Supporting information for:

How to Twist, Split and Warp a σ-Hole with Hypervalent Halogens.

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Examples of XYZ geometries with constrained coordinates, as explained in the main text:

$(PhNO_2)_3I…NCS^-$

C	0.000000	1.213004	-3.296109
C	0.000000	1.206352	-1.910496
C	0.000000	0.000000	-1.221464
C	0.000000	-1.206352	-1.910496
C	0.000000	-1.213004	-3.296109
H	0.000000	2.133900	-3.860292
H	0.000000	2.143675	-1.369994
H	0.000000	-2.143675	-1.369994
H	0.000000	-2.133900	-3.860292
I	0.000000	0.000000	0.890299
C	-2.290913	0.000000	0.588693
C	2.290913	0.000000	0.588693
N	0.000000	0.000000	3.584996
C	0.000000	0.000000	4.754841
S	0.000000	0.000000	6.391625
C	2.996222	1.197897	0.513591
C	4.373132	1.213300	0.345095
C	5.034940	0.000000	0.257887
C	4.373132	-1.213300	0.345095
C	2.996222	-1.197897	0.513591
H	2.470565	2.143999	0.594854
H	4.935354	2.133940	0.283545
H	4.935354	-2.133940	0.283545
H	2.470565	-2.143999	0.594854
C	-2.996222	-1.197897	0.513591
C	-4.373132	-1.213300	0.345095
C	-5.034940	0.000000	0.257887
C	-4.373132	1.213300	0.345095
C	-2.996222	1.197897	0.513591
H	-2.470565	-2.143999	0.594854
H	-4.935354	-2.133940	0.283545
H	-4.935354	2.133940	0.283545
H	-2.470565	2.143999	0.594854
C	0.000000	0.000000	-3.960844
N	0.000000	0.000000	-5.434514
O	0.000000	-1.072153	-5.996149
O	0.000000	1.072153	-5.996149
N	6.492968	0.000000	0.066803
N	-6.492968	0.000000	0.066803
O	7.055123	1.071219	-0.008701
O	-7.055123	1.071219	-0.008701
O	-7.055123	-1.071219	-0.008701
O	7.055123	-1.071219	-0.008701

$(PhNH_2)_2(PhNO_2)I…NCS^-$

C	0.000000	1.212793	-3.304801
C	0.000000	1.205591	-1.919955
C	0.000000	0.000000	-1.228425
C	0.000000	-1.205591	-1.919955
C	0.000000	-1.212793	-3.304801
H	0.000000	2.134213	-3.868056
H	0.000000	2.142135	-1.378437
H	0.000000	-2.142135	-1.378437
H	0.000000	-2.134213	-3.868056
I	0.000000	0.000000	0.880672
C	-2.276224	0.000000	0.581000
C	2.276224	0.000000	0.581000
N	0.000000	0.000000	3.675568
C	0.000000	0.000000	4.843671
S	0.000000	0.000000	6.488254
C	2.992849	1.188519	0.500196
C	4.370915	1.198705	0.328543
C	5.075186	0.000000	0.234361
C	4.370915	-1.198705	0.328543
C	2.992849	-1.188519	0.500196
H	2.474175	2.140258	0.579816
H	4.911641	2.138287	0.276136
H	4.911641	-2.138287	0.276136
H	2.474175	-2.140258	0.579816
C	-2.992849	-1.188519	0.500196
C	-4.370915	-1.198705	0.328543
C	-5.075186	0.000000	0.234361
C	-4.370915	1.198705	0.328543
C	-2.992849	1.188519	0.500196
H	-2.474175	-2.140258	0.579816
H	-4.911641	-2.138287	0.276136
H	-4.911641	2.138287	0.276136
H	-2.474175	2.140258	0.579816
C	0.000000	0.000000	-3.971842
N	0.000000	0.000000	-5.442037
O	0.000000	-1.071594	-6.008057
O	0.000000	1.071594	-6.008057
N	6.474826	0.000000	0.110856
N	-6.474826	0.000000	0.110856
H	6.840884	0.830943	-0.328427
H	6.840884	-0.830943	-0.328427
H	-6.840884	0.830943	-0.328427
H	-6.840884	-0.830943	-0.328427

Ph_3I…NCS^-

C	0.000000	1.200575	-3.941894
C	0.000000	1.203603	-2.553433
C	0.000000	0.000000	-1.863785
C	0.000000	-1.203603	-2.553433
C	0.000000	-1.200575	-3.941894
C	0.000000	0.000000	-4.638056
H	0.000000	2.140690	-4.479049
H	0.000000	2.140607	-2.011587
H	0.000000	-2.140607	-2.011587
H	0.000000	-2.140690	-4.479049
H	0.000000	0.000000	-5.720583
I	0.000000	0.000000	0.242261
C	-2.284901	0.000000	-0.058552
C	2.284901	0.000000	-0.058552
N	0.000000	0.000000	3.086871
C	0.000000	0.000000	4.254683
S	0.000000	0.000000	5.901375
C	2.993226	1.194171	-0.137245
C	4.373852	1.200443	-0.305115
C	5.066857	0.000000	-0.392435
C	4.373852	-1.200443	-0.305115
C	2.993226	-1.194171	-0.137245
H	2.466577	2.141303	-0.057925
H	4.910997	2.140488	-0.360937
H	6.142656	0.000000	-0.518631
H	4.910997	-2.140488	-0.360937
H	2.466577	-2.141303	-0.057925
C	-2.993226	-1.194171	-0.137245
C	-4.373852	-1.200443	-0.305115
C	-5.066857	0.000000	-0.392435
C	-4.373852	1.200443	-0.305115
C	-2.993226	1.194171	-0.137245
H	-2.466577	-2.141303	-0.057925
H	-4.910997	-2.140488	-0.360937
H	-6.142656	0.000000	-0.518631
H	-4.910997	2.140488	-0.360937
H	-2.466577	2.141303	-0.057925

Ph_3I

C	0.000000	1.201901	-3.131719
C	0.000000	1.209337	-1.743093
C	0.000000	0.000000	-1.068857
C	0.000000	-1.209337	-1.743093
C	0.000000	-1.201901	-3.131719
C	0.000000	0.000000	-3.825144
H	0.000000	2.140957	-3.669622
H	0.000000	2.146099	-1.202133
H	0.000000	-2.146099	-1.202133
H	0.000000	-2.140957	-3.669622
H	0.000000	0.000000	-4.907073
I	0.000000	0.000000	1.041972
C	-2.254316	0.000000	0.745186
C	2.254316	0.000000	0.745186
C	2.956652	1.197319	0.666933
C	4.337325	1.201347	0.501904
C	5.028554	0.000000	0.417732
C	4.337325	-1.201347	0.501904
C	2.956652	-1.197319	0.666933
H	2.429729	2.144835	0.734943
H	4.874205	2.140267	0.440411
H	6.103432	0.000000	0.289654
H	4.874205	-2.140267	0.440411
H	2.429729	-2.144835	0.734943
C	-2.956652	-1.197319	0.666933
C	-4.337325	-1.201347	0.501904
C	-5.028554	0.000000	0.417732
C	-4.337325	1.201347	0.501904
C	-2.956652	1.197319	0.666933
H	-2.429729	-2.144835	0.734943
H	-4.874205	-2.140267	0.440411
H	-6.103432	0.000000	0.289654
H	-4.874205	2.140267	0.440411
H	-2.429729	2.144835	0.734943

$(PhCN)_2(PhNO_2)I$…NCS^-

C	0.000000	1.212909	-3.293301
C	0.000000	1.206229	-1.907783
C	0.000000	0.000000	-1.218425
C	0.000000	-1.206229	-1.907783
C	0.000000	-1.212909	-3.293301
H	0.000000	2.133819	-3.857507
H	0.000000	2.143524	-1.367267
H	0.000000	-2.143524	-1.367267
H	0.000000	-2.133819	-3.857507
I	0.000000	0.000000	0.893059
C	-2.289849	0.000000	0.591593
C	2.289849	0.000000	0.591593
N	0.000000	0.000000	3.594531
C	0.000000	0.000000	4.764239
S	0.000000	0.000000	6.401599
C	2.995791	1.196873	0.516681
C	4.371975	1.209130	0.349523
C	5.061234	0.000000	0.259901
C	4.371975	-1.209130	0.349523
C	2.995791	-1.196873	0.516681
H	2.470228	2.143440	0.597360
H	4.920440	2.140647	0.290686
H	4.920440	-2.140647	0.290686
H	2.470228	-2.143440	0.597360
C	-2.995791	-1.196873	0.516681
C	-4.371975	-1.209130	0.349523
C	-5.061234	0.000000	0.259901
C	-4.371975	1.209130	0.349523
C	-2.995791	1.196873	0.516681
H	-2.470228	-2.143440	0.597360
H	-4.920440	-2.140647	0.290686
H	-4.920440	2.140647	0.290686
H	-2.470228	2.143440	0.597360
C	0.000000	0.000000	-3.958194
N	0.000000	0.000000	-5.431617
C	6.484417	0.000000	0.074851
C	-6.484417	0.000000	0.074851
N	7.622639	0.000000	-0.080132
N	-7.622639	0.000000	-0.080132
O	0.000000	-1.072232	-5.993542
O	0.000000	1.072232	-5.993542

$(PhF)_3I$…NCS^-

C	0.000000	1.209033	-3.688042
C	0.000000	1.202285	-2.299909
C	0.000000	0.000000	-1.607513
C	0.000000	-1.202285	-2.299909
C	0.000000	-1.209033	-3.688042
H	0.000000	2.131483	-4.252565
H	0.000000	2.141048	-1.761427
H	0.000000	-2.141048	-1.761427
H	0.000000	-2.131483	-4.252565
I	0.000000	0.000000	0.497817
C	-2.283572	0.000000	0.197179
C	2.283572	0.000000	0.197179
N	0.000000	0.000000	3.300362
C	0.000000	0.000000	4.468659
S	0.000000	0.000000	6.112841
C	2.993072	1.193106	0.117298
C	4.373554	1.208800	-0.055604
C	5.033972	0.000000	-0.142314
C	4.373554	-1.208800	-0.055604
C	2.993072	-1.193106	0.117298
H	2.470106	2.141528	0.199178
H	4.937989	2.130506	-0.115876
H	4.937989	-2.130506	-0.115876
H	2.470106	-2.141528	0.199178
C	-2.993072	-1.193106	0.117298
C	-4.373554	-1.208800	-0.055604
C	-5.033972	0.000000	-0.142314
C	-4.373554	1.208800	-0.055604
C	-2.993072	1.193106	0.117298
H	-2.470106	-2.141528	0.199178
H	-4.937989	-2.130506	-0.115876
H	-4.937989	2.130506	-0.115876
H	-2.470106	2.141528	0.199178
C	0.000000	0.000000	-4.353881
F	-6.374418	0.000000	-0.312820
F	6.374418	0.000000	-0.312820
F	0.000000	0.000000	-5.699329

Examples of Gaussian input files:

$(PhNH_2)_2(PhNO_2)I\ldots NCS^-$

```
%chk=I_Ph2_NH2_Ph_NO2_NCS_perp_fix.chk
%nprocshared=4
%mem=20GB
#p opt=modredundant freq def2tzvp int=ultrafine
m062x

Title

-1 1
 C   -1.21400138    0.00000000    3.28854306
 C   -1.20993028    0.00000000    1.89756805
 C    0.00000000    0.00000000    1.20184012
 C    1.20993028    0.00000000    1.89756805
 C    1.21400138    0.00000000    3.28854306
 H   -2.15467939    0.00000000    3.84007202
 H   -2.15512525    0.00000000    1.35234702
 H    2.15512525    0.00000000    1.35234702
 H    2.15467939    0.00000000    3.84007202
 I    0.00000000    0.00000000   -0.92365387
 C    0.00000000    2.30647489   -0.61999988
 C    0.00000000   -2.30647489   -0.61999988
 N    0.00000000    0.00000000   -3.62664589
 C    0.00000000    0.00000000   -4.80160789
 S    0.00000000    0.00000000   -6.44639688
 C   -1.20015914   -3.01650830   -0.53729593
 C   -1.20601676   -4.40265531   -0.36287993
 C    0.00000000   -5.09813010   -0.27292187
 C    1.20601676   -4.40265531   -0.36287993
 C    1.20015914   -3.01650830   -0.53729593
 H   -2.15575368   -2.48637425   -0.61678800
 H   -2.15355224   -4.94356724   -0.30259998
 H    2.15355224   -4.94356724   -0.30259998
 H    2.15575368   -2.48637425   -0.61678800
 C    1.20015914    3.01650830   -0.53729593
 C    1.20601676    4.40265531   -0.36287993
 C   -0.00000000    5.09813010   -0.27292187
 C   -1.20601676    4.40265531   -0.36287993
 C   -1.20015914    3.01650830   -0.53729593
 H    2.15575368    2.48637425   -0.61678800
 H    2.15355224    4.94356724   -0.30259998
 H   -2.15355224    4.94356724   -0.30259998
 H   -2.15575368    2.48637425   -0.61678800
 C    0.00000000    0.00000000    3.98826013
 N    0.00000000    0.00000000    5.52826013
 O    1.17779455   -0.00000000    6.20826013
 O   -1.17779455   -0.00000000    6.20826013
 N    0.00000000   -6.62664791   -0.08521647
 N   -0.00000000    6.62664791   -0.08521647
 H   -0.81648590   -6.90003543    0.42332069
 H    0.81648590   -6.90003543    0.42332069
 H   -0.81648590    6.90003543    0.42332069
 H    0.81648590    6.90003543    0.42332069

A 11 10 12 F
```

Ph_3I

```
%chk=I_Ph2_H_Ph_H_perp_fix
%nproc=4
%mem=20gb
#p opt=modredundant freq def2tzvp int=ultrafine
m062x

Title

0 1
C     0.000000    1.200575   -3.941894
C     0.000000    1.203603   -2.553433
C     0.000000    0.000000   -1.863785
C     0.000000   -1.203603   -2.553433
C     0.000000   -1.200575   -3.941894
C     0.000000    0.000000   -4.638056
H     0.000000    2.140690   -4.479049
H     0.000000    2.140607   -2.011587
H     0.000000   -2.140607   -2.011587
H     0.000000   -2.140690   -4.479049
H     0.000000    0.000000   -5.720583
I     0.000000    0.000000    0.242261
C    -2.284901    0.000000   -0.058552
C     2.284901    0.000000   -0.058552
C     2.993226    1.194171   -0.137245
C     4.373852    1.200443   -0.305115
C     5.066857    0.000000   -0.392435
C     4.373852   -1.200443   -0.305115
C     2.993226   -1.194171   -0.137245
H     2.466577    2.141303   -0.057925
H     4.910997    2.140488   -0.360937
H     6.142656    0.000000   -0.518631
H     4.910997   -2.140488   -0.360937
H     2.466577   -2.141303   -0.057925
C    -2.993226   -1.194171   -0.137245
C    -4.373852   -1.200443   -0.305115
C    -5.066857    0.000000   -0.392435
C    -4.373852    1.200443   -0.305115
C    -2.993226    1.194171   -0.137245
H    -2.466577   -2.141303   -0.057925
H    -4.910997   -2.140488   -0.360937
H    -6.142656    0.000000   -0.518631
H    -4.910997    2.140488   -0.360937
H    -2.466577    2.141303   -0.057925

14 12 13 F
```

$(PhCN)_2(PhNO_2)I\ldots NCS^-$

```
%chk=I_Ph2_CN_Ph_NO2_NCS_perp_fix
%nproc=4
%mem=20gb
#p opt=modredundant freq def2tzvp int=ultrafine
m062x

Title

-1 1
 C     -1.21400138    0.00000000    3.28806221
 C     -1.20993028    0.00000000    1.89708720
 C      0.00000000    0.00000000    1.20135927
 C      1.20993028    0.00000000    1.89708720
 C      1.21400138    0.00000000    3.28806221
 H     -2.15467939    0.00000000    3.83959117
 H     -2.15512525    0.00000000    1.35186617
 H      2.15512525    0.00000000    1.35186617
 H      2.15467939    0.00000000    3.83959117
 I      0.00000000    0.00000000   -0.92413472
 C      0.00000000    2.30647489   -0.62048073
 C      0.00000000   -2.30647489   -0.62048073
 N      0.00000000    0.00000000   -3.62712674
 C      0.00000000    0.00000000   -4.80208874
 S      0.00000000    0.00000000   -6.44687773
 C     -1.20015914   -3.01650830   -0.53777678
 C     -1.20601676   -4.40265531   -0.36336078
 C      0.00000000   -5.09813010   -0.27340272
 C      1.20601676   -4.40265531   -0.36336078
 C      1.20015914   -3.01650830   -0.53777678
 H     -2.15575368   -2.48637425   -0.61726885
 H     -2.15355224   -4.94356724   -0.30308083
 H      2.15355224   -4.94356724   -0.30308083
 H      2.15575368   -2.48637425   -0.61726885
 C      1.20015914    3.01650830   -0.53777678
 C      1.20601676    4.40265531   -0.36336078
 C     -0.00000000    5.09813010   -0.27340272
 C     -1.20601676    4.40265531   -0.36336078
 C     -1.20015914    3.01650830   -0.53777678
 H      2.15575368    2.48637425   -0.61726885
 H      2.15355224    4.94356724   -0.30308083
 H     -2.15355224    4.94356724   -0.30308083
 H     -2.15575368    2.48637425   -0.61726885
 C      0.00000000    0.00000000    3.98777928
 N      0.00000000    0.00000000    5.52777928
 C      0.00000000   -6.62664791   -0.08569732
 C     -0.00000000    6.62664791   -0.08569732
 N      0.00000000   -7.76469889    0.05405788
 N     -0.00000000    7.76469889    0.05405788
 O      1.27305734   -0.00000000    6.26277928
 O     -1.27305734   -0.00000000    6.26277928

A 11 10 12 F
```

$(PhF)_3I\ldots NCS^-$

```
%chk=I_Ph2_F_Ph_F_NCS_perp_fix
%nproc=4
%mem=20gb
#p opt=modredundant freq def2tzvp int=ultrafine
m062x

Title

-1 1
 C      1.21400138   -0.00000000   -3.68405096
 C      1.20993028   -0.00000000   -2.29307595
 C      0.00000000    0.00000000   -1.59734802
 C     -1.20993028   -0.00000000   -2.29307595
 C     -1.21400138   -0.00000000   -3.68405096
 H      2.15467939   -0.00000000   -4.23557991
 H      2.15512525   -0.00000000   -1.74785491
 H     -2.15512525   -0.00000000   -1.74785491
 H     -2.15467939   -0.00000000   -4.23557991
 I      0.00000000    0.00000000    0.52814598
 C      0.00000000    2.30647489    0.22449197
 C      0.00000000   -2.30647489    0.22449197
 N      0.00000000    0.00000000    3.23113799
 C      0.00000000    0.00000000    4.40609999
 S      0.00000000    0.00000000    6.05088899
 C      1.20015913   -3.01650830    0.14178804
 C      1.20601676   -4.40265531   -0.03262795
 C      0.00000000   -5.09813010   -0.12258602
 C     -1.20601676   -4.40265531   -0.03262795
 C     -1.20015913   -3.01650830    0.14178804
 H      2.15575367   -2.48637425    0.22128011
 H      2.15355223   -4.94356724   -0.09290790
 H     -2.15355223   -4.94356724   -0.09290790
 H     -2.15575367   -2.48637425    0.22128011
 C     -1.20015913    3.01650830    0.14178804
 C     -1.20601676    4.40265531   -0.03262795
 C     -0.00000000    5.09813010   -0.12258602
 C      1.20601676    4.40265531   -0.03262795
 C      1.20015913    3.01650830    0.14178804
 H     -2.15575367    2.48637425    0.22128011
 H     -2.15355223    4.94356724   -0.09290790
 H      2.15355223    4.94356724   -0.09290790
 H      2.15575367    2.48637425    0.22128011
 C      0.00000000    0.00000000   -4.38376803
 F      0.00000000    6.43697655   -0.29576269
 F      0.00000000   -6.43697655   -0.29576269
 F      0.00000000    0.00000000   -5.92376803

A 11 10 12 F
A 3 10 11 F
A 3 10 12 F
L 3 10 13 12 F
L 3 10 13 11 F
L 10 13 14 12 F
L 10 13 14 11 F
```

Iodosodilactone XYZ geometries:

x2:

I	-3.931704	2.354518	0.000000
O	-5.818310	1.518960	0.000000
C	-5.883085	0.177327	0.000000
C	-1.203151	1.249767	0.000000
O	-1.827112	2.413937	0.000000
O	0.000000	1.146481	0.000000
O	-6.911744	-0.430516	0.000000
C	-3.464414	0.384719	0.000000
C	-4.527593	-0.469430	0.000000
C	-4.214858	-1.825548	0.000000
C	-2.874650	-2.212013	0.000000
C	-1.829082	-1.285702	0.000000
C	-2.134634	0.072616	0.000000
H	-5.013836	-2.555886	0.000000
H	-2.628493	-3.265395	0.000000
H	-0.794887	-1.607500	0.000000
I	2.677126	0.142449	0.000000
O	4.512904	1.132329	0.000000
C	5.613552	0.380030	0.000000
C	1.939406	-2.723297	0.000000
O	1.385181	-1.514953	0.000000
O	1.302780	-3.742491	0.000000
O	6.727752	0.819680	0.000000
C	3.978587	-1.415446	0.000000
C	5.305552	-1.092147	0.000000
C	6.200506	-2.155556	0.000000
C	5.705947	-3.460304	0.000000
C	4.337247	-3.731541	0.000000
C	3.438296	-2.671634	0.000000
H	7.264279	-1.955091	0.000000
H	6.404346	-4.286363	0.000000
H	3.963827	-4.747479	0.000000

X3:

I	-2.186489	2.017551	0.000000
O	-4.069017	2.815268	0.000000
C	-4.170937	4.153611	0.000000
C	0.550525	3.270039	0.000000
O	0.000000	2.080463	0.000000
O	1.751782	3.456606	0.000000
O	-5.219324	4.728490	0.000000
C	-1.753659	4.005580	0.000000
C	-2.837642	4.838318	0.000000
C	-2.582373	6.204718	0.000000
C	-1.260118	6.647252	0.000000
C	-0.186112	5.756517	0.000000
C	-0.440239	4.390461	0.000000
H	-3.411171	6.901092	0.000000
H	-1.061036	7.710395	0.000000
H	0.837780	6.107857	0.000000
I	-0.654006	-2.902330	0.000000
O	-0.403585	-4.931506	0.000000
C	-1.511664	-5.688943	0.000000
C	-3.107199	-1.158251	0.000000
O	-1.801734	-1.040232	0.000000
O	-3.869400	-0.211216	0.000000
O	-1.485331	-6.884312	0.000000
C	-2.592105	-3.521503	0.000000
C	-2.771285	-4.876629	0.000000
C	-4.082256	-5.338760	0.000000
C	-5.126630	-4.414921	0.000000
C	-4.892234	-3.039436	0.000000
C	-3.582131	-2.576489	0.000000
H	-4.270935	-6.404707	0.000000
H	-6.146880	-4.774082	0.000000
H	-5.708449	-2.328390	0.000000
I	2.840495	0.884779	0.000000
O	4.472602	2.116238	0.000000
C	5.682601	1.535332	0.000000
C	2.556674	-2.111788	0.000000
O	1.801734	-1.040232	0.000000
O	2.117618	-3.245391	0.000000
O	6.704655	2.155822	0.000000
C	4.345763	-0.484077	0.000000
C	5.608927	0.038311	0.000000
C	6.664630	-0.865958	0.000000
C	6.386749	-2.232332	0.000000
C	5.078346	-2.717080	0.000000
C	4.022370	-1.813972	0.000000
H	7.682106	-0.496385	0.000000
H	7.207916	-2.936313	0.000000
H	4.870670	-3.779467	0.000000

X4:

I	2.164511	3.586887	0.000000
O	3.886262	4.696138	0.000000
C	3.759501	6.030196	0.000000
C	-0.737270	4.352190	0.000000
O	0.001890	3.278819	0.000000
O	-1.954324	4.354503	0.000000
O	4.696138	6.774906	0.000000
C	1.404883	5.474812	0.000000
C	2.330809	6.479867	0.000000
C	1.844586	7.782183	0.000000
C	0.465899	7.991085	0.000000
C	-0.439227	6.929220	0.000000
C	0.046258	5.627249	0.000000
H	2.541407	8.610531	0.000000
H	0.087108	9.004223	0.000000
H	-1.508664	7.097605	0.000000
I	3.586887	-2.164511	0.000000
O	4.696138	-3.886262	0.000000
C	6.030196	-3.759501	0.000000
C	4.352190	0.737270	0.000000
O	3.278819	-0.001890	0.000000
O	4.354503	1.954324	0.000000
O	6.774906	-4.696138	0.000000
C	5.474812	-1.404883	0.000000
C	6.479867	-2.330809	0.000000
C	7.782183	-1.844586	0.000000
C	7.991085	-0.465899	0.000000
C	6.929220	0.439227	0.000000
C	5.627249	-0.046258	0.000000
H	8.610531	-2.541407	0.000000
H	9.004223	-0.087108	0.000000
H	7.097605	1.508664	0.000000
I	-3.586887	2.164511	0.000000
O	-4.696138	3.886262	0.000000
C	-6.030196	3.759501	0.000000
C	-4.352190	-0.737270	0.000000
O	-3.278819	0.001890	0.000000
O	-4.354503	-1.954324	0.000000
O	-6.774906	4.696138	0.000000
C	-5.474812	1.404883	0.000000
C	-6.479867	2.330809	0.000000
C	-7.782183	1.844586	0.000000
C	-7.991085	0.465899	0.000000
C	-6.929220	-0.439227	0.000000
C	-5.627249	0.046258	0.000000
H	-8.610531	2.541407	0.000000
H	-9.004223	0.087108	0.000000
H	-7.097605	-1.508664	0.000000
I	-2.164511	-3.586887	0.000000
O	-3.886262	-4.696138	0.000000
C	-3.759501	-6.030196	0.000000
C	0.737270	-4.352190	0.000000
O	-0.001890	-3.278819	0.000000
O	1.954324	-4.354503	0.000000
O	-4.696138	-6.774906	0.000000
C	-1.404883	-5.474812	0.000000
C	-2.330809	-6.479867	0.000000
C	-1.844586	-7.782183	0.000000
C	-0.465899	-7.991085	0.000000
C	0.439227	-6.929220	0.000000
C	-0.046258	-5.627249	0.000000
H	-2.541407	-8.610531	0.000000
H	-0.087108	-9.004223	0.000000
H	1.508664	-7.097605	0.000000

X5:

I	2.378540	4.991541	0.000000
O	4.026769	6.223930	0.000000
C	3.802708	7.544096	0.000000
C	-0.552891	5.527967	0.000000
O	0.276311	4.518913	0.000000
O	-1.762703	5.425041	0.000000
O	4.680600	8.358010	0.000000
C	1.492674	6.818583	0.000000
C	2.342864	7.888081	0.000000
C	1.757533	9.149076	0.000000
C	0.366372	9.251682	0.000000
C	-0.457219	8.124881	0.000000
C	0.126224	6.863624	0.000000
H	2.387874	10.029089	0.000000
H	-0.088097	10.233200	0.000000
H	-1.536530	8.213172	0.000000
I	5.482247	-0.719655	0.000000
O	7.163650	-1.906385	0.000000
C	8.349963	-1.285336	0.000000
C	5.086556	2.234067	0.000000
O	4.383127	1.133634	0.000000
O	4.614815	3.352860	0.000000
O	9.395325	-1.868748	0.000000
C	6.946120	0.687441	0.000000
C	8.225996	0.209355	0.000000
C	9.244396	1.155706	0.000000
C	8.912087	2.510487	0.000000
C	7.585932	2.945567	0.000000
C	6.566699	2.000930	0.000000
H	10.276125	0.828156	0.000000
H	9.705128	3.246018	0.000000
H	7.336377	3.999336	0.000000
I	-4.012228	3.804597	0.000000
O	-4.674969	5.752985	0.000000
C	-5.999760	5.947844	0.000000
C	-5.428262	1.182405	0.000000
O	-4.212357	1.659208	0.000000
O	-5.704225	0.000000	0.000000
O	-6.502555	7.034282	0.000000
C	-6.023597	3.526675	0.000000
C	-6.778026	4.665747	0.000000
C	-8.158180	4.498733	0.000000
C	-8.685657	3.207367	0.000000
C	-7.868509	2.075885	0.000000
C	-6.488689	2.241022	0.000000
H	-8.800337	5.370163	0.000000
H	-9.759575	3.078448	0.000000
H	-8.286004	1.076683	0.000000
I	-4.858234	-2.640170	0.000000
O	-6.916059	-2.668390	0.000000
C	-7.510763	-3.868126	0.000000
C	-2.801959	-4.797201	0.000000
O	-2.879691	-3.493466	0.000000
O	-1.762703	-5.425041	0.000000
O	-8.699400	-4.010585	0.000000
C	-5.215461	-4.638978	0.000000
C	-6.531914	-5.004491	0.000000
C	-6.799566	-6.368705	0.000000
C	-5.734403	-7.269420	0.000000
C	-4.405787	-6.841913	0.000000
C	-4.136454	-5.478596	0.000000
H	-7.826782	-6.710146	0.000000
H	-5.943652	-8.330615	0.000000
H	-3.584503	-7.547745	0.000000
I	1.009674	-5.436312	0.000000
O	0.400610	-7.402141	0.000000
C	1.357853	-8.338477	0.000000
C	3.696556	-4.147238	0.000000
O	2.432610	-3.818289	0.000000
O	4.614815	-3.352860	0.000000
O	1.126030	-9.512960	0.000000
C	2.800264	-6.393721	0.000000
C	2.741081	-7.758692	0.000000
C	3.955817	-8.434810	0.000000
C	5.141601	-7.700116	0.000000
C	5.145583	-6.304420	0.000000
C	3.932220	-5.626981	0.000000
H	3.963120	-9.517261	0.000000
H	6.086196	-8.227051	0.000000
H	6.070660	-5.741446	0.000000

Benziodazole trimer XYZ geometry:

I	-2.535528	1.742154	0.000000
H	-2.423970	-7.590154	0.000000
C	-4.408484	2.665311	0.000000
C	-0.279017	-7.893229	0.000000
O	-2.760439	5.868221	0.000000
H	1.867446	-7.863658	0.000000
C	-5.629873	2.013397	0.000000
C	0.964499	-7.267074	0.000000
C	-4.307261	4.046317	0.000000
H	5.876405	5.549084	0.000000
O	0.000000	1.910354	0.000000
H	2.032714	-5.390959	0.000000
N	-1.959605	3.739541	0.000000
H	7.785251	1.695858	0.000000
C	-0.588899	4.214421	0.000000
C	-5.462810	4.816618	0.000000
C	6.975245	3.704978	0.000000
C	-2.953761	4.668266	0.000000
C	5.811222	4.468818	0.000000
H	-0.405529	4.841727	0.875914
H	7.939421	4.195562	0.000000
H	3.652351	4.455862	0.000000
H	-0.405529	4.841727	-0.875914
H	-7.743850	2.314573	0.000000
C	0.414614	3.077269	0.000000
H	-5.361282	5.894297	0.000000
O	1.645095	3.387076	0.000000
I	-0.240985	-3.066909	0.000000
C	-6.696228	4.188250	0.000000
C	-0.103986	-5.150515	0.000000
C	-6.775720	2.798257	0.000000
O	-3.701809	-5.324721	0.000000
H	-0.336247	-8.973521	0.000000
H	-5.685065	0.935098	0.000000
C	1.071284	-5.882312	0.000000
H	-7.603174	4.777959	0.000000
C	-1.350583	-5.753356	0.000000
O	-1.654416	-0.955177	0.000000
N	-2.258734	-3.566838	0.000000
C	-3.355346	-2.617212	0.000000
C	-1.439909	-7.139241	0.000000
C	-2.565956	-4.892165	0.000000
H	-3.990294	-2.772062	0.875914
H	-3.990294	-2.772062	-0.875914
C	-2.872300	-1.179568	0.000000
O	-3.755841	-0.268843	0.000000
I	2.776514	1.324755	0.000000
C	4.512469	2.485203	0.000000
O	6.462248	-0.543500	0.000000
C	4.558590	3.868915	0.000000
C	5.657844	1.707039	0.000000
O	1.654416	-0.955177	0.000000
N	4.218340	-0.172702	0.000000
C	3.944245	-1.597209	0.000000
C	6.902718	2.322623	0.000000
C	5.519717	0.223900	0.000000
H	4.395823	-2.069666	0.875914
H	4.395823	-2.069666	-0.875914
C	2.457686	-1.897701	0.000000
O	2.110746	-3.118232	0.000000