

The Cartesian coordinates of the stationary points in the potential energy profiles obtained at the B3LYP/6-31+G(d) level.

RR2 dianion

C	2.45375700	-0.58516100	-0.01257800
C	1.15042800	-0.03108600	0.02094800
C	-0.02454800	-0.85634800	0.01085400
C	0.18197000	-2.27313300	-0.01925200
C	1.49942400	-2.81756000	-0.05481100
C	2.59946900	-2.00955900	-0.05481300
C	-1.38813000	-0.36938600	0.03246800
C	-0.91699600	-3.16481700	-0.01101400
H	1.60875300	-3.89510200	-0.08118700
C	-2.19414300	-2.65959900	0.02825200
C	-2.44042100	-1.27447300	0.04787400
H	-0.73180900	-4.23288900	-0.03277600
H	-3.45555300	-0.91003500	0.06994500
N	-1.60292400	1.02213100	0.02877300
H	-0.74883100	1.57850100	0.03022900
C	-2.72558000	1.77199000	-0.00365000
C	-3.59350300	3.84341800	-0.07267700
C	-4.94352000	2.09539700	-0.03040300
Cl	-3.38269100	5.57504300	-0.11618400
Cl	-6.55827300	1.43287200	-0.02881600
N	-4.86379200	3.42210200	-0.06934100
N	-3.95800600	1.22164300	0.00733200
N	-2.50415400	3.11684500	-0.04716600
S	-3.62263600	-3.76841900	0.08451000
S	4.23919000	-2.79915600	-0.10788400
O	-4.24366400	-3.54788600	1.43173900
O	-4.51750200	-3.33657700	-1.03749900
O	-3.09121100	-5.15531900	-0.09254200
O	3.96383400	-4.27028800	-0.14524400
O	4.90317600	-2.31372300	-1.35907600
O	4.95272800	-2.38867400	1.14318700
N	3.62288000	0.16892200	-0.00144100
N	3.49686900	1.43466000	0.05158100
C	4.68014500	2.20380700	0.06567100
C	4.50107600	3.59406300	0.15274200
C	5.97634300	1.65941400	-0.00106100
C	5.61083800	4.43939200	0.17632900
H	3.49280500	3.99595100	0.20327500
C	7.07643900	2.51231800	0.02150900
H	6.11020600	0.58571400	-0.06953300

C	6.90013600	3.90149300	0.11025500
H	5.46878900	5.51427600	0.24493100
H	8.07890700	2.09606800	-0.03093500
H	7.76580000	4.55807800	0.12739600
O	1.01150000	1.30721600	0.06847900
H	1.95636800	1.71296800	0.07728000

C34-CP1

C	-2.35008200	-0.45384800	-0.19933400
C	-1.03066700	0.06047400	-0.17267100
C	0.11892800	-0.80015000	-0.15900400
C	-0.12889300	-2.21043600	-0.18406100
C	-1.46219700	-2.71590900	-0.21135700
C	-2.53636400	-1.87388700	-0.21504100
C	1.49551400	-0.35314300	-0.12058100
C	0.94347400	-3.13375900	-0.17757400
H	-1.60427000	-3.78999300	-0.22549300
C	2.23509400	-2.66565000	-0.14611000
C	2.52120700	-1.28864000	-0.11822600
H	0.72774700	-4.19611400	-0.19751700
H	3.54643900	-0.95355800	-0.09400600
N	1.75012700	1.03065600	-0.07574700
H	0.91274600	1.61191400	-0.07619500
C	2.89312400	1.74665200	-0.00685300
C	3.81689100	3.78972100	0.13498900
C	5.11858000	2.00696600	0.05234200
Cl	3.64989600	5.52430500	0.22839100
Cl	6.71444300	1.30041100	0.04506700
N	5.07509400	3.33364700	0.13260300
N	4.10980400	1.16269200	-0.02183700
N	2.70836200	3.09504600	0.07427700
S	3.63127900	-3.81537800	-0.10023400
S	-4.19549500	-2.61455400	-0.25677300
O	4.24773400	-3.63752600	1.25524100
O	4.54563800	-3.38743400	-1.20776600
O	3.06221900	-5.18288400	-0.30728800
O	-3.97378400	-4.09155500	-0.24820400
O	-4.85817900	-2.13384600	-1.50579400
O	-4.90283500	-2.14599100	0.98915100
N	-3.49631300	0.33485600	-0.20593900
N	-3.32955700	1.59700900	-0.20176900
C	-4.48531900	2.40609900	-0.19955300
C	-4.25560800	3.79160200	-0.21627600
C	-5.80079900	1.90598500	-0.17775400

C	-5.33370500	4.67715500	-0.21360300
H	-3.23287200	4.15819300	-0.23172800
C	-6.86908500	2.79878500	-0.17422600
H	-5.97382400	0.83586700	-0.16197200
C	-6.64207300	4.18335900	-0.19234400
H	-5.15282800	5.74828000	-0.22709700
H	-7.88643300	2.41728000	-0.15621000
H	-7.48382400	4.87053600	-0.18909300
O	-0.85126700	1.39420200	-0.15957900
H	-1.78404400	1.82826800	-0.17622800
O	-3.80619500	-1.91063100	3.49779300
H	-4.15252100	-2.01219800	2.56275700

C34-TS1

C	-2.32767500	-0.54426900	-0.16288000
C	-1.01937400	-0.00223000	-0.13004800
C	0.14749300	-0.83875500	-0.09944300
C	-0.07138800	-2.25398000	-0.11097200
C	-1.39332200	-2.78718900	-0.15220700
C	-2.48457000	-1.96796900	-0.17584600
C	1.51468900	-0.36372900	-0.05804700
C	1.01893500	-3.15544600	-0.08193700
H	-1.51261800	-3.86395800	-0.16481600
C	2.30034300	-2.66118700	-0.03815800
C	2.55853700	-1.27837900	-0.02706800
H	0.82437100	-4.22200400	-0.09279700
H	3.57651700	-0.92262400	0.00610800
N	1.74196300	1.02547600	-0.04204400
H	0.89325200	1.58994900	-0.04346400
C	2.87170600	1.76548200	-0.02516200
C	3.75803700	3.82947800	0.02712700
C	5.09239300	2.06976900	-0.02803400
Cl	3.56133800	5.56269000	0.06843200
Cl	6.70096200	1.39299200	-0.04731500
N	5.02453300	3.39724000	0.00895000
N	4.09893700	1.20446600	-0.05076000
N	2.66242200	3.11205700	0.01700400
S	3.71869900	-3.78199800	0.04042800
S	-4.12633400	-2.74424200	-0.25693200
O	4.32692100	-3.55935000	1.39307300
O	4.62871800	-3.36346800	-1.07428800
O	3.17725000	-5.16512700	-0.13492000
O	-3.87249000	-4.21612900	-0.26974700
O	-4.77193000	-2.25647700	-1.51278300

O	-4.86820800	-2.32168500	0.98404800
N	-3.49022600	0.22005500	-0.17010800
N	-3.35278200	1.48529500	-0.18467400
C	-4.52673000	2.26743400	-0.17603000
C	-4.32996000	3.65752700	-0.21610200
C	-5.82964300	1.73710600	-0.12622800
C	-5.42869900	4.51725800	-0.20956700
H	-3.31658300	4.04780700	-0.25302900
C	-6.91862600	2.60440500	-0.11954900
H	-5.97749700	0.66360500	-0.09299800
C	-6.72456600	3.99348100	-0.16070300
H	-5.27322700	5.59199100	-0.24097900
H	-7.92635700	2.19965300	-0.08026600
H	-7.58194700	4.66102500	-0.15426300
O	-0.86764500	1.33499800	-0.12244800
H	-1.80689800	1.75052400	-0.15440100
O	-4.20253700	-0.52820800	2.96419100
H	-4.39566600	-1.16113800	2.21350500

C34-CP2

C	-2.32204800	-0.57223700	-0.10392700
C	-1.01952200	-0.02008100	-0.10011400
C	0.15288200	-0.84819200	-0.05432600
C	-0.05639300	-2.26480600	-0.06364400
C	-1.37332400	-2.80589000	-0.12944100
C	-2.47182000	-1.99631500	-0.14409700
C	1.51770000	-0.36503000	-0.00911000
C	1.03852600	-3.16035800	-0.02667100
H	-1.48442200	-3.88248200	-0.17924000
C	2.31636200	-2.65874600	0.02680300
C	2.56564900	-1.27440600	0.03572700
H	0.84987900	-4.22792200	-0.03996200
H	3.58119000	-0.91253800	0.07568700
N	1.74148600	1.02494300	-0.00989900
H	0.89324800	1.58860300	-0.03237100
C	2.86977700	1.76791300	-0.01890500
C	3.75044500	3.83456500	-0.06104400
C	5.08959900	2.07826200	-0.01551000
Cl	3.54939300	5.56733500	-0.09487900
Cl	6.69985200	1.40563900	-0.00106700
N	5.01808100	3.40562700	-0.04577900
N	4.09837500	1.21018700	0.00365200
N	2.65677600	3.11406100	-0.05319100
S	3.74104700	-3.77095800	0.11451300

S	-4.10049300	-2.78945200	-0.32634000
O	4.34475300	-3.53850600	1.46741100
O	4.65105200	-3.35223300	-1.00010200
O	3.20758500	-5.15775900	-0.05589700
O	-3.81938800	-4.24648900	-0.48561600
O	-4.72646800	-2.17870800	-1.53811500
O	-4.87047500	-2.51085100	0.93632100
N	-3.48227400	0.19665300	-0.02595100
N	-3.38368300	1.44799100	-0.19905100
C	-4.54977100	2.23069800	-0.10855800
C	-4.34811700	3.62133100	-0.11777500
C	-5.85297500	1.70101000	-0.04726400
C	-5.44235400	4.48240600	-0.03868300
H	-3.33524700	4.00949000	-0.17909800
C	-6.93730200	2.57049100	0.02040300
H	-6.00434900	0.62805900	-0.06471800
C	-6.73768900	3.95955100	0.03153500
H	-5.28455100	5.55712900	-0.03647000
H	-7.94576300	2.16806400	0.06126100
H	-7.59200100	4.62871700	0.08654500
O	-0.86707700	1.31915900	-0.11446000
H	-1.78471600	1.74004400	-0.20457600
O	-4.35313800	-0.12838800	2.23681600
H	-4.59311800	-0.99820700	1.82152700

C34-TS2

C	-2.31093900	-0.56459800	-0.12510600
C	-1.00613400	-0.01600800	-0.07039000
C	0.16484800	-0.84678300	-0.04276500
C	-0.04633000	-2.26270700	-0.07910600
C	-1.36399100	-2.80140200	-0.15969500
C	-2.45972600	-1.98832900	-0.18333400
C	1.52956800	-0.36567500	0.01451900
C	1.04765600	-3.15952200	-0.04408000
H	-1.47691800	-3.87784900	-0.20757200
C	2.32550000	-2.65983500	0.02902900
C	2.57674000	-1.27602400	0.05633500
H	0.85869400	-4.22671700	-0.07355400
H	3.59238800	-0.91565800	0.10633500
N	1.75260100	1.02431500	0.02165700
H	0.90270100	1.58658500	0.01228900
C	2.88046600	1.76729400	-0.00196600
C	3.76122300	3.83350200	-0.05970700
C	5.10029300	2.07699300	-0.02102600

Cl	3.56037100	5.56626500	-0.09789500
Cl	6.71063900	1.40421500	-0.01765200
N	5.02882600	3.40428700	-0.05494800
N	4.10917300	1.20922100	0.01011800
N	2.66744100	3.11341300	-0.03909300
S	3.74821200	-3.77460500	0.11530600
S	-4.09210800	-2.77437600	-0.34324100
O	4.35081200	-3.54640800	1.46944300
O	4.66026500	-3.35464500	-0.99727500
O	3.21293700	-5.16023500	-0.05913200
O	-3.82181400	-4.23989900	-0.43733600
O	-4.71598800	-2.21698100	-1.58106000
O	-4.86154600	-2.43835700	0.90677600
N	-3.47635300	0.19582800	-0.10456300
N	-3.35049900	1.46101100	-0.12696200
C	-4.52789700	2.23592600	-0.10527200
C	-4.33984000	3.62496400	-0.01604500
C	-5.82692000	1.69909500	-0.18211500
C	-5.44450700	4.47668000	0.01074600
H	-3.32915300	4.02027900	0.03671500
C	-6.92139300	2.55901600	-0.16101900
H	-5.96741300	0.62743900	-0.26395500
C	-6.73661000	3.94647200	-0.06175200
H	-5.29633100	5.55032200	0.08480700
H	-7.92604700	2.14984500	-0.22499900
H	-7.59834700	4.60818800	-0.04523900
O	-0.85934300	1.32137900	-0.02962900
H	-1.79426700	1.73655200	-0.07504900
O	-4.70797400	-0.18210700	2.46586500
H	-4.73680300	-0.96866200	1.84963700

C34-CP3

C	-2.30717500	-0.56465800	-0.12957700
C	-1.00223500	-0.01671000	-0.07480000
C	0.16819300	-0.84813900	-0.04596300
C	-0.04372900	-2.26406200	-0.07902600
C	-1.36188700	-2.80245800	-0.15573400
C	-2.45697600	-1.98843100	-0.18149700
C	1.53307500	-0.36747500	0.01024200
C	1.05024400	-3.16097900	-0.04354700
H	-1.47536300	-3.87908000	-0.19862600
C	2.32839200	-2.66159200	0.02656100
C	2.58024300	-1.27778600	0.05177200
H	0.86107900	-4.22819600	-0.07048300

H	3.59602800	-0.91744900	0.10086000
N	1.75579400	1.02253000	0.01773800
H	0.90571200	1.58461800	0.00930600
C	2.88323300	1.76601900	-0.00274700
C	3.76232200	3.83324200	-0.05041500
C	5.10266000	2.07748700	-0.02060800
Cl	3.56057000	5.56604800	-0.08122200
Cl	6.71401100	1.40701200	-0.01947500
N	5.03009700	3.40483800	-0.04777300
N	4.11229400	1.20852400	0.00547300
N	2.66917500	3.11221900	-0.03264800
S	3.75121000	-3.77656500	0.10601900
S	-4.09156400	-2.77128500	-0.33031700
O	4.37619900	-3.53039600	1.44665100
O	4.64509500	-3.37254200	-1.02712000
O	3.21264900	-5.16401800	-0.04138000
O	-3.82532600	-4.23831500	-0.41267600
O	-4.71805200	-2.22318900	-1.57098100
O	-4.85627600	-2.42327000	0.91921800
N	-3.47251700	0.19556600	-0.11679300
N	-3.34544000	1.46091300	-0.13122900
C	-4.52383000	2.23506200	-0.11642800
C	-4.33730800	3.62457300	-0.03240000
C	-5.82234600	1.69687700	-0.19288600
C	-5.44270800	4.47559100	-0.01211000
H	-3.32709900	4.02109200	0.02073000
C	-6.91765800	2.55605700	-0.17706900
H	-5.96207600	0.62477800	-0.27041300
C	-6.73431000	3.94410100	-0.08428800
H	-5.29543300	5.54967300	0.05729200
H	-7.92185000	2.14562700	-0.24026500
H	-7.59661400	4.60515600	-0.07215400
O	-0.85560900	1.32073600	-0.03689100
H	-1.79177600	1.73537800	-0.07906200
O	-4.78352100	-0.17480300	2.49636900
H	-4.77109900	-0.94405800	1.85763600

C34-TS3

C	-2.30113000	-0.56365400	-0.14776300
C	-0.99702700	-0.01481300	-0.08266600
C	0.17371500	-0.84555200	-0.04685800
C	-0.03748200	-2.26173200	-0.07663600
C	-1.35487500	-2.80108200	-0.15939600
C	-2.44988100	-1.98748400	-0.19598100

C	1.53802400	-0.36410700	0.01394900
C	1.05649200	-3.15813100	-0.02992700
H	-1.46796200	-3.87795000	-0.19631100
C	2.33389500	-2.65791000	0.04752500
C	2.58507300	-1.27389900	0.06747900
H	0.86791700	-4.22553400	-0.05394100
H	3.60039000	-0.91294100	0.12025000
N	1.76066700	1.02602000	0.01053700
H	0.91054500	1.58796500	-0.00271500
C	2.88850400	1.76853700	-0.02393300
C	3.76977000	3.83361900	-0.10733500
C	5.10844900	2.07722700	-0.05113800
Cl	3.56942900	5.56604000	-0.16287800
Cl	6.71863500	1.40407000	-0.04546600
N	5.03724600	3.40408400	-0.10014900
N	4.11714000	1.21031100	-0.00665300
N	2.67572700	3.11419100	-0.07750700
S	3.75607500	-3.77217300	0.14847500
S	-4.08416500	-2.77107300	-0.34396900
O	4.35177900	-3.53578800	1.50429900
O	4.67399600	-3.35910600	-0.96188600
O	3.22175300	-5.15889300	-0.02026500
O	-3.81740200	-4.23896200	-0.41264000
O	-4.70705100	-2.23467800	-1.59155200
O	-4.85299500	-2.41197500	0.89977500
N	-3.46740200	0.19474000	-0.14780500
N	-3.34141100	1.46038300	-0.14929500
C	-4.52294500	2.23053600	-0.14248300
C	-4.34317300	3.62050300	-0.05360600
C	-5.81866500	1.68678900	-0.22743300
C	-5.45260700	4.46644600	-0.03872300
H	-3.33514500	4.02143800	0.00727100
C	-6.91810700	2.54094100	-0.21627400
H	-5.95288600	0.61421900	-0.30746200
C	-6.74148100	3.92949900	-0.12000700
H	-5.31061700	5.54104900	0.03371500
H	-7.92004700	2.12601900	-0.28575900
H	-7.60668000	4.58683500	-0.11179700
O	-0.85197800	1.32270700	-0.04180700
H	-1.78908400	1.73604300	-0.08550300
O	-4.90386300	-0.16547100	2.47965100
H	-4.83397900	-0.92179800	1.82899300

C	-2.25978500	-0.57382000	-0.12551000
C	-0.94827300	-0.02128400	-0.04661200
C	0.22220500	-0.84714700	-0.02240100
C	0.01873400	-2.26649000	-0.05004900
C	-1.29980700	-2.81199700	-0.11555300
C	-2.39631500	-2.00387300	-0.15749600
C	1.58614900	-0.36242700	0.03210900
C	1.11458800	-3.15663100	-0.00691500
H	-1.40864000	-3.89028500	-0.12662500
C	2.39322800	-2.65244000	0.06340700
C	2.63797000	-1.26804000	0.08092600
H	0.93013800	-4.22493700	-0.02696800
H	3.65184400	-0.90216300	0.12793100
N	1.80240900	1.02893200	0.02576200
H	0.94847700	1.58583800	0.01569500
C	2.92559100	1.77762700	-0.00649300
C	3.79588700	3.84783800	-0.08448200
C	5.14404100	2.09864500	-0.03112700
Cl	3.58694300	5.57960500	-0.13648300
Cl	6.75825200	1.43447600	-0.02566900
N	5.06585200	3.42531100	-0.07701300
N	4.15774200	1.22616600	0.01042100
N	2.70576500	3.12266200	-0.05753000
S	3.81799400	-3.76144200	0.16170200
S	-4.04188900	-2.76853200	-0.25394000
O	4.41571400	-3.52617700	1.51724500
O	4.73525200	-3.34569700	-0.94860800
O	3.28778300	-5.14998300	-0.00792000
O	-3.80301200	-4.23942600	-0.12959500
O	-4.60938500	-2.38921500	-1.58635400
O	-4.84141100	-2.22851200	0.89790700
N	-3.42078600	0.14745800	-0.15006000
N	-3.31616100	1.46084500	-0.06225100
C	-4.47605500	2.13376100	0.00836800
C	-4.41662000	3.54602900	0.05586900
C	-5.81419800	1.40379200	0.00686400
C	-5.56898400	4.29941000	0.10025600
H	-3.43943800	4.02143000	0.06241100
C	-6.99389800	2.32812200	0.09162900
H	-5.88192700	0.86029200	-0.95118700
C	-6.86976600	3.67576300	0.11485700
H	-5.50263500	5.38282100	0.13725000
H	-7.96864400	1.84848100	0.12660800
H	-7.75218800	4.30836100	0.15852300

O	-0.81211300	1.32089200	0.00597600
H	-1.75324400	1.72677000	-0.00828400
O	-5.92982200	0.44622600	1.07619300
H	-5.38569100	-0.34191100	0.84710900

C34-TS_{co}

C	2.27083600	-0.72485100	0.13142400
C	0.99013600	-0.12668500	0.02196700
C	-0.05903700	-2.33128100	0.13196300
C	1.23838700	-2.91869500	0.24550800
C	2.36475600	-2.15194500	0.24941400
H	1.30703800	-3.99664000	0.32958200
S	3.97159400	-2.99347700	0.41141300
O	3.63948800	-4.44889900	0.51654000
O	4.74944600	-2.67879200	-0.82874300
O	4.60153000	-2.46038000	1.66055500
N	3.46148800	-0.01445400	0.12046700
N	3.38815900	1.25081600	0.02104100
C	4.62701900	1.95342000	-0.01418300
C	4.52066600	3.34776000	0.31895900
C	5.89339200	1.29655700	0.17680500
C	5.64354500	4.06241900	0.68081300
H	3.54419800	3.81840300	0.25519800
C	7.00411100	2.03661100	0.53838500
H	5.96122300	0.22784100	0.00991400
C	6.89238500	3.41643000	0.78685900
H	5.56247800	5.12196600	0.90496700
H	7.96556300	1.54363200	0.64902900
H	7.77024800	3.98488800	1.08016100
O	0.89942300	1.20820100	-0.09233500
H	1.85067400	1.58884800	-0.07774100
O	4.72030200	2.14390500	-1.98573300
H	5.00108900	1.23339500	-2.20584400
C	-1.18434000	-3.18152500	0.12588500
C	-2.44467400	-2.63477800	0.01329400
C	-2.64034300	-1.25041400	-0.08346400
C	-1.55486900	-0.37921400	-0.07429100
C	-0.21464200	-0.91003300	0.02476700
N	-1.72426000	1.01382400	-0.16548300
H	-0.85442300	1.54414200	-0.18822600
H	-1.03227200	-4.25319400	0.20629500
C	-2.82282600	1.80076500	-0.20077400
C	-3.61674700	3.89973300	-0.30937500
C	-5.02774600	2.20366900	-0.19151700

S	-3.88058700	-3.74166800	-0.02989300
O	-5.09055200	-2.86266200	-0.05265800
O	-3.78522800	-4.57715700	1.21068200
O	-3.72233700	-4.55271000	-1.28074000
N	-2.55382200	3.13420800	-0.28993000
N	-4.07309200	1.29572400	-0.14877800
N	-4.90077400	3.52512100	-0.26638400
Cl	-3.34396300	5.62065300	-0.40464400
Cl	-6.66529400	1.60218400	-0.14861200
H	-3.64211700	-0.86143200	-0.16323200

C34-CP5

C	2.31504800	-0.45747200	-0.20329400
C	0.99543800	0.04515000	-0.14019600
C	0.12217900	-2.23266500	-0.02475600
C	1.45800400	-2.72453400	-0.09707100
C	2.52229000	-1.87344600	-0.18079500
H	1.61158700	-3.79693600	-0.08352900
S	4.18876700	-2.60197500	-0.27666500
O	3.96941700	-4.08263500	-0.25263200
O	4.77743100	-2.13775600	-1.57270200
O	4.93754700	-2.12040800	0.92660500
N	3.45716700	0.35039500	-0.27035800
N	3.28348100	1.59755700	-0.33909200
C	4.52845600	2.43904300	-0.37232900
C	4.50016000	3.24814700	0.89252600
C	5.79239700	1.64934200	-0.55384200
C	5.51524900	3.19430600	1.80933200
H	3.61876700	3.86310000	1.05090000
C	6.78953000	1.65345400	0.38163600
H	5.88427800	1.07990600	-1.47460800
C	6.66899000	2.40053300	1.58346000
H	5.44293900	3.78251400	2.72072100
H	7.69501900	1.07892200	0.20248500
H	7.46663900	2.37923000	2.31958400
O	0.79531800	1.37753500	-0.16609200
H	1.70753700	1.82778400	-0.24849000
O	4.32809700	3.35026800	-1.46851000
H	4.39614100	2.85035100	-2.30432200
C	-0.93714500	-3.16768200	0.06410700
C	-2.23184100	-2.71461800	0.13538300
C	-2.53542800	-1.34066500	0.11629600
C	-1.52386500	-0.39466500	0.02484900
C	-0.14339300	-0.82594900	-0.04446900

N	-1.79779700	0.98617300	-0.00137600
H	-0.96983300	1.57862800	-0.04720100
H	-0.70828800	-4.22727000	0.07541300
C	-2.95150800	1.68796600	-0.01818200
C	-3.90236000	3.72198000	-0.10554200
C	-5.18058400	1.92273900	-0.01607500
S	-3.60769400	-3.88452100	0.25273500
O	-4.32934600	-3.53441100	1.51927400
O	-2.99777500	-5.24884700	0.28726900
O	-4.44401700	-3.64760700	-0.96888300
N	-2.78532600	3.03936800	-0.08262000
N	-4.16054800	1.08938600	0.02279600
N	-5.15494300	3.25088900	-0.08012000
Cl	-3.75482800	5.45936900	-0.17548500
Cl	-6.76732200	1.19662600	0.01739800
H	-3.56269300	-1.01547900	0.17391900

C34-TS5

C	-2.30067200	-0.57603300	-0.25594600
C	-1.00459700	-0.04410000	-0.06530100
C	-0.04558400	-2.28142700	-0.25573900
C	-1.35893100	-2.80381500	-0.44262400
C	-2.45202300	-1.98672500	-0.45082900
H	-1.47167600	-3.87228100	-0.58168900
S	-4.08368200	-2.75506100	-0.70873000
O	-3.80512800	-4.21727000	-0.86220400
O	-4.89321700	-2.45886600	0.51524000
O	-4.64422700	-2.14916100	-1.95736500
N	-3.46814600	0.19357900	-0.26999900
N	-3.35552900	1.43242500	-0.06916000
C	-4.62562000	2.22640000	-0.11177900
C	-4.59759200	3.00807200	-1.39567200
C	-5.86651500	1.39958000	0.05936500
C	-5.60506900	2.92626000	-2.31948100
H	-3.73018900	3.64376800	-1.55029600
C	-6.85413300	1.36884000	-0.88534600
H	-5.95046800	0.84043700	0.98659500
C	-6.74231000	2.10933400	-2.09290200
H	-5.54139100	3.51050100	-3.23415800
H	-7.74611300	0.77241100	-0.70987600
H	-7.53527600	2.06439100	-2.83310600
O	-0.85462100	1.27950100	0.13339400
H	-1.77349400	1.70950800	0.11134600
O	-4.51152200	3.14762200	1.00171200

H	-3.70013100	2.93378400	1.50041400
C	1.04437700	-3.18451200	-0.25255800
C	2.31749500	-2.70137000	-0.07274700
C	2.56906100	-1.32798400	0.09820700
C	1.52667100	-0.41127100	0.09583500
C	0.16574400	-0.87723500	-0.07292800
N	1.75338100	0.96939300	0.25281100
H	0.90922700	1.53950700	0.25870300
H	0.85556400	-4.24320400	-0.39031800
C	2.88328300	1.69869600	0.37785900
C	3.77148800	3.74923300	0.60658800
C	5.10242300	1.98951000	0.50044300
S	3.73311900	-3.82814200	-0.03109400
O	4.31597000	-3.68195900	1.34256400
O	4.66409300	-3.34996900	-1.10397500
O	3.19221800	-5.19737800	-0.29407300
N	2.67503000	3.04082600	0.49803600
N	4.10858100	1.13338100	0.37736400
N	5.03626000	3.31216600	0.61831000
Cl	3.57844200	5.47748800	0.75381400
Cl	6.70862900	1.30708300	0.51141900
H	3.58192200	-0.98026400	0.22911400

C34-CP6

C	2.31479200	-0.45760500	-0.20971900
C	0.99536300	0.04453700	-0.14932100
C	0.12247400	-2.23311600	-0.03061900
C	1.45827600	-2.72470700	-0.10213500
C	2.52248400	-1.87334300	-0.18534300
H	1.61219100	-3.79704500	-0.08759300
S	4.18933000	-2.60185300	-0.27777600
O	3.96976600	-4.08252700	-0.25443300
O	4.78087500	-2.13732300	-1.57225000
O	4.93528700	-2.12071400	0.92746400
N	3.45821900	0.35013500	-0.27195300
N	3.28723900	1.59656700	-0.34427400
C	4.53212300	2.43828300	-0.37074900
C	4.50831200	3.23026500	0.90578800
C	5.79593200	1.65555900	-0.57045500
C	5.53369800	3.17902900	1.81263600
H	3.62409200	3.83898100	1.07950500
C	6.79308500	1.64566700	0.36374500
H	5.88365700	1.09853600	-1.49813300
C	6.68357200	2.38572800	1.57206000

H	5.46971900	3.76369500	2.72694000
H	7.69446500	1.06707000	0.17729900
H	7.48746100	2.35757700	2.30111400
O	0.79416300	1.37730200	-0.17828100
H	1.70402500	1.82843300	-0.25964400
O	4.37666600	3.28729200	-1.52399300
H	3.64942900	3.91488300	-1.35343600
C	-0.93656400	-3.16836100	0.06065300
C	-2.23120100	-2.71559000	0.13298800
C	-2.53506800	-1.34164300	0.11226300
C	-1.52395200	-0.39551900	0.01831800
C	-0.14335800	-0.82643000	-0.05204600
N	-1.79852200	0.98524400	-0.00839200
H	-0.97106000	1.57812100	-0.05626600
H	-0.70730700	-4.22784800	0.07345400
C	-2.95248200	1.68664400	-0.02129400
C	-3.90404800	3.72053900	-0.10437000
C	-5.18162200	1.92087700	-0.01422800
S	-3.60667600	-3.88539100	0.25546000
O	-4.32422600	-3.53417000	1.52404400
O	-2.99669900	-5.24973400	0.28920900
O	-4.44688700	-3.64937200	-0.96364100
N	-2.78680600	3.03819600	-0.08434600
N	-4.16129500	1.08773600	0.02162100
N	-5.15645400	3.24912200	-0.07692600
Cl	-3.75698200	5.45807700	-0.17194100
Cl	-6.76807300	1.19428900	0.02127900
H	-3.56232400	-1.01663600	0.17096700

C34-TS6

C	2.32967600	-0.67289500	-0.17088900
C	1.03827800	-0.09776300	-0.09446100
C	0.04471300	-2.32569800	0.02260800
C	1.35274400	-2.88984000	-0.05381200
C	2.46035800	-2.09888300	-0.15119400
H	1.44793700	-3.96889800	-0.03384900
S	4.08601700	-2.91191800	-0.25814400
O	3.79386100	-4.37870200	-0.20027600
O	4.67438700	-2.50203800	-1.57248400
O	4.87792100	-2.44310100	0.92248900
N	3.50470900	0.07336800	-0.25707400
N	3.39890400	1.33151900	-0.27013800
C	4.70032700	2.07985200	-0.38683700
C	4.37712500	3.52663400	-0.13489500

C	5.75145600	1.53583600	0.53714500
C	5.04369600	4.27320900	0.79767000
H	3.59176300	3.95898200	-0.75109600
C	6.37382900	2.32174400	1.46778100
H	5.99873200	0.48508100	0.42870000
C	6.04953000	3.69571300	1.61533700
H	4.79225800	5.32332800	0.92409900
H	7.13484800	1.88413500	2.10934600
H	6.56118500	4.29940900	2.35850200
O	0.91613900	1.24090500	-0.10076200
H	1.85988100	1.63864500	-0.17136800
O	5.18670500	1.88835300	-1.73366700
H	4.57009700	2.32474100	-2.35206400
C	-1.06204400	-3.20170100	0.12646000
C	-2.33001200	-2.67803600	0.20267900
C	-2.56019400	-1.29081300	0.16473800
C	-1.50079300	-0.40101100	0.05251100
C	-0.14584100	-0.90700800	-0.00740500
N	-1.70254700	0.99114500	-0.00552500
H	-0.84493500	1.54078800	-0.03246800
H	-0.89045100	-4.27194000	0.14971300
C	-2.81949800	1.74742400	-0.08089900
C	-3.66980500	3.82143200	-0.23191600
C	-5.03410700	2.08558300	-0.15745800
S	-3.77022200	-3.76532700	0.34140600
O	-4.50422500	-3.30223000	1.56327500
O	-3.24062300	-5.15792700	0.46987300
O	-4.55898600	-3.55216000	-0.91569000
N	-2.58632400	3.08816000	-0.16609000
N	-4.05601500	1.20678200	-0.07312900
N	-4.94301400	3.40970900	-0.23640700
Cl	-3.44545800	5.54949300	-0.32508300
Cl	-6.65371100	1.43553300	-0.16688200
H	-3.56865200	-0.91229200	0.22237100

C34-CP7

C	2.34434300	-0.72720600	-0.17145300
C	1.06311200	-0.13597000	-0.06706200
C	0.03910900	-2.35146700	0.01389400
C	1.33848400	-2.93220300	-0.07811600
C	2.45574800	-2.15473300	-0.17574800
H	1.41954200	-4.01255400	-0.07089800
S	4.06949500	-2.98903000	-0.30166600
O	3.75828900	-4.45193800	-0.24302100

O	4.64992600	-2.58570900	-1.62158000
O	4.87938100	-2.53291800	0.87177600
N	3.52866400	0.00408900	-0.27296700
N	3.44638000	1.26261700	-0.23681700
C	4.77189900	1.97892100	-0.32500800
C	4.47178200	3.43910700	-0.53132100
C	5.55318200	1.70590900	0.93000600
C	4.93350000	4.40636900	0.31722900
H	3.88792000	3.69130600	-1.41409700
C	5.97173600	2.71054000	1.75910000
H	5.76476600	0.66254800	1.14554800
C	5.68443400	4.07093400	1.47534600
H	4.71693300	5.45111800	0.10840700
H	6.53891200	2.46199000	2.65287200
H	6.03346400	4.85180500	2.14379700
O	0.96000700	1.20469400	-0.03721100
H	1.90692900	1.59108600	-0.09778600
O	5.53651500	1.45892300	-1.42483600
H	5.10614500	1.72899500	-2.25857400
C	-1.07886000	-3.21400400	0.11110700
C	-2.33920800	-2.67479100	0.20094200
C	-2.55087100	-1.28412600	0.18238300
C	-1.48009000	-0.40713400	0.07804700
C	-0.13206200	-0.93003400	0.00715000
N	-1.66416100	0.98821100	0.03509100
H	-0.79983500	1.52761400	0.01639200
H	-0.92115200	-4.28659300	0.11866100
C	-2.77135100	1.75890300	-0.03763900
C	-3.59474900	3.84479200	-0.17557700
C	-4.98126100	2.12601200	-0.11894200
S	-3.79245800	-3.74567200	0.32896600
O	-4.52566300	-3.28050100	1.55046600
O	-3.27913000	-5.14495200	0.45205400
O	-4.57425600	-3.51761600	-0.92994800
N	-2.52098800	3.09725900	-0.11164600
N	-4.01479500	1.23400900	-0.03787300
N	-4.87308700	3.44937700	-0.18827300
Cl	-3.34837600	5.57059900	-0.25441500
Cl	-6.60927400	1.49725400	-0.13671600
H	-3.55408000	-0.89329900	0.24789200
C34-TS7			
C	2.35404400	-0.74179400	-0.18970400
C	1.07591800	-0.14634300	-0.07450600

C	0.04370400	-2.35810100	0.00492500
C	1.34002500	-2.94331100	-0.09917000
C	2.45969600	-2.16961200	-0.20153000
H	1.41715500	-4.02396500	-0.09637800
S	4.06908200	-3.01044000	-0.34049400
O	3.75142900	-4.47225300	-0.28900000
O	4.64462200	-2.60199600	-1.66101700
O	4.88719700	-2.56542600	0.83143200
N	3.54184200	-0.01418400	-0.28955100
N	3.46326900	1.24382900	-0.24062500
C	4.78922600	1.96365500	-0.30394200
C	4.49096100	3.41072100	-0.59621800
C	5.49251000	1.75714800	1.00926800
C	4.87262900	4.41838500	0.24490200
H	3.97257700	3.61800300	-1.53000900
C	5.83164100	2.80119900	1.82597800
H	5.70903100	0.72714600	1.27829000
C	5.53908900	4.14303200	1.46904300
H	4.65824300	5.45016000	-0.02254800
H	6.34037800	2.59955200	2.76554600
H	5.82289600	4.95653500	2.12934200
O	0.97760300	1.19467800	-0.03597100
H	1.92590400	1.57753400	-0.09515700
O	5.62167700	1.39773200	-1.32510600
H	5.22775500	1.59535600	-2.19603600
C	-1.07686600	-3.21650900	0.11007300
C	-2.33412700	-2.67255900	0.21289400
C	-2.54048600	-1.28098000	0.19852800
C	-1.46728400	-0.40805700	0.08615100
C	-0.12187700	-0.93605900	0.00388000
N	-1.64645700	0.98811500	0.04640200
H	-0.78017500	1.52434400	0.02587500
H	-0.92328100	-4.28971500	0.11418200
C	-2.75090400	1.76286800	-0.02391700
C	-3.56661000	3.85204200	-0.15872400
C	-4.95951300	2.13842000	-0.10260300
S	-3.79027100	-3.73801600	0.35309900
O	-4.51221200	-3.26891400	1.57978300
O	-3.28108600	-5.13905700	0.47367400
O	-4.58100600	-3.50861800	-0.90001500
N	-2.49563900	3.10040900	-0.09666400
N	-3.99636500	1.24263100	-0.02350100
N	-4.84646000	3.46146700	-0.17059400
Cl	-3.31372600	5.57701100	-0.23630400

Cl	-6.58999800	1.51597900	-0.11926900
H	-3.54156700	-0.88644600	0.27368100
C34-CP8			
C	-2.35532800	-0.79051700	-0.01553200
C	-1.08259800	-0.18254300	-0.03803000
C	-0.03206500	-2.38696200	-0.03649800
C	-1.32761700	-2.98331600	-0.02357700
C	-2.45615500	-2.21678300	-0.00914300
H	-1.39634900	-4.06461400	-0.01914400
S	-4.07389300	-3.05065400	0.03597100
O	-3.76226800	-4.51301500	0.00574400
O	-4.72072200	-2.62803500	1.31864000
O	-4.82170700	-2.59769300	-1.17907800
N	-3.55361400	-0.07362800	-0.00077800
N	-3.52313500	1.18223500	-0.01155800
C	-4.89509500	1.81177100	0.00075200
C	-4.97432500	2.65622000	1.24813300
C	-5.01101200	2.61676600	-1.27021100
C	-5.11687500	4.01555900	1.19877300
H	-4.92313000	2.11763400	2.19060000
C	-5.15371900	3.97698000	-1.25968100
H	-4.98830600	2.04873400	-2.19641800
C	-5.19812400	4.70565000	-0.04074000
H	-5.18715500	4.57964200	2.12571800
H	-5.25304200	4.51135300	-2.20148600
H	-5.31632800	5.78456000	-0.05589700
O	-0.99081500	1.16195500	-0.05410100
H	-1.92272400	1.55130400	-0.04060100
O	-5.90612200	0.80552100	0.03305500
H	-5.43853500	-0.06312700	0.01506300
C	1.09884900	-3.23791900	-0.03459800
C	2.35662900	-2.68594900	-0.03437200
C	2.55235300	-1.29290400	-0.03875500
C	1.46857900	-0.42588800	-0.04127100
C	0.12337900	-0.96268300	-0.04097100
N	1.63535900	0.97204200	-0.03420900
H	0.76512900	1.50132100	-0.02814700
H	0.95241500	-4.31212100	-0.03005800
C	2.73185600	1.76131200	-0.01759000
C	3.52382700	3.86356200	0.03615300
C	4.93661600	2.16577700	-0.01320100
S	3.82577400	-3.74211300	0.01019800
O	4.46834300	-3.47156400	1.33776400

O	4.67777900	-3.30102100	-1.14090300
O	3.33957900	-5.14982900	-0.12694600
N	2.46157700	3.09733300	0.02237600
N	3.98311200	1.25600900	-0.04020700
N	4.80847600	3.48862400	0.02391800
Cl	3.25061000	5.58646500	0.07665400
Cl	6.57491700	1.56438800	-0.02654500
H	3.55395200	-0.89255900	-0.03817100

C34-TS_{CN}

C	-3.57244600	0.28032800	-1.58501800
C	-3.33602500	0.61329500	-2.92958700
C	-0.97467700	0.96154400	-2.41687800
C	-1.23991900	0.62483900	-1.05766000
C	-2.49963700	0.29500100	-0.64593600
H	-0.41593800	0.63655000	-0.35395000
S	-2.76605900	-0.12891400	1.10286500
O	-1.43438300	0.04442000	1.75811600
O	-3.79153000	0.83381600	1.61511000
O	-3.23676700	-1.55049000	1.11614300
N	-4.85329400	-0.07562400	-1.11104800
N	-5.84093700	-0.10251100	-1.83969800
C	-7.31207400	-0.53708100	-0.77913000
C	-8.00948400	0.74406800	-0.77906000
C	-7.93217600	-1.61839000	-1.52895200
C	-9.03206900	0.97908800	-1.67340100
H	-7.65445700	1.51487800	-0.10065100
C	-8.95650600	-1.35198700	-2.41278200
H	-7.52252700	-2.61767100	-1.41234900
C	-9.49995200	-0.05114900	-2.52133100
H	-9.50893900	1.95561700	-1.70265600
H	-9.37524800	-2.15830600	-3.00966800
H	-10.31212300	0.14276400	-3.21553800
O	-4.35698200	0.59552000	-3.81408600
H	-5.20459600	0.33725500	-3.34456400
O	-6.70738600	-0.92050400	0.41906800
H	-5.77387700	-0.58444600	0.41108400
C	0.35408600	1.28812200	-2.78179200
C	0.63343300	1.61765400	-4.08505800
C	-0.37091700	1.64807700	-5.07094600
C	-1.68581400	1.34104800	-4.75094200
C	-2.02466100	0.97258100	-3.39209400
N	-2.71201200	1.37806500	-5.71461200
H	-3.63190100	1.11601600	-5.36554200

H	1.12966900	1.27017700	-2.02444400
C	-2.72828100	1.73087600	-7.01825600
C	-3.97965800	2.01838900	-8.86228800
C	-1.81044800	2.42980100	-8.93995600
S	2.32091300	2.04663800	-4.58012100
O	2.26052900	3.48099200	-5.01359100
O	2.65933100	1.11971900	-5.70813900
O	3.17864300	1.83736400	-3.37325800
N	-3.95995300	1.66929600	-7.59998400
N	-1.61327700	2.11190800	-7.67605500
N	-2.95182900	2.41540800	-9.62231900
Cl	-5.53045700	1.97272100	-9.66218900
Cl	-0.40191200	2.94026500	-9.83431400
H	-0.12078400	1.91460700	-6.08623300

P1

C	-0.93569000	-0.02809500	0.00005000
C	-0.26901100	1.20221000	-0.00003000
C	-0.21629200	-1.22803800	0.00001000
C	1.12940300	1.22514600	0.00004500
H	-0.84160400	2.12706200	-0.00023000
C	1.18043900	-1.19053100	0.00002300
H	-0.75167500	-2.17355800	0.00000800
C	1.86170900	0.03285900	-0.00004700
H	1.64502200	2.18209100	-0.00017800
H	1.73714800	-2.12422500	-0.00000800
H	2.94793900	0.05599800	0.00020600
O	-2.31703400	-0.11575200	-0.00015300
H	-2.70390600	0.77734900	0.00112000

P1-CPLT

C	3.00483700	-1.58725100	-0.02837400
C	1.61178000	-1.45573100	-0.09582700
C	1.86764000	0.97133900	-0.03496600
C	3.28137500	0.80349300	0.03110800
C	3.84329000	-0.44141600	0.03960500
H	3.90470900	1.68848700	0.07893800
S	5.65193500	-0.60085600	0.13176700
O	6.16570200	0.79915300	0.22349800
O	5.93031700	-1.40132100	1.36508400
O	6.06718000	-1.29116000	-1.12937000
N	3.61749400	-2.87075500	-0.02802600
N	3.09643300	-3.94192300	-0.07584400
O	0.82122900	-2.55056100	-0.17193600

H	1.35247500	-3.38358300	-0.16175700
C	1.34822200	2.28924700	-0.03679200
C	-0.00999200	2.47809500	-0.09686400
C	-0.90430100	1.39280300	-0.14845900
C	-0.43659000	0.08674100	-0.13903200
C	0.98970700	-0.16088500	-0.09232500
N	-1.31609000	-1.01247100	-0.18141400
H	-0.86451100	-1.92133200	-0.25301300
H	2.03361500	3.12787900	0.00846800
C	-2.66012800	-1.10826500	-0.07915000
C	-4.43537800	-2.48397000	-0.02745700
C	-4.73716300	-0.30420200	0.16664000
S	-0.70748200	4.14835700	-0.09644000
O	-1.54624200	4.23284600	1.14351400
O	-1.52597100	4.24361300	-1.34857100
O	0.45424900	5.08928800	-0.08231900
N	-3.13419800	-2.38471600	-0.13789300
N	-3.45178400	-0.02651300	0.07398400
N	-5.32499300	-1.49624300	0.12781000
Cl	-5.10559300	-4.09417100	-0.08610300
Cl	-5.80559400	1.06048300	0.36599500
H	-1.96689800	1.57472800	-0.19422000

C1-CP1

C	2.34980000	-0.45435900	-0.16321700
C	1.03057300	0.05999200	-0.13148800
C	-0.11901000	-0.80066500	-0.11759500
C	0.12897700	-2.21107700	-0.13438500
C	1.46239700	-2.71662600	-0.15535600
C	2.53631900	-1.87443600	-0.16941400
C	-1.49581800	-0.35361300	-0.09156800
C	-0.94344700	-3.13427000	-0.13567400
H	1.60457400	-3.79076800	-0.16184500
C	-2.23541000	-2.66601500	-0.12282800
C	-2.52167800	-1.28897300	-0.10065900
H	-0.72752800	-4.19671500	-0.14826300
H	-3.54704000	-0.95384300	-0.08445600
N	-1.75066800	1.03015700	-0.04793800
H	-0.91322800	1.61132500	-0.04399400
C	-2.89395800	1.74625400	0.01511900
C	-3.81821000	3.78943100	0.15265100
C	-5.11961300	2.00658000	0.06703900
Cl	-3.65140400	5.52408800	0.24490000
Cl	-6.71538600	1.29991500	0.05592700

N	-5.07640200	3.33331700	0.14677800
N	-4.11059300	1.16230300	-0.00399500
N	-2.70951800	3.09468700	0.09616800
S	-3.63175300	-3.81545900	-0.17349200
S	4.19565500	-2.61475600	-0.21077700
O	-4.54225300	-3.39863800	0.94123500
O	-4.25321200	-3.62498700	-1.52511200
O	-3.06155300	-5.18471000	0.01836400
O	3.97441000	-4.09172300	-0.18985600
O	4.85481300	-2.14426900	-1.46546800
O	4.90613900	-2.13587900	1.02947500
N	3.49581000	0.33401500	-0.19239800
N	3.32979100	1.59625700	-0.19069800
C	4.48589100	2.40415100	-0.22816800
C	4.25829800	3.79002600	-0.21370300
C	5.79982600	1.90231600	-0.28058400
C	5.33703000	4.67411100	-0.24999200
H	3.23678200	4.15818100	-0.17368200
C	6.86873600	2.79362200	-0.31692000
H	5.97139300	0.83193000	-0.29305500
C	6.64385200	4.17857300	-0.30195600
H	5.15773500	5.74553000	-0.23861300
H	7.88484800	2.41059100	-0.35806300
H	7.48598700	4.86467500	-0.33087700
O	0.85112400	1.39375400	-0.11933200
H	1.78330000	1.82804000	-0.14394000
O	3.81328800	-1.88447600	3.53871400
H	4.15786300	-1.99142100	2.60365100

C1-TS1

C	2.36644600	-0.53748900	-0.07003400
C	1.05431000	0.00723000	-0.07412800
C	-0.11297800	-0.82876000	-0.08254400
C	0.10547300	-2.24403700	-0.09443600
C	1.42818400	-2.77923200	-0.07322900
C	2.52066600	-1.96356000	-0.05931800
C	-1.47985400	-0.35186500	-0.09263300
C	-0.98459600	-3.14383000	-0.12194000
H	1.54545900	-3.85627800	-0.05771200
C	-2.26703700	-2.64803100	-0.14324100
C	-2.52493300	-1.26620200	-0.12821600
H	-0.79091500	-4.21056100	-0.12751700
H	-3.54302900	-0.90953000	-0.13939700
N	-1.70680800	1.03593100	-0.05853100

H	-0.85881800	1.60111800	-0.04745600
C	-2.83758300	1.77524000	-0.02169500
C	-3.72436300	3.83720100	0.07116700
C	-5.05827300	2.07758100	-0.00259600
Cl	-3.52822200	5.56950900	0.13660500
Cl	-6.66618200	1.40000900	-0.01850600
N	-4.99050900	3.40426800	0.05468500
N	-4.06410800	1.21374200	-0.04806700
N	-2.62824200	3.12047800	0.04307200
S	-3.68591500	-3.76899700	-0.22580400
S	4.16123300	-2.73793800	0.05709500
O	-4.59872700	-3.35017700	0.88601200
O	-4.28898600	-3.54575300	-1.58053900
O	-3.14423800	-5.15165400	-0.04901900
O	3.90761900	-4.20927900	0.09883000
O	4.95158000	-2.32478500	-1.14069200
O	4.73913700	-2.22509800	1.35081900
N	3.52810600	0.22634000	-0.14183500
N	3.38906600	1.49076200	-0.17295000
C	4.56115100	2.26887100	-0.27440800
C	4.37077600	3.66048300	-0.26754400
C	5.85694600	1.73051800	-0.38522900
C	5.47018000	4.51360900	-0.36813200
H	3.36270000	4.05693800	-0.18243000
C	6.94627300	2.59117700	-0.48646700
H	5.99852100	0.65572100	-0.39555400
C	6.75905400	3.98186300	-0.47778000
H	5.32047600	5.58957900	-0.36182600
H	7.94841200	2.18020800	-0.57406500
H	7.61631900	4.64475800	-0.55752900
O	0.90626800	1.34126400	-0.09161200
H	1.84827000	1.75597600	-0.11856300
O	2.96791800	-0.72532700	2.95103200
H	3.63045400	-1.28782500	2.46232500
C1-CP2			
C	2.40851400	-0.55492900	0.05893500
C	1.08229600	-0.00140500	0.00165700
C	-0.08461100	-0.83669400	-0.05217000
C	0.13627100	-2.24990700	-0.08390500
C	1.46183500	-2.78831200	-0.01501500
C	2.55711200	-1.98460400	0.05259700
C	-1.44609700	-0.35556800	-0.09535800
C	-0.94635000	-3.14691200	-0.16863600

H	1.57208900	-3.86638900	-0.00032000
C	-2.23142900	-2.64858200	-0.22888500
C	-2.49096100	-1.27214000	-0.19162300
H	-0.75457400	-4.21371600	-0.18666100
H	-3.50806000	-0.91435500	-0.23011500
N	-1.67676300	1.02673500	-0.03283100
H	-0.83392600	1.59822400	-0.01304900
C	-2.81349200	1.76089300	0.03303800
C	-3.70679300	3.81562100	0.17687100
C	-5.03407800	2.05102800	0.09003400
Cl	-3.51628800	5.54617800	0.27190700
Cl	-6.63778100	1.36640500	0.08384200
N	-4.97025500	3.37650500	0.17046000
N	-4.03552700	1.19338800	0.01507000
N	-2.60750100	3.10365400	0.11895200
S	-3.64519000	-3.77231500	-0.38539300
S	4.18673500	-2.75855100	0.27896600
O	-4.59237100	-3.37995500	0.70600900
O	-4.20202100	-3.51720000	-1.75337800
O	-3.10240700	-5.15549500	-0.22284500
O	3.91223900	-4.22407900	0.38706900
O	5.02069200	-2.42386100	-0.91596400
O	4.70636800	-2.17171900	1.55713900
N	3.56926600	0.20047000	-0.09672800
N	3.42378800	1.46293700	-0.15285800
C	4.57829700	2.24443900	-0.33491200
C	4.37182500	3.63435400	-0.37321200
C	5.87512100	1.71165700	-0.47112700
C	5.45762600	4.49192500	-0.54648400
H	3.36290900	4.02295800	-0.26566500
C	6.94986200	2.57737700	-0.64416100
H	6.02661900	0.63859800	-0.44288000
C	6.74673700	3.96607100	-0.68162100
H	5.29862200	5.56602700	-0.57506000
H	7.95307200	2.17395700	-0.75035100
H	7.59378900	4.63305100	-0.81647700
O	0.94563800	1.31782200	-0.03919200
H	1.89490100	1.73171900	-0.06757400
O	2.21145100	-0.26746000	2.43361800
H	3.00114800	-0.84626100	2.47300900
C1-TS _{CO}			
C	-2.41430200	-0.55922800	-0.29149000
C	-1.07810500	-0.01475300	-0.12627700

C	0.07852700	-0.84629300	-0.00715900
C	-0.14398600	-2.26023800	0.04197400
C	-1.47120200	-2.79621200	-0.05341200
C	-2.56134700	-1.99903500	-0.18347200
C	1.44030600	-0.36669600	0.08183300
C	0.93104000	-3.15546500	0.18385200
H	-1.58312400	-3.87409500	-0.02346200
C	2.21581200	-2.65809800	0.28197000
C	2.47854100	-1.28249600	0.23187200
H	0.73706000	-4.22158600	0.21592900
H	3.49416700	-0.92535200	0.30259000
N	1.67495600	1.01479600	0.00924500
H	0.83420300	1.58832600	-0.02787800
C	2.81425100	1.74427800	-0.05880100
C	3.71610400	3.79443600	-0.21455300
C	5.03599600	2.02478900	-0.11934400
Cl	3.53218600	5.52531200	-0.31982000
Cl	6.63705300	1.33360400	-0.11158500
N	4.97785700	3.35021200	-0.20671200
N	4.03414300	1.17174200	-0.03908400
N	2.61393700	3.08760100	-0.15135600
S	3.62076900	-3.78022500	0.50305800
S	-4.18951300	-2.78376700	-0.37654900
O	4.59845100	-3.41386100	-0.57084600
O	4.14259600	-3.49668700	1.87933600
O	3.07934400	-5.16583100	0.35613600
O	-3.90771200	-4.24407200	-0.52378500
O	-4.98974200	-2.48135400	0.84995600
O	-4.76010700	-2.17619900	-1.62448200
N	-3.57325200	0.18841300	0.03229300
N	-3.42685000	1.44421000	0.08889200
C	-4.55112500	2.22430000	0.42418200
C	-4.33651400	3.61222800	0.45163700
C	-5.82304900	1.69216600	0.70908600
C	-5.39135400	4.47135700	0.75909000
H	-3.34585300	3.99923900	0.22936900
C	-6.86701300	2.55906800	1.01571900
H	-5.98115400	0.61972300	0.68817600
C	-6.65687600	3.94683600	1.04080700
H	-5.22621100	5.54472500	0.77838100
H	-7.85177500	2.15638400	1.23599900
H	-7.48051600	4.61387800	1.28004200
O	-0.94531800	1.30743700	-0.11190600
H	-1.89053600	1.72061600	-0.08142100

O	-2.47657200	-0.28722800	-2.28248200
H	-3.24696900	-0.87801300	-2.41677300
C1-CP3			
C	-2.55640700	-0.36565800	-0.89312400
C	-1.10082500	0.01738800	-0.74241000
C	-0.06806700	-0.85330000	-0.34549800
C	-0.42169200	-2.22947600	-0.10616100
C	-1.79441500	-2.65842200	-0.24910600
C	-2.79491000	-1.82116700	-0.57810500
C	1.32641500	-0.48686700	-0.17478400
C	0.53926600	-3.17168700	0.26656600
H	-2.00099300	-3.71066700	-0.07477200
C	1.86451300	-2.78168400	0.41418200
C	2.25631100	-1.45357800	0.19732400
H	0.24008400	-4.19983200	0.43807800
H	3.29025000	-1.17009100	0.32121500
N	1.69091000	0.85435900	-0.39577600
H	0.92186100	1.46134200	-0.67561700
C	2.87108600	1.50686700	-0.33177400
C	3.94417600	3.46063300	-0.61688100
C	5.07660700	1.67717300	0.02937400
Cl	3.91716100	5.15369600	-1.04200100
Cl	6.58765400	0.93218700	0.48535000
N	5.14348200	2.96936600	-0.28064200
N	4.01782800	0.89299800	0.03183500
N	2.79952300	2.82742300	-0.66473000
S	3.13013300	-3.98180400	0.87328600
S	-4.48042300	-2.46308600	-0.70412400
O	4.06014100	-4.06595100	-0.30164300
O	3.80223000	-3.42482600	2.09286400
O	2.41242700	-5.26760300	1.13940900
O	-4.36109100	-3.89034100	-1.13031500
O	-5.12783500	-2.31671400	0.63630700
O	-5.13168900	-1.59478400	-1.75197900
N	-3.37474800	0.46713700	0.08042500
N	-3.30388800	1.69006500	-0.17999600
C	-4.01225900	2.58644800	0.66124200
C	-3.79310300	3.94821900	0.40523000
C	-4.89899000	2.18397500	1.67624500
C	-4.44810200	4.91321900	1.17188700
H	-3.10963000	4.23377800	-0.38941900
C	-5.55119400	3.15416900	2.43173100
H	-5.07430000	1.12971000	1.86007900

C	-5.32722500	4.51758800	2.18439200
H	-4.27529400	5.96779500	0.97719200
H	-6.23995300	2.85200800	3.21580600
H	-5.84231300	5.26667600	2.77962000
O	-0.83764600	1.31174300	-1.05409100
H	-1.68619200	1.83302200	-1.01793200
O	-2.92333200	-0.04609000	-2.23673100
H	-3.82524900	-0.42145700	-2.36814800

C1-TS3

C	-2.47611500	-0.14231000	-0.96316300
C	-0.98921000	0.12727800	-0.90246500
C	-0.01545800	-0.78829600	-0.46925500
C	-0.45827300	-2.13646500	-0.21043500
C	-1.84849400	-2.49245200	-0.40026300
C	-2.79453300	-1.60247300	-0.74961500
C	1.39837600	-0.50819100	-0.29877400
C	0.43681800	-3.12743000	0.19496000
H	-2.11297100	-3.53562400	-0.25290600
C	1.78229000	-2.81650300	0.35574100
C	2.26010700	-1.52201300	0.11001600
H	0.07304900	-4.13287500	0.37616600
H	3.30875300	-1.30199700	0.23885000
N	1.85112900	0.80185400	-0.54724600
H	1.13680800	1.45207600	-0.86754300
C	3.06887700	1.37959900	-0.46592600
C	4.27044800	3.25594500	-0.75759700
C	5.27120800	1.41709600	-0.05134700
Cl	4.36450300	4.93834200	-1.21378300
Cl	6.71693300	0.58919300	0.46916300
N	5.42761400	2.69592500	-0.38311200
N	4.16514900	0.70088700	-0.06430900
N	3.08886300	2.69594900	-0.82221200
S	2.96317300	-4.08006000	0.86695600
S	-4.51108400	-2.13814600	-0.90965600
O	3.92499300	-4.23023300	-0.27487900
O	3.62591400	-3.54775600	2.10271500
O	2.16593500	-5.32066800	1.12121600
O	-4.47994600	-3.59318600	-1.23871900
O	-5.19198000	-1.84925800	0.39097000
O	-5.06294300	-1.29554800	-2.03420200
N	-3.05328700	0.64112900	0.21135500
N	-3.33812900	1.81875600	-0.08978800
C	-3.79606000	2.65469300	0.97011500

C	-4.26178600	3.91646600	0.57339400
C	-3.78773100	2.29753000	2.33026400
C	-4.73609100	4.81785700	1.52848000
H	-4.25227000	4.17463600	-0.48180300
C	-4.25496700	3.20543900	3.27724400
H	-3.41282700	1.32716800	2.63646600
C	-4.73231700	4.46389300	2.88087100
H	-5.10200600	5.79255100	1.21819000
H	-4.24583100	2.93662700	4.33007900
H	-5.09557100	5.16481500	3.62763200
O	-0.64525400	1.39246900	-1.26160000
H	-1.42437700	1.88534100	-1.59012600
O	-2.91164600	0.34329700	-2.22127600
H	-3.82232800	-0.00808900	-2.36551100

C1-CP4

C	-2.49261300	-0.14146900	-1.06442700
C	-0.99562800	0.08908800	-1.10053100
C	-0.03618500	-0.79683500	-0.58762300
C	-0.49779600	-2.11050600	-0.20732100
C	-1.88990500	-2.46657800	-0.38300000
C	-2.82504300	-1.59426200	-0.80319700
C	1.38167000	-0.52478200	-0.44900200
C	0.38689900	-3.07469600	0.27759900
H	-2.16411800	-3.49629400	-0.17163800
C	1.73976600	-2.77455100	0.39379200
C	2.23439900	-1.51358800	0.03046300
H	0.01093100	-4.05570600	0.54672700
H	3.28889900	-1.30229400	0.12344800
N	1.84992000	0.75308400	-0.81396800
H	1.17329600	1.33488900	-1.30307800
C	3.01709400	1.39141600	-0.58693400
C	4.20702300	3.27588600	-0.86963500
C	5.08689400	1.58607200	0.24980100
Cl	4.34814900	4.89956100	-1.49553600
Cl	6.42029500	0.90009000	1.14343400
N	5.27452900	2.82425800	-0.19994600
N	4.02480800	0.81975700	0.10802200
N	3.08097000	2.65105100	-1.10697000
S	2.90624700	-4.00754300	1.00148600
S	-4.54641400	-2.12198300	-0.92820500
O	3.92466700	-4.17918700	-0.08628600
O	3.50334700	-3.43298900	2.25235200
O	2.11004300	-5.24908600	1.25486300

O	-4.52729000	-3.58312400	-1.22877800
O	-5.20394700	-1.80400600	0.37785600
O	-5.11247200	-1.29778100	-2.05913200
N	-2.97851700	0.64504900	0.15223000
N	-3.68120600	1.63181100	-0.13554100
C	-4.13741500	2.42305000	0.96291800
C	-4.97475000	3.49216200	0.61620500
C	-3.80233800	2.19271600	2.30870900
C	-5.48556100	4.33047900	1.60987200
H	-5.21835700	3.65430000	-0.43004600
C	-4.31387600	3.03408000	3.29346500
H	-3.15016300	1.36775600	2.57370400
C	-5.15654100	4.10191500	2.94895500
H	-6.13599300	5.15737300	1.33890300
H	-4.05765800	2.86058100	4.33519800
H	-5.55132300	4.75230000	3.72492900
O	-0.63308700	1.29113100	-1.62605300
H	-1.38423100	1.68014900	-2.11829800
O	-2.98631900	0.34689800	-2.29299500
H	-3.90178000	-0.00219800	-2.40865400

C1-TS_{CN}

C	-2.49861100	-0.01515900	-1.30485700
C	-1.05095900	0.13888800	-1.27058500
C	-0.20217200	-0.79278500	-0.64409100
C	-0.79906100	-2.04958200	-0.25667000
C	-2.17686800	-2.31889000	-0.56496100
C	-2.98412600	-1.38775000	-1.13413700
C	1.21336200	-0.61419700	-0.38208400
C	-0.03519300	-3.04618200	0.37239800
H	-2.55365200	-3.31438700	-0.35036100
C	1.30649200	-2.82412100	0.62472700
C	1.93147200	-1.62035700	0.24861300
H	-0.50785300	-3.98229500	0.64935300
H	2.97995000	-1.47211300	0.45766700
N	1.80164700	0.60889300	-0.76613700
H	1.17429000	1.25471600	-1.24050400
C	3.04792900	1.10515400	-0.62559400
C	4.42338700	2.84864700	-0.96966100
C	5.18964800	1.03586800	0.03374200
Cl	4.70215900	4.46554700	-1.56839300
Cl	6.50392200	0.16437600	0.78362900
N	5.48223100	2.25871700	-0.40018700
N	4.03752300	0.40149600	-0.03290100

N	3.21703400	2.36413500	-1.12519700
S	2.31266800	-4.08334200	1.43130100
S	-4.70912000	-1.77220500	-1.47270100
O	3.37304600	-4.46411200	0.43928200
O	2.88875700	-3.43017900	2.65333600
O	1.39174400	-5.21708500	1.75865200
O	-4.78743000	-3.24033500	-1.71336400
O	-5.50721800	-1.32142300	-0.29107600
O	-5.02443900	-0.95616900	-2.70613700
N	-2.90854800	0.74425200	0.35678500
N	-3.27252700	1.89197200	0.20527700
C	-3.55257300	2.70937700	1.36083500
C	-3.94628300	4.02436200	1.09301300
C	-3.44882500	2.24435100	2.68068900
C	-4.23636700	4.88798700	2.15265700
H	-4.01989300	4.35890100	0.06213600
C	-3.74097800	3.11224000	3.73100500
H	-3.14382100	1.22127800	2.87538300
C	-4.13395900	4.43319500	3.47059900
H	-4.54030400	5.91081000	1.94844200
H	-3.66333400	2.76069300	4.75634600
H	-4.35952300	5.10308500	4.29595800
O	-0.57145300	1.31081500	-1.77885200
H	-1.28609900	1.75512000	-2.27935700
O	-3.07394900	0.81479800	-2.24617200
H	-3.90726300	0.39238700	-2.57734400
FRG1			
C	0.44537100	-2.12013200	0.00000000
C	1.53187500	-1.23999500	0.00000000
C	1.31161800	0.13981300	0.00000000
C	0.00000000	0.61717700	0.00000000
C	-1.09935200	-0.25057500	0.00000000
C	-0.86664000	-1.62474700	0.00000000
H	0.61687400	-3.19305300	0.00000000
H	2.54786800	-1.62406700	0.00000000
H	2.14038500	0.84179300	0.00000000
H	-2.11009800	0.14592900	0.00000000
H	-1.70818900	-2.31208100	0.00000000
N	-0.16038800	2.05977100	0.00000000
N	-1.18590900	2.65626300	0.00000000
FRG1-CPLT			
C	3.00019700	-1.76187400	0.00677800

C	1.62293200	-1.56359900	0.06063600
C	1.04701700	-0.26390000	0.05849700
C	1.96071300	0.84677000	-0.00520500
C	3.35648500	0.62558000	-0.06661200
C	3.87383200	-0.65185800	-0.06012000
C	-0.37162900	0.03420600	0.10621300
C	1.47617800	2.18326300	-0.00720200
H	4.01608300	1.48576500	-0.11994400
C	0.12777200	2.41366100	0.05565100
C	-0.80092300	1.34878800	0.11280700
H	2.18764900	3.00013300	-0.05751700
H	-1.85744600	1.56297000	0.15999300
N	-1.27448800	-1.05242300	0.14574500
H	-0.83622300	-1.97097900	0.18538300
C	-2.61833600	-1.11973600	0.07514200
C	-4.42630500	-2.45366500	0.00945000
C	-4.68341500	-0.26241900	-0.08632900
Cl	-5.13315600	-4.05076500	0.02707000
Cl	-5.72765700	1.13237500	-0.20646100
N	-5.29803400	-1.44198400	-0.08759600
N	-3.39231800	-0.01492200	-0.00738900
N	-3.12196000	-2.38841800	0.09202000
S	-0.52138100	4.09735300	0.04769100
S	5.66565100	-0.87954500	-0.06064500
O	-1.37163200	4.20230900	-1.18505300
O	-1.32886800	4.23447300	1.30496600
O	0.66426800	5.01044200	0.01503500
O	6.23660700	0.16951900	-0.95156600
O	6.11199300	-0.75674800	1.36057200
O	5.86586700	-2.27654100	-0.60088000
O	0.82150800	-2.68240500	0.11711000
H	1.38297800	-3.48114100	0.08913000
O	3.40986600	-3.06882300	0.02031500
H	4.37608300	-3.09391000	-0.20182400

C7-CP1

C	-2.52099700	-0.59232900	-0.07086100
C	-1.24068800	0.00230700	0.04074700
C	-0.03661400	-0.77829700	-0.01050600
C	-0.18995700	-2.19608300	-0.13982400
C	-1.48508600	-2.78245000	-0.24214200
C	-2.61345800	-2.01434400	-0.21793000
C	1.30648000	-0.24438900	0.06103000
C	0.94098100	-3.04669700	-0.16816400

H	-1.55547000	-3.85867700	-0.34397500
C	2.19632900	-2.49848500	-0.06556000
C	2.39119200	-1.10968400	0.04758400
H	0.79671900	-4.11712000	-0.26263900
H	3.39183300	-0.71272100	0.11883700
N	1.47634800	1.15023000	0.15902000
H	0.61453400	1.67284200	0.30933100
C	2.55634300	1.94232900	-0.01539600
C	3.35580000	4.04181800	-0.03734200
C	4.71210900	2.35308200	-0.47166700
Cl	3.10805500	5.75879400	0.15650400
Cl	6.30062900	1.75858000	-0.88227800
N	4.60486100	3.67301300	-0.34525800
N	3.77150800	1.44231300	-0.32443800
N	2.30842600	3.27407400	0.13636600
S	3.66237100	-3.55462500	-0.07255300
S	-4.21988700	-2.85791600	-0.37786600
O	3.18115800	-4.96291700	-0.18131700
O	4.49079900	-3.11416800	-1.23669600
O	4.35378600	-3.27679100	1.23977300
O	-3.88524300	-4.31164000	-0.50128900
O	-4.99136300	-2.56043800	0.87055200
O	-4.85984500	-2.31412000	-1.61761800
N	-3.71703600	0.11844900	-0.04088800
N	-3.63978200	1.38041700	0.10534100
C	-4.85178300	2.10290400	0.13858000
C	-4.72856200	3.49088200	0.31397300
C	-6.12430000	1.51523400	0.01213600
C	-5.87061900	4.29078000	0.36504600
H	-3.73778100	3.92662900	0.41001500
C	-7.25696300	2.32288700	0.06402800
H	-6.21502200	0.44346000	-0.12377500
C	-7.13658400	3.70970700	0.24046400
H	-5.77185700	5.36400000	0.50177900
H	-8.24114300	1.87262100	-0.03387600
H	-8.02730200	4.33085200	0.27935600
O	-1.14957100	1.33489900	0.20764000
H	-2.10601600	1.70820000	0.21277900
O	3.14017600	-2.46685300	3.57790900
H	3.53294600	-2.77304700	2.70923900
C7-TS1			
C	-2.52173100	-0.59642300	-0.07597600
C	-1.24033700	-0.00440900	0.03743700

C	-0.03777000	-0.78738400	-0.01297100
C	-0.19375100	-2.20467000	-0.14451000
C	-1.48981700	-2.78827400	-0.24947400
C	-2.61676500	-2.01799600	-0.22505000
C	1.30625500	-0.25632900	0.06197200
C	0.93544800	-3.05776400	-0.17066900
H	-1.56223000	-3.86421800	-0.35282300
C	2.19163000	-2.51252600	-0.06387300
C	2.38928700	-1.12409700	0.05076100
H	0.78895100	-4.12781300	-0.26596800
H	3.39061400	-0.72925100	0.12426600
N	1.47882100	1.13768900	0.16082800
H	0.61761300	1.66204400	0.30869100
C	2.56108300	1.92767700	-0.00994300
C	3.36446500	4.02563200	-0.02997400
C	4.71880100	2.33426800	-0.46037000
Cl	3.11935600	5.74299800	0.16336700
Cl	6.30719700	1.73684100	-0.86697800
N	4.61358400	3.65442300	-0.33470800
N	3.77619300	1.42523500	-0.31495900
N	2.31518300	3.25983100	0.14087600
S	3.65499500	-3.57242600	-0.05809600
S	-4.22466200	-2.85849900	-0.38678400
O	3.17178200	-4.97910800	-0.17890100
O	4.49897900	-3.12955100	-1.21020800
O	4.32871900	-3.30162300	1.26467600
O	-3.89254400	-4.31265000	-0.51176600
O	-4.99613700	-2.56109600	0.86162900
O	-4.86302300	-2.31209000	-1.62620600
N	-3.71649600	0.11652900	-0.04521300
N	-3.63687700	1.37814600	0.10262100
C	-4.84757500	2.10269300	0.13808100
C	-4.72175800	3.49023000	0.31513600
C	-6.12125800	1.51730800	0.01282500
C	-5.86241000	4.29193800	0.36918400
H	-3.73010900	3.92419800	0.41026600
C	-7.25250200	2.32674900	0.06768900
H	-6.21397200	0.44585600	-0.12427100
C	-7.12953200	3.71312100	0.24587800
H	-5.76164400	5.36479500	0.50729200
H	-8.23759300	1.87825400	-0.02917100
H	-8.01915300	4.33568200	0.28716800
O	-1.14672400	1.32776500	0.20592600
H	-2.10238800	1.70298100	0.21088800

O	3.12315300	-2.21606600	3.50202600
H	3.51369800	-2.61293600	2.67053700

C7-CP2

C	-2.53570800	-0.59217100	-0.00046000
C	-1.24465200	-0.00889400	0.08563800
C	-0.04701700	-0.80462900	0.08566000
C	-0.22836400	-2.22677300	0.00291700
C	-1.50928700	-2.79369500	-0.08669500
C	-2.64673500	-2.01000000	-0.09283000
C	1.27925000	-0.28282500	0.13575900
C	0.91647700	-3.10602700	-0.03756300
H	-1.59627400	-3.87116900	-0.16126100
C	2.16626100	-2.62560200	0.07961300
C	2.46759700	-1.18098300	0.35905800
H	0.73446000	-4.16673200	-0.18271200
H	3.29749400	-0.84607100	-0.26545400
N	1.48721100	1.08653700	0.07026300
H	0.62750900	1.63884800	0.07034300
C	2.59795500	1.86184700	-0.02609600
C	3.40599500	3.95279000	-0.17034300
C	4.79934500	2.23724900	-0.19297300
Cl	3.14852600	5.67826500	-0.22118000
Cl	6.43006500	1.61741900	-0.26759900
N	4.68424300	3.56345400	-0.24313600
N	3.84153200	1.34144300	-0.09188100
N	2.33885500	3.19949600	-0.06509500
S	3.60144400	-3.69705400	-0.04646300
S	-4.25497300	-2.84384500	-0.23742500
O	3.12249600	-5.10852600	0.05086300
O	4.23758700	-3.38087400	-1.36697000
O	4.47450100	-3.28924500	1.11196700
O	-3.92836300	-4.30253400	-0.32283100
O	-5.03072200	-2.51099800	0.99983800
O	-4.89017700	-2.32908900	-1.49206500
N	-3.72422500	0.13707000	0.00226500
N	-3.62739900	1.40131000	0.09647800
C	-4.82809900	2.14328700	0.09958700
C	-4.68343500	3.53411000	0.22967300
C	-6.10871300	1.57110600	-0.01661900
C	-5.81308700	4.35278100	0.24634800
H	-3.68647500	3.95703100	0.31830100
C	-7.22861300	2.39745000	-0.00017100
H	-6.21504600	0.49695500	-0.11820000

C	-7.08700300	3.78733200	0.13153300
H	-5.69856700	5.42826400	0.34827500
H	-8.21923400	1.96006000	-0.09084200
H	-7.96800500	4.42328300	0.14349800
O	-1.13155200	1.32894800	0.18538600
H	-2.07947400	1.71836700	0.17859400
O	2.86516200	-1.01381000	1.75420500
H	3.63805800	-1.60533900	1.87330100

C7-TS2

C	-2.52945300	-0.58923700	-0.00172800
C	-1.23970900	-0.00297900	0.08322700
C	-0.04100500	-0.79644100	0.07355500
C	-0.21782400	-2.21663200	-0.02855800
C	-1.49723400	-2.78742800	-0.11929100
C	-2.63674000	-2.00706400	-0.10631000
C	1.28539400	-0.27745000	0.12817600
C	0.93075500	-3.08753700	-0.08406500
H	-1.58127000	-3.86416900	-0.20680200
C	2.18303500	-2.61450900	0.05934700
C	2.47792800	-1.17604000	0.35742300
H	0.75414400	-4.14317400	-0.26584000
H	3.31052200	-0.83829000	-0.25747900
N	1.49179600	1.09143400	0.06073500
H	0.63126400	1.64236200	0.04892200
C	2.60155000	1.87132000	-0.01733700
C	3.40180900	3.96445700	-0.16805000
C	4.80442000	2.25618800	-0.13480600
Cl	3.13650700	5.68765000	-0.24540900
Cl	6.43907000	1.64431800	-0.17108300
N	4.68334800	3.58100200	-0.20510200
N	3.84879700	1.35693600	-0.04198600
N	2.33619800	3.20653000	-0.08155900
S	3.59274100	-3.73144400	-0.01922300
S	-4.24387400	-2.84413300	-0.24313500
O	3.08659600	-5.03280000	-0.55304800
O	4.58503400	-3.06863400	-0.92599200
O	4.09087100	-3.83934800	1.39520300
O	-3.91455800	-4.30168900	-0.33682600
O	-5.01117100	-2.51813200	1.00126500
O	-4.88976600	-2.32576300	-1.49086000
N	-3.71948600	0.13714800	0.01013600
N	-3.62469400	1.40134000	0.10899500
C	-4.82650100	2.14125900	0.11924000

C	-4.68307000	3.53277600	0.24345100
C	-6.10710600	1.56680200	0.01441500
C	-5.81373200	4.34991900	0.26440000
H	-3.68613600	3.95748800	0.32334900
C	-7.22807600	2.39158800	0.03572500
H	-6.21261100	0.49208200	-0.08186000
C	-7.08759700	3.78223000	0.16047600
H	-5.70003000	5.42599900	0.36079200
H	-8.21868700	1.95240600	-0.04590800
H	-7.96941000	4.41698300	0.17571700
O	-1.12874500	1.33413200	0.18993300
H	-2.07777600	1.72160500	0.18763700
O	2.90868600	-0.99045200	1.74780200
H	2.90072300	-1.85808100	2.19057200

C7-CP3

C	-2.52836100	-0.58458400	-0.01106400
C	-1.23956700	0.00244400	0.08538800
C	-0.04123700	-0.79035400	0.08882200
C	-0.21507900	-2.21147300	-0.00365400
C	-1.49306100	-2.78247800	-0.11144300
C	-2.63294400	-2.00228200	-0.11743400
C	1.28616600	-0.27101000	0.15036400
C	0.93539100	-3.08236100	-0.04476600
H	-1.57587100	-3.85935400	-0.19851300
C	2.18545000	-2.60931600	0.12019800
C	2.46554900	-1.16995400	0.44324800
H	0.76033900	-4.13561800	-0.24089900
H	3.33827700	-0.83050900	-0.10730100
N	1.49359800	1.09749700	0.06522300
H	0.63453900	1.65063700	0.05676900
C	2.60521300	1.87055800	-0.03560100
C	3.41771800	3.95799100	-0.19956500
C	4.80797500	2.23963500	-0.20434800
Cl	3.16438600	5.68340700	-0.26666700
Cl	6.43678200	1.61538600	-0.27296400
N	4.69528500	3.56519900	-0.26745400
N	3.84756800	1.34703600	-0.09556400
N	2.34880600	3.20815500	-0.08778300
S	3.59713600	-3.72183700	-0.02641300
S	-4.23720600	-2.84044700	-0.28037800
O	3.07301100	-4.99165600	-0.62091500
O	4.56322200	-3.00974500	-0.92673100
O	4.14605000	-3.92079200	1.35591700

O	-3.90471800	-4.29675700	-0.38150000
O	-5.02031100	-2.52531100	0.95696100
O	-4.86824800	-2.31301400	-1.53188400
N	-3.71921000	0.14016300	-0.00312000
N	-3.62683800	1.40406400	0.10195800
C	-4.83052900	2.14108900	0.11562200
C	-4.69127000	3.53107400	0.25997700
C	-6.10925500	1.56496800	-0.00187600
C	-5.82422800	4.34479600	0.29007800
H	-3.69573900	3.95720200	0.34940600
C	-7.23251700	2.38639800	0.02799000
H	-6.21164400	0.49154000	-0.11453300
C	-7.09626200	3.77533800	0.17432300
H	-5.71374400	5.41956700	0.40340900
H	-8.22163500	1.94577900	-0.06350300
H	-7.97985300	4.40738800	0.19678700
O	-1.12978000	1.33969300	0.19467500
H	-2.07861800	1.72641000	0.18771300
O	2.85795800	-0.99655900	1.83664400
H	2.13840100	-1.34054900	2.39735100

C7-TS_{CO}

C	-2.52230100	0.59723900	-0.07083500
C	-1.22218300	0.02732300	-0.20357400
C	-0.05030700	0.83137300	-0.15240200
C	-0.22405700	2.23861900	0.00115900
C	-1.52131100	2.80058300	0.11625500
C	-2.64053000	2.00752100	0.08868800
C	1.31622500	0.31585500	-0.28433200
C	0.89627000	3.11082100	0.05285000
H	-1.61326600	3.87373000	0.23154700
C	2.17715900	2.59965300	-0.03279000
C	2.40372100	1.23112200	-0.17137800
H	0.72436800	4.17482000	0.17334400
H	3.40906100	0.84070300	-0.19209100
N	1.50903300	-1.05169100	-0.08282000
H	0.64848100	-1.59701400	-0.04014500
C	2.62512900	-1.82501200	-0.10587800
C	3.46266500	-3.89927100	0.07301200
C	4.82589300	-2.19737500	-0.28663300
Cl	3.22495000	-5.60876000	0.31666100
Cl	6.43528000	-1.58097600	-0.54415600
N	4.72931300	-3.51164800	-0.10803700
N	3.85216100	-1.30750200	-0.29882700

N	2.38639600	-3.14823500	0.08858200
S	3.60734400	3.71144200	0.00922100
S	-4.26253300	2.82460900	0.26799200
O	3.10437000	5.00445500	0.56490300
O	4.61376200	3.04129700	0.89094500
O	4.06694500	3.82446000	-1.41309000
O	-3.94542700	4.28093400	0.39574600
O	-5.03619100	2.51947000	-0.97569800
O	-4.87838400	2.26282100	1.51052200
N	-3.70540200	-0.13696400	-0.09035600
N	-3.59966000	-1.39572000	-0.24660300
C	-4.79108700	-2.14687400	-0.26771400
C	-4.63253200	-3.53148400	-0.44780600
C	-6.07742200	-1.59150300	-0.12674200
C	-5.75344000	-4.36044900	-0.48774200
H	-3.63154100	-3.94015100	-0.55533300
C	-7.18821500	-2.42831500	-0.16796500
H	-6.19411600	-0.52261800	0.01175200
C	-7.03232600	-3.81154600	-0.34852000
H	-5.62896000	-5.43045200	-0.62785800
H	-8.18316800	-2.00521200	-0.05952100
H	-7.90693500	-4.45558300	-0.37944400
O	-1.10167300	-1.29948900	-0.38944900
H	-2.04327800	-1.69763300	-0.37844100
O	1.55610100	0.33943300	-2.38873200
H	1.27809600	1.24988000	-2.60594400

C7-CP4

C	2.48628400	-0.53167400	-0.03668300
C	1.17623800	-0.01994300	-0.33550800
C	0.04174400	-0.84413900	-0.27131400
C	0.20475500	-2.20592000	0.09532800
C	1.49735000	-2.71079300	0.40213900
C	2.60498700	-1.90069700	0.33902900
C	-1.34172300	-0.29232700	-0.62925100
C	-0.90474600	-3.08713800	0.15420600
H	1.59615900	-3.75100500	0.68809700
C	-2.19783400	-2.62207000	-0.17244900
C	-2.43793700	-1.32938700	-0.52662600
H	-0.73831600	-4.12049500	0.43919400
H	-3.43325600	-0.99119300	-0.78179200
N	-1.62907700	0.83410300	0.27075000
H	-0.87786100	1.12010200	0.88920400
C	-2.69657800	1.65214400	0.28424000

C	-3.69010200	3.45198600	1.18750300
C	-4.70377500	2.34219500	-0.43060400
Cl	-3.67879600	4.77238400	2.33048300
Cl	-6.07251200	2.14834600	-1.49846900
N	-4.77294600	3.37460200	0.40834900
N	-3.73786100	1.45844300	-0.55732600
N	-2.64282300	2.66388300	1.19472200
S	-3.56588900	-3.81165500	-0.11077000
S	4.21699000	-2.64314800	0.76536300
O	-3.64615600	-4.25135700	1.32030700
O	-4.78680000	-3.08146800	-0.56907000
O	-3.16492800	-4.92284300	-1.03282900
O	3.90574000	-4.06305400	1.12153500
O	5.07551500	-2.54011100	-0.45684600
O	4.74273600	-1.86830800	1.93336000
N	3.65494600	0.20879700	-0.10017700
N	3.54517300	1.44161700	-0.41721900
C	4.73913600	2.18239400	-0.50675100
C	4.58761400	3.54981000	-0.79642900
C	6.02606600	1.63454700	-0.33817300
C	5.71191700	4.36688700	-0.91390100
H	3.58771700	3.95522500	-0.92495800
C	7.14097600	2.45852000	-0.46092900
H	6.13979900	0.57852200	-0.12093900
C	6.99050000	3.82417000	-0.74757100
H	5.59042100	5.42343000	-1.13583100
H	8.13506800	2.03806800	-0.33453900
H	7.86766300	4.45856800	-0.84132300
O	1.02487200	1.27597000	-0.67679600
H	1.94265100	1.69652000	-0.65636700
O	-1.34737400	0.24288700	-1.96751400
H	-1.21537300	-0.49855500	-2.58687200

C7-TS4

C	-2.50359300	0.53565600	-0.06585000
C	-1.21114800	0.01856100	-0.42633100
C	-0.06297300	0.82237100	-0.35773300
C	-0.18990300	2.16938200	0.07493200
C	-1.46458900	2.67715200	0.44318100
C	-2.58642800	1.88649000	0.37860600
C	1.30607900	0.25116900	-0.72771100
C	0.93536900	3.02833300	0.14122700
H	-1.53813200	3.70440800	0.77902800
C	2.20969700	2.55756600	-0.24672800

C	2.41553400	1.27595400	-0.65532200
H	0.79511300	4.05043800	0.47654200
H	3.39445300	0.93378800	-0.96312700
N	1.59384100	-0.84818400	0.22142700
H	0.89369900	-1.03213100	0.93265400
C	2.66643600	-1.65504400	0.26511500
C	3.73971100	-3.33769500	1.29393000
C	4.63920500	-2.39922200	-0.49196100
Cl	3.82276400	-4.52099000	2.57641600
Cl	5.94695300	-2.30499900	-1.64730600
N	4.77546800	-3.33117600	0.45035800
N	3.65151800	-1.54748600	-0.65783000
N	2.68075500	-2.56528600	1.27902000
S	3.59480800	3.72722600	-0.20335300
S	-4.17166800	2.63411600	0.88939300
O	3.69721800	4.16790600	1.22599400
O	4.79955600	2.97828200	-0.67435100
O	3.20075600	4.84370200	-1.12226400
O	-3.82657600	4.03306300	1.29374900
O	-5.06966900	2.59461900	-0.30772100
O	-4.67095800	1.81798900	2.04053700
N	-3.68384100	-0.18545200	-0.12299100
N	-3.60605000	-1.39651200	-0.52353700
C	-4.81186000	-2.12011500	-0.59066000
C	-4.70528300	-3.43925800	-1.06513900
C	-6.06917400	-1.60144400	-0.22235000
C	-5.84569300	-4.23436300	-1.17846600
H	-3.72780500	-3.82368400	-1.34321200
C	-7.19993500	-2.40449600	-0.33740900
H	-6.14802700	-0.58506300	0.14629800
C	-7.09493600	-3.71978800	-0.81559500
H	-5.75978400	-5.25225200	-1.54829100
H	-8.17078000	-2.00716700	-0.05373400
H	-7.98436800	-4.33793500	-0.90216900
O	-1.08784800	-1.26015900	-0.83824400
H	-2.01334000	-1.66454000	-0.82690900
O	1.33154200	-0.27968000	-2.06385900
H	0.50976300	-0.03468200	-2.52272300

C7-CP5

C	-2.50722200	0.52021800	-0.03446700
C	-1.22967600	0.01471800	-0.44403800
C	-0.07333600	0.79658300	-0.35675600
C	-0.17255900	2.12238600	0.13606900

C	-1.43283300	2.62394000	0.56026700
C	-2.56515100	1.84805600	0.48033400
C	1.28081000	0.21009200	-0.76716300
C	0.96709300	2.96491000	0.18027800
H	-1.48897900	3.63616800	0.94243900
C	2.20303500	2.51036600	-0.33542200
C	2.37474800	1.25088300	-0.82269100
H	0.86267700	3.97091500	0.57249200
H	3.31851700	0.93058800	-1.24327800
N	1.61694800	-0.81362100	0.26327400
H	0.92639500	-0.96911300	0.99132300
C	2.70350200	-1.59981200	0.34136000
C	3.79776500	-3.22789300	1.43470400
C	4.69279600	-2.33761800	-0.37753400
Cl	3.89012400	-4.37004700	2.75384800
Cl	6.00696300	-2.26006700	-1.52699200
N	4.83740200	-3.23524400	0.59602900
N	3.69242800	-1.50853300	-0.57894500
N	2.72862300	-2.47089500	1.38911400
S	3.58159500	3.68940700	-0.37728600
S	-4.13507800	2.58313900	1.05189300
O	3.73774200	4.15915500	1.03741800
O	4.77056500	2.93754600	-0.88213500
O	3.14263900	4.78401300	-1.30201500
O	-3.77323700	3.95918000	1.51557300
O	-5.05041500	2.60486100	-0.13233400
O	-4.62241100	1.71657000	2.17075200
N	-3.69345100	-0.19067800	-0.10669900
N	-3.62532500	-1.38112000	-0.56549200
C	-4.83406000	-2.09797300	-0.64965400
C	-4.73279800	-3.40681100	-1.15267600
C	-6.08929900	-1.58099600	-0.27204400
C	-5.87624400	-4.19533400	-1.28050000
H	-3.75704400	-3.78925500	-1.43938600
C	-7.22331900	-2.37671000	-0.40380600
H	-6.16434400	-0.57087400	0.11419000
C	-7.12324600	-3.68309200	-0.90692900
H	-5.79442000	-5.20612400	-1.67012900
H	-8.19286800	-1.98055500	-0.11419300
H	-8.01513900	-4.29581700	-1.00571700
O	-1.11591400	-1.24203500	-0.93749000
H	-2.04292900	-1.64711200	-0.93693400
O	1.23883900	-0.37854100	-2.06122500
H	0.47452400	-0.98846000	-2.08639400

C7-TS_{CN}

C	-2.53263600	0.47609500	-0.08707000
C	-1.28963900	-0.03301000	-0.57369200
C	-0.10239400	0.71197900	-0.45680200
C	-0.14598300	1.98989700	0.16570800
C	-1.37951200	2.49191300	0.65583000
C	-2.53783400	1.75850000	0.53338600
C	1.19295300	0.19626300	-0.91271700
C	1.03100500	2.77700700	0.26762600
H	-1.39718300	3.46798000	1.12563700
C	2.24095500	2.31528100	-0.26710200
C	2.33560800	1.07846200	-0.87067400
H	0.96765800	3.75144700	0.74069500
H	3.25877600	0.72090800	-1.31276600
N	1.69238800	-0.83746400	0.80664200
H	1.77139300	-0.08416800	1.49215400
C	2.78722100	-1.59420300	0.84161900
C	4.77421400	-2.17718100	1.76086700
C	3.96195900	-3.37510400	0.09548200
Cl	6.04445800	-1.89500700	2.94004700
Cl	4.12563600	-4.73092600	-1.00840500
N	4.96882800	-3.23249800	0.96366000
N	2.87899400	-2.65271200	-0.02731800
N	3.77549900	-1.33253100	1.76585700
S	3.71202800	3.36878500	-0.13652700
S	-4.07721500	2.49088100	1.18877400
O	4.14190200	3.27136100	1.29531000
O	4.71213500	2.79947600	-1.08919000
O	3.25114500	4.74173800	-0.51111200
O	-3.66562800	3.81313800	1.75403500
O	-5.00172700	2.63293000	0.02132100
O	-4.57449600	1.55087800	2.24049300
N	-3.74378200	-0.19996100	-0.17807900
N	-3.70981000	-1.35237300	-0.72243100
C	-4.92715400	-2.04863400	-0.83112400
C	-4.84149900	-3.33567300	-1.39027800
C	-6.17327600	-1.53209000	-0.42426700
C	-5.99333200	-4.10747200	-1.53898100
H	-3.87150000	-3.71463800	-1.69999000
C	-7.31586700	-2.31015600	-0.58033900
H	-6.23460500	-0.53671200	0.00082700
C	-7.23147200	-3.59707400	-1.13484400
H	-5.92520400	-5.10283800	-1.96852000

H	-8.27983500	-1.91631900	-0.27021800
H	-8.13035700	-4.19631900	-1.25100400
O	-1.22708600	-1.24615300	-1.15661800
H	-2.16942100	-1.63169000	-1.15497700
O	1.26651600	-0.74534200	-1.86914600
H	0.43344300	-1.26639700	-1.88293200

FRG2 (anion)

N	-0.00554400	3.04855000	0.00058400
H	-0.97091500	3.38336300	0.00087700
C	-0.02169000	1.75091000	-0.00021800
C	-1.08730500	-0.27349900	-0.00020600
C	1.11113700	-0.23082400	-0.00020600
Cl	-2.59091000	-1.21520900	0.00011000
Cl	2.64841500	-1.11426000	0.00012000
N	0.02598700	-1.02250500	0.00027100
N	1.19707800	1.06237500	-0.00048900
N	-1.22030900	1.01702000	-0.00051000

FRG2-CPLT(anion)

C	1.10081100	0.19541700	0.00000500
C	0.25134800	-0.97622100	0.00011700
C	-1.16144300	-0.85506100	0.00009500
C	-1.73601500	0.45519900	0.00003400
C	-0.88937600	1.59671900	0.00001900
C	0.48704000	1.47232200	-0.00003000
C	-2.03751200	-1.98248800	0.00015600
C	-3.13081500	0.61326700	0.00003000
H	-1.34320400	2.58087800	0.00000100
C	-3.96397300	-0.51816900	0.00004800
C	-3.44083100	-1.79671700	0.00008400
H	-3.54929600	1.61436300	-0.00006800
H	-4.07812000	-2.67391000	0.00007400
S	-5.76195500	-0.26415600	-0.00001200
S	1.48017200	3.01020400	-0.00006800
O	-6.03429700	0.51437900	-1.24710600
O	-6.37296000	-1.62422100	0.00009000
O	-6.03438700	0.51458300	1.24694200
O	0.46777000	4.10777100	0.00017700
O	2.29396200	2.97233000	1.25171800
O	2.29364100	2.97249500	-1.25207500
N	2.48371500	0.14344100	-0.00014900
N	2.99649900	-1.02885300	-0.00021000
C	4.38609500	-1.13035300	-0.00004500

C	4.89620700	-2.44526300	-0.00032000
C	5.26089000	-0.02055400	0.00034900
C	6.27208700	-2.65206100	-0.00027800
H	4.20206300	-3.28076200	-0.00058900
C	6.63066200	-0.24258700	0.00043500
H	4.86012600	0.98645400	0.00055400
C	7.13999200	-1.55325600	0.00009900
H	6.66860400	-3.66282300	-0.00049200
H	7.31316700	0.60233100	0.00072700
H	8.21462600	-1.71258600	0.00015100
O	0.78682000	-2.18599800	0.00002600
H	1.81599000	-2.07162300	-0.00008000
O	-1.61515300	-3.24622900	0.00006900
H	-0.63109600	-3.28324800	-0.00000300

FRG1-OH-CP

C	0.03454200	-0.20482900	-0.03068600
C	-0.45827400	1.11197700	-0.03611800
C	-1.83472800	1.32624800	-0.00605700
C	-2.72419400	0.24251900	0.02791400
C	-2.22987200	-1.06454900	0.02664700
C	-0.85141900	-1.28970600	-0.00759600
H	0.22491700	1.95386600	-0.07142700
H	-2.21767600	2.34317500	-0.01374200
H	-3.79595900	0.42030400	0.04938000
H	-2.91301000	-1.90907500	0.04831800
H	-0.45299900	-2.30015800	-0.01300900
N	1.41673900	-0.55235400	-0.06565000
N	2.20568800	0.38890000	0.07174100
O	3.51436200	-0.09890600	-0.00117600
H	4.06651100	0.69734900	0.12263300

FRG1-2OH-CP1

C	-3.06232800	0.18905000	0.00003700
C	-2.23528900	1.31512900	0.00004600
C	-0.84725000	1.16010600	0.00003300
C	-0.28815100	-0.12476500	-0.00002800
C	-1.11527100	-1.26126400	-0.00004900
C	-2.49830100	-1.09517900	-0.00000800
H	-4.14251000	0.30656900	0.00005800
H	-2.66555400	2.31254000	0.00008200
H	-0.19092900	2.02595100	0.00004200
H	-0.68387000	-2.25636100	-0.00009200
H	-3.14190200	-1.97066300	-0.00002500

N	1.65724100	-1.28503300	-0.00010200
O	3.03930500	-1.14229100	-0.00000800
H	3.37317500	-2.06063400	-0.00022100
N	1.13532600	-0.16221600	-0.00006200
O	2.71061600	2.29603100	0.00013500
H	2.18380900	1.44497600	0.00010100

FRG1-2OH-TS1

C	-3.05373100	0.10541800	0.00211000
C	-2.26332000	1.25666900	0.04966600
C	-0.87106900	1.14645000	0.05137100
C	-0.27076200	-0.11886700	0.01268500
C	-1.06116700	-1.28061500	-0.03933800
C	-2.44883600	-1.15918000	-0.04409200
H	-4.13710300	0.18846600	-0.00271900
H	-2.72607300	2.23889100	0.08229200
H	-0.24075700	2.03068300	0.08374600
H	-0.59667900	-2.26001400	-0.07956300
H	-3.06386600	-2.05399100	-0.08549000
N	1.71388100	-1.21123600	0.07864500
O	3.09316200	-1.00596900	0.06334400
H	3.47278400	-1.90464100	0.11684300
N	1.15183200	-0.11189500	0.01958400
O	2.66045000	2.35759800	-0.16470600
H	2.77678700	1.37856800	-0.14207700

FRG1-2OH-CP2

C	3.06325700	0.06183100	0.00024700
C	2.31087600	1.23169600	-0.13612400
C	0.91598000	1.16970000	-0.13695600
C	0.27815400	-0.07113500	-0.01322800
C	1.02738500	-1.25210000	0.13329600
C	2.41800200	-1.17557500	0.13732600
H	4.14864800	0.11028600	0.00658700
H	2.80631600	2.19297300	-0.23756500
H	0.31684400	2.06880700	-0.23682400
H	0.52857900	-2.20831500	0.24925000
H	3.00245200	-2.08415700	0.25250500
N	-1.74644300	-1.10868300	-0.12778400
O	-3.11324500	-0.87498800	-0.09485600
H	-3.51479000	-1.76075000	-0.19472000
N	-1.14117700	-0.03949600	-0.02932100
O	-2.38868900	1.95063700	0.24235200
H	-3.14116000	1.32671100	0.17316300

FRG1-2OH-TS2

C	-2.97254400	-0.15858500	0.07418400
C	-2.33217300	1.07777200	0.20352200
C	-0.94063600	1.17287200	0.12165500
C	-0.19055200	0.01065500	-0.08760800
C	-0.82067500	-1.23550300	-0.22723400
C	-2.21119800	-1.31264100	-0.13948600
H	-4.05534600	-0.22219000	0.13554500
H	-2.91451000	1.97935000	0.37251700
H	-0.44646000	2.12976700	0.22686300
H	-0.22933700	-2.12566600	-0.41469200
H	-2.69777300	-2.27799500	-0.24800600
N	1.88414300	-0.72966800	0.54195900
O	3.22958200	-0.69537000	0.18274600
H	3.65376900	-1.31377500	0.80881500
N	1.23502200	0.04850900	-0.22814300
O	1.78935300	1.65198000	-0.25741600
H	2.41366500	1.57317400	-1.00431800

FRG1-2OH-CP3

C	2.97805900	-0.20878700	-0.09604700
C	2.37938800	1.04950300	-0.20311000
C	0.99215100	1.19303200	-0.10276000
C	0.19908500	0.05916200	0.11034700
C	0.79050100	-1.20824000	0.23520400
C	2.17540700	-1.33453400	0.12249300
H	4.05663700	-0.31205900	-0.17587700
H	2.99045300	1.93239200	-0.37096100
H	0.53544200	2.17082800	-0.19079700
H	0.17417800	-2.07983100	0.42724500
H	2.62704900	-2.31830400	0.21829500
N	-1.91384500	-0.76142600	-0.43607800
O	-3.25299900	-0.61565300	-0.06739100
H	-3.70376500	-1.31388600	-0.57916900
N	-1.22016300	0.16040500	0.25958200
O	-1.71866900	1.50386900	0.12884600
H	-2.05614400	1.72146100	1.01834100

FRG1-3OH-CP1

C	-3.49118200	-0.33602400	-0.03660400
C	-2.64193500	-1.40998200	0.24841500
C	-1.25790900	-1.22854400	0.26840600
C	-0.74766500	0.04309000	0.00572200

C	-1.57513800	1.12902800	-0.29149000
C	-2.95600000	0.92823800	-0.30760500
H	-4.56711400	-0.48492200	-0.05445400
H	-3.05330500	-2.39321600	0.45698200
H	-0.58888300	-2.05180500	0.49029900
H	-1.15419200	2.10165100	-0.51863500
H	-3.61159600	1.76124700	-0.54376300
N	1.12198100	1.37727500	0.31747900
O	2.48946500	1.38314700	0.26695600
H	2.72129600	2.30788300	0.48302700
O	1.44539800	-0.80183000	-0.20386100
H	3.35377600	-0.85112000	-0.19411300
O	4.30034900	-1.10666900	-0.23868900
H	4.28789600	-2.03870100	-0.51257000
N	0.69936100	0.20800500	0.03636700

FRG1-3OH-CP2

C	-2.94221100	-0.21287700	-0.05732800
C	-2.36633800	1.05038200	-0.22821900
C	-0.97981900	1.20534400	-0.18086000
C	-0.18888500	0.07560300	0.03112900
C	-0.74106300	-1.19457200	0.21161300
C	-2.12945000	-1.33005100	0.16362300
H	-4.02212200	-0.32629700	-0.08994400
H	-2.99434100	1.91949500	-0.40064000
H	-0.52105300	2.17844900	-0.31456600
H	-0.10641700	-2.05242100	0.40212100
H	-2.57371000	-2.31007000	0.31133700
N	1.95349600	-0.72897100	-0.31875300
O	3.28378900	-0.42860500	-0.17203100
H	3.73223600	-1.23193200	-0.50134100
N	1.25578700	0.26224900	0.08115000
O	1.72958900	1.36946300	0.49909400

FRG1-3OH-TS

C	-2.22160200	-2.27591700	-2.45813600
C	-1.15102100	-3.01427100	-2.97328600
C	0.16201300	-2.66941700	-2.64997800
C	0.37651300	-1.58400900	-1.79955600
C	-0.67585600	-0.82774500	-1.27705600
C	-1.98172700	-1.18493300	-1.61529800
H	-3.24140700	-2.54589700	-2.71741300
H	-1.33420900	-3.86123200	-3.62778800
H	1.00113500	-3.23379100	-3.04011300

H	-0.48263500	0.02659000	-0.63923700
H	-2.81069900	-0.60189100	-1.22521100
N	1.93174600	-0.64806300	-0.34998400
O	3.29413700	-0.41706500	-0.13420900
H	3.49163000	0.47392600	-0.49337100
N	1.76170800	-1.24501800	-1.47768100
O	2.66758700	-1.55945300	-2.29501800

FRG1-3OH-CP3

C	-2.94822900	-0.15999500	-0.04167500
C	-2.34264600	1.09368700	-0.17158900
C	-0.95210200	1.21188800	-0.13609000
C	-0.18798300	0.05533900	0.02594500
C	-0.77043600	-1.20755400	0.16516900
C	-2.16142500	-1.30529100	0.12681200
H	-4.03088300	-0.24528700	-0.06635400
H	-2.94957200	1.98465400	-0.30246900
H	-0.47042200	2.17690100	-0.24181500
H	-0.15732200	-2.08877800	0.31439000
H	-2.62917300	-2.27876200	0.24075500
N	1.96024200	-0.81820500	-0.27435200
O	3.28384300	-0.54008300	-0.17913000
H	3.35233100	0.41303000	0.10622900
N	1.25410800	0.19929600	0.05434300
O	1.78634800	1.32035400	0.38886800

FRG1-4OH-CP1

C	3.11324100	0.24989100	0.00410600
C	2.56785900	-0.87446800	0.63305400
C	1.20064500	-1.13669000	0.54370300
C	0.39823100	-0.25001300	-0.17743000
C	0.92105400	0.87575800	-0.82198400
C	2.29044000	1.11966000	-0.72094200
H	4.17934800	0.44606900	0.07416200
H	3.20460400	-1.54959600	1.19689200
H	0.76144600	-1.99951400	1.03109300
H	0.28157900	1.53191500	-1.40122900
H	2.71506200	1.98457200	-1.22165400
O	-1.72710100	1.58479900	1.59797500
H	-0.95372400	2.09634100	1.27611500
N	-1.01538400	-0.53756400	-0.25387900
O	-1.44356900	-1.73262700	-0.12471200
N	-1.82252300	0.45698900	-0.44732100
O	-3.10150300	0.03469800	-0.53044500

H	-3.09440600	-0.94554700	-0.35255700
---	-------------	-------------	-------------

FRG1-4OH-TS1

C	3.09486900	-0.38492700	-0.12249700
C	2.62894100	0.92315400	-0.29687900
C	1.27250900	1.21223900	-0.15807900
C	0.39230500	0.16992600	0.15453300
C	0.83919400	-1.14553000	0.34121000
C	2.19889500	-1.41289200	0.19552000
H	4.15353800	-0.60270400	-0.23059100
H	3.32092300	1.72229000	-0.54516900
H	0.89746700	2.21932100	-0.29886300
H	0.14704500	-1.93560200	0.60689800
H	2.55967900	-2.42663400	0.34145500
O	-1.91976300	-0.85702200	-1.64669200
H	-1.69240700	-1.80475200	-1.57040900
N	-0.99440500	0.48732200	0.30167300
O	-1.40253100	1.68370100	0.43260100
N	-1.87457700	-0.52422500	0.23151500
O	-3.11178000	-0.08094700	0.50865500
H	-3.08928000	0.91326300	0.45513500

FRG1-4OH-CP2

C	-3.19846800	-0.34620500	-0.00505500
C	-2.73275800	0.96313900	0.17272800
C	-1.36915000	1.24070100	0.13813300
C	-0.46114800	0.18817100	-0.07960400
C	-0.91517800	-1.13144600	-0.26350400
C	-2.28494900	-1.38469100	-0.22210000
H	-4.26407900	-0.55456400	0.02460600
H	-3.43533800	1.77421500	0.34178800
H	-1.00213500	2.25086000	0.27755600
H	-0.21291200	-1.93758200	-0.43562100
H	-2.63880500	-2.40211200	-0.36194000
O	2.22175400	-0.79982500	1.20394700
H	2.26650500	-1.77164300	1.29289700
N	0.91080900	0.49314600	-0.11983000
O	1.39047800	1.66334500	0.02810700
N	1.84226700	-0.61717700	-0.17661500
O	2.96415100	-0.16365800	-0.85820400
H	3.17407200	0.73213500	-0.49855800

FRG1-4OH-TS2

C	-3.13049500	-0.32376900	0.29812200
---	-------------	-------------	------------

C	-2.54623200	0.88764100	0.69688400
C	-1.22792700	1.17743200	0.35672900
C	-0.49637900	0.23748000	-0.39169900
C	-1.07370400	-0.97978200	-0.79200500
C	-2.39399600	-1.25566700	-0.44446900
H	-4.16024600	-0.54032700	0.56864900
H	-3.12283200	1.60338200	1.27605200
H	-0.76189300	2.10997100	0.65725000
H	-0.48479200	-1.68846700	-1.36659800
H	-2.84958900	-2.19296300	-0.75018100
O	1.90739900	-0.80112200	1.39801800
H	1.18042100	-1.43785200	1.56150500
N	0.83884200	0.45875900	-0.79513900
O	1.37820800	1.54848500	-0.49620500
N	2.20543500	-0.95385400	0.04880200
O	3.26952700	-0.15362500	-0.17153200
H	2.92990800	0.79878900	-0.16572700

FRG1-4OH-CP3

C	-3.90436800	0.41490600	0.00003400
C	-2.92571400	1.42687700	0.00002000
C	-1.57966800	1.09489700	-0.00001000
C	-1.21645800	-0.26951300	-0.00004700
C	-2.19324500	-1.28389600	-0.00009100
C	-3.54173900	-0.93653100	-0.00002300
H	-4.95557500	0.68952900	0.00006200
H	-3.22907100	2.46956800	0.00003800
H	-0.81140800	1.86069100	-0.00001500
H	-1.87643600	-2.32269800	-0.00015200
H	-4.30515400	-1.70842400	-0.00002100
O	3.97950900	1.09978700	0.00005900
H	4.75539400	1.69457600	-0.00046800
N	0.10827900	-0.73311700	-0.00006300
O	0.99434300	0.13799100	0.00012900
N	4.52762500	-0.18352100	-0.00028100
O	3.46854900	-1.03915800	0.00024600
H	2.59886300	-0.53616900	0.00019500

P2

C	2.17312800	0.26155500	-0.00014700
C	1.27228800	1.34209700	0.00040800
C	-0.09599700	1.10980400	-0.00035400
C	-0.56081200	-0.22122500	0.00036000
C	0.33638500	-1.30350900	0.00090200

C	1.70830900	-1.05801300	-0.00065100
H	3.24221500	0.45580800	0.00037400
H	1.65053400	2.36026000	0.00040500
H	-0.80421900	1.93180200	-0.00079900
H	-0.05561900	-2.31662300	0.00064500
H	2.41096900	-1.88584600	-0.00091300
N	-1.92824000	-0.58456600	-0.00059400
O	-2.74325000	0.34528800	0.00016600

P2-OH-CP

C	2.58069500	-0.05262800	0.00001000
C	1.91650200	1.18170300	-0.00009000
C	0.52585500	1.24048700	-0.00010500
C	-0.20833100	0.03796800	-0.00001000
C	0.44488600	-1.21035500	0.00008600
C	1.83781200	-1.23992000	0.00009500
H	3.66626700	-0.08827400	0.00001600
H	2.48571100	2.10702800	-0.00017100
H	0.00649800	2.19176200	-0.00020800
H	-0.12568500	-2.13082600	0.00016300
H	2.34554300	-2.20032000	0.00018100
O	-2.29777800	1.16938400	0.00024300
O	-2.26940000	-1.11443200	-0.00021400
H	-3.21641400	-0.86148800	-0.00015700
N	-1.60128700	0.11413900	0.00000400

P2-2OH-CP

C	-3.20633700	-0.21683500	-0.00006300
C	-2.64046800	1.06401800	-0.00034200
C	-1.25604500	1.21862000	-0.00027600
C	-0.45942200	0.06891400	0.00000300
C	-1.00276800	-1.22046800	0.00024200
C	-2.38938500	-1.35384600	0.00024000
H	-4.28675300	-0.32924800	-0.00008000
H	-3.27698200	1.94354000	-0.00059800
H	-0.80370600	2.20286400	-0.00049900
H	-0.35779100	-2.09075500	0.00048800
H	-2.83101300	-2.34557200	0.00048000
O	1.47328000	1.35853200	0.00077900
O	1.69284000	-0.80283700	-0.00045700
H	3.61318500	-0.46104600	-0.00024200
N	0.98870400	0.22126700	0.00010800
O	4.58668700	-0.35982000	-0.00020500
H	4.72622700	0.60193200	-0.00006700

P3

C	2.51726400	-0.00000500	-0.00002500
C	1.82147600	1.21511700	-0.00010700
C	0.42808700	1.22568100	-0.00002700
C	-0.24530100	0.00003800	0.00023600
C	0.42820400	-1.22558900	-0.00013000
C	1.82162800	-1.21516200	0.00013300
H	3.60355800	0.00013600	-0.00012800
H	2.36369200	2.15567900	0.00002200
H	-0.12435000	2.15758400	-0.00012200
H	-0.12446600	-2.15733300	-0.00004000
H	2.36385200	-2.15570900	0.00010500
O	-2.29907000	1.08561200	0.00002800
O	-2.29914400	-1.08561200	-0.00012600
N	-1.70353100	-0.00011900	0.00006800

FRG2-anion-H₂O-CP1

N	-1.86840800	-1.72333800	0.00002500
H	-1.57257000	-2.70025300	0.00021400
C	-0.82406200	-0.94739900	-0.00001000
C	1.42678900	-0.57697100	0.00030500
C	0.06321600	1.15017100	-0.00014700
Cl	3.08155200	-1.20437200	0.00012100
Cl	-0.15442100	2.90531700	-0.00016700
N	1.34739600	0.76097400	0.00005600
N	-1.01950000	0.43440400	-0.00015200
N	0.47639000	-1.46318800	0.00025000
O	-4.56447500	-1.08201700	-0.00014700
H	-4.64348300	-0.11405200	-0.00030000
H	-3.57617800	-1.26239400	-0.00008800

FRG2-anion-H₂O-TS

N	-1.84310400	-1.76702800	-0.00011600
H	-1.60788800	-2.75526000	-0.00004900
C	-0.81700500	-0.94643100	-0.00009100
C	1.40687400	-0.54491900	0.00000700
C	0.00504900	1.15712500	-0.00017900
Cl	3.06124500	-1.14021200	0.00010500
Cl	-0.25554100	2.89513000	-0.00027900
N	1.29084700	0.78726600	-0.00009500
N	-1.06403800	0.40845600	-0.00019500
N	0.46581500	-1.45064000	0.00003700
O	-4.29779700	-1.16029700	-0.00037900

H	-4.38974500	-0.19343100	-0.00039800
H	-2.96578200	-1.42882500	-0.00024200

FRG2-anion-H₂O-CP2

N	-1.81950400	-1.77651800	-0.03198600
H	-1.60754800	-2.76850000	-0.02969500
C	-0.79626500	-0.94342800	-0.01806900
C	1.42057000	-0.54304700	0.00117300
C	0.01421200	1.15750400	-0.00331500
Cl	3.07155100	-1.13600500	0.01324700
Cl	-0.25258300	2.89061600	-0.00146700
N	1.29865400	0.78762000	0.00563200
N	-1.05387500	0.40282200	-0.01325300
N	0.47799600	-1.45046100	-0.01102100
O	-4.39008300	-1.14963100	0.03802600
H	-4.49319200	-0.18413300	0.01419700
H	-2.85504600	-1.44913000	-0.01330300

P4

N	0.00002600	2.97266300	-0.00021600
H	-0.87497800	3.48327500	0.00093000
C	0.00001000	1.64193200	-0.00005300
C	-1.10475400	-0.30890500	0.00010900
C	1.10474600	-0.30892000	-0.00021200
Cl	-2.61310000	-1.19154900	0.00000100
Cl	2.61308400	-1.19157400	0.00007800
N	-0.00000800	-1.05843600	-0.00006400
N	1.19920200	1.00015900	-0.00009000
N	-1.19919300	1.00017200	0.00005800
H	0.87504800	3.48324800	0.00084800

FRG3

N	1.74610100	-1.98412000	0.11943200
H	1.46305600	-2.92368800	-0.14901400
C	0.83810900	-0.98946400	0.03054800
C	-1.31381100	-0.38619400	0.00073000
C	0.26401300	1.16504700	0.00770500
Cl	-3.00434200	-0.81191300	-0.01345900
Cl	0.72208500	2.84784800	-0.00486200
N	-1.04577100	0.92289000	-0.00175300
N	1.25274700	0.29412000	0.02745700
N	-0.45948500	-1.38316900	0.00695100
O	3.07500800	-1.70688500	-0.18791400
H	3.55025500	-1.71650400	0.66527700

FRG3-CPLT1(dianion)

C	-1.01886600	-0.04300400	-0.02249200
C	-0.18819000	1.09677100	-0.03147300
C	1.23080000	0.95958200	-0.02791000
C	1.81569400	-0.34699100	-0.02106100
C	0.96254400	-1.48853600	-0.02075400
C	-0.39959200	-1.34152100	-0.02036800
C	2.12093800	2.04026000	-0.02721600
C	3.23088600	-0.46645300	-0.01147300
H	1.40819300	-2.47639000	-0.01966000
C	4.03266300	0.65619000	-0.00797500
C	3.47692600	1.97110800	-0.01714600
H	3.67336400	-1.45678300	-0.00519900
H	4.11284900	2.85187900	-0.01639300
S	5.83602100	0.49818200	0.02960200
S	-1.40894900	-2.85905000	-0.02266500
O	6.33052100	1.25914300	-1.16304600
O	6.26138600	1.12166800	1.32486100
O	6.13865600	-0.96442500	-0.04068000
O	-0.42561900	-3.98787900	-0.03113300
O	-2.22748200	-2.83128100	1.23158200
O	-2.23513500	-2.81828600	-1.27165600
N	-2.41208700	0.00520500	-0.00731400
N	-2.93957200	1.16209700	-0.02081900
C	-4.35069800	1.22099200	0.00815300
C	-4.90518100	2.50898900	-0.06808100
C	-5.18871200	0.09473200	0.11064400
C	-6.29063500	2.67479300	-0.04857300
H	-4.24157900	3.36606000	-0.14408700
C	-6.56947900	0.27139700	0.13309800
H	-4.75713900	-0.89777800	0.17500200
C	-7.12536400	1.55726500	0.05243100
H	-6.71572100	3.67263500	-0.11082700
H	-7.21984600	-0.59545700	0.21412200
H	-8.20449200	1.68354900	0.07010800
O	-0.68467600	2.34692200	-0.03934500
H	-1.69076700	2.25472800	-0.04060500

FRG3-CPLT2

C	1.02113200	0.00683300	-0.02865700
C	0.18153500	-1.19175500	-0.04734700
C	-1.26808400	-0.99930100	-0.03816200
C	-1.83175400	0.30805000	-0.02353700

C	-0.96236100	1.45749600	-0.02177900
C	0.38959700	1.31639200	-0.02274800
C	-2.16581600	-2.06163000	-0.03969100
C	-3.23793500	0.45040800	-0.00893900
H	-1.41245000	2.44355900	-0.01909200
C	-4.06091500	-0.66548700	-0.00786800
C	-3.52825700	-1.98000800	-0.02472100
H	-3.66831200	1.44594200	0.00258000
H	-4.17226800	-2.85475400	-0.02558400
S	-5.86358300	-0.47442800	0.03757400
S	1.39732800	2.83371800	-0.02631600
O	-6.37640400	-1.23561600	-1.14657200
O	-6.29207500	-1.07865600	1.34045900
O	-6.13788300	0.99291600	-0.04323900
O	0.41685500	3.96507700	-0.03350500
O	2.21934100	2.80425000	1.22603300
O	2.22308000	2.79081800	-1.27594800
N	2.35869700	-0.02834500	-0.00921500
N	2.99432300	-1.15650600	-0.02128500
C	4.40052300	-1.21938100	0.01165200
C	4.98506700	-2.49282200	-0.06365800
C	5.19650900	-0.06934100	0.11670900
C	6.37434000	-2.61332100	-0.03617600
H	4.35287300	-3.37339200	-0.14426200
C	6.58360700	-0.20741700	0.14404800
H	4.73514300	0.90955600	0.17781100
C	7.17896000	-1.47335600	0.06751200
H	6.82609900	-3.59944300	-0.09650200
H	7.20384100	0.68094100	0.22597600
H	8.26087000	-1.56910100	0.08927100
O	0.68278300	-2.35173000	-0.06485600
H	2.44067500	-2.02661600	-0.05562800

FRG4

N	1.83278200	-0.56162500	-0.29904200
C	0.46408500	-0.24456800	-0.10621900
C	-0.46057500	-1.29687600	-0.00103100
C	0.00835200	1.08177900	-0.11623500
C	-1.82710900	-1.02155800	0.07686900
H	-0.10582200	-2.32513100	0.01790200
C	-1.36133100	1.34515600	-0.02111500
H	0.71895500	1.89803100	-0.19635300
C	-2.28774200	0.30064200	0.06985000
H	-2.53190200	-1.84547300	0.15684800

H	-1.70379800	2.37702000	-0.02389700
H	-3.35115200	0.51254400	0.13980700
H	2.05613900	-1.46522700	0.11575800
O	2.70630000	0.37794900	0.35512900
H	3.22364000	0.76857100	-0.37051600

FRG4-CPLT

C	-3.05351700	-1.92772900	-0.01663000
C	-1.52875000	-1.70543200	-0.05180300
C	-1.03125700	-0.32626100	-0.05022300
C	-1.97346100	0.73749700	-0.01962000
C	-3.40680200	0.48035300	0.01292400
C	-3.93533900	-0.75778500	0.01590900
C	0.36391300	-0.01367100	-0.07709300
C	-1.54993900	2.06691000	-0.01844600
H	-4.06159900	1.34589000	0.03732200
C	-0.18445100	2.34418500	-0.05443700
C	0.76745200	1.33332300	-0.08490200
H	-2.28033000	2.86759100	0.00424200
H	1.81927600	1.57246300	-0.11901700
N	1.27441300	-1.06946900	-0.10115200
H	0.82993000	-1.99258800	-0.11965900
C	2.63012000	-1.11180400	-0.05378100
C	4.45710000	-2.41333000	-0.00282700
C	4.67836100	-0.21503600	0.05668400
Cl	5.18598900	-3.99630600	-0.01016400
Cl	5.69739300	1.19626400	0.13981800
N	5.30910600	-1.38527900	0.06146100
N	3.37892700	0.00578800	-0.00073400
N	3.14699700	-2.36834100	-0.06054600
S	0.39067000	4.06725300	-0.02673500
S	-5.72772600	-1.00534900	0.05415500
O	0.95680200	4.26894800	1.34535900
O	1.42451500	4.15987700	-1.10312400
O	-0.81630200	4.90664200	-0.29144800
O	-6.32127300	0.36366000	0.08810100
O	-6.05087800	-1.75913800	-1.19736100
O	-5.99501500	-1.79512600	1.29656900
N	-3.46553000	-3.13235800	-0.01779000
O	-0.80282900	-2.70521400	-0.08171100

FRG5

C	0.00011900	-1.39839900	0.00000500
C	-1.23017800	-0.77439900	-0.00058800

C	1.23026100	-0.77432100	0.00061300
C	-1.21698700	0.63349300	0.00046200
H	-2.16752400	-1.32495800	-0.00035700
C	1.21685700	0.63370400	-0.00047600
H	2.16780800	-1.32453400	0.00024500
C	-0.00006800	1.32636400	0.00001100
H	-2.15813100	1.17874800	0.00073200
H	2.15802100	1.17892000	-0.00081100
H	-0.00020400	2.41317100	0.00002900

FRG5-CPLT

C	-2.96404200	-1.20727500	-0.01552500
C	-1.51564100	-1.18004000	-0.02774400
C	-0.83565500	0.11516500	-0.02230700
C	-1.63421800	1.29453100	-0.02138800
C	-3.07062200	1.21676400	-0.02448600
C	-3.71654900	0.02166500	-0.01893400
C	0.59530700	0.25575000	-0.01625700
C	-1.02768600	2.56908300	-0.01288400
H	-3.63073700	2.14424400	-0.02669800
C	0.34905900	2.66317900	-0.00356300
C	1.16884800	1.52594800	-0.00581900
H	-1.65007900	3.45682500	-0.01148800
H	2.24344600	1.62832600	0.00112500
N	1.35828200	-0.92246500	-0.01847700
H	0.77556800	-1.77003900	-0.02535000
C	2.68677200	-1.14925400	-0.01079700
C	4.32559000	-2.68681300	-0.00423400
C	4.84429200	-0.53943500	0.00290000
Cl	4.83785100	-4.35599800	-0.00436300
Cl	6.05130900	0.72093100	0.01177600
N	5.31375900	-1.78410500	0.00357200
N	3.58771100	-0.14226000	-0.00377200
N	3.03473900	-2.46780600	-0.01196100
S	1.15374400	4.28606900	0.01381100
S	-5.53497000	0.01771700	-0.00323900
O	1.98140800	4.31245900	1.26379100
O	1.99184000	4.33492500	-1.22859700
O	0.05599300	5.30076400	0.01831300
O	-5.93690200	1.45912200	-0.03775200
O	-5.96781600	-0.72525500	-1.22926200
O	-5.93899500	-0.65708000	1.27149700
N	-3.65910500	-2.36836800	0.01071800
N	-3.07140800	-3.47895800	0.01055900

O	-0.87576000	-2.29040900	-0.03653800
H	-2.03626600	-3.57511600	0.01392500
O	-3.88610300	-4.58930400	0.09322000
H	-3.28791800	-5.35833000	-0.01229100

FRG6

N	2.88080400	0.43359200	-0.00012900
N	1.98561600	-0.40330000	0.00005900
C	0.54181400	-0.16492100	0.00004100
C	-0.29677200	-1.27888300	0.00000200
C	0.03628700	1.13488700	0.00004500
C	-1.68139300	-1.08686600	-0.00003800
H	0.12603700	-2.28162000	0.00000700
C	-1.34666400	1.31670100	0.00001600
H	0.71873500	1.97906900	0.00009200
C	-2.20640700	0.20922200	-0.00003300
H	-2.34509400	-1.94697900	-0.00006700
H	-1.75598500	2.32321400	0.00004000
H	-3.28265600	0.35879700	-0.00005600
H	2.19283500	-1.42537200	0.00027600

FRG6-CPLT

C	2.99266300	-1.82788000	-0.04028900
C	1.54012100	-1.63732900	-0.06183700
C	1.01995300	-0.27179200	-0.05535800
C	1.94810100	0.81066600	-0.03480700
C	3.35269000	0.55869900	-0.01516200
C	3.86673100	-0.72510700	-0.01654800
C	-0.37937500	0.03199300	-0.06905800
C	1.49943100	2.14754400	-0.02666100
H	4.02140300	1.41394300	0.00247900
C	0.14067300	2.40262000	-0.04231100
C	-0.80014800	1.36657600	-0.06582800
H	2.22258000	2.95511600	-0.00748600
H	-1.85570100	1.59144400	-0.08159000
N	-1.27083300	-1.04782400	-0.08673000
H	-0.79053100	-1.95824900	-0.10444300
C	-2.61908600	-1.11917200	-0.04415000
C	-4.42414000	-2.45467200	0.00183200
C	-4.68708500	-0.26190100	0.05716300
Cl	-5.12606700	-4.05213100	-0.00780300
Cl	-5.73526800	1.13124300	0.13324000
N	-5.29772300	-1.44334500	0.06291200
N	-3.39367600	-0.01495600	0.00318200

N	-3.11645900	-2.38693700	-0.05134000
S	-0.47219500	4.10736900	-0.02611100
S	5.66699900	-0.92017600	0.06991200
O	-1.27282700	4.26163500	-1.28323700
O	-1.31540600	4.21811800	1.20809700
O	0.73718900	4.98606900	0.01014800
O	6.24332300	-0.01507300	-0.96295500
O	6.06275100	-0.55748300	1.46165400
O	5.89993000	-2.38054200	-0.23623400
O	0.80639000	-2.66932300	-0.08728700
O	3.38759300	-3.10434100	-0.05476200
H	4.38419900	-3.12473800	-0.10367400

HC1-CP1

C	2.32609000	-0.44064700	-0.14675600
C	0.97265200	0.11689700	-0.10350500
C	-0.17299700	-0.79859100	-0.10228800
C	0.08045600	-2.19871500	-0.13077700
C	1.42845400	-2.70753200	-0.15618100
C	2.50031400	-1.87793100	-0.16555700
C	-1.53809300	-0.35126500	-0.07375700
C	-0.98319200	-3.12132400	-0.13693100
H	1.56346900	-3.78272400	-0.16951200
C	-2.28384500	-2.65395200	-0.11564600
C	-2.57518800	-1.28597900	-0.08408000
H	-0.76908700	-4.18400900	-0.15736400
H	-3.59999000	-0.94890000	-0.06351400
N	-1.76711400	1.03192700	-0.02794900
H	-0.89434600	1.57593300	-0.02090000
C	-2.89679800	1.76835100	0.02212300
C	-3.79300100	3.82512200	0.13948400
C	-5.11944900	2.06062700	0.05570200
Cl	-3.60367100	5.55809200	0.22032600
Cl	-6.72538100	1.37693900	0.04115900
N	-5.05726200	3.38732900	0.12633400
N	-4.12233100	1.20194300	-0.00364100
N	-2.69348100	3.11407800	0.09819700
S	-3.67345500	-3.81521200	-0.17388200
S	4.15417500	-2.62780000	-0.21367100
O	-4.60754800	-3.38633400	0.91564600
O	-4.26755600	-3.65153900	-1.54093300
O	-3.09588500	-5.17596800	0.05205800
O	3.92892900	-4.10435500	-0.19865000
O	4.81394200	-2.15370200	-1.46712800

O	4.87046900	-2.15625100	1.02656900
N	3.43867200	0.30251100	-0.17717600
N	3.39672800	1.59578200	-0.16030200
C	4.56623000	2.37817400	-0.21471300
C	4.40393400	3.77103000	-0.17124000
C	5.84334200	1.80713700	-0.31464300
C	5.52737100	4.59536400	-0.22935300
H	3.40589200	4.19511700	-0.09276500
C	6.95601000	2.64525200	-0.37159500
H	5.95793800	0.72988800	-0.34903500
C	6.80664900	4.03774800	-0.33016200
H	5.40062600	5.67382100	-0.19640900
H	7.94720400	2.20720400	-0.45083800
H	7.68060700	4.68140900	-0.37596300
O	0.82689600	1.38039900	-0.07397500
H	2.47530300	2.05397100	-0.11466800
O	3.77502200	-1.86204800	3.52909700
H	4.12051100	-1.98422100	2.59611200

HC1-TS_{CO}

C	2.32454600	-0.49873500	-0.07736500
C	0.97242900	0.07183200	-0.06438700
C	-0.18050100	-0.83405100	-0.07180100
C	0.06171600	-2.23621200	-0.08574200
C	1.40593300	-2.75667900	-0.08848600
C	2.48587400	-1.93812600	-0.08666100
C	-1.54163900	-0.37473900	-0.07155200
C	-1.00867700	-3.14987800	-0.09711900
H	1.53126600	-3.83318800	-0.08988100
C	-2.30614800	-2.67158800	-0.09585500
C	-2.58651300	-1.30160500	-0.08353000
H	-0.80315300	-4.21440600	-0.10488200
H	-3.60871100	-0.95606100	-0.08051700
N	-1.75979400	1.01024900	-0.05453600
H	-0.88333200	1.54751900	-0.04255900
C	-2.88406400	1.75763000	-0.05092900
C	-3.76380100	3.82442300	-0.01296700
C	-5.10401500	2.06910200	-0.06758400
Cl	-3.56147500	5.55708800	0.02200700
Cl	-6.71504800	1.39827700	-0.09161000
N	-5.03130500	3.39667500	-0.03596500
N	-4.11343300	1.20063700	-0.08141500
N	-2.67010700	3.10306000	-0.01436500
S	-3.70471000	-3.82248800	-0.15517400

S	4.13473900	-2.70174700	-0.06422000
O	-4.64090400	-3.37938300	0.92666300
O	-4.28968700	-3.66216400	-1.52641500
O	-3.13854500	-5.18599400	0.08211000
O	3.89877800	-4.17658300	-0.05314100
O	4.85728100	-2.24106600	-1.28791400
O	4.78202400	-2.22550400	1.21088000
N	3.44435400	0.23663100	-0.12747200
N	3.41254200	1.52846000	-0.15013400
C	4.58722000	2.29983100	-0.23349000
C	4.43631700	3.69455900	-0.21192300
C	5.85750800	1.71557200	-0.34358800
C	5.56557600	4.50784000	-0.30199100
H	3.44308800	4.12829100	-0.12579200
C	6.97590300	2.54288800	-0.43265700
H	5.96210500	0.63696800	-0.36394600
C	6.83830000	3.93717000	-0.41279600
H	5.44871200	5.58774200	-0.28579400
H	7.96200500	2.09524400	-0.52060800
H	7.71668800	4.57241200	-0.48374100
O	0.83914800	1.33517600	-0.05707800
H	2.49565800	1.99618500	-0.10808700
O	3.34382400	-0.59424900	2.95322000
H	3.87743600	-1.20591100	2.37184800

HC1-CP2

C	-2.67938000	-0.21875200	-0.90784400
C	-1.15313400	0.03266100	-1.07155900
C	-0.18240300	-0.94242200	-0.55316700
C	-0.65553100	-2.23252600	-0.20358100
C	-2.07710100	-2.55916100	-0.28267000
C	-3.01970500	-1.65972400	-0.58973600
C	1.21544100	-0.66919800	-0.45618600
C	0.22909000	-3.22586700	0.22522900
H	-2.35149500	-3.58487300	-0.05443400
C	1.58683100	-2.93388200	0.30826000
C	2.08797000	-1.67822000	-0.02343700
H	-0.14569600	-4.20947300	0.48455100
H	3.14623800	-1.47681300	0.04369600
N	1.66284800	0.60694900	-0.82018300
H	0.94077900	1.17821200	-1.26986900
C	2.83807900	1.24593100	-0.62175600
C	4.01800700	3.13218200	-0.91990800
C	4.92806500	1.43329400	0.16147800

Cl	4.14107500	4.75818600	-1.53862700
Cl	6.28291800	0.74109700	1.01400600
N	5.10118100	2.67513700	-0.28259800
N	3.86171700	0.66787500	0.03964900
N	2.88451500	2.50737600	-1.13049600
S	2.76131000	-4.20621400	0.85052400
S	-4.76137100	-2.15594200	-0.53625000
O	3.73845700	-4.35081300	-0.27495600
O	3.38972000	-3.66365700	2.09706600
O	1.95445400	-5.44112300	1.08960900
O	-4.79320600	-3.62482700	-0.79165700
O	-5.27992400	-1.78486200	0.81565000
O	-5.41498900	-1.35619200	-1.63621600
N	-3.02524800	0.60455400	0.26060300
N	-3.25605100	1.85937800	-0.09194200
C	-3.42845900	2.89845400	0.82203300
C	-3.77328300	4.16614500	0.31573600
C	-3.27187800	2.70863300	2.20650100
C	-3.95938400	5.23365900	1.19097400
H	-3.89129100	4.30220900	-0.75684800
C	-3.46392700	3.78930000	3.06824800
H	-3.00392500	1.73274800	2.59498700
C	-3.80727100	5.05331100	2.57245800
H	-4.22480800	6.20922500	0.79249600
H	-3.34251800	3.64031800	4.13803400
H	-3.95390000	5.88710000	3.25325500
O	-0.82730600	1.10780300	-1.59673800
H	-3.39103800	2.06389600	-1.08522300
O	-3.26758600	0.21726000	-2.12414000
H	-4.18108300	-0.15638400	-2.15108300

HC1-TS_{CN}

C	-2.77339400	0.09350100	-1.08468800
C	-1.30884400	0.20047500	-1.14607800
C	-0.51920500	-0.89946400	-0.59689800
C	-1.19024500	-2.09563600	-0.20813400
C	-2.62047800	-2.20762700	-0.32711900
C	-3.38709500	-1.17878500	-0.77563700
C	0.90904100	-0.84943100	-0.47322300
C	-0.46670300	-3.19536400	0.29214400
H	-3.07594700	-3.15226800	-0.04553500
C	0.90856800	-3.10733200	0.40506900
C	1.60403400	-1.95029000	0.02844900
H	-0.99548300	-4.09665400	0.58187300

H	2.67821400	-1.90536600	0.12625700
N	1.54259800	0.33631200	-0.88141000
H	0.88409900	1.00645800	-1.30558400
C	2.81779700	0.76004700	-0.79146400
C	4.29128900	2.39976500	-1.22709900
C	4.96786600	0.57709100	-0.17961200
Cl	4.65574900	3.97431900	-1.88923200
Cl	6.24003100	-0.34795900	0.57960500
N	5.32582900	1.76342800	-0.66407600
N	3.77765200	0.01482400	-0.19933100
N	3.05226200	1.98914600	-1.33532400
S	1.86618600	-4.50511600	1.03922600
S	-5.18542300	-1.35466500	-0.78048500
O	2.77194000	-4.91843800	-0.08217800
O	2.62294200	-3.97554400	2.22017100
O	0.87488400	-5.56283200	1.40862800
O	-5.48743700	-2.76464600	-1.15204200
O	-5.65667200	-0.98694900	0.58872800
O	-5.65072800	-0.36197400	-1.82272200
N	-2.69524100	0.98641100	0.82397700
N	-2.90306900	2.19281300	0.57696400
C	-2.41863900	3.31748100	1.32223800
C	-2.79060800	4.59169900	0.88119900
C	-1.62159500	3.13765200	2.45785700
C	-2.34788300	5.70984700	1.58970200
H	-3.41373100	4.70114800	-0.00325900
C	-1.18609000	4.26424500	3.15393500
H	-1.34811600	2.13835400	2.77983100
C	-1.54652100	5.54905400	2.72520000
H	-2.62943800	6.70368300	1.25374100
H	-0.56328500	4.13962400	4.03527200
H	-1.20307200	6.42064000	3.27529200
O	-0.80528300	1.25078600	-1.65367300
H	-3.43595100	2.43030700	-0.28636000
O	-3.42576200	1.04811200	-1.79099500
H	-4.37245000	0.75949200	-1.90920600

HC34-CP1

C	-2.32600600	-0.43999800	-0.17958900
C	-0.97251100	0.11773600	-0.14051500
C	0.17325700	-0.79758100	-0.14014100
C	-0.07995500	-2.19755100	-0.17486000
C	-1.42773400	-2.70645700	-0.20686700
C	-2.49986000	-1.87712600	-0.20833400

C	1.53825100	-0.35024400	-0.10309300
C	0.98374500	-3.12027400	-0.17456700
H	-1.56250800	-3.78157300	-0.22698900
C	2.28404200	-2.65302700	-0.14118300
C	2.57522700	-1.28498600	-0.10672200
H	0.76995900	-4.18284900	-0.20168700
H	3.59995000	-0.94775300	-0.08323600
N	1.76706600	1.03299000	-0.05648600
H	0.89434400	1.57707900	-0.05280200
C	2.89660800	1.76924000	-0.00142600
C	3.79266000	3.82586200	0.11929300
C	5.11917100	2.06131800	0.03816000
Cl	3.60334000	5.55881000	0.20074400
Cl	6.72513000	1.37758700	0.02680800
N	5.05690500	3.38798900	0.10909800
N	4.12215100	1.20272300	-0.02378300
N	2.69316900	3.11495800	0.07459700
S	3.67368100	-3.81486000	-0.10172800
S	-4.15360400	-2.62722100	-0.25628500
O	4.27011700	-3.67154400	1.26632000
O	4.60571200	-3.36872200	-1.18639500
O	3.09638400	-5.17219600	-0.34781400
O	-3.92775400	-4.10376200	-0.25319700
O	-4.81799600	-2.14363700	-1.50370300
O	-4.86573100	-2.16565000	0.99004500
N	-3.43914800	0.30289000	-0.19194500
N	-3.39738700	1.59592200	-0.16306700
C	-4.56807100	2.37812600	-0.18499800
C	-4.40552300	3.77041600	-0.12619000
C	-5.84686300	1.80760100	-0.26530400
C	-5.53026700	4.59464400	-0.14741300
H	-3.40625800	4.19415700	-0.06323300
C	-6.96080500	2.64567500	-0.28593100
H	-5.96175800	0.73076600	-0.31122000
C	-6.81123000	4.03756200	-0.22785400
H	-5.40328200	5.67261000	-0.10184400
H	-7.95335000	2.20812800	-0.34936700
H	-7.68631800	4.68110700	-0.24496700
O	-0.82691400	1.38124700	-0.10938500
H	-2.47543500	2.05394500	-0.12605300
O	-3.76300500	-1.88066800	3.49032700
H	-4.11117000	-1.99955700	2.55794500

HC34-TS1

C	-2.30307200	-0.53244500	-0.17529800
C	-0.96112600	0.05218700	-0.10886700
C	0.20132300	-0.84076300	-0.06652900
C	-0.02480800	-2.24553900	-0.08341400
C	-1.36100700	-2.78068400	-0.14918300
C	-2.44854500	-1.97295400	-0.19540400
C	1.55662300	-0.36699100	-0.00981000
C	1.05525200	-3.14793000	-0.04136100
H	-1.47420400	-3.85825500	-0.16539200
C	2.34538400	-2.65562200	0.01778600
C	2.61030100	-1.28191500	0.03207000
H	0.86184800	-4.21462700	-0.05659200
H	3.62759000	-0.92485400	0.07553200
N	1.75913200	1.02094600	0.00748100
H	0.87629000	1.54811700	-0.00522600
C	2.87512100	1.77972500	0.02201100
C	3.73410900	3.85542000	0.05986500
C	5.09211600	2.11352600	0.02003800
Cl	3.51557800	5.58641200	0.08906800
Cl	6.71029500	1.45924100	0.00621500
N	5.00601300	3.44040000	0.04646500
N	4.11058000	1.23503800	0.00356700
N	2.64758200	3.12339300	0.05325400
S	3.75553700	-3.78982900	0.11153100
S	-4.08280600	-2.75816200	-0.31696500
O	4.33696700	-3.58758600	1.47871500
O	4.68936600	-3.36538700	-0.98032400
O	3.20533500	-5.16555900	-0.09068400
O	-3.82541800	-4.22958300	-0.31566100
O	-4.69660000	-2.27822500	-1.59202800
O	-4.86131500	-2.33235500	0.90043200
N	-3.42949000	0.18934400	-0.21717300
N	-3.41363100	1.48314800	-0.20665700
C	-4.59892600	2.24106500	-0.25231100
C	-4.46468500	3.63717200	-0.21537300
C	-5.86506400	1.64331200	-0.33565200
C	-5.60543200	4.43781400	-0.26475300
H	-3.47500900	4.08219600	-0.14822900
C	-6.99515100	2.45830700	-0.38567600
H	-5.95792400	0.56379900	-0.36390800
C	-6.87399600	3.85365500	-0.35114300
H	-5.50077100	5.51875500	-0.23641000
H	-7.97775000	1.99948200	-0.45297900
H	-7.76140700	4.47905100	-0.39063700

O	-0.84076900	1.31813000	-0.08944500
H	-2.50202600	1.96008000	-0.15871600
O	-4.40059300	-0.41933900	2.81509700
H	-4.51255000	-1.09226200	2.08245400

HC34-CP2

C	-2.22518300	-0.57628100	-0.10123200
C	-0.89422200	0.02040300	-0.04514900
C	0.27307000	-0.85841300	-0.02536700
C	0.06593300	-2.26919600	-0.04176300
C	-1.26166000	-2.81685000	-0.09029100
C	-2.35707100	-2.01220900	-0.12429700
C	1.62671600	-0.37197500	0.01389300
C	1.15954700	-3.15805300	-0.00820200
H	-1.36882800	-3.89542800	-0.09533800
C	2.44355800	-2.65172500	0.04058900
C	2.69075600	-1.27220300	0.04999200
H	0.97811200	-4.22705500	-0.02004000
H	3.70390200	-0.90229700	0.08247600
N	1.80985200	1.02032100	0.00860700
H	0.91481200	1.53058000	-0.00408500
C	2.91170100	1.79568700	-0.00936600
C	3.73802600	3.88512400	-0.06859900
C	5.12377900	2.16567200	-0.01942900
Cl	3.49314000	5.61326300	-0.11130000
Cl	6.75381100	1.53891600	-0.00977000
N	5.01693200	3.49092200	-0.05849000
N	4.15744600	1.27142200	0.01170600
N	2.66347200	3.13687900	-0.05127500
S	3.86692900	-3.76604900	0.12719600
S	-4.00197400	-2.78055900	-0.20989200
O	4.46235500	-3.54935800	1.48685400
O	4.78696400	-3.33935400	-0.97637100
O	3.33335400	-5.15109800	-0.06009700
O	-3.76469300	-4.25055900	-0.07359500
O	-4.57303600	-2.41008200	-1.54373300
O	-4.80410100	-2.23182900	0.93760200
N	-3.37621000	0.11401100	-0.11090900
N	-3.37406000	1.42961600	-0.02663700
C	-4.53308300	2.11972100	0.01989200
C	-4.49292400	3.52320700	0.10244800
C	-5.83416700	1.34295900	-0.04460300
C	-5.66761200	4.24780600	0.10297700
H	-3.52888800	4.02184500	0.16888300

C	-7.03768800	2.24017600	-0.03228000
H	-5.83426700	0.77376900	-0.98899700
C	-6.94789000	3.59032200	0.02498700
H	-5.63004100	5.33080500	0.16944200
H	-7.99975600	1.73686300	-0.07387100
H	-7.84774400	4.19933200	0.02333100
O	-0.78896400	1.29859700	-0.01513900
H	-2.45590800	1.90519900	0.01252100
O	-5.96638400	0.40505100	1.04294600
H	-5.42435400	-0.39310100	0.84304700

HC34-TS_{CO}

C	2.25886800	-0.70708200	0.11057700
C	0.93067500	-0.07149900	0.02838800
C	-0.09184800	-2.33185100	0.09127500
C	1.22764500	-2.91436000	0.17347000
C	2.34728900	-2.15440300	0.18643800
H	1.29782500	-3.99458700	0.22553200
S	3.95551600	-2.99895800	0.29864800
O	3.62965500	-4.45840500	0.36248700
O	4.71429700	-2.64131100	-0.94201100
O	4.60467700	-2.50384200	1.55382000
N	3.40313800	-0.03178000	0.11068900
N	3.43683100	1.26840200	0.04560000
C	4.65740900	1.96216000	-0.01554600
C	4.54984400	3.39373100	0.11567100
C	5.87906200	1.31945800	0.39613800
C	5.65623100	4.13456100	0.46647300
H	3.59466500	3.86526100	-0.09960700
C	6.97110600	2.09277900	0.74387500
H	5.92742300	0.23699800	0.40316400
C	6.87687000	3.49544600	0.77400500
H	5.58252100	5.21626100	0.52796600
H	7.90325800	1.60706900	1.01708800
H	7.74037600	4.08967000	1.05778300
O	0.86000700	1.19105800	-0.03515300
H	2.55112700	1.78158400	-0.04844200
O	4.99627700	1.90939100	-1.96460000
H	5.30132500	0.98498400	-2.05105700
C	-1.20079700	-3.18996600	0.08050000
C	-2.47686600	-2.64953600	0.00074100
C	-2.68975600	-1.27434600	-0.06085200
C	-1.59816100	-0.39643300	-0.04911400
C	-0.26581700	-0.91965200	0.02279000

N	-1.75169100	0.99374800	-0.11510500
H	-0.85313000	1.49171800	-0.12399500
H	-1.04259700	-4.26250600	0.13144600
C	-2.83954500	1.79496500	-0.14531900
C	-3.61059400	3.90292300	-0.23699200
C	-5.04014400	2.22077800	-0.14297800
S	-3.89935900	-3.77482200	-0.03773700
O	-5.12000800	-2.91207200	-0.07134400
O	-3.79416400	-4.59695900	1.21048200
O	-3.72320400	-4.59215900	-1.28138900
N	-2.55562500	3.12558800	-0.21756400
N	-4.09538700	1.30226900	-0.10411100
N	-4.89823000	3.54157700	-0.20602200
Cl	-3.31799200	5.62133500	-0.31463300
Cl	-6.68449500	1.63771900	-0.11108100
H	-3.69433900	-0.88815900	-0.11932100

HC34-CP3

C	-2.29718900	-0.64322100	0.16455600
C	-0.96858800	-0.02712900	0.09754200
C	0.01434900	-2.30526800	-0.01353700
C	-1.31242800	-2.86940600	0.04925800
C	-2.41530000	-2.08848000	0.13553100
H	-1.40293100	-3.94913300	0.02867300
S	-4.03815700	-2.90543200	0.22871700
O	-3.74797600	-4.37281000	0.16610600
O	-4.63683200	-2.50187800	1.54144500
O	-4.82640000	-2.43119700	-0.95302000
N	-3.43148700	0.05625600	0.25069800
N	-3.45510500	1.34632800	0.27956600
C	-4.74095900	2.07199000	0.44218600
C	-4.48831500	3.49881200	0.03845400
C	-5.84214600	1.41133600	-0.34150800
C	-5.24115100	4.12582700	-0.91423100
H	-3.68413500	4.01277600	0.55937000
C	-6.56797900	2.09309500	-1.27941900
H	-6.05523000	0.37329200	-0.10699100
C	-6.29044000	3.44938100	-1.58985100
H	-5.03211900	5.16392500	-1.15962300
H	-7.37492600	1.58338100	-1.79983300
H	-6.87663600	3.96711800	-2.34247200
O	-0.87398000	1.23896000	0.11459900
H	-2.56652800	1.86319000	0.26162100
O	-5.06690100	2.09078800	1.84963800

H	-5.35242200	1.19498300	2.11272300
C	1.11023200	-3.17966500	-0.09610300
C	2.39314900	-2.65759000	-0.15424900
C	2.62980900	-1.28347600	-0.12738200
C	1.55457200	-0.39191100	-0.04042000
C	0.21302500	-0.89459700	0.01331500
N	1.73057900	0.99836200	-0.00099700
H	0.83746900	1.50637800	0.04199300
H	0.93395400	-4.25048000	-0.11336800
C	2.83067600	1.78014800	0.02964200
C	3.64206300	3.87295600	0.12959600
C	5.03957900	2.16416900	0.04070600
S	3.79615000	-3.80159000	-0.26479500
O	5.02794700	-2.95565100	-0.32325200
O	3.56817700	-4.59350300	-1.51638600
O	3.72279200	-4.64678800	0.97111100
N	2.57242400	3.11674500	0.10300800
N	4.07819500	1.26443400	-0.00750000
N	4.92297800	3.48739100	0.10610600
Cl	3.38415700	5.59731100	0.20679400
Cl	6.67289800	1.54892000	0.01935400
H	3.64019900	-0.91079800	-0.17199100

HC34-TS3

C	-2.29499700	-0.63914300	0.16220600
C	-0.96578700	-0.02420200	0.09284200
C	0.01483600	-2.30353400	-0.01380300
C	-1.31265000	-2.86632800	0.04851900
C	-2.41471300	-2.08435400	0.13433500
H	-1.40417800	-3.94597900	0.02814900
S	-4.03866600	-2.89919500	0.22644100
O	-3.75040600	-4.36685800	0.16227000
O	-4.63731900	-2.49636000	1.53937100
O	-4.82577800	-2.42242900	-0.95504000
N	-3.42764100	0.06163000	0.25172300
N	-3.45125100	1.35181800	0.28034000
C	-4.74085800	2.07115100	0.44128400
C	-4.47459600	3.51909100	0.13219600
C	-5.81150600	1.45968600	-0.42130400
C	-5.20157500	4.20565700	-0.79910700
H	-3.68687300	3.99792400	0.70874800
C	-6.51147900	2.19986300	-1.33448300
H	-6.02377900	0.40651500	-0.26596200
C	-6.23063900	3.57426800	-1.54607100

H	-4.98691700	5.25714000	-0.97207700
H	-7.29771100	1.72292700	-1.91425500
H	-6.79584400	4.13999300	-2.27998600
O	-0.87050800	1.24166400	0.10667800
H	-2.56411400	1.87041700	0.25379300
O	-5.11950700	2.01131700	1.83452600
H	-5.41939300	1.10519300	2.03973400
C	1.10977900	-3.17920800	-0.09400100
C	2.39338400	-2.65859000	-0.15129900
C	2.63148700	-1.28475400	-0.12613000
C	1.55707700	-0.39183900	-0.04185800
C	0.21502400	-0.89303000	0.01116900
N	1.73456600	0.99826900	-0.00403900
H	0.84208600	1.50749700	0.03672400
H	0.93234300	-4.24984900	-0.10996100
C	2.83567100	1.77869200	0.02742400
C	3.64985300	3.87040800	0.12675600
C	5.04507800	2.15962100	0.04035300
S	3.79530100	-3.80424800	-0.25858700
O	5.02806100	-2.95967300	-0.31609100
O	3.56827700	-4.59714800	-1.50972000
O	3.71913900	-4.64809700	0.97805100
N	2.57917300	3.11565500	0.09962000
N	4.08247200	1.26122300	-0.00809700
N	4.93023500	3.48304000	0.10476900
Cl	3.39436900	5.59515400	0.20241800
Cl	6.67749600	1.54198200	0.02082000
H	3.64233800	-0.91325400	-0.17004100

HC34-CP4

C	2.30253100	-0.72969800	-0.13680700
C	0.98919900	-0.08469900	-0.07043500
C	-0.04082000	-2.34285000	0.02036800
C	1.27454400	-2.93500400	-0.03103200
C	2.39331500	-2.17640700	-0.11019500
H	1.34265200	-4.01635900	-0.00891600
S	4.00346700	-3.02014000	-0.18415900
O	3.68865600	-4.48229600	-0.12277700
O	4.62555400	-2.62777200	-1.48936500
O	4.78376000	-2.55525100	1.00670400
N	3.44757900	-0.05093000	-0.23235500
N	3.50806600	1.23500800	-0.27055100
C	4.85446400	1.87720400	-0.33985800
C	4.66080000	3.31649700	-0.72833200

C	5.55776400	1.70254100	0.98181500
C	5.15071800	4.34073700	0.03138100
H	4.13698900	3.49803600	-1.66306900
C	6.02723800	2.76735000	1.70190100
H	5.68425900	0.67934200	1.32668700
C	5.84115700	4.09857600	1.24978400
H	5.00876800	5.36533000	-0.30287900
H	6.54793700	2.59062800	2.63976300
H	6.21892900	4.93140200	1.83443500
O	0.92489200	1.18318600	-0.08085300
H	2.64852300	1.79166200	-0.19033200
O	5.59093500	1.24224700	-1.39462500
H	5.71314800	0.30129300	-1.16142500
C	-1.15543700	-3.19449400	0.08717500
C	-2.42804000	-2.64646700	0.13293300
C	-2.63643500	-1.26761300	0.11009300
C	-1.54200300	-0.39833900	0.03943100
C	-0.21061300	-0.92819700	-0.00201300
N	-1.68731800	0.99543500	0.00218000
H	-0.78280500	1.48380800	-0.03270200
H	-1.00129000	-4.26877800	0.10161500
C	-2.76894000	1.80228300	-0.02900000
C	-3.52935700	3.91450100	-0.12583500
C	-4.96780300	2.23970600	-0.04505800
S	-3.85408800	-3.76373200	0.22054000
O	-5.07040100	-2.89523300	0.27343600
O	-3.65318700	-4.56929400	1.46809600
O	-3.78451900	-4.60085600	-1.02104900
N	-2.47853000	3.13265900	-0.09666500
N	-4.02868500	1.31640700	0.00251400
N	-4.81934900	3.55996200	-0.10744500
Cl	-3.22754100	5.63202100	-0.20132300
Cl	-6.61595000	1.66496000	-0.02736500
H	-3.63939400	-0.87448400	0.14426400

HC34-TS4

C	2.30961200	-0.74221300	-0.17010700
C	0.99913800	-0.09236300	-0.09789000
C	-0.03876600	-2.34633900	0.00684500
C	1.27360400	-2.94354200	-0.05668600
C	2.39479900	-2.18933300	-0.14408400
H	1.33776100	-4.02514100	-0.03504400
S	4.00031300	-3.04076300	-0.22834400
O	3.67898200	-4.50148300	-0.16755800

O	4.61696400	-2.64913800	-1.53634800
O	4.78945100	-2.58153900	0.95888300
N	3.45748100	-0.06711200	-0.26292800
N	3.52252900	1.21840600	-0.30185400
C	4.87335200	1.85880800	-0.32741500
C	4.70164700	3.28304500	-0.77680000
C	5.50381900	1.73190400	1.03575500
C	5.14199400	4.33468100	-0.02421700
H	4.23389900	3.42989300	-1.74662900
C	5.92542000	2.82272200	1.74661200
H	5.61649700	0.72101400	1.41967000
C	5.75958200	4.13712700	1.24064900
H	5.01731500	5.34680000	-0.40076800
H	6.39277500	2.68002200	2.71775800
H	6.09842400	4.99129100	1.81834300
O	0.93902200	1.17576500	-0.11293800
H	2.66542500	1.77787300	-0.21471300
O	5.66126000	1.18620400	-1.31649100
H	5.75530800	0.25124000	-1.04952000
C	-1.15590900	-3.19362200	0.08644900
C	-2.42572300	-2.64067500	0.14620700
C	-2.62896900	-1.26100000	0.12463700
C	-1.53202600	-0.39609900	0.04043800
C	-0.20321100	-0.93113400	-0.01530600
N	-1.67233600	0.99828000	0.00488000
H	-0.76623900	1.48297000	-0.03956400
H	-1.00577700	-4.26848200	0.10022900
C	-2.75114900	1.80908200	-0.02019600
C	-3.50445100	3.92405600	-0.11348800
C	-4.94851400	2.25441600	-0.02699300
S	-3.85449100	-3.75282600	0.25121800
O	-5.06775600	-2.88041100	0.30949400
O	-3.64605800	-4.55277700	1.50114600
O	-3.79739200	-4.59633300	-0.98670800
N	-2.45631000	3.13849100	-0.08844600
N	-4.01253600	1.32773000	0.01673400
N	-4.79564400	3.57415700	-0.08983700
Cl	-3.19635200	5.64042100	-0.19081200
Cl	-6.59866100	1.68561300	-0.00346500
H	-3.62989000	-0.86386100	0.17017400

HC34-CP5

C	-2.32557500	-0.75194000	0.17451800
C	-1.01254200	-0.10731900	0.11870700

C	0.01488600	-2.36277400	-0.00391000
C	-1.29860500	-2.95583300	0.05513500
C	-2.41767000	-2.19723300	0.14309000
H	-1.36679200	-4.03707500	0.02912500
S	-4.02787000	-3.04009600	0.22445000
O	-3.71419000	-4.50243400	0.16520500
O	-4.64364800	-2.64301700	1.53116500
O	-4.81307700	-2.57707100	-0.96386200
N	-3.47316600	-0.07094900	0.24718800
N	-3.53060400	1.21342900	0.29149000
C	-4.87701100	1.86853200	0.24110800
C	-4.74523700	3.24419800	0.83305100
C	-5.35374800	1.87460500	-1.18943300
C	-5.07349000	4.36747300	0.12847400
H	-4.39417700	3.29402800	1.86012800
C	-5.67041600	3.03249500	-1.84649600
H	-5.44081300	0.90220400	-1.66796000
C	-5.54015000	4.29442400	-1.21250900
H	-4.97783200	5.34046300	0.60369500
H	-6.02689000	2.98544200	-2.87243400
H	-5.79466000	5.20310800	-1.74891300
O	-0.94661500	1.16097400	0.14793900
H	-2.66762000	1.76645500	0.21519000
O	-5.76153600	1.11705900	1.07459900
H	-5.77939000	0.19443200	0.75183500
C	1.13086600	-3.21727100	-0.09353300
C	2.39894500	-2.67047600	-0.15042800
C	2.60877600	-1.28740300	-0.11287300
C	1.51942500	-0.42003000	-0.01889200
C	0.18541700	-0.95084300	0.03106800
N	1.66333700	0.97448200	0.02963100
H	0.75848300	1.46111500	0.07820900
H	0.98175700	-4.29077900	-0.12073800
C	2.74441700	1.78116200	0.05835200
C	3.50635000	3.89262400	0.16072900
C	4.94376700	2.21783500	0.06437800
S	3.85484700	-3.74317600	-0.26674700
O	4.62185300	-3.51948700	1.00153800
O	4.60084400	-3.27464400	-1.47882800
O	3.34083400	-5.14111900	-0.40011000
N	2.45506800	3.11151300	0.13440400
N	4.00413700	1.29511100	0.01756600
N	4.79623500	3.53785400	0.13273100
Cl	3.20563400	5.61003400	0.24640500

Cl	6.59174100	1.64258900	0.03771500
H	3.60974000	-0.88715500	-0.15688300

HC34-TS_{CN}

C	-2.14653300	-0.71293700	0.15524700
C	-0.86048400	-0.05550600	0.10560500
C	0.18972000	-2.30291900	-0.02954700
C	-1.11169700	-2.90751000	0.02797500
C	-2.23597000	-2.14722400	0.11796800
H	-1.17601400	-3.98866100	-0.00166500
S	-3.84305000	-2.99615700	0.19759200
O	-3.52862300	-4.45778200	0.11616400
O	-4.45144500	-2.62016600	1.51443500
O	-4.63953200	-2.52079000	-0.97950400
N	-3.31339700	-0.00489800	0.22834100
N	-3.39683000	1.23742900	0.25775200
C	-5.19612200	2.01620100	0.11632800
C	-5.15889800	2.91580600	1.25151800
C	-5.04587400	2.58261600	-1.21067400
C	-4.75845300	4.22133500	1.07377000
H	-5.40071400	2.51249100	2.22993600
C	-4.64888500	3.89547800	-1.35162300
H	-5.19944800	1.93215100	-2.06762100
C	-4.47781800	4.72134800	-0.21883200
H	-4.68063900	4.88156100	1.93292800
H	-4.48803200	4.30405700	-2.34529700
H	-4.16518000	5.75343400	-0.34402300
O	-0.80133000	1.22416400	0.14372700
H	-2.53053700	1.80128700	0.17522400
O	-5.95131400	0.89676400	0.30224900
H	-5.96749300	0.35106300	-0.50639500
C	1.32075700	-3.14492200	-0.12415700
C	2.57921900	-2.58505500	-0.18204200
C	2.77330300	-1.19594100	-0.14237000
C	1.67581400	-0.34440400	-0.04426400
C	0.34448300	-0.88750000	0.00962000
N	1.79944300	1.05444400	0.00359600
H	0.88202200	1.52207700	0.05912900
H	1.18301300	-4.21998900	-0.15380100
C	2.86494600	1.87711300	0.02259400
C	3.59417500	4.00196900	0.11306600
C	5.05767500	2.35072100	0.01578500
S	4.04629600	-3.63878700	-0.30425600
O	4.82159600	-3.40331100	0.95766200

O	4.78057700	-3.16652700	-1.52290200
O	3.55081800	-5.04480700	-0.42973800
N	2.55583900	3.20502400	0.09364800
N	4.13429400	1.41219500	-0.02229900
N	4.89017500	3.66885900	0.08027700
Cl	3.26481700	5.71543700	0.19600100
Cl	6.71599600	1.80298700	-0.01815700
H	3.76962400	-0.78447800	-0.18824700

Figure S1. Structures of some degradation fragments

Figure S2. The Gibbs free energy profiles of the reaction channels for RR2 obtained at the B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d) level with the thermal corrections at 298.15 K and 1 Atm. (Energies in kcal/mol)

Figure S3. The Gibbs free energy profiles of the reaction channels for HRR2 obtained at the B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d) level with the thermal corrections at 298.15 K and 1 Atm. (Energies in kcal/mol)

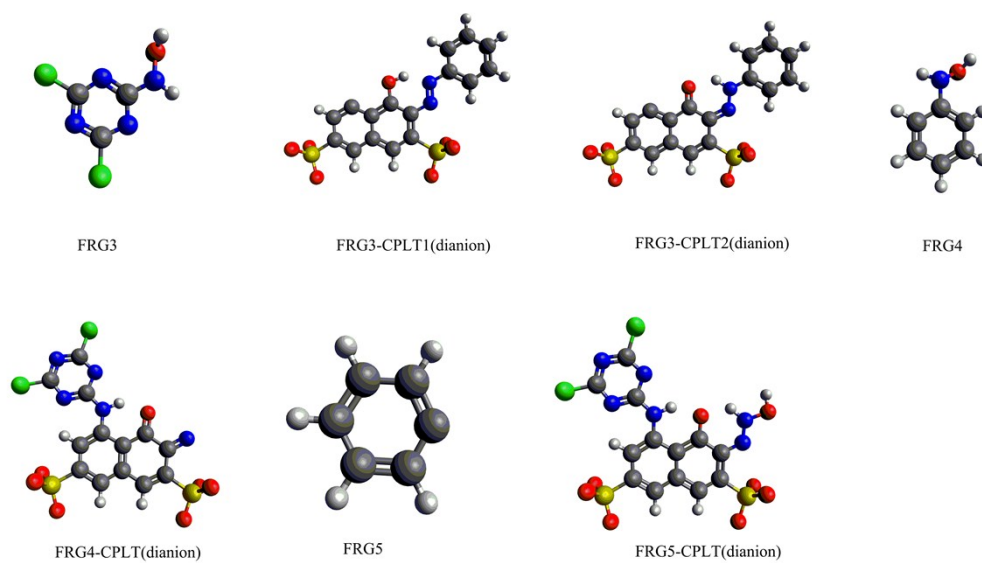


Figure S1

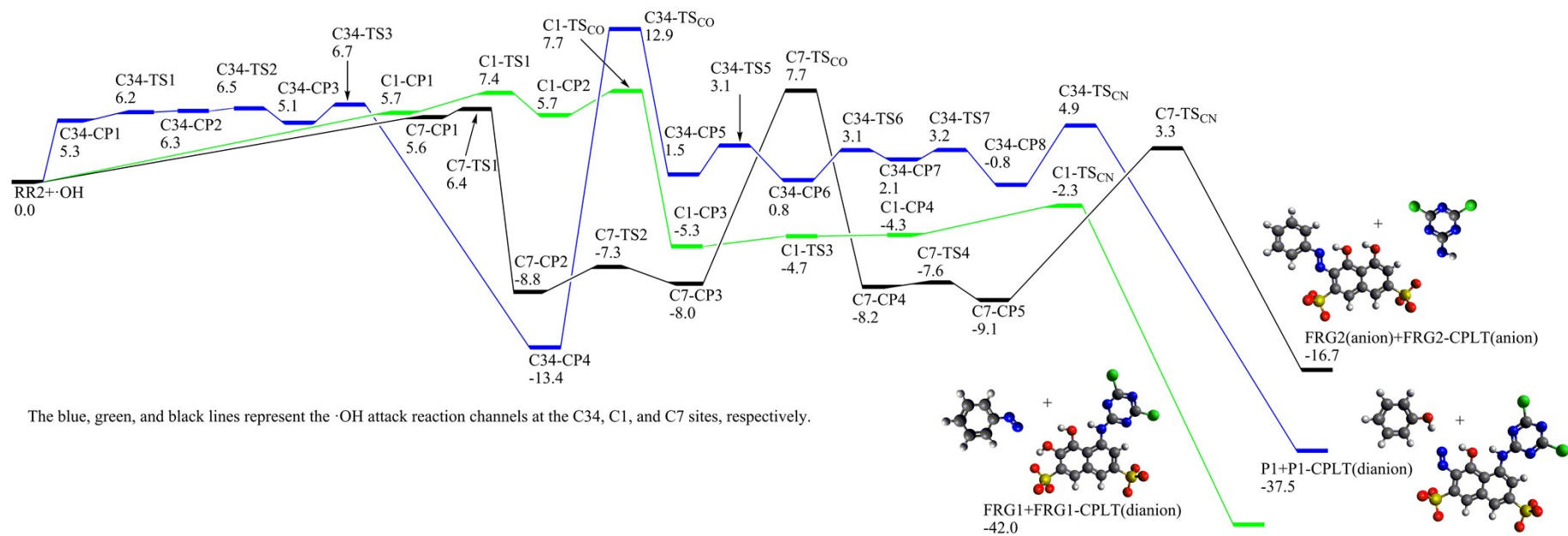


Figure S2

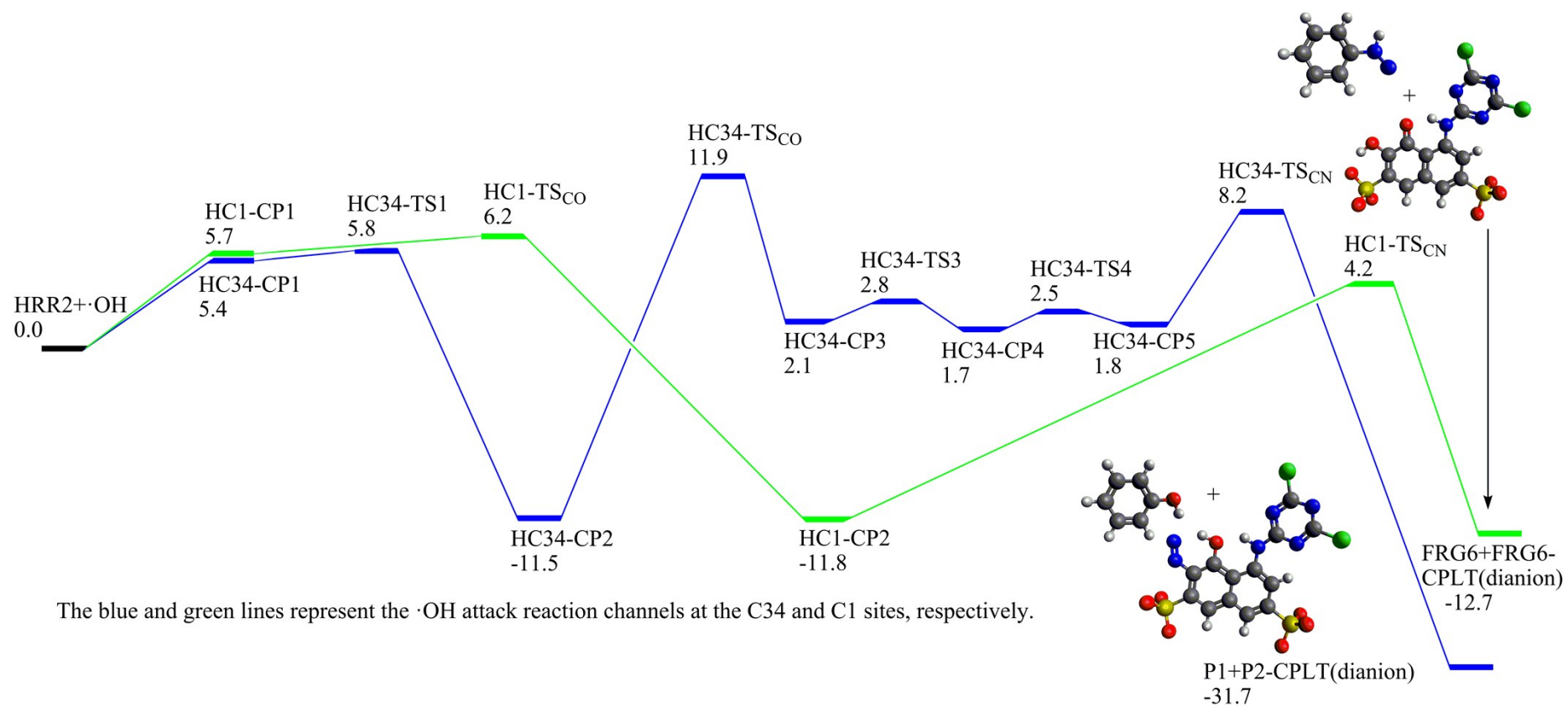


Figure S3