

# **Electronic Supplementary Information for**

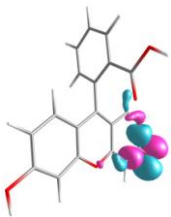
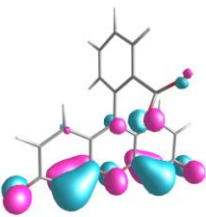
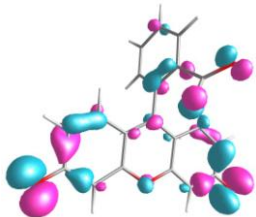
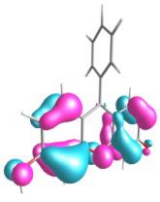
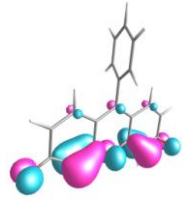
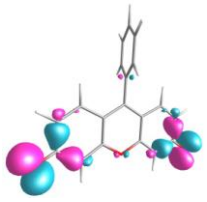
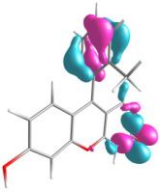
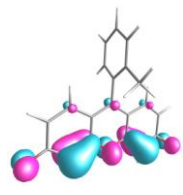
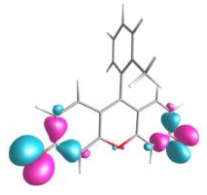
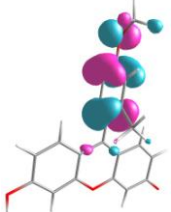
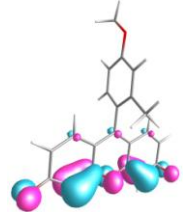
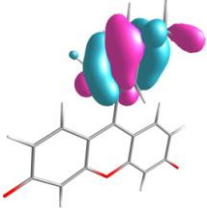
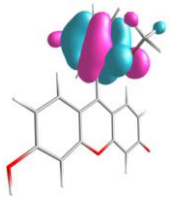
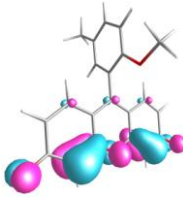
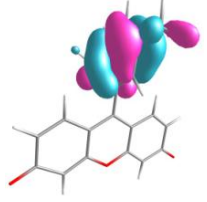
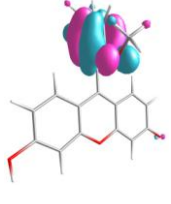
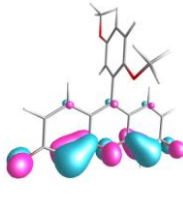
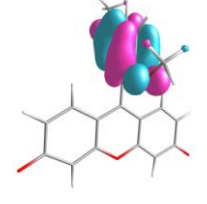
## **The invalidity of the Photo-induced Electron Transfer Mechanism for Fluorescein Derivatives**

Panwang Zhou, Jianyong Liu, Songqiu Yang, Junsheng Chen, Keli Han<sup>\*</sup>, Guozhong

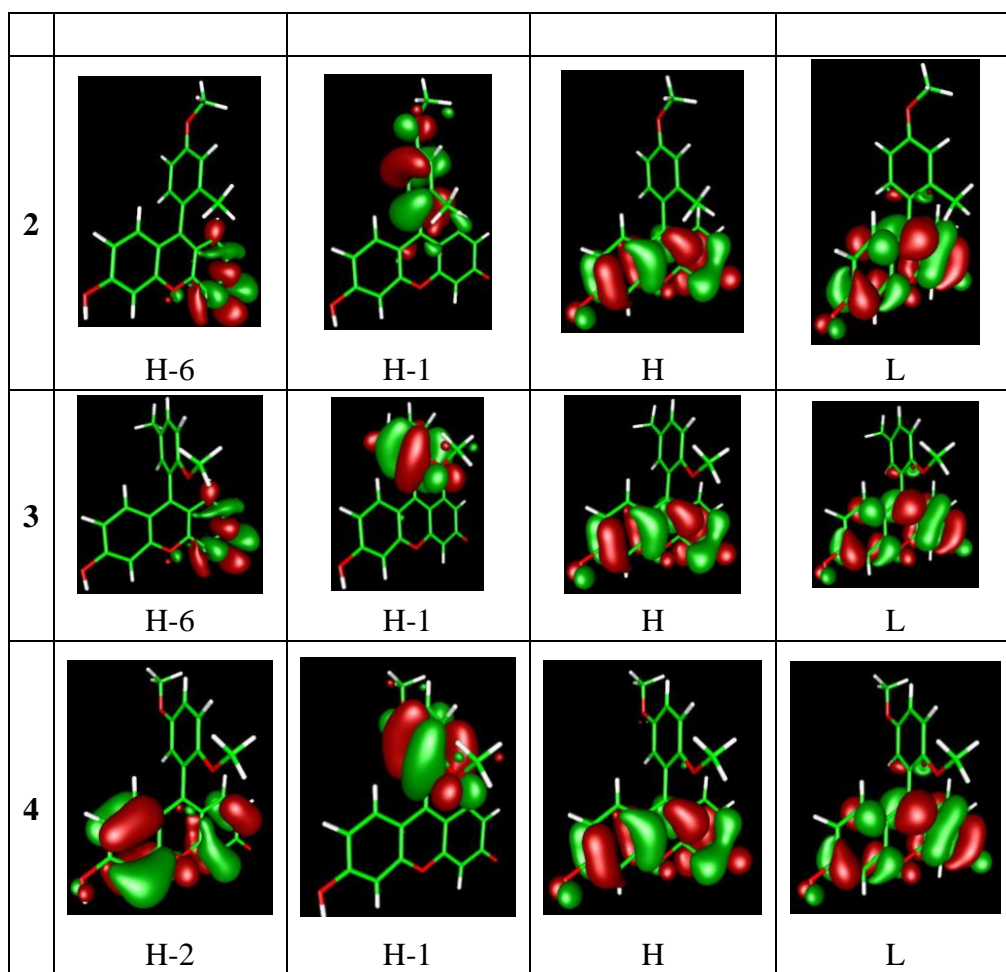
He

State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical  
Physics, Chinese Academy of Science, Dalian 116023, Liaoning, China

Email: [klhan@dipc.ac.cn](mailto:klhan@dipc.ac.cn)

	Acidic Condition	Alkaline Condition	
Fluorescein	 H-2	 H-1	 H-3
HPFluorone	 H-2	 H-1	 H-2
1	 H-3	 H-1	 H-2
2	 H-1	 H-1	 H-2
3	 H-1	 H-1	 H-2
4	 H-1	 H-2	 H-1

**Figure S1** Calculated frontier molecular orbitals (MOs) of the neutral and anionic form of the six fluorescein derivatives from DFT/CAM-B3LYP calculations.



**Figure S2.** Calculated frontier molecular orbitals (MOs) of the neutral form of compounds **2~4** from RI-CC2/TZVP calculations.

**Table S1.** All the optimized geometric coordinates for anionic and neutral form of all the six fluorescein derivatives.

Anionic form of Fluorescein S0 B3LYP/TZVP/IEFPCM

C	-2.914580000	-2.620178000	0.141182000
C	-2.920168000	-3.245665000	-1.099232000
C	-1.989212000	-2.869237000	-2.062659000
C	-1.058646000	-1.880851000	-1.766244000
C	-1.030232000	-1.264198000	-0.509321000
C	-1.974955000	-1.635424000	0.463155000
C	-0.012091000	-0.193156000	-0.291448000
C	1.347459000	-0.523590000	-0.159036000
C	2.312100000	0.517245000	-0.008254000

O	1.913789000	1.827776000	-0.009008000
C	0.597312000	2.173537000	-0.160296000
C	-0.395496000	1.158941000	-0.312109000
C	0.304998000	3.512406000	-0.163669000
C	-1.043828000	3.980800000	-0.329888000
C	-2.049998000	2.944049000	-0.498816000
C	-1.735265000	1.619509000	-0.490579000
C	1.856771000	-1.856451000	-0.110453000
C	3.184037000	-2.119269000	0.041035000
C	4.173188000	-1.060919000	0.175143000
C	3.653531000	0.278711000	0.141221000
O	-1.342812000	5.205667000	-0.337526000
C	-2.010558000	-1.024505000	1.869019000
O	5.401090000	-1.311796000	0.314647000
O	-0.905611000	-0.830285000	2.432996000
O	-3.151783000	-0.792751000	2.343190000
H	-3.648911000	-2.890825000	0.889010000
H	-3.650176000	-4.016431000	-1.315928000
H	-1.987881000	-3.336984000	-3.039627000
H	-0.342373000	-1.575200000	-2.519647000
H	1.101628000	4.236405000	-0.045525000
H	-3.075593000	3.266472000	-0.636951000
H	-2.515748000	0.881503000	-0.622554000
H	1.153230000	-2.674080000	-0.198582000
H	3.544048000	-3.141153000	0.074332000
H	4.338208000	1.110887000	0.248558000

Anionic form of Fluorescein S1 B3LYP/TZVP/IEFPCM

C	-2.916575000	-2.648890000	0.125987000
C	-2.798317000	-3.417840000	-1.025799000
C	-1.764804000	-3.152289000	-1.921618000
C	-0.872082000	-2.123290000	-1.652610000
C	-0.969031000	-1.345599000	-0.485709000
C	-2.008730000	-1.628903000	0.426847000
C	-0.002956000	-0.243947000	-0.292047000
C	1.393530000	-0.505913000	-0.131019000
C	2.317202000	0.571312000	-0.004426000
O	1.888993000	1.878400000	-0.036696000
C	0.551350000	2.166585000	-0.186458000
C	-0.414107000	1.127300000	-0.316850000
C	0.224923000	3.501219000	-0.216419000
C	-1.134939000	3.939473000	-0.398182000
C	-2.113015000	2.882538000	-0.554612000
C	-1.759575000	1.559382000	-0.518213000

C	1.955847000	-1.814187000	-0.021725000
C	3.298826000	-2.029627000	0.141441000
C	4.242337000	-0.934445000	0.236349000
C	3.668601000	0.384534000	0.159304000
O	-1.450392000	5.164965000	-0.428231000
C	-2.157398000	-0.913743000	1.773391000
O	5.484806000	-1.121598000	0.387819000
O	-1.110057000	-0.748196000	2.448386000
O	-3.325900000	-0.589138000	2.108978000
H	-3.721518000	-2.841153000	0.824581000
H	-3.506639000	-4.213185000	-1.225266000
H	-1.662722000	-3.732651000	-2.830956000
H	-0.087453000	-1.898104000	-2.365608000
H	1.005070000	4.245203000	-0.113026000
H	-3.145771000	3.173037000	-0.709137000
H	-2.522034000	0.802592000	-0.644649000
H	1.283587000	-2.660220000	-0.073612000
H	3.690186000	-3.037203000	0.221788000
H	4.321159000	1.244212000	0.248041000

Neutral form of Fluorescein S0 B3LYP/TZVP/IEFPCM

C	-3.874283000	-0.678885000	0.025863000
C	-4.259981000	-0.654825000	-1.305990000
C	-3.313252000	-0.399600000	-2.291242000
C	-1.987888000	-0.170726000	-1.939339000
C	-1.582981000	-0.191785000	-0.603874000
C	-2.542487000	-0.452581000	0.393982000
C	-0.135515000	0.057147000	-0.328428000
C	0.770927000	-1.051871000	-0.271260000
C	2.141105000	-0.794294000	-0.074453000
O	2.610007000	0.475341000	0.045683000
C	1.770846000	1.551967000	-0.033679000
C	0.358858000	1.341753000	-0.238158000
C	2.326971000	2.788208000	0.084364000
C	1.510936000	3.976874000	0.021305000
C	0.075504000	3.762250000	-0.177272000
C	-0.457057000	2.525953000	-0.295622000
C	0.381176000	-2.403813000	-0.386353000
C	1.298082000	-3.424350000	-0.308352000
C	2.657894000	-3.127566000	-0.107110000
C	3.084121000	-1.809599000	0.004964000
O	1.987271000	5.125723000	0.127316000
C	-2.154730000	-0.478995000	1.830679000
O	3.508732000	-4.178997000	-0.034359000

O	-1.030503000	-0.312691000	2.252469000
O	-3.198490000	-0.712848000	2.653332000
H	-4.606429000	-0.873504000	0.795865000
H	-5.293726000	-0.832845000	-1.572198000
H	-3.601913000	-0.376770000	-3.334433000
H	-1.253646000	0.027978000	-2.709583000
H	3.393581000	2.893522000	0.233165000
H	-0.550041000	4.645248000	-0.223890000
H	-1.522313000	2.404472000	-0.440847000
H	-0.662858000	-2.638475000	-0.541285000
H	0.993589000	-4.458400000	-0.396169000
H	4.126557000	-1.559368000	0.155794000
H	4.415904000	-3.879396000	0.113174000
H	-2.864315000	-0.716262000	3.564729000

Neutral form of Fluorescein S1(121.04) B3LYP/TZVP/IEFPCM

C	-3.186058000	-2.360120000	-0.012065000
C	-3.084814000	-3.108411000	-1.173301000
C	-1.969269000	-2.952401000	-1.994190000
C	-0.979180000	-2.042458000	-1.654605000
C	-1.066808000	-1.253660000	-0.496566000
C	-2.190901000	-1.440929000	0.348619000
C	-0.016643000	-0.246041000	-0.270911000
C	1.329682000	-0.620984000	-0.112760000
C	2.339647000	0.385186000	0.034970000
O	2.017110000	1.703952000	0.016574000
C	0.726609000	2.095110000	-0.163582000
C	-0.320146000	1.179299000	-0.310941000
C	0.537411000	3.474973000	-0.212594000
C	-0.783037000	4.038671000	-0.433400000
C	-1.847835000	3.082547000	-0.610593000
C	-1.610222000	1.735298000	-0.551141000
C	1.792336000	-1.968670000	-0.010798000
C	3.117761000	-2.268414000	0.159658000
C	4.079443000	-1.237554000	0.264779000
C	3.681897000	0.091403000	0.209428000
O	-0.944968000	5.284956000	-0.466564000
C	-2.274920000	-0.756149000	1.659371000
O	5.368004000	-1.619120000	0.431484000
O	-1.387817000	-0.100577000	2.168692000
O	-3.462752000	-0.940937000	2.283077000
H	-4.036433000	-2.493737000	0.640930000
H	-3.865098000	-3.811321000	-1.434707000
H	-1.876635000	-3.529368000	-2.905832000

H	-0.133829000	-1.902713000	-2.316037000
H	1.382608000	4.139165000	-0.093270000
H	-2.844713000	3.462411000	-0.794074000
H	-2.437309000	1.053033000	-0.698105000
H	1.071979000	-2.771427000	-0.066550000
H	3.448093000	-3.296202000	0.234690000
H	4.392165000	0.902416000	0.309093000
H	5.949505000	-0.849415000	0.500829000
H	-3.416681000	-0.489215000	3.140684000

Neutral form of Fluorescein S1(67.07) B3LYP/TZVP/IEFPCM

C	-3.836048000	-0.967404000	-0.034178000
C	-4.308041000	-0.602941000	-1.285018000
C	-3.445159000	0.005448000	-2.193854000
C	-2.120134000	0.232559000	-1.848761000
C	-1.614131000	-0.142634000	-0.596750000
C	-2.503973000	-0.731212000	0.331077000
C	-0.173176000	0.055443000	-0.341470000
C	0.715673000	-1.026607000	-0.217485000
C	2.115886000	-0.779868000	-0.034479000
O	2.598696000	0.490386000	0.003900000
C	1.760025000	1.551837000	-0.119447000
C	0.378779000	1.398181000	-0.290249000
C	2.378254000	2.799139000	-0.050754000
C	1.598671000	4.024865000	-0.139461000
C	0.176117000	3.850443000	-0.284425000
C	-0.384982000	2.601079000	-0.345311000
C	0.344727000	-2.401843000	-0.296970000
C	1.266075000	-3.408560000	-0.170740000
C	2.632452000	-3.111874000	0.038163000
C	3.054242000	-1.790390000	0.095019000
O	2.171077000	5.142255000	-0.080967000
C	-2.079386000	-1.016521000	1.727931000
O	3.474046000	-4.166824000	0.162455000
O	-1.147257000	-0.495942000	2.303142000
O	-2.874004000	-1.924349000	2.338830000
H	-4.504821000	-1.421762000	0.682901000
H	-5.341575000	-0.786858000	-1.548312000
H	-3.800291000	0.292644000	-3.175665000
H	-1.448756000	0.680372000	-2.570620000
H	3.450205000	2.863250000	0.078102000
H	-0.441538000	4.738083000	-0.331587000
H	-1.459150000	2.512663000	-0.441793000
H	-0.691802000	-2.653721000	-0.469704000

H	0.964454000	-4.446006000	-0.233475000
H	4.096521000	-1.531100000	0.232500000
H	4.382057000	-3.868535000	0.309190000
H	-2.571452000	-2.012859000	3.257139000

Anionic form of HPFluorone S0 B3LYP/TZVP/IEFPCM

C	0.000042000	4.712453000	0.000000000
C	-0.270188000	4.013164000	1.172992000
C	-0.273645000	2.621464000	1.173019000
C	0.000018000	1.912715000	0.000008000
C	0.273698000	2.621453000	-1.173006000
C	0.270262000	4.013153000	-1.172987000
C	0.000003000	0.420428000	0.000013000
C	-1.214622000	-0.284227000	-0.008433000
C	-1.195571000	-1.713468000	-0.009515000
O	-0.000023000	-2.381861000	0.000109000
C	1.195538000	-1.713489000	0.009590000
C	1.214614000	-0.284248000	0.008466000
C	2.333425000	-2.474666000	0.019936000
C	3.636981000	-1.866432000	0.042939000
C	3.650870000	-0.410979000	0.055994000
C	2.506545000	0.324962000	0.042792000
C	-2.506542000	0.325005000	-0.042810000
C	-3.650878000	-0.410917000	-0.056065000
C	-3.637013000	-1.866372000	-0.043126000
C	-2.333469000	-2.474626000	-0.019926000
O	4.700505000	-2.540555000	0.054632000
O	-4.700550000	-2.540476000	-0.054654000
H	0.000051000	5.795466000	-0.000002000
H	-0.479201000	4.549906000	2.090273000
H	-0.485342000	2.081572000	2.087978000
H	0.485385000	2.081553000	-2.087962000
H	0.479284000	4.549887000	-2.090271000
H	2.258716000	-3.554882000	0.019127000
H	4.619069000	0.075265000	0.082368000
H	2.561708000	1.405789000	0.056731000
H	-2.561687000	1.405833000	-0.056727000
H	-4.619070000	0.075343000	-0.082440000
H	-2.258778000	-3.554843000	-0.019051000

Anionic form of HPFluorone S1(52.86) B3LYP/TZVP/IEFPCM

C	0.000269000	4.768776000	-0.000008000
C	-0.741608000	4.062310000	0.945884000
C	-0.744697000	2.673679000	0.945241000



C	0.000101000	1.940021000	0.000008000
C	0.744990000	2.673579000	-0.945229000
C	0.742065000	4.062211000	-0.945891000
C	0.000019000	0.472613000	0.000020000
C	-1.224405000	-0.280523000	-0.023348000
C	-1.192116000	-1.704643000	-0.009797000
O	-0.000129000	-2.388142000	0.000023000
C	1.191928000	-1.704767000	0.009834000
C	1.224363000	-0.280650000	0.023387000
C	2.324435000	-2.483526000	0.026156000
C	3.638343000	-1.899114000	0.084209000
C	3.670526000	-0.451125000	0.152479000
C	2.525847000	0.298215000	0.131014000
C	-2.525826000	0.298470000	-0.131048000
C	-3.670582000	-0.450753000	-0.152520000
C	-3.638553000	-1.898738000	-0.084109000
C	-2.324703000	-2.483286000	-0.026116000
O	4.690153000	-2.599147000	0.092162000
O	-4.690426000	-2.598674000	-0.092281000
H	0.000334000	5.851601000	-0.000015000
H	-1.314472000	4.596442000	1.694801000
H	-1.309278000	2.144276000	1.702509000
H	1.309515000	2.144100000	-1.702487000
H	1.314994000	4.596266000	-1.694812000
H	2.230939000	-3.562153000	0.012409000
H	4.639724000	0.026724000	0.235548000
H	2.601969000	1.374216000	0.200857000
H	-2.601836000	1.374475000	-0.200955000
H	-4.639727000	0.027188000	-0.235680000
H	-2.231316000	-3.561923000	-0.012401000

Anionic form of HPFluorone S1(127.17) B3LYP/TZVP/IEFPCM

C	0.000254000	4.768857000	-0.000020000
C	0.669873000	4.062264000	0.998250000
C	0.672865000	2.673648000	0.997821000
C	0.000105000	1.939980000	-0.000019000
C	-0.672579000	2.673717000	-0.997859000
C	-0.669440000	4.062333000	-0.998288000
C	0.000027000	0.472672000	-0.000016000
C	-1.222720000	-0.280541000	-0.067975000
C	-1.189516000	-1.704646000	-0.079056000
O	-0.000126000	-2.388159000	0.000010000
C	1.189338000	-1.704772000	0.079056000
C	1.222695000	-0.280671000	0.067947000

C	2.319905000	-2.483548000	0.147234000
C	3.634494000	-1.899168000	0.187104000
C	3.671675000	-0.451169000	0.121358000
C	2.528586000	0.298162000	0.057452000
C	-2.528550000	0.298431000	-0.057478000
C	-3.671719000	-0.450779000	-0.121376000
C	-3.634691000	-1.898781000	-0.187142000
C	-2.320166000	-2.483302000	-0.147230000
O	4.683974000	-2.599201000	0.257364000
O	-4.684249000	-2.598705000	-0.257324000
H	0.000310000	5.851677000	-0.000020000
H	1.185694000	4.596298000	1.787609000
H	1.179656000	2.144238000	1.794918000
H	-1.179426000	2.144361000	-1.794954000
H	-1.185206000	4.596421000	-1.787647000
H	2.225601000	-3.562172000	0.153990000
H	4.644355000	0.026705000	0.110629000
H	2.609760000	1.374154000	-0.006650000
H	-2.609609000	1.374432000	0.006622000
H	-4.644348000	0.027198000	-0.110633000
H	-2.225978000	-3.561936000	-0.153954000

Neutral form of HPFluorone S0 B3LYP/TZVP/IEFPCM

C	-0.847669000	4.656994000	0.003842000
C	-0.362275000	4.032461000	-1.141869000
C	-0.125640000	2.661864000	-1.144550000
C	-0.385164000	1.898804000	-0.001791000
C	-0.875210000	2.531248000	1.144494000
C	-1.100878000	3.904174000	1.146674000
C	-0.135244000	0.430891000	-0.004636000
C	1.214286000	-0.058761000	0.009401000
C	1.431051000	-1.451656000	0.007370000
O	0.392515000	-2.326800000	-0.007668000
C	-0.903259000	-1.891155000	-0.017114000
C	-1.179515000	-0.474234000	-0.016789000
C	-1.879215000	-2.838883000	-0.025067000
C	-3.273469000	-2.467214000	-0.053428000
C	-3.554345000	-1.029735000	-0.075888000
C	-2.570538000	-0.103540000	-0.064299000
C	2.360652000	0.766105000	0.056393000
C	3.628252000	0.235973000	0.075500000
C	3.802526000	-1.159073000	0.057825000
C	2.702301000	-2.007301000	0.024470000
O	-4.193834000	-3.309910000	-0.063659000

O	5.076045000	-1.618562000	0.078658000
H	-1.027409000	5.724854000	0.005739000
H	-0.166420000	4.611467000	-2.035785000
H	0.251532000	2.180934000	-2.038719000
H	-1.073183000	1.949219000	2.036088000
H	-1.475891000	4.383727000	2.042268000
H	-1.617857000	-3.888969000	-0.022782000
H	-4.595819000	-0.734404000	-0.113204000
H	-2.814499000	0.949595000	-0.090389000
H	2.232912000	1.838953000	0.076785000
H	4.500820000	0.874028000	0.110990000
H	2.815362000	-3.083870000	0.020155000
H	5.092770000	-2.585132000	0.066980000

Neutral form of HPFluorone S1(56.35) B3LYP/TZVP/IEFPCM

C	0.000150000	4.758466000	0.012117000
C	-0.622176000	4.054403000	1.039688000
C	-0.630056000	2.664647000	1.032932000
C	-0.009171000	1.943772000	-0.001029000
C	0.624233000	2.669690000	-1.024409000
C	0.620846000	4.058491000	-1.020928000
C	-0.018251000	0.472153000	-0.011595000
C	-1.218813000	-0.264786000	0.032390000
C	-1.180167000	-1.698259000	0.031895000
O	0.005349000	-2.362679000	-0.016034000
C	1.178115000	-1.678481000	-0.060739000
C	1.232495000	-0.279717000	-0.063786000
C	2.317952000	-2.482081000	-0.091568000
C	3.647421000	-1.893770000	-0.107580000
C	3.689659000	-0.454986000	-0.074012000
C	2.539558000	0.291111000	-0.045952000
C	-2.529139000	0.303158000	0.016097000
C	-3.658546000	-0.473160000	0.050321000
C	-3.562737000	-1.881900000	0.086259000
C	-2.315250000	-2.490937000	0.069715000
O	4.665485000	-2.631272000	-0.141148000
O	-4.727057000	-2.576028000	0.121758000
H	0.004454000	5.841285000	0.016885000
H	-1.098344000	4.587796000	1.853361000
H	-1.102061000	2.129043000	1.847099000
H	1.099698000	2.139687000	-1.840279000
H	1.101520000	4.596364000	-1.828984000
H	2.216390000	-3.558878000	-0.095209000
H	4.660037000	0.024574000	-0.062043000

H	2.619801000	1.368760000	-0.006040000
H	-2.629421000	1.377068000	-0.030568000
H	-4.641111000	-0.019690000	0.034374000
H	-2.208435000	-3.568501000	0.072962000
H	-4.558518000	-3.528081000	0.133389000

Neutral form of HPFluorone S1(123.79) B3LYP/TZVP/IEFPCM

C	-0.874008000	4.699361000	0.008915000
C	-1.347771000	3.902006000	-1.031365000
C	-1.105175000	2.534551000	-1.033688000
C	-0.366306000	1.930791000	-0.001697000
C	0.103996000	2.748766000	1.039445000
C	-0.149922000	4.115155000	1.044925000
C	-0.096673000	0.484064000	-0.010821000
C	1.214787000	-0.028709000	0.048727000
C	1.430620000	-1.446312000	0.049441000
O	0.382141000	-2.310109000	-0.011988000
C	-0.892553000	-1.844371000	-0.072208000
C	-1.193769000	-0.477355000	-0.077794000
C	-1.871609000	-2.837024000	-0.116176000
C	-3.283872000	-2.493491000	-0.149532000
C	-3.580733000	-1.084940000	-0.118466000
C	-2.581351000	-0.146988000	-0.077106000
C	2.403881000	0.762401000	0.047791000
C	3.652423000	0.198330000	0.096645000
C	3.807188000	-1.205161000	0.133011000
C	2.687589000	-2.025517000	0.101889000
O	-4.154765000	-3.399602000	-0.194778000
O	5.075533000	-1.682094000	0.183425000
H	-1.070014000	5.764302000	0.012682000
H	-1.905773000	4.347414000	-1.845956000
H	-1.468848000	1.929900000	-1.855126000
H	0.653054000	2.304043000	1.859994000
H	0.213946000	4.723273000	1.864133000
H	-1.580907000	-3.878824000	-0.117143000
H	-4.620806000	-0.784944000	-0.119312000
H	-2.851620000	0.899402000	-0.039673000
H	2.312873000	1.837133000	0.001116000
H	4.539255000	0.818676000	0.092211000
H	2.773283000	-3.104964000	0.105068000
H	5.078172000	-2.648950000	0.194504000

Anionic form of Complex 1 S0 B3LYP/TZVP/IEFPCM

C	0.001886000	3.983172000	0.834292000
---	-------------	-------------	-------------

C	0.001971000	4.597764000	-0.413774000
C	0.001405000	3.820483000	-1.566458000
C	0.000774000	2.434000000	-1.456700000
C	0.000703000	1.813109000	-0.205517000
C	0.001252000	2.592103000	0.965637000
C	0.000090000	0.319377000	-0.140189000
C	-1.213795000	-0.384738000	-0.116346000
C	-1.196319000	-1.812267000	-0.052102000
O	-0.001052000	-2.480853000	-0.023860000
C	1.194758000	-1.813242000	-0.052129000
C	1.213399000	-0.385733000	-0.116385000
C	2.333388000	-2.572855000	-0.020642000
C	3.636400000	-1.963229000	-0.040899000
C	3.649578000	-0.508834000	-0.104989000
C	2.504317000	0.225066000	-0.137711000
C	-2.504208000	0.227126000	-0.137529000
C	-3.650069000	-0.505833000	-0.104770000
C	-3.638079000	-1.960242000	-0.040801000
C	-2.335572000	-2.570946000	-0.020612000
O	4.700777000	-2.635369000	-0.007203000
C	0.001181000	1.958804000	2.334239000
O	-4.703009000	-2.631503000	-0.007093000
H	0.002314000	4.593734000	1.730004000
H	0.002464000	5.678778000	-0.483273000
H	0.001452000	4.286089000	-2.544218000
H	0.000340000	1.821912000	-2.350839000
H	2.260204000	-3.652172000	0.026029000
H	4.617878000	-0.022347000	-0.123011000
H	2.556491000	1.305531000	-0.184639000
H	-2.555490000	1.307637000	-0.184376000
H	-4.617966000	-0.018543000	-0.122664000
H	-2.263294000	-3.650327000	0.026032000
H	0.001153000	2.721399000	3.112783000
H	-0.876993000	1.325799000	2.481821000
H	0.879346000	1.325798000	2.481906000

Anionic form of Complex **1** S1(71.78) B3LYP/TZVP/IEFPCM

C	-0.254389000	4.025337000	0.802708000
C	0.074328000	4.630143000	-0.406159000
C	0.412338000	3.838962000	-1.500120000
C	0.408593000	2.455605000	-1.371577000
C	0.065967000	1.831683000	-0.162665000
C	-0.262335000	2.635842000	0.951355000
C	0.059132000	0.352120000	-0.087592000

C	-1.166658000	-0.381297000	-0.003914000
C	-1.146611000	-1.804429000	0.055639000
O	0.041906000	-2.496620000	0.023932000
C	1.234973000	-1.824825000	-0.114676000
C	1.271911000	-0.400580000	-0.167685000
C	2.362963000	-2.605015000	-0.184624000
C	3.675554000	-2.021628000	-0.298553000
C	3.713614000	-0.572812000	-0.328709000
C	2.572569000	0.181621000	-0.258836000
C	-2.461127000	0.220914000	-0.013376000
C	-3.615354000	-0.512411000	0.067281000
C	-3.595649000	-1.958706000	0.157234000
C	-2.287832000	-2.564699000	0.137102000
O	4.723509000	-2.726628000	-0.360106000
C	-0.591221000	2.027478000	2.290728000
O	-4.653962000	-2.646280000	0.236833000
H	-0.499882000	4.644393000	1.658559000
H	0.072739000	5.710203000	-0.489949000
H	0.671940000	4.294238000	-2.448277000
H	0.662040000	1.838242000	-2.225477000
H	2.272199000	-3.683160000	-0.139172000
H	4.685630000	-0.098118000	-0.396469000
H	2.644596000	1.261130000	-0.276350000
H	-2.517547000	1.299086000	-0.092819000
H	-4.582258000	-0.023041000	0.060163000
H	-2.211730000	-3.644046000	0.178904000
H	-0.594357000	2.788915000	3.070999000
H	-1.575103000	1.550266000	2.287182000
H	0.132422000	1.256705000	2.564145000

Anionic form of Complex **1** S1(111.61) B3LYP/TZVP/IEFPCM

C	0.332286000	4.020706000	0.790833000
C	-0.029414000	4.627383000	-0.407639000
C	-0.404510000	3.838114000	-1.490842000
C	-0.404407000	2.454752000	-1.362342000
C	-0.028953000	1.828862000	-0.164230000
C	0.337153000	2.631184000	0.939307000
C	-0.028063000	0.349304000	-0.089083000
C	-1.246753000	-0.396799000	-0.132926000
C	-1.216033000	-1.821199000	-0.079820000
O	-0.023135000	-2.499404000	0.024701000
C	1.169599000	-1.813790000	0.019731000
C	1.195676000	-0.390859000	-0.041769000
C	2.308549000	-2.580337000	0.066979000

C	3.619714000	-1.981572000	0.047543000
C	3.644643000	-0.535478000	-0.044572000
C	2.492551000	0.204171000	-0.090795000
C	-2.546369000	0.192410000	-0.186465000
C	-3.693018000	-0.555840000	-0.222221000
C	-3.661980000	-2.004850000	-0.192201000
C	-2.349818000	-2.595285000	-0.116023000
O	4.676127000	-2.674886000	0.096270000
C	0.702810000	2.020970000	2.268276000
O	-4.715117000	-2.704150000	-0.222663000
H	0.606842000	4.638348000	1.638839000
H	-0.024456000	5.707421000	-0.491575000
H	-0.690092000	4.294878000	-2.430782000
H	-0.686820000	1.838844000	-2.208165000
H	2.227761000	-3.659206000	0.112173000
H	4.613549000	-0.051438000	-0.081238000
H	2.552488000	1.281953000	-0.172968000
H	-2.612999000	1.272279000	-0.202673000
H	-4.664029000	-0.075927000	-0.261887000
H	-2.263591000	-3.673873000	-0.072338000
H	0.735222000	2.782630000	3.047658000
H	-0.017524000	1.255400000	2.564184000
H	1.682720000	1.536813000	2.234787000

Neutral form of Complex 1 S0 B3LYP/TZVP/IEFPCM

C	1.101369000	3.853807000	0.824135000
C	1.238476000	4.444147000	-0.427658000
C	1.021552000	3.691114000	-1.576002000
C	0.668632000	2.351508000	-1.458796000
C	0.532863000	1.756051000	-0.202487000
C	0.748515000	2.509262000	0.965389000
C	0.145477000	0.315682000	-0.131145000
C	-1.243079000	-0.042109000	-0.103992000
C	-1.592385000	-1.406265000	-0.047717000
O	-0.641515000	-2.376332000	-0.024135000
C	0.690176000	-2.066291000	-0.052400000
C	1.097732000	-0.682997000	-0.111920000
C	1.574257000	-3.099797000	-0.028960000
C	2.997339000	-2.857491000	-0.050213000
C	3.411068000	-1.452922000	-0.109389000
C	2.516954000	-0.440472000	-0.135529000
C	-2.302491000	0.891881000	-0.123401000
C	-3.615719000	0.488877000	-0.091797000
C	-3.924278000	-0.882311000	-0.036790000

C	-2.911827000	-1.834568000	-0.017763000
O	3.836414000	-3.780547000	-0.022058000
C	0.614353000	1.898073000	2.337313000
O	-5.237305000	-1.212162000	-0.005956000
H	1.271888000	4.446005000	1.715697000
H	1.513910000	5.488884000	-0.503795000
H	1.125083000	4.139331000	-2.556184000
H	0.496982000	1.757983000	-2.348718000
H	1.218036000	-4.120651000	0.013660000
H	4.476223000	-1.256841000	-0.127584000
H	2.854367000	0.586636000	-0.179563000
H	-2.067967000	1.946414000	-0.166947000
H	-4.422855000	1.208634000	-0.106320000
H	-3.128374000	-2.894422000	0.022940000
H	0.764514000	2.651176000	3.110239000
H	-0.372770000	1.454442000	2.486324000
H	1.349090000	1.104696000	2.494855000
H	-5.352788000	-2.171042000	0.037317000

Neutral form of Complex 1 S1(110.19) B3LYP/TZVP/IEFPCM

C	-2.256615000	-3.378836000	0.764639000
C	-2.188956000	-4.100129000	-0.423409000
C	-1.444420000	-3.606264000	-1.488994000
C	-0.781569000	-2.392123000	-1.355439000
C	-0.853389000	-1.652087000	-0.167694000
C	-1.599679000	-2.156231000	0.918893000
C	-0.149706000	-0.350872000	-0.087871000
C	1.250933000	-0.271844000	-0.046567000
C	1.894976000	1.010060000	-0.003564000
O	1.159445000	2.155093000	-0.006872000
C	-0.196936000	2.104628000	-0.071618000
C	-0.899490000	0.895023000	-0.114583000
C	-0.830691000	3.346536000	-0.106500000
C	-2.280282000	3.443468000	-0.199321000
C	-2.986561000	2.190603000	-0.267178000
C	-2.317076000	0.993775000	-0.228656000
C	2.128346000	-1.398158000	-0.003288000
C	3.490636000	-1.251128000	0.046191000
C	4.075612000	0.035008000	0.066832000
C	3.268991000	1.166458000	0.045619000
O	-2.835841000	4.571292000	-0.219424000
C	-1.663592000	-1.424047000	2.234550000
O	5.430084000	0.092369000	0.113683000
H	-2.824772000	-3.776318000	1.597981000



H	-2.711538000	-5.044756000	-0.512173000
H	-1.381642000	-4.157862000	-2.418903000
H	-0.207763000	-1.998454000	-2.185879000
H	-0.243017000	4.253598000	-0.064727000
H	-4.065364000	2.220215000	-0.350946000
H	-2.880473000	0.071441000	-0.293095000
H	1.698055000	-2.389204000	-0.009958000
H	4.139823000	-2.116536000	0.079448000
H	3.689126000	2.164026000	0.070876000
H	-2.190854000	-2.017084000	2.981601000
H	-0.663172000	-1.206106000	2.615660000
H	-2.182802000	-0.466697000	2.140276000
H	5.734354000	1.010081000	0.127399000

Neutral form of Complex 1 S1(75.37) B3LYP/TZVP/IEFPCM

C	-1.555444000	-3.756766000	0.760887000
C	-2.132778000	-4.129761000	-0.447410000
C	-2.057902000	-3.273620000	-1.541809000
C	-1.401495000	-2.056011000	-1.413058000
C	-0.801909000	-1.678912000	-0.204308000
C	-0.887149000	-2.537853000	0.909937000
C	-0.102387000	-0.372727000	-0.128988000
C	1.297012000	-0.282412000	-0.119626000
C	1.932380000	1.003521000	-0.060452000
O	1.186957000	2.140837000	-0.016441000
C	-0.170354000	2.079413000	-0.034237000
C	-0.863999000	0.864177000	-0.095201000
C	-0.815848000	3.314360000	0.012440000
C	-2.269645000	3.397955000	0.015524000
C	-2.967464000	2.139485000	-0.031838000
C	-2.286581000	0.949202000	-0.079126000
C	2.182869000	-1.400130000	-0.190264000
C	3.545087000	-1.242923000	-0.181199000
C	4.120850000	0.045534000	-0.106989000
C	3.306030000	1.170407000	-0.051373000
O	-2.835093000	4.520043000	0.061180000
C	-0.289517000	-2.166959000	2.243904000
O	5.475769000	0.111212000	-0.102283000
H	-1.629011000	-4.420702000	1.614731000
H	-2.643492000	-5.081320000	-0.531428000
H	-2.504709000	-3.550731000	-2.488660000
H	-1.338323000	-1.387017000	-2.263194000
H	-0.235219000	4.226009000	0.053193000
H	-4.049692000	2.158804000	-0.022172000

H	-2.844091000	0.021974000	-0.108395000
H	1.758935000	-2.391995000	-0.259888000
H	4.201878000	-2.101397000	-0.236824000
H	3.719412000	2.170409000	-0.006070000
H	-0.674130000	-2.815430000	3.031119000
H	0.799568000	-2.265762000	2.237728000
H	-0.514681000	-1.132914000	2.510986000
H	5.774793000	1.029464000	-0.055886000

Anionic form of Complex 2 S0 B3LYP/TZVP/IEFPCM

C	-3.301922000	0.001964000	1.216869000
C	-4.024582000	-0.000412000	0.019845000
C	-3.343054000	-0.003163000	-1.195142000
C	-1.949833000	-0.003009000	-1.185315000
C	-1.222091000	-0.000351000	0.001158000
C	-1.911906000	0.002131000	1.230715000
C	0.271191000	-0.000197000	-0.054530000
C	0.977395000	-1.213263000	-0.086848000
C	2.405330000	-1.195354000	-0.140417000
O	3.073695000	0.000128000	-0.166143000
C	2.405013000	1.195458000	-0.140937000
C	0.977102000	1.213007000	-0.087325000
C	3.164112000	2.334618000	-0.172797000
C	2.554157000	3.637256000	-0.145268000
C	1.099550000	3.649477000	-0.088265000
C	0.366176000	2.503642000	-0.060055000
C	0.366895000	-2.504119000	-0.058658000
C	1.100616000	-3.649736000	-0.086207000
C	2.555251000	-3.637161000	-0.143144000
C	3.164760000	-2.334286000	-0.171684000
O	3.226184000	4.702174000	-0.170573000
C	-1.173686000	0.004479000	2.545672000
O	3.227574000	-4.701847000	-0.168742000
H	-3.853762000	0.003513000	2.149316000
H	-3.868346000	-0.005873000	-2.139086000
H	-1.421440000	-0.005156000	-2.131309000
H	4.243687000	2.261968000	-0.214767000
H	0.612611000	4.617512000	-0.066946000
H	-0.714589000	2.554027000	-0.018953000
H	-0.713831000	-2.554862000	-0.017460000
H	0.613974000	-4.617917000	-0.064300000
H	4.244306000	-2.261277000	-0.213796000
H	-1.871168000	0.005215000	3.382761000
H	-0.530117000	-0.873105000	2.641496000

H	-0.531247000	0.883133000	2.638980000
O	-5.382997000	-0.001152000	0.145433000
C	-6.176509000	-0.000865000	-1.042509000
H	-7.210887000	0.000080000	-0.708348000
H	-5.988265000	0.891678000	-1.644397000
H	-5.990365000	-0.894059000	-1.643943000

Anionic form of Complex **2** S1(74.25) B3LYP/TZVP/IEFPCM

C	3.342757000	0.315970000	1.177967000
C	4.052916000	0.000442000	0.016372000
C	3.357197000	-0.329536000	-1.145203000
C	1.964876000	-0.327319000	-1.118113000
C	1.237496000	-0.003822000	0.029656000
C	1.952445000	0.317129000	1.207250000
C	-0.244440000	-0.009251000	-0.012615000
C	-0.992131000	1.210196000	-0.025989000
C	-2.415080000	1.177680000	-0.081698000
O	-3.093598000	-0.018691000	-0.131101000
C	-2.403396000	-1.209580000	-0.162757000
C	-0.978901000	-1.231800000	-0.100534000
C	-3.165791000	-2.348834000	-0.244926000
C	-2.563324000	-3.657905000	-0.262411000
C	-1.116653000	-3.679919000	-0.179363000
C	-0.379542000	-2.527718000	-0.099310000
C	-0.401235000	2.509800000	-0.015643000
C	-1.147858000	3.658906000	-0.031440000
C	-2.595826000	3.627241000	-0.065666000
C	-3.188005000	2.313119000	-0.098957000
O	-3.253115000	-4.715703000	-0.338031000
C	1.235880000	0.639419000	2.493986000
O	-3.296799000	4.680297000	-0.074220000
H	3.904769000	0.551863000	2.074130000
H	3.872411000	-0.580101000	-2.061364000
H	1.428017000	-0.577335000	-2.025761000
H	-4.244991000	-2.270451000	-0.288980000
H	-0.628952000	-4.647899000	-0.174418000
H	0.699051000	-2.585940000	-0.033760000
H	0.679441000	2.574010000	-0.000210000
H	-0.667097000	4.630282000	-0.020459000
H	-4.266602000	2.227229000	-0.141864000
H	1.933797000	0.672239000	3.330607000
H	0.732562000	1.608487000	2.439755000
H	0.467337000	-0.104373000	2.714270000
O	5.414418000	0.037016000	0.121597000

C	6.194423000	-0.285023000	-1.030306000
H	7.232651000	-0.193417000	-0.721136000
H	6.004600000	-1.307937000	-1.365336000
H	5.997833000	0.410080000	-1.850521000

Anionic form of Complex 2 S1 (108.52) B3LYP/TZVP/IEFPCM

C	-3.354343000	0.206260000	1.178811000
C	-4.053314000	-0.080943000	0.003150000
C	-3.346473000	-0.349533000	-1.167472000
C	-1.954671000	-0.315604000	-1.134827000
C	-1.238626000	-0.019463000	0.027349000
C	-1.964563000	0.239002000	1.213611000
C	0.243135000	0.011517000	-0.009229000
C	1.006484000	-1.189171000	-0.141214000
C	2.430250000	-1.131181000	-0.197057000
O	3.092075000	0.073458000	-0.116961000
C	2.385419000	1.250748000	-0.023465000
C	0.961935000	1.247754000	0.027729000
C	3.131440000	2.403780000	0.006555000
C	2.508377000	3.701383000	0.088648000
C	1.059969000	3.697801000	0.118001000
C	0.340575000	2.531777000	0.086164000
C	0.437855000	-2.497874000	-0.192214000
C	1.202166000	-3.628527000	-0.313725000
C	2.648145000	-3.569401000	-0.390447000
C	3.219535000	-2.248229000	-0.319984000
O	3.184404000	4.770068000	0.124100000
C	-1.259767000	0.528221000	2.514621000
O	3.362894000	-4.607006000	-0.504328000
H	-3.924526000	0.394170000	2.081137000
H	-3.852835000	-0.576774000	-2.094586000
H	-1.409310000	-0.517815000	-2.049290000
H	4.211890000	2.344916000	-0.035275000
H	0.556433000	4.656493000	0.164739000
H	-0.741356000	2.570032000	0.099616000
H	-0.639246000	-2.583877000	-0.133023000
H	0.737414000	-4.607145000	-0.347985000
H	4.296710000	-2.142918000	-0.356873000
H	-1.960752000	0.511885000	3.349160000
H	-0.474207000	-0.204941000	2.708978000
H	-0.779746000	1.510427000	2.499890000
O	-5.415618000	-0.080539000	0.104381000
C	-6.184309000	-0.376340000	-1.062073000
H	-7.225344000	-0.321051000	-0.753714000

H	-6.001693000	0.354153000	-1.854283000
H	-5.969382000	-1.380907000	-1.435285000

Neutral form of Complex 2 S0 B3LYP/TZVP/IEFPCM

C	-3.419485000	-0.077870000	0.800559000
C	-4.021153000	-0.025866000	-0.456782000
C	-3.223754000	0.064001000	-1.600528000
C	-1.846667000	0.098481000	-1.470896000
C	-1.232966000	0.044847000	-0.214270000
C	-2.028003000	-0.045452000	0.937685000
C	0.256473000	0.072769000	-0.132812000
C	0.989027000	-1.160868000	-0.108463000
C	2.395724000	-1.117894000	-0.038505000
O	3.062532000	0.065153000	0.002854000
C	2.394100000	1.257728000	-0.027625000
C	0.952570000	1.264752000	-0.100476000
C	3.140850000	2.394310000	0.009666000
C	2.512986000	3.694015000	-0.010700000
C	1.049383000	3.701168000	-0.079425000
C	0.325769000	2.560799000	-0.117967000
C	0.387594000	-2.437936000	-0.151976000
C	1.139836000	-3.587533000	-0.126621000
C	2.541953000	-3.503228000	-0.056653000
C	3.174525000	-2.266287000	-0.013315000
O	3.166629000	4.756482000	0.027526000
C	-1.416615000	-0.093021000	2.315981000
O	3.224092000	-4.672999000	-0.037555000
H	-4.022690000	-0.143116000	1.695063000
H	-3.693996000	0.105098000	-2.574492000
H	-1.232326000	0.167348000	-2.360532000
H	4.220092000	2.335933000	0.062282000
H	0.564354000	4.669624000	-0.093719000
H	-0.754339000	2.598352000	-0.166736000
H	-0.690100000	-2.504187000	-0.209082000
H	0.673695000	-4.562893000	-0.161066000
H	4.252533000	-2.180631000	0.038391000
H	-2.186631000	-0.200045000	3.079182000
H	-0.722490000	-0.930146000	2.418564000
H	-0.853746000	0.818360000	2.531925000
H	4.177144000	-4.516599000	0.003132000
O	-5.366937000	-0.055841000	-0.666529000
C	-6.237641000	-0.149974000	0.463045000
H	-7.246186000	-0.161528000	0.057963000
H	-6.060729000	-1.070887000	1.023811000

H	-6.122153000	0.711305000	1.125405000
---	--------------	-------------	-------------

Neutral form of Complex 2 S1(75.05) CAM-B3LYP/TZVP/IEFPCM

C	-3.436022000	-0.252811000	0.745686000
C	-4.033550000	0.157274000	-0.437449000
C	-3.238640000	0.539213000	-1.514814000
C	-1.867509000	0.499284000	-1.392236000
C	-1.248859000	0.076142000	-0.213506000
C	-2.048109000	-0.296265000	0.870703000
C	0.228630000	0.044353000	-0.138107000
C	0.944043000	-1.158361000	-0.187019000
C	2.372472000	-1.148605000	-0.096141000
O	3.050333000	0.010705000	0.033046000
C	2.381616000	1.205280000	0.060932000
C	0.981925000	1.264827000	-0.027303000
C	3.169517000	2.319412000	0.175748000
C	2.581239000	3.647402000	0.230760000
C	1.143332000	3.699022000	0.153319000
C	0.400096000	2.564177000	0.036131000
C	0.342826000	-2.439718000	-0.340705000
C	1.086153000	-3.581799000	-0.383156000
C	2.490631000	-3.521017000	-0.277554000
C	3.128804000	-2.299751000	-0.137618000
O	3.303224000	4.659461000	0.340336000
C	-1.441059000	-0.734618000	2.174796000
O	3.153073000	-4.691908000	-0.328013000
H	-4.039425000	-0.538795000	1.595001000
H	-3.711137000	0.860408000	-2.433538000
H	-1.252670000	0.795926000	-2.233182000
H	4.244857000	2.222291000	0.234681000
H	0.671887000	4.672076000	0.197386000
H	-0.677907000	2.633833000	-0.015480000
H	-0.732462000	-2.493350000	-0.433567000
H	0.617658000	-4.549299000	-0.502951000
H	4.206167000	-2.228471000	-0.062354000
H	-2.192604000	-0.765773000	2.961872000
H	-1.003597000	-1.731736000	2.093298000
H	-0.643871000	-0.059635000	2.487301000
H	4.107083000	-4.558755000	-0.258090000
O	-5.375207000	0.223261000	-0.631960000
C	-6.236428000	-0.151703000	0.433223000
H	-7.248105000	-0.026489000	0.058538000
H	-6.082821000	-1.194326000	0.718559000
H	-6.091635000	0.490240000	1.304454000

Neutral form of Complex 2 S1(109.80) CAM-B3LYP/TZVP/IEFPCM

C	-3.463798000	0.052427000	0.732319000
C	-4.010315000	-0.410529000	-0.457472000
C	-3.171231000	-0.758988000	-1.511755000
C	-1.807794000	-0.632077000	-1.362871000
C	-1.240702000	-0.155808000	-0.178004000
C	-2.085615000	0.183265000	0.884208000
C	0.227383000	-0.020157000	-0.078203000
C	1.065459000	-1.142333000	-0.015226000
C	2.485324000	-0.975527000	0.024945000
O	3.040964000	0.254362000	-0.000084000
C	2.250972000	1.369572000	-0.078205000
C	0.851375000	1.276409000	-0.117921000
C	2.919880000	2.564054000	-0.121831000
C	2.198233000	3.821485000	-0.221581000
C	0.762681000	3.716186000	-0.285301000
C	0.140283000	2.506229000	-0.235974000
C	0.599313000	-2.486203000	0.045866000
C	1.458400000	-3.542919000	0.115286000
C	2.850529000	-3.327073000	0.137083000
C	3.358511000	-2.039554000	0.092656000
O	2.812314000	4.907589000	-0.251609000
C	-1.527600000	0.656320000	2.196935000
O	3.633661000	-4.420226000	0.209078000
H	-4.101661000	0.310438000	1.565246000
H	-3.603836000	-1.120320000	-2.435193000
H	-1.158256000	-0.898161000	-2.187649000
H	4.000303000	2.584208000	-0.081923000
H	0.194271000	4.632922000	-0.371650000
H	-0.938947000	2.457304000	-0.294363000
H	-0.466676000	-2.660127000	0.039503000
H	1.091087000	-4.559001000	0.165283000
H	4.423812000	-1.849701000	0.116422000
H	-2.315710000	0.762977000	2.940271000
H	-0.785341000	-0.044217000	2.582229000
H	-1.030486000	1.622924000	2.093788000
H	4.568913000	-4.180234000	0.227365000
O	-5.340638000	-0.559606000	-0.677605000
C	-6.246334000	-0.213548000	0.360478000
H	-7.240185000	-0.403754000	-0.033947000
H	-6.085747000	-0.829020000	1.247792000
H	-6.158514000	0.841608000	0.626850000

Anionic form of Complex **3** S0 B3LYP/TZVP/IEFPCM

C	-3.587789000	-0.001384000	1.027784000
C	-4.260647000	-0.000383000	-0.193433000
C	-3.575464000	0.000621000	-1.404489000
C	-2.177244000	0.000713000	-1.355117000
C	-1.477485000	-0.000278000	-0.153221000
C	-2.194990000	-0.001351000	1.056330000
C	0.015895000	0.000040000	-0.151765000
C	0.720435000	-1.213227000	-0.161088000
C	2.149093000	-1.194970000	-0.168961000
O	2.817795000	0.000689000	-0.174694000
C	2.148548000	1.196039000	-0.168504000
C	0.719876000	1.213643000	-0.160594000
C	2.907866000	2.335550000	-0.172301000
C	2.296866000	3.637926000	-0.161765000
C	0.841230000	3.649675000	-0.150364000
C	0.107685000	2.503636000	-0.149328000
C	0.108829000	-2.503502000	-0.150403000
C	0.842892000	-3.649208000	-0.151959000
C	2.298527000	-3.636791000	-0.163189000
C	2.908932000	-2.334129000	-0.173320000
O	2.969046000	4.703138000	-0.162916000
O	2.971196000	-4.701690000	-0.164596000
H	-4.158864000	-0.002035000	1.945195000
H	-5.344682000	-0.000322000	-0.190420000
H	-1.612216000	0.001680000	-2.280973000
H	3.988249000	2.263295000	-0.179760000
H	0.353486000	4.617472000	-0.142280000
H	-0.973851000	2.554065000	-0.142436000
H	-0.972686000	-2.554418000	-0.143602000
H	0.355597000	-4.617236000	-0.144278000
H	3.989281000	-2.261371000	-0.180683000
O	-1.448768000	-0.002144000	2.199548000
C	-2.125455000	-0.002537000	3.456954000
H	-2.744273000	-0.895564000	3.574085000
H	-1.344385000	-0.002764000	4.212942000
H	-2.744293000	0.890404000	3.574617000
C	-4.300716000	0.000749000	-2.726883000
H	-4.050960000	-0.884045000	-3.318298000
H	-5.381416000	0.011407000	-2.581871000
H	-4.034442000	0.874490000	-3.327293000

Anionic form of Complex **3** S1(65.00)TZVP/IEFPCM

C	-3.660796000	-0.499304000	0.786024000
---	--------------	--------------	-------------



C	-4.288227000	0.226163000	-0.226336000
C	-3.549875000	0.911018000	-1.188772000
C	-2.157982000	0.842657000	-1.105432000
C	-1.487276000	0.119994000	-0.111773000
C	-2.270834000	-0.553384000	0.854214000
C	-0.013248000	0.077464000	-0.082629000
C	0.702013000	-1.149546000	-0.288004000
C	2.124326000	-1.155960000	-0.292591000
O	2.840151000	0.004683000	-0.113040000
C	2.187553000	1.204173000	0.055378000
C	0.762749000	1.266945000	0.080880000
C	2.989463000	2.309142000	0.206339000
C	2.433088000	3.618705000	0.426122000
C	0.985535000	3.676899000	0.487621000
C	0.209586000	2.560150000	0.331054000
C	0.076814000	-2.405332000	-0.549072000
C	0.789564000	-3.558113000	-0.744350000
C	2.238189000	-3.573108000	-0.713677000
C	2.867036000	-2.297294000	-0.482785000
O	3.156965000	4.646070000	0.566786000
O	2.908630000	-4.631163000	-0.888059000
H	-4.267442000	-1.004922000	1.523815000
H	-5.371542000	0.255107000	-0.255334000
H	-1.561040000	1.356750000	-1.850807000
H	4.066107000	2.196787000	0.176556000
H	0.530086000	4.642016000	0.677561000
H	-0.866694000	2.647295000	0.394621000
H	-1.003829000	-2.434599000	-0.588750000
H	0.281115000	-4.495467000	-0.937847000
H	3.948391000	-2.241071000	-0.474899000
O	-1.585426000	-1.205757000	1.839713000
C	-2.322882000	-1.926257000	2.825635000
H	-2.925618000	-2.717837000	2.373000000
H	-1.580822000	-2.369989000	3.484813000
H	-2.969749000	-1.261772000	3.404440000
C	-4.222268000	1.670950000	-2.305639000
H	-4.203472000	1.102912000	-3.240643000
H	-5.266987000	1.877087000	-2.068838000
H	-3.723790000	2.623443000	-2.497263000

Anionic form of Complex **3** S1(118.74)/IEFPCM

C	-3.634313000	0.523243000	0.959559000
C	-4.288454000	0.200958000	-0.228406000
C	-3.577240000	-0.180078000	-1.364812000

C	-2.185215000	-0.214576000	-1.274723000
C	-1.487074000	0.109572000	-0.104419000
C	-2.243888000	0.472965000	1.033092000
C	-0.013232000	0.068921000	-0.076671000
C	0.702460000	-1.144524000	-0.320223000
C	2.128776000	-1.146410000	-0.336925000
O	2.840668000	0.008421000	-0.107778000
C	2.183987000	1.197471000	0.108038000
C	0.763109000	1.259364000	0.123024000
C	2.983238000	2.300662000	0.294228000
C	2.419502000	3.610989000	0.498395000
C	0.972136000	3.677700000	0.476601000
C	0.202308000	2.560601000	0.291208000
C	0.084766000	-2.419683000	-0.502701000
C	0.803716000	-3.562309000	-0.728710000
C	2.252823000	-3.557659000	-0.781949000
C	2.874382000	-2.277358000	-0.564671000
O	3.142293000	4.633784000	0.673737000
O	2.924232000	-4.608148000	-0.993722000
H	-4.220457000	0.803550000	1.823209000
H	-5.370973000	0.250640000	-0.260337000
H	-1.608534000	-0.483834000	-2.152716000
H	4.060437000	2.192227000	0.273655000
H	0.511728000	4.650544000	0.603805000
H	-0.875236000	2.653966000	0.272309000
H	-0.994900000	-2.470371000	-0.460618000
H	0.300034000	-4.512924000	-0.861313000
H	3.955433000	-2.214097000	-0.566001000
O	-1.535803000	0.735683000	2.171695000
C	-2.244865000	1.136160000	3.342940000
H	-2.933488000	0.356277000	3.678459000
H	-1.487735000	1.300201000	4.105777000
H	-2.798533000	2.063757000	3.176210000
C	-4.282669000	-0.557238000	-2.644176000
H	-4.472596000	-1.634088000	-2.689678000
H	-5.246847000	-0.053153000	-2.728612000
H	-3.685539000	-0.296321000	-3.519696000

Neutral form of Complex 3 S0 B3LYP/TZVP/IEFPCM

C	-3.578280000	-0.523939000	0.995410000
C	-4.268108000	-0.314800000	-0.197559000
C	-3.609189000	0.031942000	-1.373563000
C	-2.218307000	0.165660000	-1.318814000
C	-1.502431000	-0.041221000	-0.143666000

C	-2.192449000	-0.390129000	1.031328000
C	-0.018316000	0.092129000	-0.134175000
C	0.799129000	-1.083815000	-0.215765000
C	2.200064000	-0.938783000	-0.221546000
O	2.781800000	0.287344000	-0.154376000
C	2.029095000	1.426486000	-0.082840000
C	0.589046000	1.330151000	-0.072706000
C	2.693698000	2.612285000	-0.027079000
C	1.975265000	3.860806000	0.065187000
C	0.513825000	3.762058000	0.091815000
C	-0.128005000	2.574604000	0.030643000
C	0.289605000	-2.397768000	-0.304001000
C	1.122711000	-3.487647000	-0.381752000
C	2.516861000	-3.302241000	-0.379021000
C	3.059883000	-2.025598000	-0.299150000
O	2.552917000	4.965714000	0.122206000
O	3.282367000	-4.416846000	-0.460337000
H	-4.130183000	-0.785977000	1.886538000
H	-5.346441000	-0.424818000	-0.200459000
H	-1.672761000	0.433773000	-2.216832000
H	3.775553000	2.631094000	-0.040214000
H	-0.038336000	4.690689000	0.170042000
H	-1.208674000	2.534386000	0.055186000
H	-0.781858000	-2.542003000	-0.311437000
H	0.726801000	-4.491880000	-0.449082000
H	4.130073000	-1.862213000	-0.299771000
H	4.222223000	-4.190759000	-0.454978000
C	-4.354842000	0.251393000	-2.665862000
H	-4.075316000	-0.492381000	-3.416779000
H	-5.432274000	0.182452000	-2.513506000
H	-4.136683000	1.234717000	-3.089304000
O	-1.427502000	-0.563938000	2.146641000
C	-2.070614000	-0.935751000	3.367544000
H	-2.582639000	-1.895743000	3.267904000
H	-1.276356000	-1.023466000	4.104242000
H	-2.781621000	-0.170996000	3.688820000

Neutral form of Complex **3** S1(67.20) CAM-B3LYP/TZVP/IEFPCM

C	1.133294000	3.759516000	0.811017000
C	1.515080000	4.299214000	-0.407234000
C	1.493724000	3.546598000	-1.573784000
C	1.077895000	2.224936000	-1.476816000
C	0.678598000	1.650953000	-0.273798000
C	0.715625000	2.436920000	0.887108000

C	0.245909000	0.241047000	-0.229581000
C	-1.076185000	-0.116835000	0.069247000
C	-1.457584000	-1.494515000	0.093263000
O	-0.561320000	-2.468043000	-0.169758000
C	0.738261000	-2.151852000	-0.462857000
C	1.178338000	-0.819683000	-0.508852000
C	1.560677000	-3.219445000	-0.707411000
C	2.967921000	-3.024063000	-1.010664000
C	3.417797000	-1.655538000	-1.033293000
C	2.563056000	-0.625182000	-0.786781000
C	-2.117961000	0.816665000	0.329849000
C	-3.389500000	0.415395000	0.611966000
C	-3.712310000	-0.956618000	0.641443000
C	-2.741294000	-1.907811000	0.379963000
O	3.715103000	-3.999427000	-1.230184000
O	-4.989766000	-1.272579000	0.926410000
H	1.173112000	4.375926000	1.696728000
H	1.840647000	5.332120000	-0.441861000
H	1.050669000	1.612297000	-2.370725000
H	1.169873000	-4.226860000	-0.666366000
H	4.463498000	-1.473562000	-1.243659000
H	2.934521000	0.389934000	-0.804038000
H	-1.882271000	1.870265000	0.301097000
H	-4.172343000	1.135622000	0.807550000
H	-2.967227000	-2.966302000	0.385478000
H	-5.124387000	-2.228877000	0.918046000
C	1.875513000	4.147418000	-2.898269000
H	1.024772000	4.654085000	-3.359832000
H	2.669937000	4.884931000	-2.782803000
H	2.219136000	3.383694000	-3.595661000
O	0.347776000	1.826894000	2.043358000
C	0.357625000	2.582983000	3.244850000
H	-0.327735000	3.430827000	3.185403000
H	0.025526000	1.905983000	4.026494000
H	1.361839000	2.941188000	3.480118000

Neutral form of Complex 3 S1(119.15) CAM-B3LYP/TZVP/IEFPCM

C	-3.691682000	-0.197392000	0.779371000
C	-4.166569000	-1.014872000	-0.235863000
C	-3.317267000	-1.553955000	-1.192550000
C	-1.967559000	-1.236416000	-1.107004000
C	-1.453911000	-0.413166000	-0.108711000
C	-2.338847000	0.100100000	0.853861000
C	-0.021122000	-0.081545000	-0.070798000

C	0.961688000	-1.073292000	0.080020000
C	2.344788000	-0.719108000	0.045457000
O	2.732517000	0.561059000	-0.137940000
C	1.799587000	1.549067000	-0.300416000
C	0.424693000	1.275679000	-0.266130000
C	2.306390000	2.807694000	-0.494990000
C	1.426159000	3.943147000	-0.706427000
C	0.015793000	3.649348000	-0.698602000
C	-0.442311000	2.384227000	-0.494930000
C	0.686364000	-2.448701000	0.322846000
C	1.681752000	-3.368520000	0.473619000
C	3.031420000	-2.972258000	0.407842000
C	3.356727000	-1.644152000	0.194711000
O	1.892045000	5.087602000	-0.884032000
O	3.957385000	-3.937666000	0.568509000
H	-4.383810000	0.195909000	1.509032000
H	-5.227020000	-1.233032000	-0.277099000
H	-1.284342000	-1.623042000	-1.854284000
H	3.375872000	2.967215000	-0.503238000
H	-0.669820000	4.469744000	-0.865670000
H	-1.506847000	2.197831000	-0.502182000
H	-0.344352000	-2.763408000	0.390611000
H	1.455232000	-4.409328000	0.661257000
H	4.385542000	-1.310883000	0.153318000
H	4.851905000	-3.577011000	0.520280000
C	-3.831968000	-2.461560000	-2.275392000
H	-3.738610000	-3.510722000	-1.985365000
H	-4.884831000	-2.271308000	-2.482147000
H	-3.273916000	-2.328978000	-3.202326000
O	-1.781334000	0.859680000	1.829697000
C	-2.632078000	1.459782000	2.795811000
H	-3.157151000	0.703898000	3.382902000
H	-1.983148000	2.035875000	3.448735000
H	-3.357443000	2.125749000	2.324520000

Anionic form of Complex 4 S0 B3LYP/TZVP/IEFPCM

C	3.192625000	-0.000742000	1.491133000
C	4.009541000	-0.000332000	0.357917000
C	3.439134000	0.000195000	-0.909748000
C	2.046067000	0.000288000	-1.031084000
C	1.226444000	-0.000114000	0.087911000
C	1.807548000	-0.000647000	1.370329000
C	-0.258711000	0.000035000	-0.073449000
C	-0.956776000	1.213872000	-0.157148000
C	-2.377215000	1.195873000	-0.312436000

O	-3.042185000	0.000364000	-0.384654000
C	-2.377470000	-1.195268000	-0.312795000
C	-0.957013000	-1.213602000	-0.157516000
C	-3.132259000	-2.334446000	-0.397556000
C	-2.525531000	-3.636996000	-0.327166000
C	-1.078287000	-3.649325000	-0.167845000
C	-0.348777000	-2.503653000	-0.087282000
C	-0.348306000	2.503771000	-0.086507000
C	-1.077612000	3.649618000	-0.166724000
C	-2.524834000	3.637614000	-0.326073000
C	-3.131813000	2.335208000	-0.396855000
O	-3.194109000	-4.701853000	-0.398772000
O	-3.193229000	4.702629000	-0.397360000
H	3.660708000	-0.001119000	2.464839000
H	5.081682000	-0.000446000	0.491439000
H	1.608250000	0.000675000	-2.021499000
H	-4.206183000	-2.262000000	-0.515544000
H	-0.594132000	-4.617492000	-0.113975000
H	0.726479000	-2.554377000	0.029328000
H	0.726956000	2.554309000	0.030123000
H	-0.593247000	4.617660000	-0.112561000
H	-4.205745000	2.262976000	-0.514884000
O	0.938644000	-0.001025000	2.426540000
C	1.476474000	-0.001972000	3.748271000
H	2.079625000	0.890850000	3.932586000
H	0.619326000	-0.002478000	4.416928000
H	2.079673000	-0.895022000	3.931291000
O	4.141206000	0.000550000	-2.084876000
C	5.566590000	0.000538000	-2.018110000
H	5.912945000	0.001044000	-3.048621000
H	5.941043000	0.892994000	-1.509618000
H	5.941087000	-0.892386000	-1.510462000

Anionic form of Complex 4 S1(64.40) B3LYP/TZVP/IEFPCM

C	3.237599000	0.429523000	1.426849000
C	4.040737000	0.009575000	0.361909000
C	3.444052000	-0.429774000	-0.814805000
C	2.051952000	-0.435328000	-0.916109000
C	1.230374000	-0.015197000	0.131601000
C	1.851934000	0.417511000	1.329242000
C	-0.236243000	-0.034825000	-0.017554000
C	-1.003779000	1.177414000	0.013175000
C	-2.414979000	1.134843000	-0.159214000

O	-3.068969000	-0.057046000	-0.365608000
C	-2.360358000	-1.233623000	-0.443979000
C	-0.944567000	-1.251016000	-0.269966000
C	-3.101173000	-2.365727000	-0.681997000
C	-2.487329000	-3.666057000	-0.750516000
C	-1.052498000	-3.687515000	-0.540125000
C	-0.337946000	-2.543960000	-0.306951000
C	-0.436459000	2.478686000	0.156147000
C	-1.197306000	3.616489000	0.178813000
C	-2.639114000	3.572510000	0.038587000
C	-3.205628000	2.259570000	-0.139531000
O	-3.152893000	-4.718705000	-0.968933000
O	-3.353006000	4.615844000	0.059043000
H	3.720769000	0.752833000	2.337682000
H	5.114531000	0.031526000	0.477823000
H	1.605135000	-0.760325000	-1.847347000
H	-4.174129000	-2.286024000	-0.805218000
H	-0.557555000	-4.651502000	-0.560155000
H	0.729508000	-2.608772000	-0.145019000
H	0.638164000	2.555002000	0.253677000
H	-0.732947000	4.589175000	0.291609000
H	-4.275829000	2.165630000	-0.275440000
O	1.013843000	0.772728000	2.351459000
C	1.587719000	1.242541000	3.568710000
H	2.185106000	2.143752000	3.406236000
H	0.750268000	1.477690000	4.221129000
H	2.208101000	0.474986000	4.039416000
O	4.126168000	-0.861549000	-1.923840000
C	5.551480000	-0.856731000	-1.880758000
H	5.880817000	-1.227230000	-2.848548000
H	5.942484000	0.152992000	-1.727929000
H	5.929132000	-1.515526000	-1.093985000

Anionic form of Complex 4 S1(119.02) B3LYP/TZVP/IEFPCM

C	-3.313724000	-0.174997000	1.328861000
C	-4.001943000	-0.664885000	0.214493000
C	-3.305936000	-0.924841000	-0.960996000
C	-1.932174000	-0.683290000	-1.011184000
C	-1.225279000	-0.189019000	0.086707000
C	-1.945215000	0.058843000	1.281805000
C	0.225515000	0.054264000	-0.009255000
C	1.142244000	-1.003967000	-0.299680000
C	2.537321000	-0.731633000	-0.420391000

O	3.026803000	0.543258000	-0.254407000
C	2.169197000	1.589671000	-0.008817000
C	0.768253000	1.377154000	0.114125000
C	2.750214000	2.831168000	0.099564000
C	1.958331000	4.013536000	0.326173000
C	0.527816000	3.798922000	0.416090000
C	-0.021457000	2.549936000	0.305188000
C	0.772391000	-2.378079000	-0.426773000
C	1.681919000	-3.365068000	-0.693594000
C	3.096127000	-3.083358000	-0.849456000
C	3.470870000	-1.702552000	-0.690569000
O	2.477896000	5.161694000	0.427710000
O	3.941223000	-3.990454000	-1.097717000
H	-3.870384000	0.006052000	2.237127000
H	-5.065740000	-0.836050000	0.291827000
H	-1.410414000	-0.871094000	-1.941228000
H	3.823599000	2.931838000	-0.002145000
H	-0.102329000	4.668230000	0.563372000
H	-1.095084000	2.433321000	0.367374000
H	-0.271237000	-2.636058000	-0.307729000
H	1.363998000	-4.397392000	-0.782372000
H	4.516259000	-1.431158000	-0.769852000
O	-1.210186000	0.493716000	2.351446000
C	-1.889715000	0.782586000	3.570677000
H	-2.378227000	-0.107925000	3.975547000
H	-1.124083000	1.119671000	4.265258000
H	-2.631298000	1.574661000	3.436011000
O	-3.871771000	-1.402766000	-2.115643000
C	-5.276532000	-1.647572000	-2.124688000
H	-5.509734000	-2.012397000	-3.122120000
H	-5.554053000	-2.406639000	-1.388178000
H	-5.842273000	-0.731571000	-1.933207000

Neutral form of Complex 4 S0 B3LYP/TZVP/IEFPCM

C	-3.194270000	-0.506373000	1.448541000
C	-4.016918000	-0.339704000	0.332476000
C	-3.460483000	-0.030718000	-0.903954000
C	-2.073688000	0.109357000	-1.011890000
C	-1.249320000	-0.056995000	0.091860000
C	-1.814847000	-0.369220000	1.342432000
C	0.227502000	0.085240000	-0.053372000
C	1.039277000	-1.086577000	-0.207065000
C	2.430735000	-0.932489000	-0.362658000



O	3.007006000	0.298089000	-0.369632000
C	2.258337000	1.433044000	-0.225706000
C	0.827683000	1.327556000	-0.064996000
C	2.916262000	2.623490000	-0.246975000
C	2.201830000	3.867787000	-0.087980000
C	0.751352000	3.759719000	0.089126000
C	0.115264000	2.567845000	0.102000000
C	0.532970000	-2.404678000	-0.223612000
C	1.361341000	-3.490108000	-0.377434000
C	2.746331000	-3.295652000	-0.526881000
C	3.285133000	-2.014671000	-0.519769000
O	2.774078000	4.976712000	-0.096907000
O	3.507788000	-4.405675000	-0.677526000
H	-3.652530000	-0.743003000	2.397883000
H	-5.084349000	-0.454355000	0.453531000
H	-1.646046000	0.348369000	-1.977426000
H	3.990676000	2.649764000	-0.372800000
H	0.203402000	4.685284000	0.217074000
H	-0.956973000	2.521020000	0.237061000
H	-0.531976000	-2.555929000	-0.113604000
H	0.968272000	-4.497619000	-0.389785000
H	4.347981000	-1.844791000	-0.635618000
H	4.440597000	-4.172497000	-0.778425000
O	-0.937451000	-0.506670000	2.380761000
C	-1.456176000	-0.828439000	3.671758000
H	-1.974696000	-1.790387000	3.662200000
H	-0.593548000	-0.889334000	4.330253000
H	-2.133570000	-0.050019000	4.031506000
O	-4.169489000	0.154660000	-2.058436000
C	-5.590281000	0.025687000	-2.006475000
H	-5.942657000	0.212712000	-3.017703000
H	-5.886961000	-0.980689000	-1.699522000
H	-6.031282000	0.759931000	-1.327253000

Neutral form of Complex **4** S1(67.15) CAM-B3LYP/TZVP/IEFPCM

C	-3.199758000	-0.650003000	1.407372000
C	-4.028973000	-0.313327000	0.342334000
C	-3.477326000	0.133453000	-0.846397000
C	-2.094981000	0.235753000	-0.957822000
C	-1.254447000	-0.102171000	0.090406000
C	-1.823603000	-0.547093000	1.297032000
C	0.207337000	0.027642000	-0.063203000
C	1.050960000	-1.091992000	-0.061536000
C	2.462114000	-0.924882000	-0.216685000

O	3.003200000	0.301304000	-0.370876000
C	2.206230000	1.414212000	-0.379181000
C	0.812762000	1.322004000	-0.234862000
C	2.863548000	2.605034000	-0.541103000
C	2.138797000	3.863942000	-0.545418000
C	0.711718000	3.763295000	-0.372575000
C	0.100433000	2.556906000	-0.218868000
C	0.597646000	-2.435371000	0.057263000
C	1.462161000	-3.488964000	0.052818000
C	2.848679000	-3.271463000	-0.082470000
C	3.342783000	-1.985741000	-0.219646000
O	2.741920000	4.947224000	-0.688220000
O	3.636060000	-4.363441000	-0.076444000
H	-3.653874000	-0.988887000	2.326504000
H	-5.097625000	-0.405649000	0.466333000
H	-1.675840000	0.578922000	-1.895018000
H	3.938677000	2.620783000	-0.655757000
H	0.140612000	4.682271000	-0.357922000
H	-0.971406000	2.517429000	-0.084014000
H	-0.463164000	-2.613603000	0.154707000
H	1.104276000	-4.505569000	0.143720000
H	4.401119000	-1.792963000	-0.337227000
H	4.567243000	-4.126514000	-0.174604000
O	-0.956297000	-0.837733000	2.303959000
C	-1.483959000	-1.296721000	3.538124000
H	-2.035114000	-2.231007000	3.411166000
H	-0.628291000	-1.468989000	4.184544000
H	-2.135884000	-0.548346000	3.993706000
O	-4.194338000	0.487094000	-1.949814000
C	-5.608389000	0.394243000	-1.885293000
H	-5.976248000	0.715942000	-2.855356000
H	-5.930783000	-0.632703000	-1.699403000
H	-6.014317000	1.048431000	-1.110483000

Neutral form of Complex **4** S1(118.54) CAM-B3LYP/TZVP/IEFPCM

C	3.250024000	-0.694876000	1.306617000
C	4.041943000	-0.163237000	0.293621000
C	3.448207000	0.445835000	-0.799519000
C	2.061477000	0.511399000	-0.872751000
C	1.256295000	-0.020022000	0.123121000
C	1.870405000	-0.624792000	1.235889000
C	-0.210085000	0.043133000	0.012409000
C	-0.893519000	1.268291000	-0.043364000
C	-2.310869000	1.286554000	-0.219057000

O	-3.013267000	0.139885000	-0.338440000
C	-2.374851000	-1.069708000	-0.296256000
C	-0.987534000	-1.163511000	-0.116127000
C	-3.185048000	-2.166029000	-0.440461000
C	-2.632017000	-3.508833000	-0.441652000
C	-1.202643000	-3.595276000	-0.283027000
C	-0.438176000	-2.479126000	-0.136354000
C	-0.277580000	2.542084000	0.113400000
C	-0.993604000	3.701172000	0.059245000
C	-2.387105000	3.667028000	-0.142137000
C	-3.040965000	2.455027000	-0.277919000
O	-3.373209000	-4.504082000	-0.576658000
O	-3.024613000	4.852900000	-0.185238000
H	3.735459000	-1.155631000	2.153943000
H	5.115701000	-0.234999000	0.381528000
H	1.610259000	0.973022000	-1.741460000
H	-4.251462000	-2.039743000	-0.567180000
H	-0.754422000	-4.580146000	-0.290458000
H	0.632354000	-2.579771000	-0.026573000
H	0.788328000	2.581780000	0.281238000
H	-0.510720000	4.661028000	0.182737000
H	-4.112587000	2.401003000	-0.419990000
H	-3.973740000	4.735395000	-0.318885000
O	1.031481000	-1.086507000	2.200025000
C	1.590630000	-1.763892000	3.314884000
H	2.243227000	-1.104401000	3.890567000
H	0.751163000	-2.067932000	3.933175000
H	2.149862000	-2.647694000	3.000992000
O	4.128321000	0.994063000	-1.845158000
C	5.545576000	0.932112000	-1.826965000
H	5.879903000	1.413340000	-2.741533000
H	5.955762000	1.466829000	-0.967400000
H	5.897455000	-0.101862000	-1.813685000