

**Electronic Supplementary Information**  
**Intermolecular Proton Shuttling in Excited State Proton Transfer**  
**Reactions : Insights from Theory**

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C	-4.06643800	-0.89778500	-0.04254900
C	-1.68477000	-0.94216300	-0.49427000
C	-1.55212900	-2.26157400	-0.00101600
C	-2.75220600	-2.89778900	0.47733600
C	-3.95101900	-2.25384700	0.45809900
H	-0.75703700	0.79187400	-1.36208800
C	-0.61279000	-0.21572700	-0.98961600
C	-0.25416300	-2.82541600	-0.02502700
C	0.82990500	-2.11793200	-0.50826900
C	0.66386900	-0.79732000	-1.00028100
H	-0.09873700	-3.83218400	0.34348100
H	1.81709200	-2.56596000	-0.51046600
O	-2.90444800	-0.30885300	-0.50324800
C	-2.69396100	-4.31323600	1.01645200
O	1.67691900	-0.07163500	-1.47874900
H	2.58195400	-0.55083900	-1.44080000
F	-3.89880500	-4.76542800	1.42446800
F	-2.24177500	-5.18524900	0.07928200
F	-1.85599900	-4.40757800	2.08033200
H	-4.86314400	-2.71297100	0.81335100
O	-5.08956300	-0.23662800	-0.08991200
N	4.09712000	-1.13489200	-1.36614900
C	5.01489600	-0.59032800	-0.57615400
N	6.22042900	-1.19197600	-0.74713900
C	6.05918400	-2.17705700	-1.70316100
C	4.73955000	-2.12731500	-2.07652800
H	4.22210200	-2.73403700	-2.80549900
H	4.84507400	0.23085200	0.11530400
C	7.45806600	-0.85447400	-0.05200700
H	7.81749600	-1.71285600	0.52142500
H	8.22418800	-0.55082100	-0.76995400
H	7.26168300	-0.02689300	0.63015000
H	6.87719100	-2.80433100	-2.02263500
C	3.28873800	3.71610300	2.58349400
H	3.16541200	4.50937400	3.30545700
C	4.30791900	2.82057900	2.35796300
H	5.24390100	2.72853800	2.89137200
C	2.78934100	2.38629500	0.90158600
H	2.22375400	1.95166900	0.08746900
N	3.98898800	1.99128000	1.30388500

N	2.32018200	3.42892500	1.64361900
C	1.03772000	4.10996400	1.49016000
H	0.43492600	3.98839400	2.39433600
H	1.19872700	5.17582800	1.30732300
H	0.48796700	3.69118600	0.64663100
C	-3.78235000	5.17749500	-1.11321200
H	-4.52318300	5.90649500	-1.40575000
N	-4.11021900	3.85920100	-0.87244400
N	-1.91253100	4.04262600	-0.53590300
C	-2.95306200	3.22401200	-0.52998000
C	-2.42554500	5.26948600	-0.90103700
H	-1.79592300	6.14370100	-0.99332700
H	-2.93395900	2.16831200	-0.29926600
C	-5.43491500	3.25369300	-0.96388500
H	-6.11929500	3.73050300	-0.25642100
H	-5.83176700	3.36323200	-1.97707000
H	-5.35528500	2.19201800	-0.72415300

**Ground state minimum energy Cartesian coordinate of 1, Reagent.**

C	-4.15073600	-0.55446200	-0.33575100
C	-1.76924300	-0.91005300	-0.60183500
C	-1.80324700	-2.17519700	-0.01501300
C	-3.13289400	-2.68750900	0.42451400
C	-4.22547900	-1.85127000	0.25282000
H	-0.57333000	0.64684700	-1.50922500
C	-0.56686500	-0.33779600	-1.05556200
C	-0.56474000	-2.86352300	0.11429100
C	0.63841600	-2.33514600	-0.31715000
C	0.68135200	-1.04084800	-0.92320200
H	-0.56577600	-3.84660100	0.57169800
H	1.56006400	-2.89415200	-0.19397100
O	-2.87328200	-0.12870500	-0.77918800
C	-3.26522100	-4.01142000	1.04089300
O	1.76108400	-0.47498900	-1.34866500
H	3.17234400	-1.05603100	-1.31599200
F	-4.54275100	-4.33221100	1.35599600
F	-2.79107700	-5.04258200	0.24571800
F	-2.53372100	-4.15361000	2.21287400
H	-5.21564000	-2.15757500	0.56834300
O	-5.07101000	0.25379000	-0.50906500
N	4.21583900	-1.33576800	-1.29858400
C	5.13086700	-0.72920100	-0.54135200
N	6.31985600	-1.31621600	-0.76006200
C	6.14897500	-2.32984200	-1.68996300
C	4.82459200	-2.33615500	-2.02460600
H	4.27849600	-2.96178600	-2.71237300
H	4.93372000	0.10810100	0.13426200
C	7.58280700	-0.94498300	-0.11895900
H	7.97153500	-1.79262700	0.44881800
H	8.30764600	-0.64455800	-0.87795500
H	7.39920400	-0.11002900	0.55626100
H	6.97006100	-2.94352100	-2.02436100
C	3.48291600	3.33000800	2.63151300
H	3.39244900	4.08502000	3.39777200
C	4.50131600	2.46849600	2.30000400
H	5.47169000	2.37215000	2.76665400
C	2.89695200	2.07473700	0.92109300
H	2.28801300	1.66405800	0.12583400
N	4.12815100	1.68556300	1.22788200

N	2.46214000	3.07045900	1.74030000
C	1.15064500	3.71506300	1.71970600
H	0.55125700	3.38402800	2.57259200
H	1.27578500	4.79930000	1.76828500
H	0.62289700	3.46838700	0.79717400
C	-3.27159400	5.41967700	-0.90431200
H	-3.93469800	6.25974800	-1.04728400
N	-3.73679000	4.12191300	-0.85601000
N	-1.52461800	4.01717500	-0.59233200
C	-2.64974200	3.32107700	-0.66822700
C	-1.90775100	5.33377300	-0.74013000
H	-1.18798000	6.14071100	-0.72262200
H	-2.74329300	2.24577100	-0.60458300
C	-5.12188500	3.67801200	-0.98682700
H	-5.74081200	4.14797400	-0.21732500
H	-5.51207100	3.94364800	-1.97362700
H	-5.15664900	2.59348800	-0.86435000

**Excited state minimum energy Cartesian coordinate of 2\*.**

6	-4.024550	0.071749	-1.085469
6	-1.812933	-0.681596	-0.394512
6	-2.355920	-1.823407	0.263583
6	-3.767208	-1.990544	0.202751
6	-4.578544	-1.089460	-0.444581
1	-0.109964	0.474893	-0.961575
6	-0.465072	-0.402293	-0.430595
6	-1.418799	-2.679156	0.914565
6	-0.072319	-2.411929	0.907569
6	0.485696	-1.252755	0.232952
1	-1.778766	-3.559603	1.435453
1	0.619254	-3.069633	1.427172
8	-2.647687	0.214026	-1.034743
6	-4.413637	-3.191261	0.861123
8	1.733005	-1.000585	0.238925
9	-5.758048	-3.216678	0.709380
9	-3.946243	-4.362625	0.351063
9	-4.176255	-3.229512	2.199885
1	-5.651516	-1.206437	-0.494504
8	-4.649155	0.951335	-1.668979
6	4.784991	-3.292116	-1.545959
1	4.780161	-4.257879	-2.025881
6	4.397914	2.504197	2.368576
1	4.873159	3.242257	2.996329
6	4.858254	1.334853	1.815979
1	5.838970	0.889561	1.902526
6	2.792132	1.540636	1.205354
1	1.826532	1.347244	0.766200
7	3.844934	0.742112	1.092152
7	3.081643	2.623622	1.966265
6	2.151100	3.690170	2.335849
1	1.297915	3.681279	1.652746
1	1.802913	3.549247	3.363106
1	2.659215	4.653907	2.256885
6	-1.761718	5.759750	-1.033627
1	-2.184591	6.646678	-1.481260
7	-2.331061	4.514905	-1.202854
7	-0.533190	4.225890	0.084555
6	-1.555810	3.631102	-0.512468
6	-0.656653	5.560701	-0.238392

1	0.049140	6.299257	0.116361
1	-1.783870	2.574397	-0.487896
6	-3.527547	4.201451	-1.979646
1	-4.378856	4.776040	-1.604257
1	-3.367156	4.444921	-3.033939
1	-3.749960	3.136627	-1.887549
7	4.354360	-1.432188	-0.424210
1	3.860131	-0.570512	0.249030
6	3.842603	-2.655247	-0.784490
1	2.850586	-2.940686	-0.478693
6	5.570665	-1.318803	-0.947091
1	6.223283	-0.465409	-0.847723
7	5.869364	-2.434701	-1.640167
6	7.109400	-2.691206	-2.371362
1	6.892879	-2.834276	-3.432049
1	7.773484	-1.834661	-2.253402
1	7.598054	-3.582576	-1.972506

**Ground state minimum energy Cartesian coordinate of 3, TS.**



C	-3.87013400	0.05235300	-0.59557700
C	-1.75226600	-0.83507000	0.20913600
C	-2.30200500	-2.14023800	0.36273700
C	-3.67356400	-2.30612400	0.01839300
C	-4.43583300	-1.26154400	-0.44262800
H	-0.07920500	0.48036900	0.35428800
C	-0.43972300	-0.53200500	0.50098700
C	-1.41450600	-3.14514800	0.84653600
C	-0.10388000	-2.86472600	1.14545700
C	0.45893600	-1.53888600	0.98747700
H	-1.78262200	-4.15563900	0.98529800
H	0.55295600	-3.64455600	1.52026500
O	-2.53853700	0.20202300	-0.25356700
C	-4.32628900	-3.66594000	0.15195500
O	1.68198400	-1.28954500	1.26361800
F	-5.63344200	-3.65992100	-0.19767600
F	-3.72108500	-4.59793800	-0.63298200
F	-4.26946800	-4.13627200	1.42635000
H	-5.47709400	-1.37539900	-0.70816200
O	-4.45606800	1.05099400	-0.99969900
C	4.90153300	-3.13375900	-0.74110500
H	4.63117100	-4.17658400	-0.78612100
C	3.86435700	3.58462000	1.04092200
H	3.85491800	4.65007000	1.21148700
C	4.76822200	2.76368600	0.41386400
H	5.70494300	3.02759800	-0.05537500
C	3.14515500	1.50038600	1.10191400
H	2.50945500	0.63643900	1.29113000
N	4.30954000	1.46323400	0.45645000
N	2.84089800	2.76602900	1.47538300
C	1.62271000	3.19170700	2.16700100
H	1.11456500	2.30476100	2.54783300
H	1.88879600	3.83434100	3.00973700
H	0.95672900	3.72621200	1.48206100
C	-2.24511100	6.09712500	-0.93604600
H	-2.79507400	6.93627300	-1.33505300
N	-2.73882900	4.81026300	-0.98942600
N	-0.75396600	4.69178300	0.01934200
C	-1.80611000	4.00647200	-0.40383500
C	-1.02278100	6.00302700	-0.31114600

H	-0.32871800	6.80019400	-0.08283700
H	-1.95077800	2.93790500	-0.31693000
C	-4.01049800	4.38533100	-1.56735700
H	-4.83687300	4.91401500	-1.08409100
H	-4.02725800	4.59712200	-2.64046900
H	-4.13048100	3.31248800	-1.40876000
N	5.05427700	-0.95642700	-0.41598000
H	4.81516200	0.06527300	-0.08765300
C	4.26591400	-2.06301300	-0.17502200
H	3.32435000	-1.98069200	0.36712600
C	6.13053000	-1.33383700	-1.10282800
H	6.92852000	-0.68945300	-1.43744400
N	6.06880300	-2.65870100	-1.31842500
C	7.05640700	-3.46341500	-2.03850900
H	6.58302500	-3.94517500	-2.89617600
H	7.85835200	-2.81332400	-2.38782700
H	7.47063800	-4.22211100	-1.37173000

**Ground state minimum energy Cartesian coordinate of 4.**

C	-3.76560700	0.25546700	-0.91089500
C	-1.78758700	-0.71865000	0.11954600
C	-2.46745400	-1.94072800	0.38596500
C	-3.82697300	-2.02437400	-0.02938500
C	-4.45945000	-0.97784900	-0.65366900
H	-0.00638500	0.44781400	0.21139500
C	-0.46840800	-0.50249100	0.45669400
C	-1.70804600	-2.95503800	1.03966600
C	-0.39484700	-2.75921600	1.38946600
C	0.29986800	-1.51832600	1.11629200
H	-2.17825900	-3.90495900	1.26833000
H	0.16433200	-3.54343400	1.89119500
O	-2.44430700	0.32337000	-0.50489900
C	-4.61464000	-3.29446500	0.21594500
O	1.52415400	-1.34871500	1.44699000
F	-5.88302900	-3.22561800	-0.25015800
F	-4.04139100	-4.37226700	-0.38303600
F	-4.70463600	-3.58738900	1.54066700
H	-5.49027500	-1.03007700	-0.97349500
O	-4.23135800	1.25208800	-1.45278800
C	4.78795800	-3.32014300	-0.90231300
H	4.45833300	-4.34527500	-0.97354600
C	3.76681900	3.27746800	1.35335500
H	3.76058400	4.32729200	1.59848700
C	4.66271100	2.52292700	0.65031700
H	5.58959500	2.79815200	0.17341100
C	3.01686500	1.19200400	1.29801500
H	2.38963100	0.29533300	1.42118500
N	4.17403700	1.23413000	0.62949000
N	2.74938700	2.42619000	1.75093300
C	1.54695500	2.81693300	2.49807000
H	1.01973100	1.91100300	2.79664800
H	1.84596400	3.37007500	3.39067800
H	0.90347000	3.43034900	1.85887500
C	-1.54157400	6.04267300	-0.99217800
H	-1.93393300	6.93205700	-1.46206600
N	-2.13464800	4.80840800	-1.15673500
N	-0.37500200	4.49876600	0.17598600
C	-1.39686700	3.91729400	-0.43653900
C	-0.46034000	5.83138600	-0.16820200

H	0.25285700	6.55922500	0.19361500
H	-1.65226200	2.86667700	-0.39890200
C	-3.32067800	4.50782100	-1.95443600
H	-4.16400700	5.11471900	-1.61369700
H	-3.12906700	4.71960400	-3.01035300
H	-3.56912400	3.45183100	-1.83582700
N	5.06161000	-1.12815700	-0.48987100
H	4.60473600	0.37863900	0.16573700
C	4.24354800	-2.22361900	-0.28131700
H	3.32718500	-2.14517700	0.29304500
C	6.07603400	-1.56277900	-1.22329900
H	6.90749800	-0.96840500	-1.57514900
N	5.95702100	-2.88711100	-1.49932100
C	6.87787900	-3.69705800	-2.28886600
H	6.38143500	-4.06930000	-3.18869900
H	7.72942000	-3.08129900	-2.58172700
H	7.23830600	-4.54232600	-1.69759400

**Ground state minimum energy Cartesian coordinate of 5.**

C	4.14127900	0.28303300	-0.12706500
C	1.98064400	-0.75422100	0.29505400
C	2.53935100	-2.06134800	0.23116900
C	3.93940000	-2.15113500	-0.01531200
C	4.71744800	-1.03355900	-0.18841700
H	0.28589700	0.50461000	0.57734900
C	0.64274900	-0.51873700	0.53156500
C	1.63260600	-3.14454900	0.42426100
C	0.29595400	-2.93302400	0.65668800
C	-0.27401800	-1.60421900	0.72190700
H	2.00624800	-4.16168500	0.38603700
H	-0.37823300	-3.77208500	0.80000600
O	2.78044400	0.35655800	0.11596400
C	4.60731900	-3.50868300	-0.08650400
O	-1.52327400	-1.42180700	0.93422200
F	5.93604200	-3.42926800	-0.32811100
F	4.46565000	-4.20325300	1.07356900
F	4.08074900	-4.28385600	-1.07175100
H	5.78026600	-1.08930300	-0.37560100
O	4.73683200	1.34523500	-0.26925700
C	-5.42185100	-2.88256900	-0.81675800
H	-5.14230400	-3.85349700	-1.19745600
C	-3.66276900	3.16628500	0.66571300
H	-3.79380000	4.07147000	0.09547200
C	-4.13917200	2.80622600	1.89092300
H	-4.77121300	3.33009000	2.58878500
C	-2.90108900	1.12635400	1.10388400
H	-2.36579400	0.16185100	1.02400700
N	-3.64308300	1.54136800	2.13945500
N	-2.89844200	2.10855200	0.19793500
C	-2.17774700	2.07672800	-1.08237700
H	-1.77575300	1.07382000	-1.22257800
H	-2.87955700	2.29982800	-1.88821200
H	-1.36528600	2.81024900	-1.05739300
C	1.87330200	6.01509300	-0.64361200
H	2.36693900	6.97383800	-0.69699100
N	2.57679300	4.84027800	-0.47808400
N	0.42176100	4.28308100	-0.59286500
C	1.66073300	3.83183000	-0.45359400
C	0.54846300	5.65115600	-0.71268100

H	-0.31188700	6.29312100	-0.84295900
H	1.95576200	2.79826200	-0.33075100
C	4.02465400	4.69942300	-0.34638300
H	4.52315100	5.12887500	-1.21972300
H	4.37288100	5.21224700	0.55480100
H	4.27161000	3.63873500	-0.27824600
N	-5.52719900	-0.83589500	0.13497000
H	-3.84431200	0.96919700	2.94842800
C	-4.71372200	-1.92070100	-0.13411100
H	-3.67572200	-1.94648200	0.17446700
C	-6.70417300	-1.14809900	-0.38075500
H	-7.59186500	-0.53001700	-0.35864000
N	-6.69844400	-2.37853900	-0.97111900
C	-7.81803200	-3.03383400	-1.63336600
H	-8.06463000	-3.97306400	-1.13050700
H	-8.68672000	-2.37443800	-1.59428600
H	-7.57736900	-3.23874300	-2.68022700

**Ground state minimum energy Cartesian coordinate of 6, TS.**

C	-4.06862700	0.67456000	-0.78560000
C	-2.00001500	-0.57921500	-0.45835000
C	-2.71692600	-1.74773700	-0.06895600
C	-4.13387400	-1.66153700	-0.07297900
C	-4.79575100	-0.50369300	-0.41982100
H	-0.13857800	0.39082700	-0.84524600
C	-0.62747900	-0.51851300	-0.51248700
C	-1.92226500	-2.88253100	0.28251200
C	-0.55182700	-2.83914000	0.26004400
C	0.18145300	-1.64384000	-0.12367200
H	-2.41594900	-3.80083700	0.58065000
H	0.03184200	-3.71133300	0.53973100
O	-2.68478300	0.57472400	-0.79672100
C	-4.96395100	-2.86801200	0.31557200
O	1.44994500	-1.58711500	-0.10087500
F	-6.29501800	-2.63278100	0.25125200
F	-4.72072800	-3.93370600	-0.49203000
F	-4.70448100	-3.27446900	1.58699100
H	-5.87371200	-0.43158700	-0.42206900
O	-4.53642400	1.77113200	-1.08565000
C	5.47082700	-2.09840600	-1.86399800
H	5.07118000	-2.56940400	-2.74953500
C	2.21379700	2.75745400	2.88986100
H	2.06130400	3.75276700	3.28153500
C	2.93606700	1.72389900	3.43210200
H	3.51415700	1.64666500	4.33994400
C	2.02917300	1.08075700	1.52872300
H	1.77605300	0.41660100	0.70943700
N	2.80318600	0.66510500	2.55729400
N	1.64985600	2.34577200	1.69826600
C	-0.58104800	5.48544000	-1.18287400
H	-0.71039700	6.40103200	-1.73755600
N	-1.54157500	4.48944200	-1.18218300
N	0.09759900	3.79817300	0.07849600
C	-1.10267300	3.48157500	-0.41064000
C	0.44361200	5.04594400	-0.39231100
H	1.37948200	5.51513300	-0.13364000
H	-1.64113100	2.55845300	-0.24874600
C	-2.81778800	4.51963400	-1.90805300
H	-3.39294400	5.39068000	-1.58760900

H	-2.62154900	4.58169100	-2.98048000
H	-3.37461100	3.60760900	-1.68433100
N	5.82134400	-1.09772000	0.13083400
C	4.86775900	-1.61008600	-0.72799400
H	3.81201900	-1.60302200	-0.48871500
C	6.97704500	-1.27814300	-0.48468800
H	7.94971800	-0.99622400	-0.10400700
N	6.82516500	-1.88121500	-1.69998600
C	7.88177400	-2.23074100	-2.63882700
H	7.73506200	-1.71433500	-3.59166500
H	8.84232100	-1.92764000	-2.21867900
H	7.89839300	-3.31014600	-2.81395500
C	3.41139300	-0.66259600	2.67413000
H	2.83829200	-1.35398400	2.05397100
H	4.44475800	-0.64124400	2.31851900
H	3.37227100	-0.98402000	3.71684700
H	0.72107900	3.17365200	0.74643000

**Ground state minimum energy Cartesian coordinate of 7.**



C	-3.84741200	0.37112400	-0.60920800
C	-1.73419300	-0.81611700	-0.59723100
C	-2.37905400	-2.03936900	-0.23593600
C	-3.78498100	-2.00490500	-0.10427100
C	-4.51359600	-0.84057900	-0.28837500
H	0.03932800	0.26404400	-1.05989800
C	-0.38016200	-0.69118200	-0.76695800
C	-1.51502100	-3.16463100	-0.03939300
C	-0.15601700	-3.05723500	-0.16617400
C	0.50231400	-1.80211500	-0.51206600
H	-1.94755700	-4.12277200	0.22628800
H	0.48245200	-3.91936600	0.00244200
O	-2.48855800	0.32926400	-0.78022600
C	-4.54160000	-3.26727200	0.25786900
O	1.76072200	-1.69155500	-0.56523000
F	-5.87715800	-3.06918300	0.34887300
F	-4.35723600	-4.24933500	-0.66267200
F	-4.14306200	-3.77288200	1.45457900
H	-5.58710900	-0.80413500	-0.17546000
O	-4.36889000	1.49531900	-0.74773100
C	6.04378700	-1.79093800	-1.57926500
H	5.85941500	-2.38917100	-2.45901000
C	1.04831600	2.64950200	2.95404100
H	0.58225400	3.47746700	3.47029500
C	1.80357400	1.63314700	3.49146000
H	2.10925800	1.41363700	4.50322400
C	1.61305600	1.37727300	1.31617200
H	1.74006200	0.91816100	0.34651900
N	2.15349400	0.82326300	2.43185400
N	0.93055100	2.48374800	1.58795100
C	-1.85049200	5.54634600	-1.50111800
H	-1.64796000	6.52896100	-1.89592600
N	5.92651000	-0.56512900	0.31511500
C	5.19925100	-1.26267100	-0.63023000
H	4.12168900	-1.35103200	-0.57952400
C	7.18741000	-0.67605700	-0.06507400
H	8.04334200	-0.25133200	0.44239800
N	7.31895200	-1.40975900	-1.20908200
C	8.55786300	-1.72865300	-1.90392000
H	8.54818500	-1.31537800	-2.91658600

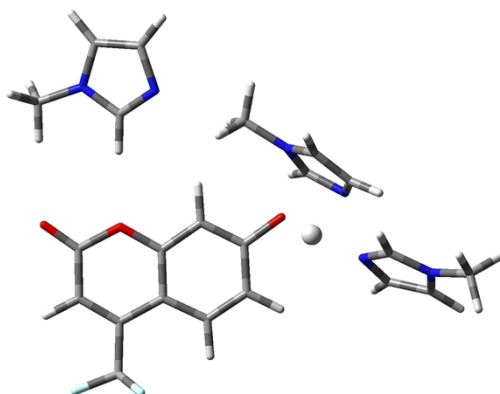
H	9.39399500	-1.29323300	-1.35397400
H	8.69877300	-2.81179800	-1.95946700
C	2.97337900	-0.38869400	2.47182100
H	2.70273900	-1.01838800	1.62182700
H	4.03610500	-0.14163800	2.40699800
H	2.77095000	-0.92683600	3.40003400
C	-2.93264900	4.72509200	-1.64327200
C	-1.46177500	3.68524400	-0.36404100
H	-0.95177400	2.96380400	0.26522900
H	-3.85339600	4.85979800	-2.18757100
N	-2.66711000	3.57749000	-0.92848200
H	-3.30788000	2.73855700	-0.85434800
N	-0.94326200	4.87707900	-0.69728800
C	0.37301800	5.37132000	-0.27597600
H	0.24793100	6.29076800	0.29944000
H	0.84083400	4.60190100	0.34023300
H	0.98521500	5.56775300	-1.15829800

**Ground state minimum energy Cartesian coordinate of 8.**

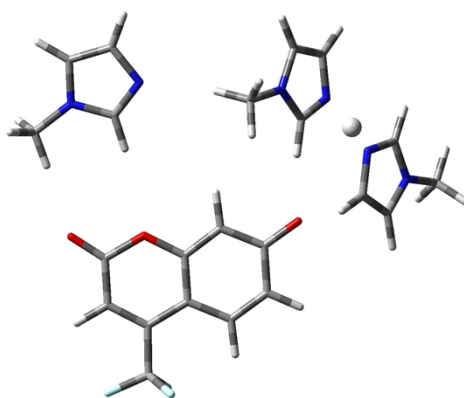
C	-2.664740	1.611737	-0.734330
C	-1.780056	-0.495239	-0.002829
C	-3.025733	-1.120539	-0.020615
C	-4.192820	-0.290145	-0.428308
C	-3.960564	1.026670	-0.767481
H	0.343493	-0.638699	0.364874
C	-0.601190	-1.170235	0.361950
C	-3.056526	-2.494890	0.351423
C	-1.926670	-3.198897	0.717936
C	-0.631253	-2.566998	0.742669
H	-4.011163	-3.010383	0.346109
H	-1.989338	-4.245897	0.995787
O	-1.596938	0.819478	-0.339919
C	-5.552094	-0.859299	-0.472528
O	0.443896	-3.162715	1.072795
F	-6.493965	0.035860	-0.860639
F	-5.663439	-1.933311	-1.331786
F	-5.970913	-1.358684	0.743205
H	-4.766392	1.681100	-1.076263
O	-2.378778	2.804135	-1.028216
C	3.749490	-3.291750	-1.919733
H	3.383934	-4.197574	-2.379516
C	1.529690	1.427925	3.376440
H	0.993404	2.262998	3.805552
C	1.729118	0.180012	3.918310
H	1.414833	-0.264898	4.850261
C	2.688030	0.317152	1.939599
H	3.241211	-0.002123	1.062782
N	2.475988	-0.517478	2.992890
N	2.132214	1.508396	2.137344
C	1.664745	5.278432	-1.313744
H	2.317162	6.064633	-1.658644
N	4.111744	-1.452949	-0.659382
C	3.280073	-2.536447	-0.870607
H	2.402144	-2.713884	-0.260935
C	5.063875	-1.561183	-1.570839
I	5.896653	-0.883471	-1.703429
N	4.894055	-2.658623	-2.363323
C	5.753462	-3.084497	-3.459601
H	5.192199	-3.113263	-4.397626
H	6.574605	-2.373005	-3.561530

H	6.168360	-4.075936	-3.258092
C	2.867409	-1.924433	3.069775
H	2.052114	-2.561186	2.714002
H	3.741420	-2.080047	2.435675
H	3.124255	-2.171525	4.101923
C	0.378377	4.962583	-1.649343
C	1.052817	3.502631	-0.138861
H	1.111310	2.678404	0.566312
H	-0.301762	5.427328	-2.344857
N	0.022083	3.857452	-0.907205
H	-0.931217	3.367318	-0.934774
N	2.067563	4.352393	-0.366268
C	3.376351	4.291463	0.292690
H	3.561338	5.228160	0.822658
H	3.358961	3.461471	1.000187
H	4.155616	4.129834	-0.454982

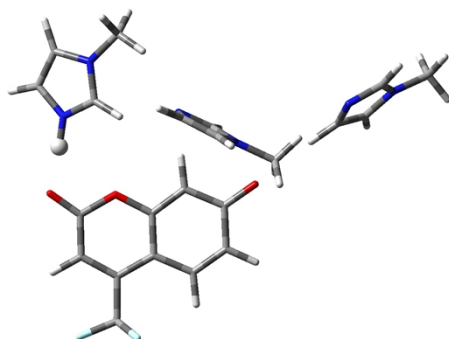
**Excited state minimum energy Cartesian coordinate of 9\*.**



**Ground state minimum energy arrangement of structure 1.**



**Ground state minimum energy arrangement of structure 4.**



**Ground state minimum energy arrangement of structure 8.**