-1.97343100	0.44553600	0.02399500
C	-2.96220900	1.41918400	0.10406300
C	-2.63117200	2.76363200	0.03283700
C	-1.30829500	3.15658200	-0.11332900
H	0.73218100	2.49543300	-0.28828500
H	-3.99661300	1.12718300	0.22534000
H	-3.41154700	3.51028700	0.08889200
H	-1.05509300	4.20585500	-0.17820200
C	-2.23566400	-1.05360000	0.12511700
C	-3.45422200	-1.47557800	-0.68459200
H	-3.55651800	-2.55991100	-0.63997400
H	-4.36547300	-1.03406100	-0.28212700
H	-3.34567900	-1.17491600	-1.72642600
C	-2.39894500	-1.44010400	1.59654800
H	-2.55748400	-2.51581100	1.67847100
H	-1.50874500	-1.17276300	2.16868800
H	-3.25463700	-0.92610500	2.03547600
O	-1.11886300	-1.72433600	-0.44468500

I	0.64893800	-0.76490700	-0.17305700
O	2.22059600	0.74792100	0.08652400
C	3.40641000	0.21452300	0.13187700
O	3.60249500	-0.98985100	0.02045900
C	4.51664000	1.20942100	0.34084500
H	4.47808900	1.97384600	-0.43484400
H	4.37958200	1.70680900	1.30142500
H	5.48264900	0.71267400	0.32155500

The acyclic isomer form, ωB97X-D, **X** = **-OAc**

C	2.81426800	0.63292000	-0.62636800
C	1.55127900	0.30950100	-0.14193500
C	0.62834400	1.31471700	0.18489300
C	1.04787800	2.63425400	0.00781900
C	2.30729200	2.95930700	-0.46428600
C	3.19736600	1.95303000	-0.78817200
H	3.50894200	-0.15538300	-0.87864700
H	0.37352800	3.44053100	0.25024400
H	2.58171600	3.99864000	-0.58172900
H	4.18477700	2.18224200	-1.16497300
C	-0.76922300	1.06627400	0.76639100
C	-1.66810900	2.29560100	0.76916200
H	-2.67343900	1.99548400	1.06231000
H	-1.32627700	3.02706300	1.49920000
H	-1.71724100	2.76576100	-0.21160200
C	-0.67231900	0.50560100	2.18390500
H	-1.66418700	0.36401700	2.60939300
H	-0.13752300	-0.44022500	2.21732200
H	-0.13702300	1.22604900	2.80170900
O	-1.31376500	0.10279400	-0.17219900
I	1.23278500	-1.77934700	0.02989400
O	-2.53606700	-0.41049300	0.34211100
C	-3.57423900	-0.27654600	-0.52611000
O	-4.62454300	-0.71385000	-0.13894700
C	-3.32294200	0.36000600	-1.85005800
H	-2.93986500	1.37053200	-1.72165300
H	-2.57540300	-0.20588000	-2.40438300
H	-4.25815900	0.38094800	-2.40074100

Hypervalent iodine form **1**, BP86, **X** = **-SCF_3**

C	-0.36465100	2.06482400	-0.64007700
C	-0.90224600	0.82415200	-0.33982600
C	-2.19404900	0.60685200	0.13044400
C	-2.99176200	1.74908600	0.30494300

C	-2.49608900	3.02129400	0.00468300
C	-1.19008800	3.18330500	-0.46705600
H	0.66019800	2.16698200	-0.99784700
H	-4.01019400	1.63924300	0.68040800
H	-3.13641800	3.89370900	0.14127000
H	-0.80481400	4.17533600	-0.70534600
C	-2.63484900	-0.82279200	0.47036800
C	-4.08525000	-1.09805700	0.05232700
H	-4.32231800	-2.15369400	0.24406000
H	-4.78871600	-0.48317400	0.63121200
H	-4.23065500	-0.89262000	-1.01655700
C	-2.44686600	-1.06848200	1.98116300
H	-2.72729100	-2.10374600	2.22261200
H	-1.39937100	-0.91251600	2.27929100
H	-3.07312500	-0.38695400	2.57506400
O	-1.82825800	-1.73101300	-0.29789800
I	0.16755200	-1.04028500	-0.53704100
S	2.49013400	0.10106500	-1.06224300
C	3.14807800	0.30008400	0.60480300
F	2.43426000	1.16774200	1.38462000
F	4.42112800	0.79361800	0.54019600
F	3.22050100	-0.86557800	1.31712300

The acyclic isomer form **2**, BP86, **X** = - **SCF_3**

C	3.20081300	0.69772700	-0.80615200
C	1.98135900	0.35772300	-0.20755500
C	1.05906100	1.34996400	0.19732200
C	1.44082000	2.68699900	-0.02903100
C	2.65822100	3.03536900	-0.61415900
C	3.54452100	2.03516600	-1.00977600
H	3.88775200	-0.09002600	-1.11370000
H	0.76368600	3.48592700	0.26692600
H	2.90440400	4.08754900	-0.76189500
H	4.49978200	2.28198400	-1.47515800
C	-0.28231000	1.07583600	0.89589300
C	-1.20625600	2.28439000	0.98519400
H	-2.17145900	1.95989900	1.39673700
H	-0.80436900	3.03847400	1.67499700
H	-1.37785100	2.74901300	0.00585200
C	-0.06980700	0.48104300	2.29043100
H	-1.03521800	0.25674700	2.76643700
H	0.53835500	-0.43108200	2.26697500
H	0.44463100	1.22391600	2.91580800
O	-0.91848700	0.07121800	-0.04155400

I	1.70904200	-1.75866500	0.00702000
S	-2.24863000	-0.77343500	0.46588200
C	-3.58769200	-0.05240200	-0.55690100
F	-4.64963000	-0.88855500	-0.38895600
F	-3.99477200	1.19737300	-0.21346600
F	-3.28174800	-0.00424600	-1.87628200

Hypervalent iodine form **1**, M06-2X, **X** = **-SCF_3**

C	-0.25167300	1.99959200	-0.74806300
C	-0.80746500	0.78817400	-0.39867000
C	-2.08196100	0.63212200	0.10925000
C	-2.83789600	1.78777200	0.28286100
C	-2.31855900	3.02714000	-0.06202300
C	-1.03418600	3.13486500	-0.57903900
H	0.75292400	2.06952200	-1.13829700
H	-3.83738300	1.71493500	0.69174400
H	-2.91969600	3.91610800	0.07390100
H	-0.63343400	4.10108900	-0.85337700
C	-2.54865800	-0.76703800	0.49340100
C	-4.00003900	-1.00632900	0.10274700
H	-4.25480700	-2.04506300	0.31224300
H	-4.67117600	-0.36843900	0.67773100
H	-4.14839100	-0.81376400	-0.95927000
C	-2.35286800	-0.96089000	1.99758900
H	-2.65844700	-1.96958500	2.27693000
H	-1.30467400	-0.82387300	2.27103200
H	-2.94876800	-0.24153200	2.56045000
O	-1.76283100	-1.69759500	-0.23055000
I	0.17347200	-1.08833800	-0.54585500
S	2.47025600	0.00261300	-1.04312300
C	2.95049100	0.33615700	0.64635900
F	2.08883800	1.13668500	1.29926300
F	4.14431400	0.94848300	0.68393900
F	3.06743200	-0.76827300	1.40403600

The acyclic isomer form **2**, M06-2X, **X** = **- SCF_3**

C	3.16279900	0.63495700	-0.79639600
C	1.94427000	0.32545600	-0.20315400
C	1.05434000	1.33438100	0.19085200
C	1.45657000	2.65177800	-0.03585400
C	2.67294800	2.96774600	-0.62023900
C	3.53184000	1.95430700	-1.00602300
H	3.82807800	-0.16188800	-1.09691400
H	0.80235300	3.46188400	0.24838100

H	2.93824300	4.00453300	-0.77661100
H	4.48322900	2.17695900	-1.47019600
C	-0.28753500	1.07763000	0.87736600
C	-1.19462700	2.29243300	0.93939300
H	-2.15135800	1.98917300	1.36279900
H	-0.77919600	3.05266900	1.59858400
H	-1.36337800	2.72033000	-0.04804100
C	-0.07348700	0.53962100	2.28803600
H	-1.02951100	0.37917100	2.78665500
H	0.49523200	-0.38672600	2.29743500
H	0.47747800	1.28821200	2.85715000
O	-0.91545100	0.08283400	-0.00368000
I	1.61515500	-1.75458400	0.01551200
S	-2.21204700	-0.75273900	0.51149200
C	-3.47056800	-0.03682900	-0.57013800
F	-4.57103300	-0.77892300	-0.41122400
F	-3.79396700	1.22970900	-0.30220900
F	-3.12025700	-0.07291000	-1.85532900

Hypervalent iodine form **1**, ωB97X-D, **X** = **-SCF$_3$**

C	-0.29379100	2.01757100	-0.69194400
C	-0.84256400	0.79658400	-0.36826000
C	-2.12430500	0.62760200	0.11520400
C	-2.89080200	1.77529800	0.28683900
C	-2.37549200	3.02114800	-0.03275600
C	-1.08414900	3.14503700	-0.52415700
H	0.71649000	2.10068800	-1.06435000
H	-3.89575000	1.69286300	0.67817900
H	-2.98591500	3.90344700	0.10301400
H	-0.68358700	4.11696400	-0.77636900
C	-2.59269600	-0.77783100	0.47611000
C	-4.02584800	-1.03310400	0.02512600
H	-4.27945800	-2.07463200	0.22187800
H	-4.73037700	-0.40426300	0.56936700
H	-4.13467800	-0.84227100	-1.04203300
C	-2.45704800	-0.97788600	1.98818600
H	-2.74906300	-1.99556300	2.24878200
H	-1.42629000	-0.81887400	2.31017200
H	-3.09355300	-0.27940800	2.53247300
O	-1.77438900	-1.69963200	-0.22027700
I	0.15822700	-1.06828300	-0.52478100
S	2.44765600	0.02217400	-1.04499000
C	3.05742500	0.31681900	0.61414300
F	2.29572000	1.16519500	1.32694600

F	4.28588600	0.85562000	0.55832800
F	3.16110100	-0.79916000	1.35732800

The acyclic isomer form **2**, ωB97X-D, **X** = - **SCF_3**

C	3.12403500	0.68769600	-0.83936600
C	1.93012400	0.34649900	-0.21435600
C	1.02902900	1.33660000	0.20427900
C	1.40117400	2.66107100	-0.02756600
C	2.59191600	3.00499700	-0.64308400
C	3.45948700	2.01277500	-1.05651400
H	3.80205200	-0.09010400	-1.16009200
H	0.74104700	3.45723000	0.27836800
H	2.82930600	4.04794400	-0.80169500
H	4.39274800	2.25610100	-1.54563400
C	-0.29704500	1.06305200	0.92142900
C	-1.21785600	2.26869800	0.99535500
H	-2.17029000	1.95885300	1.42279700
H	-0.80815400	3.02850100	1.65850700
H	-1.39828900	2.70522700	0.01490700
C	-0.05166800	0.52916300	2.32926800
H	-0.99719900	0.35178500	2.84240700
H	0.52835700	-0.39047400	2.32754000
H	0.49798300	1.28032600	2.89560900
O	-0.92373500	0.04574800	0.06120800
I	1.67041400	-1.74480800	0.01095200
S	-2.25896200	-0.73351400	0.55963400
C	-3.47926800	-0.06698600	-0.60112900
F	-4.61111600	-0.74226400	-0.37043700
F	-3.73946700	1.23393900	-0.46047600
F	-3.13339900	-0.24964100	-1.87651800

bimolecular decomposition (symmetry restricted), optimization: B3LYP, 6-31(d) for C, H, O, F, SDD for I; single point energy: aug-cc-pVTZ for C, H, O, F, aug-cc-pVTZ-pp for I, SMD solvation model (Acetonitrile).

C	3.60881000	4.13978900	0.56526900
C	2.33136600	3.62544200	0.76328300
C	1.15624400	4.15197100	0.25193600
C	1.34288700	5.31924400	-0.51600700
C	2.60020400	5.87533900	-0.75385800
C	3.74372900	5.28859700	-0.21595200
H	4.48114500	3.66073300	0.99738800
H	0.47513400	5.80382300	-0.94794100
H	2.68204000	6.76905500	-1.36704500
H	4.72972100	5.70600600	-0.39917100

C	-0.27645900	3.51736800	0.49817600
C	-1.26871600	4.05521600	-0.57223700
H	-2.23381200	3.57351700	-0.39041200
H	-1.43646500	5.13833100	-0.53243200
H	-0.93388600	3.78423600	-1.58026200
C	-0.75849000	4.04607500	1.88878700
H	-1.76298900	3.64834500	2.07537700
H	-0.10666700	3.68577000	2.69030900
H	-0.79937600	5.14228300	1.93964800
O	-0.22175600	2.16668800	0.45426500
I	2.33474300	1.85363500	2.09558700
C	1.51814100	-0.43542600	0.94668100
F	1.39160000	0.03354600	-0.22735700
F	0.50728800	-0.63522400	1.71065600
F	2.54646300	-1.19372400	1.16287200
C	-3.60881000	-4.13978900	-0.56526900
C	-2.33136600	-3.62544200	-0.76328300
C	-1.15624400	-4.15197100	-0.25193600
C	-1.34288700	-5.31924400	0.51600700
C	-2.60020400	-5.87533900	0.75385800
C	-3.74372900	-5.28859700	0.21595200
H	-4.48114500	-3.66073300	-0.99738800
H	-0.47513400	-5.80382300	0.94794100
H	-2.68204000	-6.76905500	1.36704500
H	-4.72972100	-5.70600600	0.39917100
C	0.27645900	-3.51736800	-0.49817600
C	1.26871600	-4.05521600	0.57223700
H	2.23381200	-3.57351700	0.39041200
H	1.43646500	-5.13833100	0.53243200
H	0.93388600	-3.78423600	1.58026200
C	0.75849000	-4.04607500	-1.88878700
H	1.76298900	-3.64834500	-2.07537700
H	0.10666700	-3.68577000	-2.69030900
H	0.79937600	-5.14228300	-1.93964800
O	0.22175600	-2.16668800	-0.45426500
I	-2.33474300	-1.85363500	-2.09558700
C	-1.51814100	0.43542600	-0.94668100
F	-1.39160000	-0.03354600	0.22735700
F	-0.50728800	0.63522400	-1.71065600
F	-2.54646300	1.19372400	-1.16287200

bimolecular decomposition, optimization: B3LYP, 6-31(d) for C, H, O, F, SDD for I; single point energy: aug-cc-pVTZ for C, H, O, F, aug-cc-pVTZ-pp for I, SMD solvation model (Acetonitrile).

C	-5.78671000	-0.04903900	0.20872600

C	-4.40932300	0.14699100	0.09287300
C	-3.78054400	1.37367300	0.17389000
C	-4.65167600	2.46617400	0.38835800
C	-6.02920700	2.32218500	0.50764400
C	-6.60849600	1.05519100	0.41752500
H	-6.21555000	-1.04361300	0.13788200
H	-4.22410800	3.46085100	0.46509300
H	-6.65001800	3.19899400	0.67255500
H	-7.68290500	0.92143500	0.50882500
C	-2.22469300	1.65130400	0.06422300
C	-1.80408700	2.30319100	1.41940100
H	-0.74513600	2.57569500	1.35905600
H	-2.36844500	3.20493900	1.68654100
H	-1.92303700	1.56807200	2.22290300
C	-2.03566400	2.66971600	-1.10378800
H	-0.97398700	2.93133300	-1.16337000
H	-2.32284600	2.19029400	-2.04551900
H	-2.60586500	3.60038300	-0.99671700
O	-1.50376000	0.53458900	-0.16837900
I	-3.35494400	-1.77493900	-0.24265600
C	-0.47555100	-2.09189500	-0.19795100
F	-0.43492600	-1.53580300	0.94553300
F	-0.41563000	-1.46895100	-1.30156500
F	-0.36737400	-3.37975600	-0.23140800
C	4.89705100	1.02785800	-0.27908200
C	3.86596100	0.11866200	-0.08139900
C	4.06171300	-1.22577200	0.21047500
C	5.39388100	-1.64640700	0.34679500
C	6.45655100	-0.76189600	0.16988600
C	6.21174000	0.57207400	-0.15266000
H	4.71123800	2.06074200	-0.53832100
H	5.60110100	-2.68392700	0.58917400
H	7.47712200	-1.11904900	0.27474500
H	7.03360200	1.26407900	-0.31205000
C	2.86157800	-2.18415700	0.38996800
C	3.15822000	-3.56008200	-0.24258700
H	2.25659800	-4.17695900	-0.17766800
H	3.96623400	-4.09610100	0.26710200
H	3.41891900	-3.44310300	-1.29860300
C	2.57336800	-2.34543100	1.90321900
H	1.72912600	-3.02898000	2.04786000
H	2.31463800	-1.38312800	2.35803300
H	3.43848500	-2.75133800	2.43943900
O	1.76286900	-1.64377400	-0.29127800

I	1.74319000	0.69408200	-0.19786700
C	2.29136000	2.92981400	-0.07030800
F	2.93146300	3.36987500	-1.17106600
F	1.14912700	3.62056800	0.04698300
F	3.06201400	3.20243500	0.99338600