

Electronic Supplementary Information (ESI)

Understanding Roles of Novel Electron Donors in Ziegler–Natta Catalyzed Propylene Polymerization

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Reaction coordinate (.xyz) of all structures

Dibenzoyl sulfide (Mono mode)

Cl	13.77390700	-2.63919100	-1.04710200
Cl	10.47512500	-4.18012900	-1.07565000
Mg	11.64423700	-2.40583800	0.25187500
Cl	10.79247400	-0.55534600	-1.20669100
Cl	9.51456100	-2.17238200	1.55094900
Mg	8.34555000	-3.94667100	0.22332400
Cl	7.49368800	-2.09618500	-1.23524200
Cl	6.21577900	-3.71332000	1.52240100
Cl	4.19500600	-3.63711800	-1.26379000
Mg	8.66289900	-0.32188600	0.09238300
Cl	6.53312800	-0.08853700	1.39136000
Mg	5.36411700	-1.86282700	0.06373500
Cl	4.51235400	-0.01233500	-1.39483100
Cl	3.23434100	-1.62937600	1.36280900
Mg	2.06533000	-3.40366500	0.03518400
Cl	1.21356800	-1.55317400	-1.42338200
Cl	-0.06434000	-3.17031100	1.33416100
Cl	-2.08521900	-3.09401200	-1.45193200
Mg	2.32667200	0.13578600	-0.16942800
Cl	1.53091600	2.07160900	-1.55442200
Cl	0.25300800	0.45447400	1.20322000
Mg	-0.91610300	-1.31982000	-0.12440500
Cl	-1.76786600	0.53067100	-1.58297100
Cl	-3.04577800	-1.08636700	1.17456900
Mg	-4.21479000	-2.86065400	-0.15295600
Cl	-5.06655200	-1.01016300	-1.61152100
Cl	-6.34456500	-2.62720500	1.14601800
Cl	-8.36533900	-2.55100100	-1.64007200
Ti	-0.59875500	2.30496500	-0.25534600
Cl	-2.72843000	2.53841900	1.04362800
Mg	-3.89744100	0.76412900	-0.28399700
Cl	-6.02721600	0.99758000	1.01507700
Mg	-7.19622700	-0.77670900	-0.31254700

Cl	-8.04799000	1.07378200	-1.77111300
Cl	-9.32589800	-0.54335600	0.98642900
Mg	-10.49500900	-2.31764800	-0.34109600
Cl	-11.34677200	-0.46715600	-1.79966200
Cl	-12.62468500	-2.08419400	0.95787900
Mg	-10.17766100	1.30713500	-0.47213700
Cl	-12.30733600	1.54058900	0.82683800
Mg	-13.47634700	-0.23369800	-0.50068700
Cl	-15.60611800	-0.00034900	0.79828900
Cl	0.73361000	4.11774000	-0.28962300
Cl	-1.71489000	4.25576400	-0.36016800
S	4.54856600	4.34983300	0.88611400
C	3.85076600	2.83218600	1.63133800
O	3.32933100	1.90976300	1.01573600
C	4.75296900	4.00896600	-0.93981500
O	4.36761200	2.99365000	-1.46166200
C	5.45527100	5.10098000	-1.67561500
C	3.92289600	2.87665600	3.12185200
C	5.85753600	6.32257100	-1.10805800
C	6.50295400	7.27952300	-1.89650400
C	6.76261800	7.02355200	-3.24794900
C	6.36623600	5.80697900	-3.81800100
C	5.71885800	4.85166300	-3.03730000
C	4.68632000	3.82922000	3.82456800
C	4.68375300	3.84797300	5.21899900
C	3.92510200	2.91253800	5.93027900
C	3.17337300	1.95311500	5.24155800
C	3.17078200	1.93332600	3.84713400
H	5.66422900	6.54040100	-0.05691800
H	6.80595800	8.22997400	-1.45527700
H	7.26768300	7.77284200	-3.86011000
H	6.56427000	5.59972800	-4.87136500
H	5.40291900	3.89869800	-3.46190800
H	5.29401700	4.55273900	3.28233400
H	5.28029000	4.59196000	5.74974700
H	3.92448400	2.92708900	7.02133200
H	2.58786100	1.21681900	5.79385300
H	2.58690900	1.18869800	3.30683900

Dibenzoyl sulfide (Chelate mode)

Cl	-12.96633700	-2.54844200	1.20485200
Cl	-9.64352400	-4.02825300	1.36713700
Mg	-10.84701200	-2.41485300	-0.12477400
Cl	-10.01744800	-0.41398400	1.13442300
Cl	-8.72769000	-2.28116800	-1.45450900
Mg	-7.52429300	-3.89456000	0.03749900
Cl	-6.69464300	-1.89369700	1.29670400
Cl	-5.40487200	-3.76098000	-1.29222600
Cl	-3.37191900	-3.37350200	1.45898300
Mg	-7.89821100	-0.28029200	-0.19531900
Cl	-5.77880000	-0.14670800	-1.52494400
Mg	-4.57540800	-1.76009900	-0.03292800
Cl	-3.74584400	0.24076900	1.22626800
Cl	-2.45598100	-1.62642000	-1.36266400
Mg	-1.25259100	-3.23981200	0.12934800
Cl	-0.42302700	-1.23894200	1.38854500
Cl	0.86673300	-3.10622100	-1.20028000
Cl	2.89978900	-2.71865400	1.55082200

Mg	-1.56880900	0.29784300	-0.02193800
Cl	-0.79695300	2.37532900	1.15583000
Cl	0.49280700	0.50804300	-1.43309400
Mg	1.69629700	-1.10535100	0.05891800
Cl	2.52586100	0.89551800	1.31811500
Cl	3.81562400	-0.97166100	-1.27071800
Mg	5.01901400	-2.58506000	0.22119400
Cl	5.84857800	-0.58419100	1.48039200
Cl	7.13844100	-2.45137300	-1.10844100
Cl	9.17139400	-2.06390300	1.64266800
Ti	1.32237100	2.50891200	-0.17389700
Cl	3.44169900	2.64260300	-1.50353300
Mg	4.64508800	1.02921100	-0.01152100
Cl	6.76451500	1.16289100	-1.34125600
Mg	7.96790500	-0.45050000	0.15075600
Cl	8.79746900	1.55036900	1.40995300
Cl	10.08722900	-0.31691000	-1.17887100
Mg	11.29071800	-1.93031200	0.31304100
Cl	12.12028200	0.07055800	1.57223800
Cl	13.41004600	-1.79662100	-1.01659400
Mg	10.91679300	1.68396000	0.08032600
Cl	13.03612000	1.81765000	-1.24930900
Mg	14.23951000	0.20425100	0.24260300
Cl	16.35893400	0.33783900	-1.08702500
Cl	-0.03828000	4.29541200	-0.31378400
Cl	2.40805000	4.47710200	-0.27334500
S	-9.17810700	3.27496300	-0.01962200
C	-9.67368300	1.93665600	-1.13464900
O	-8.90704000	1.03715400	-1.46793000
C	-7.64796400	2.64670700	0.75971400
O	-7.37788000	1.45428300	0.78348700
C	-6.78826900	3.65626600	1.39925300
C	-11.03698400	2.04121600	-1.68142100
C	-7.01128600	5.04299900	1.29659400
C	-6.13714200	5.93185900	1.91468600
C	-5.03563200	5.44908500	2.63044500
C	-4.80603400	4.07283700	2.73064400
C	-5.67685700	3.17561200	2.12169100
C	-12.06044800	2.76745500	-1.04698500
C	-13.34281600	2.77200000	-1.59001700
C	-13.60916500	2.06457500	-2.76592300
C	-12.59295000	1.34117600	-3.40210300
C	-11.31227700	1.32016100	-2.86078900
H	-7.84818900	5.43203100	0.72621900
H	-6.30845100	7.00038800	1.83230600
H	-4.35384600	6.14814100	3.10615800
H	-3.94725700	3.69715400	3.27758000
H	-5.50141000	2.10850800	2.18043200
H	-11.86983900	3.28733300	-0.11433300
H	-14.13743900	3.31418300	-1.08803900
H	-14.61146800	2.07009600	-3.18371400
H	-12.80322600	0.79455800	-4.31609300
H	-10.51121900	0.76421200	-3.33636000

Dibenzoyl sulfide (Bridge mode)

Cl	-13.43278800	-2.76452400	0.70424300
Cl	-10.11246900	-4.14323600	1.28035200
Mg	-11.24968500	-2.82788900	-0.52349300

Cl	-10.49876100	-0.62839800	0.41223400
Cl	-9.06657500	-2.89118100	-1.75135100
Mg	-7.92946300	-4.20650200	0.05258500
Cl	-7.17843900	-2.00701300	0.98831700
Cl	-5.74625500	-4.26989400	-1.17524300
Cl	-3.85821900	-3.38572400	1.56442000
Mg	-8.31575000	-0.69168900	-0.81562900
Cl	-6.13254700	-0.75505600	-2.04336000
Mg	-4.99543500	-2.07037700	-0.23942400
Cl	-4.24451000	0.12911400	0.69630300
Cl	-2.81222500	-2.13367100	-1.46727700
Mg	-1.67511300	-3.44899200	0.33665900
Cl	-0.92418800	-1.24950200	1.27238600
Cl	0.50799000	-3.51235700	-0.89107700
Cl	2.39613400	-2.62811700	1.84847000
Mg	-2.00738200	0.00520300	-0.43535900
Cl	-1.31048000	2.26533600	0.40426900
Cl	0.12170300	0.00245600	-1.75929200
Mg	1.25891500	-1.31286700	0.04465000
Cl	2.00984000	0.88662400	0.98037700
Cl	3.44202000	-1.37613500	-1.18311100
Mg	4.57913700	-2.69148000	0.62072800
Cl	5.33006200	-0.49199000	1.55645500
Cl	6.76234200	-2.75475000	-0.60702800
Cl	8.65038400	-1.87060500	2.13253900
Ti	0.87262800	2.20194700	-0.82356500
Cl	3.05573400	2.13867900	-2.05132600
Mg	4.19284500	0.82335700	-0.24739000
Cl	6.37605600	0.76006300	-1.47524200
Mg	7.51316700	-0.55525800	0.32869400
Cl	8.26409200	1.64423300	1.26442100
Cl	9.69627100	-0.61862300	-0.89904200
Mg	10.83348700	-1.93397000	0.90480200
Cl	11.58441200	0.26552000	1.84052900
Cl	13.01659300	-1.99723800	-0.32295900
Mg	10.44719500	1.58086800	0.03668500
Cl	12.63030100	1.51760000	-1.19107600
Mg	13.76741800	0.20225400	0.61276300
Cl	15.95062100	0.13888800	-0.61496800
Cl	-0.49133200	3.91689600	-1.33452800
Cl	1.94849800	4.14055700	-1.20652300
S	-5.99229700	2.63886600	-1.37533300
C	-5.23636600	4.31177000	-0.83414100
O	-4.89894100	5.03843400	-1.74330100
C	-7.57166900	2.45327000	-0.59354100
O	-8.14765400	1.34567100	-0.62064300
C	-8.22118800	3.60755600	0.05762000
C	-4.94131600	4.54958900	0.59805900
C	-8.18163400	4.89787700	-0.50078200
C	-8.82033100	5.95352800	0.15056300
C	-9.48112200	5.73238300	1.36506900
C	-9.53851800	4.44340800	1.91302300
C	-8.92783900	3.37722600	1.25292900
C	-4.47902100	5.83623400	0.94839300
C	-4.08760000	6.10852400	2.25820400
C	-4.13621000	5.09631900	3.22694100
C	-4.60467900	3.82351600	2.88690800
C	-5.01385400	3.54681300	1.58011700

H	-7.68900400	5.06081700	-1.45930400
H	-8.79981000	6.94870200	-0.29609000
H	-9.96048600	6.56346400	1.88296300
H	-10.06009100	4.26647700	2.85681500
H	-8.98188400	2.36656200	1.66185300
H	-4.42190100	6.60774600	0.17931000
H	-3.73617100	7.10838600	2.51939000
H	-3.79423100	5.29644400	4.24442900
H	-4.64110700	3.03026000	3.63449700
H	-5.33006900	2.53848300	1.31751200

Dibenzoyl sulfide (Zip mode)

Cl	14.79939000	-0.60115300	-1.88280900
Cl	11.53096500	-0.24400300	-3.44701200
Mg	12.74558400	-2.01084500	-2.15074100
Cl	11.77914500	-1.26801600	0.03830200
Cl	10.69167800	-3.42054100	-2.41866800
Mg	9.47715900	-1.65369500	-3.71494400
Cl	8.51071300	-0.91083700	-1.52599700
Cl	7.42325300	-3.06339100	-3.98287100
Cl	5.24228800	-0.55368700	-3.09020000
Mg	9.72533900	-2.67770700	-0.22963000
Cl	7.67143300	-4.08740400	-0.49755700
Mg	6.45704800	-2.32076500	-1.79376900
Cl	5.43573400	-1.48142800	0.33721600
Cl	4.40304300	-3.73037300	-2.06177800
Mg	3.18852600	-1.96334300	-3.35812500
Cl	2.22218200	-1.22063600	-1.16947500
Cl	1.13457600	-3.37307500	-3.62605900
Cl	-1.04638900	-0.86337200	-2.73338800
Mg	3.37838600	-2.89222100	0.07078800
Cl	2.47001400	-2.24420900	2.31586900
Cl	1.32442000	-4.30641700	-0.19966400
Mg	0.16835700	-2.63034200	-1.43741100
Cl	-0.79820900	-1.88738400	0.75192600
Cl	-1.88567700	-4.03991000	-1.70504400
Mg	-3.10019600	-2.27306300	-3.00132000
Cl	-4.06664100	-1.53020600	-0.81237300
Cl	-5.15410200	-3.68276000	-3.26924700
Cl	-7.33506600	-1.17305600	-2.37657600
Ti	0.41623300	-3.65392200	2.04795300
Cl	-1.63750400	-5.06389400	1.78017400
Mg	-2.85201600	-3.29707600	0.48399400
Cl	-4.90592200	-4.70677200	0.21606700
Mg	-6.12044800	-2.93989800	-1.08030500
Cl	-7.08688700	-2.19706900	1.10873800
Cl	-8.17435400	-4.34959400	-1.34823200
Mg	-9.38887300	-2.58274700	-2.64450800
Cl	-10.35531900	-1.83989000	-0.45556100
Cl	-11.44277900	-3.99244400	-2.91243500
Mg	-9.14069300	-3.60676000	0.84080600
Cl	-11.19459900	-5.01645600	0.57287900
Mg	-12.40912500	-3.24958200	-0.72349300
Cl	-14.46303100	-4.65927800	-0.99142000
Cl	1.71391900	-4.13735700	3.82191400
Cl	-0.73658400	-4.23710500	3.89027200
Cl	12.95954200	5.62126300	-0.39141900
Cl	9.69111700	5.97841300	-1.95562200

Mg	10.90573500	4.21157200	-0.65935200
Cl	9.93929000	4.95442900	1.52959600
Cl	8.85182900	2.80187500	-0.92727800
Mg	7.63731000	4.56872200	-2.22355500
Cl	6.67086400	5.31157900	-0.03460700
Cl	5.58340400	3.15902600	-2.49148200
Cl	3.40243900	5.66872900	-1.59881000
Mg	7.88548300	3.54473800	1.26166400
Cl	5.83157700	2.13504100	0.99373700
Mg	4.61706900	3.90186800	-0.30252700
Cl	3.59639700	4.74021300	1.82875700
Cl	2.56307200	2.49222100	-0.57051600
Mg	1.34819600	4.25868200	-1.86681500
Cl	0.38275200	5.00437800	0.32503500
Cl	-0.70527300	2.84934100	-2.13466900
Cl	-2.88623800	5.35904500	-1.24199800
Mg	1.54016700	3.32494800	1.55578300
Cl	-0.51646300	1.91743300	1.29211100
Mg	-1.67185600	3.59244400	0.05482000
Cl	-2.63806500	4.33506000	2.24322000
Cl	-3.72552500	2.18250700	-0.21365400
Mg	-4.94004400	3.94935300	-1.50993100
Cl	-5.90649000	4.69221100	0.67901700
Cl	-6.99395100	2.53965700	-1.77785700
Cl	-9.17491500	5.04936100	-0.88518600
Mg	-4.69187100	2.92536900	1.97528800
Cl	-6.74577800	1.51567200	1.70736100
Mg	-7.96029700	3.28251900	0.41108400
Cl	-8.92674200	4.02537600	2.60003200
Cl	-10.01420300	1.87282300	0.14315800
Mg	-11.22872200	3.63966900	-1.15311900
Cl	-12.19516700	4.38252600	1.03582900
Cl	-13.28262800	2.22997300	-1.42104500
Mg	-10.98054900	2.61568500	2.33210000
Cl	-13.03445500	1.20598800	2.06417300
Mg	-14.24897400	2.97283500	0.76789700
Cl	-16.30288000	1.56313800	0.49997000
S	7.05743900	-1.99994900	5.22650400
C	6.04529200	-0.45781700	4.90116700
O	6.38238500	0.35984700	4.10937100
C	8.11544300	-2.02654300	3.71849000
O	7.99156600	-1.16967500	2.90793800
C	9.03444000	-3.23418700	3.56502300
C	4.75592100	-0.33305800	5.66432500
C	8.76296100	-4.53265400	4.01273300
C	9.67202400	-5.57082400	3.79519600
C	10.87952300	-5.33027900	3.14505100
C	11.16985600	-4.04084200	2.69404400
C	10.25130500	-3.01924000	2.90227300
C	4.24563400	-1.30461500	6.53002400
C	3.00930700	-1.10944000	7.14673100
C	2.26782600	0.04314700	6.88590400
C	2.75522200	0.99818700	5.98665700
C	3.99193300	0.81067900	5.37308600
H	7.83398400	-4.73965600	4.51615300
H	9.43961600	-6.56475100	4.14715900
H	11.58847700	-6.12984000	2.99126500
H	12.11725400	-3.84795900	2.21021400

H	10.47104200	-1.99817600	2.61557400
H	4.80145900	-2.20936300	6.72388900
H	2.62393600	-1.85716700	7.82105100
H	1.31064800	0.18932500	7.36397300
H	2.18122100	1.88636500	5.76678100
H	4.35176700	1.50136700	4.62381200

Diisobutyl phthalate (Mono mode)

Cl	-13.50777000	-2.41431800	0.56153100
Cl	-10.22318400	-3.98546800	0.57739000
Mg	-11.35103000	-2.13706500	-0.68301600
Cl	-10.51275200	-0.36875300	0.88146300
Cl	-9.19428300	-1.85970600	-1.92765600
Mg	-8.06653900	-3.70811000	-0.66715100
Cl	-7.22816100	-1.93980400	0.89733000
Cl	-5.90969700	-3.43085600	-1.91179600
Cl	-3.94367500	-3.51094900	0.91318700
Mg	-8.41888300	-0.05021800	0.09814200
Cl	-6.50472100	0.17250000	-1.50313700
Mg	-5.07152100	-1.66254600	-0.34721900
Cl	-4.23324300	0.10576600	1.21725900
Cl	-2.91467400	-1.38519200	-1.59185700
Mg	-1.78693000	-3.23359700	-0.33135300
Cl	-0.94865100	-1.46528500	1.23312600
Cl	0.36980900	-2.95634400	-1.57590000
Cl	2.33594000	-3.03633500	1.24899300
Mg	-2.10612800	0.22468400	-0.59796600
Cl	-1.23821900	2.15143000	1.53719800
Cl	0.08024400	0.66037800	-1.27192700
Mg	1.20808800	-1.18803200	-0.01142100
Cl	2.04636700	0.58028000	1.55305800
Cl	3.36483300	-0.91068000	-1.25596100
Mg	4.49257900	-2.75907700	0.00444400
Cl	5.33085800	-0.99076500	1.56892300
Cl	6.64942400	-2.48173000	-1.24009400
Cl	8.61544900	-2.56181600	1.58478900
Ti	0.91852200	2.42869000	0.29255200
Cl	3.07526700	2.70604200	-0.95198800
Mg	4.20301100	0.85763700	0.30851600
Cl	6.35985800	1.13499100	-0.93612100
Mg	7.48760200	-0.71341300	0.32438300
Cl	8.32588100	1.05489900	1.88886200
Cl	9.64434200	-0.43616100	-0.92016400
Mg	10.77218800	-2.28456300	0.34024200
Cl	11.61046700	-0.51625100	1.90472100
Cl	12.92893300	-2.00721100	-0.90429700
Mg	10.48262000	1.33215100	0.64431500
Cl	12.63936500	1.60950400	-0.60022500
Mg	13.76711200	-0.23889400	0.66018000
Cl	15.92395100	0.03835300	-0.58436600
Cl	-0.39906300	4.24990900	0.39078300
Cl	2.04863800	4.36146100	0.51525500
C	-4.32468900	2.53613900	-1.51783400
O	-3.40775800	1.88048700	-1.01260500
C	-6.53642700	2.34980800	1.12615800
O	-7.49198900	1.57004600	0.97317300
C	-5.04869300	4.84525000	-1.46920900
C	-5.21026800	3.58353200	-0.85668900

C	-6.17908800	3.47649600	0.17660200
C	-6.97226300	4.60164500	0.47894100
C	-6.80181200	5.83160700	-0.15481400
C	-5.80599000	5.96128800	-1.12086400
H	-7.43908800	6.67635700	0.11349400
H	-4.29927900	4.94777000	-2.25267800
H	-7.73713900	4.50418100	1.25268900
H	-5.62418000	6.91567300	-1.61835600
O	-5.88099900	2.48576000	2.26218700
C	-6.17508900	1.53673700	3.35406500
H	-5.24983300	1.55602200	3.94268600
H	-6.29705300	0.54322900	2.91205300
C	-7.37687700	1.95358200	4.19294000
C	-7.11859400	3.25899600	4.95139600
C	-7.70671600	0.79123100	5.14176800
H	-8.23321600	2.09474400	3.51146600
H	-6.83060600	4.07624000	4.27439700
H	-6.30758900	3.13345300	5.68589700
H	-8.01765700	3.57155500	5.50074800
H	-6.83294100	0.52377900	5.75799100
H	-8.01461000	-0.10714400	4.58727500
H	-8.52570400	1.06607800	5.82103100
O	-4.57707300	2.55575600	-2.83169400
C	-3.73636100	1.74870200	-3.71705700
C	-2.40551400	2.42364000	-4.05021900
H	-4.35839500	1.63145600	-4.61338900
H	-3.59739800	0.75895000	-3.26512800
C	-1.58263900	1.48909000	-4.94617800
H	-1.85666500	2.57472900	-3.10581000
C	-2.59934700	3.78821500	-4.72222700
H	-2.05948900	1.38274800	-5.93323400
H	-1.47077200	0.48592900	-4.50928100
H	-0.57590300	1.90251400	-5.09748200
H	-1.62691200	4.26523200	-4.91327100
H	-3.19339500	4.47700700	-4.10562800
H	-3.11696700	3.67459700	-5.68838700

Diisobutyl phthalate (Chelate mode)

Cl	12.77985700	-2.95287700	-1.02911700
Cl	9.43434900	-4.38975900	-1.01460100
Mg	10.66841700	-2.63676000	0.28205900
Cl	9.86397200	-0.77861800	-1.19354500
Cl	8.55697600	-2.32054100	1.59333100
Mg	7.32300700	-4.07354200	0.29657100
Cl	6.51846200	-2.21540100	-1.17903300
Cl	5.21146800	-3.75742300	1.60784700
Cl	3.17305400	-3.65228200	-1.16451700
Mg	7.75263100	-0.46239700	0.11772600
Cl	5.64109100	-0.14628300	1.42890300
Mg	4.40712200	-1.89928300	0.13214300
Cl	3.60267700	-0.04114100	-1.34346200
Cl	2.29558100	-1.58306500	1.44341500
Mg	1.06161200	-3.33606600	0.14665500
Cl	0.25716700	-1.47792400	-1.32894900
Cl	-1.04982800	-3.01995000	1.45783100
Cl	-3.08834300	-2.91470700	-1.31443600
Mg	1.43203100	0.19064000	-0.10437700
Cl	0.68679000	2.13321700	-1.50789400

Cl	-0.62020400	0.59119400	1.27898600
Mg	-1.85427300	-1.16180800	-0.01777300
Cl	-2.65871800	0.69633400	-1.49337800
Cl	-3.96571500	-0.84559200	1.29339900
Mg	-5.19968300	-2.59858900	-0.00326100
Cl	-6.00412800	-0.74044700	-1.47886500
Cl	-7.31122400	-2.28237400	1.30791200
Cl	-9.34963800	-2.17723000	-1.46435300
Ti	-1.42464900	2.44933600	-0.19661800
Cl	-3.53609100	2.76555300	1.11455400
Mg	-4.77006000	1.01255200	-0.18220600
Cl	-6.88160100	1.32877000	1.12906700
Mg	-8.11557000	-0.42423100	-0.16769300
Cl	-8.92001500	1.43391100	-1.64329800
Cl	-10.22701000	-0.10811500	1.14348300
Mg	-11.46107800	-1.86111300	-0.15317700
Cl	-12.26552300	-0.00297100	-1.62878100
Cl	-13.57252000	-1.54489700	1.15799500
Mg	-11.03145500	1.75002700	-0.33212200
Cl	-13.14289600	2.06624300	0.97905100
Mg	-14.37686500	0.31324600	-0.31761000
Cl	-16.48840500	0.62936100	0.99356700
Cl	-0.03650800	4.21884000	-0.26327300
Cl	-2.47995300	4.43275900	-0.31798700
C	9.01130800	3.29044000	0.79484500
C	9.79530200	4.28984300	1.39744500
C	10.31436500	5.35384100	0.65998900
C	10.05079600	5.43831500	-0.70738700
C	9.26247300	4.46502200	-1.31988500
C	8.73573900	3.37884900	-0.59812300
C	7.88247600	2.39503800	-1.33290000
O	7.68998100	2.68969800	-2.61704400
C	6.88771200	1.68909100	-3.36099700
C	6.88666700	2.05451700	-4.83551100
C	8.62341400	2.16841200	1.71588200
O	8.71630900	0.96273300	1.47948100
O	8.27031600	2.63499100	2.91648900
C	7.98151700	1.61900400	3.94437600
C	7.59148900	2.33221400	5.23339000
H	10.01085500	4.21413100	2.46286800
H	10.92897700	6.10558200	1.15565400
H	10.46026200	6.25585800	-1.30156600
H	9.05588600	4.52860200	-2.38683000
H	5.87993100	1.67649900	-2.92066200
H	7.35587200	0.71066300	-3.19200800
H	8.88946700	1.00825700	4.07503300
H	7.17568500	0.98034000	3.55919200
C	8.71429300	3.22504000	5.77306100
C	7.18526200	1.28069900	6.27542600
C	8.28863100	1.92895400	-5.44341600
C	6.23276200	3.41439600	-5.10858000
H	6.25012300	1.27722400	-5.29444700
H	6.71148700	2.96030400	5.01192700
H	9.60691400	2.62444000	6.01420900
H	8.39283900	3.72740600	6.69618000
H	9.00682200	4.00174900	5.05252600
H	6.87180100	1.77275700	7.20667100
H	8.03264100	0.61993400	6.51751200

H	6.35207000	0.65376700	5.92799400
H	8.70286600	0.92526000	-5.27066500
H	8.98576400	2.65779900	-5.00420300
H	8.26274200	2.09929800	-6.52822800
H	6.80534100	4.23625500	-4.65368200
H	5.20804400	3.45202900	-4.70734200
H	6.17954400	3.60187400	-6.19005100
O	7.36438900	1.39663600	-0.82629000

Diisobutyl phthalate (Bridge mode)

Cl	13.51166100	-2.40840400	-0.57276900
Cl	10.22740700	-3.97996900	-0.60630200
Mg	11.35397200	-2.14371300	0.67286600
Cl	10.51645900	-0.36040600	-0.87491300
Cl	9.19627500	-1.87891700	1.91859500
Mg	8.06981200	-3.71517300	0.63932900
Cl	7.23219900	-1.93187200	-0.90845200
Cl	5.91202000	-3.45048100	1.88506200
Cl	3.94804400	-3.50343100	-0.94198300
Mg	8.42196400	-0.04992900	-0.09003500
Cl	6.50660600	0.15680200	1.51195900
Mg	5.07461000	-1.66717500	0.33718500
Cl	4.23709600	0.11613100	-1.21059400
Cl	2.91681300	-1.40238400	1.58291100
Mg	1.79035000	-3.23864100	0.30364500
Cl	0.95283700	-1.45533400	-1.24413400
Cl	-0.36734000	-2.97395000	1.54928000
Cl	-2.33142300	-3.02679900	-1.27767400
Mg	2.10865400	0.21694100	0.60417000
Cl	1.24188900	2.16422900	-1.51274500
Cl	-0.07829000	0.64561900	1.28076900
Mg	-1.20485300	-1.19064300	0.00150100
Cl	-2.04236600	0.59266400	-1.54627800
Cl	-3.36254700	-0.92585300	1.24713000
Mg	-4.48901300	-2.76210300	-0.03203600
Cl	-5.32652600	-0.97879600	-1.57981600
Cl	-6.64680700	-2.49731800	1.21359000
Cl	-8.61078600	-2.55026100	-1.61335500
Ti	-0.91580300	2.42892500	-0.26701000
Cl	-3.07349800	2.69371600	0.97861900
Mg	-4.19996100	0.85746000	-0.30064700
Cl	-6.35775800	1.12225100	0.94507900
Mg	-7.48422100	-0.71400600	-0.33418700
Cl	-8.32173400	1.06930100	-1.88196600
Cl	-9.64191000	-0.44931500	0.91144800
Mg	-10.76847500	-2.28557000	-0.36772000
Cl	-11.60598800	-0.50226400	-1.91549900
Cl	-12.92617000	-2.02078000	0.87790900
Mg	-10.47942300	1.33399200	-0.63633100
Cl	-12.63711800	1.59878200	0.60929800
Mg	-13.76358300	-0.23746800	-0.66986900
Cl	-15.92137200	0.02721700	0.57576400
Cl	0.40148300	4.25127400	-0.34654300
Cl	-2.04615000	4.36355300	-0.47168500
C	4.32154400	2.50158100	1.56437000
O	3.39972500	1.83494900	1.08353500
C	6.52829200	2.38908500	-1.10439400
O	7.48878500	1.63535000	-0.87872700

C	4.90872500	4.83686900	1.47227800
C	5.14475700	3.58026600	0.87298200
C	6.07347000	3.52338200	-0.19944100
C	6.72809500	4.71286700	-0.58183800
C	6.48342400	5.93850900	0.03340900
C	5.54491100	6.00437700	1.06124200
H	7.01797600	6.82904300	-0.29978100
H	4.19316700	4.88982600	2.29126000
H	7.45106100	4.66793000	-1.39773500
H	5.31338300	6.95295400	1.54982100
O	5.93447800	2.49207900	-2.27903000
C	6.29017500	1.53661400	-3.34470200
H	5.37397600	1.49642700	-3.94585900
H	6.45104000	0.55755900	-2.88176700
C	7.48795300	1.98407700	-4.17869800
C	7.27290400	3.35968600	-4.81873400
C	7.73991700	0.90524700	-5.24247800
H	8.36885000	2.02595000	-3.51635200
H	7.09856900	4.14091700	-4.06521700
H	6.40203000	3.34406700	-5.49329900
H	8.15234400	3.64890800	-5.41305800
H	6.88125600	0.81873500	-5.92657200
H	7.91592600	-0.08126800	-4.78974200
H	8.62297300	1.16118700	-5.84567000
O	4.60726400	2.52320800	2.87182600
C	3.79054200	1.70137000	3.76887900
C	2.46903900	2.38109900	4.13892600
H	4.43260300	1.57331200	4.65017100
H	3.64065500	0.72031700	3.30207900
C	1.58863900	1.38994500	4.91240000
H	1.95156600	2.64358400	3.20053000
C	2.69568100	3.66455600	4.94623400
H	2.06382200	1.09173500	5.85972600
H	1.38412500	0.47633800	4.33406500
H	0.62134600	1.85041700	5.15781900
H	1.74168900	4.18129100	5.12933900
H	3.36325800	4.36599100	4.42694000
H	3.14650000	3.43377800	5.92366100

Diisobutyl phthalate (Zip mode)

Cl	14.61789800	-2.14131800	-1.63821600
Cl	11.37266400	-2.08978200	-3.28827300
Mg	12.48768900	-3.45358400	-1.50667000
Cl	11.56747800	-2.04158300	0.34729200
Cl	10.35737900	-4.76584700	-1.37511900
Mg	9.24245500	-3.40204800	-3.15672700
Cl	8.32223800	-1.99004800	-1.30286600
Cl	7.11214500	-4.71431100	-3.02517600
Cl	5.07700400	-1.93851200	-2.95292300
Mg	9.43726800	-3.35384800	0.47883800
Cl	7.30695800	-4.66611100	0.61038900
Mg	6.19202800	-3.30231300	-1.17132000
Cl	5.22298000	-1.81357400	0.59811100
Cl	4.06171900	-4.61457700	-1.03976800
Mg	2.94679400	-3.25077700	-2.82137700
Cl	2.02657800	-1.83877700	-0.96751500
Cl	0.81648500	-4.56304000	-2.68982600
Cl	-1.21865600	-1.78724100	-2.61757300

Mg	3.08962900	-3.12776400	0.72985000
Cl	2.22138600	-1.79057900	2.66795000
Cl	0.95719000	-4.44137600	0.86153400
Mg	-0.10363200	-3.15104300	-0.83596900
Cl	-1.02384300	-1.73904200	1.01799200
Cl	-2.23394100	-4.46330600	-0.70441800
Mg	-3.34886600	-3.09950700	-2.48602700
Cl	-4.26908200	-1.68750700	-0.63216500
Cl	-5.47917600	-4.41177000	-2.35447600
Cl	-7.51431700	-1.63597100	-2.28222300
Ti	0.09117600	-3.10284500	2.79949600
Cl	-2.03913300	-4.41510800	2.93104700
Mg	-3.15405300	-3.05130700	1.14953800
Cl	-5.28436200	-4.36357000	1.28108900
Mg	-6.39929200	-2.99977200	-0.50061900
Cl	-7.31950300	-1.58777100	1.35334200
Cl	-8.52960200	-4.31203600	-0.36906800
Mg	-9.64452600	-2.94823600	-2.15067700
Cl	-10.56474300	-1.53623600	-0.29681500
Cl	-11.77483600	-4.26049900	-2.01912600
Mg	-9.44971300	-2.90003700	1.48488800
Cl	-11.58002200	-4.21230000	1.61644000
Mg	-12.69495200	-2.84850200	-0.16526900
Cl	-14.82526200	-4.16076500	-0.03371800
Cl	1.36173000	-3.10545700	4.65657400
Cl	-1.09032700	-3.04760700	4.71358900
Cl	13.71392600	4.13200300	-1.80014000
Cl	10.46869100	4.18353900	-3.45019700
Mg	11.58371600	2.81973700	-1.66859400
Cl	10.66349900	4.23173700	0.18526800
Cl	9.45340600	1.50747400	-1.53704300
Mg	8.33848200	2.87127300	-3.31865100
Cl	7.41826500	4.28327300	-1.46479000
Cl	6.20817200	1.55901000	-3.18710000
Cl	4.17303100	4.33481000	-3.11484700
Mg	8.53329000	2.91947200	0.31681400
Cl	6.40298000	1.60720900	0.44836500
Mg	5.28805600	2.97100800	-1.33324400
Cl	4.31900700	4.45974800	0.43618700
Cl	3.15774600	1.65874500	-1.20169200
Mg	2.04282100	3.02254400	-2.98330100
Cl	1.12260500	4.43454400	-1.12943900
Cl	-0.08748800	1.71028100	-2.85175000
Cl	-2.12262900	4.48608000	-2.77949700
Mg	2.18565600	3.14555700	0.56792600
Cl	0.05321800	1.83194500	0.69961000
Mg	-1.00760500	3.12227800	-0.99789300
Cl	-1.92782100	4.53427800	0.85596800
Cl	-3.13791400	1.81001500	-0.86634200
Mg	-4.25283900	3.17381500	-2.64795100
Cl	-5.17305500	4.58581500	-0.79408900
Cl	-6.38314800	1.86155100	-2.51640000
Cl	-8.41828900	4.63735100	-2.44414700
Mg	-4.05803100	3.22201300	0.98751400
Cl	-6.18834000	1.90975000	1.11906600
Mg	-7.30326500	3.27354900	-0.66254300
Cl	-8.22348100	4.68554900	1.19131900
Cl	-9.43357500	1.96128600	-0.53099200

Mg	-10.54849900	3.32508500	-2.31260100
Cl	-11.46871600	4.73708500	-0.45873900
Cl	-12.67880900	2.01282200	-2.18104900
Mg	-10.35369100	3.37328300	1.32286500
Cl	-12.48400100	2.06102000	1.45441600
Mg	-13.59892500	3.42482000	-0.32719300
Cl	-15.72923500	2.11255600	-0.19564200
C	3.53714700	2.43075800	6.07104400
C	2.50970400	2.90507100	6.89529000
C	1.78363000	2.02563200	7.70310800
C	2.08698600	0.66154800	7.69482200
C	3.09895000	0.17414300	6.86046100
C	3.81820900	1.04523700	6.03188800
C	4.76569400	0.50736100	5.00084600
O	5.52940200	-0.51041600	5.48078700
C	6.47027700	-1.10582000	4.52838100
C	6.56305800	-2.61999800	4.72475900
C	4.43068300	3.41395800	5.38147300
O	5.64683100	3.32924900	5.37411400
O	3.72020000	4.43978500	4.83838100
C	4.50991500	5.43652100	4.11553500
C	3.87534000	6.81838900	4.24639400
H	2.29860900	3.97450100	6.91055100
H	0.99953500	2.41772200	8.35255700
H	1.52426500	-0.02586100	8.32719100
H	3.32223100	-0.89245200	6.83950200
H	7.44070500	-0.62016300	4.71691700
H	6.13113700	-0.86217000	3.51275700
H	4.53900000	5.11066800	3.06339300
H	5.53057200	5.41972900	4.51836100
C	2.36785500	6.81168800	3.97452600
C	4.61378100	7.77803200	3.29793900
C	5.18232500	-3.27973600	4.64284300
C	7.33261600	-3.04096600	5.98557400
H	7.14058300	-2.96438500	3.84658300
H	4.04124900	7.17025600	5.28043100
H	1.96955500	7.83738000	3.99849500
H	2.14773000	6.39083700	2.98056300
H	1.82559600	6.21165400	4.71841200
H	4.45551100	7.49284600	2.24558300
H	5.69858700	7.77534600	3.48642000
H	4.25142400	8.81004400	3.42215400
H	5.27231200	-4.37481200	4.60336400
H	4.64230800	-2.94755400	3.74647600
H	4.56476300	-3.01984400	5.51457000
H	8.31765900	-2.54996600	6.04175600
H	7.49658400	-4.12992900	5.98952200
H	6.78268100	-2.77718400	6.90280000
O	4.79386000	0.92152500	3.85341200

Dibenzoyl sulfide (Reactant 1,2-sj)

C	7.33025800	2.23210600	-0.70358900
C	8.70869400	1.50828600	1.76407400
O	8.35461700	0.34965500	1.55006500
O	7.08451300	1.03723200	-0.84688400
Cl	-12.39808600	-2.59087100	1.32462500
Mg	-10.40854200	-2.43826400	0.11525200
Cl	-6.35334300	-2.75201300	1.31292500

Mg	-4.56890900	-2.84920400	-0.06220200
Cl	-8.60045800	-2.53777700	-1.22853800
Cl	-2.79209400	-2.94558600	-1.44739700
Cl	-0.69281100	-3.15098400	1.16429700
Mg	1.08395200	-3.24726000	-0.22086400
Cl	5.42252200	-3.98756600	0.69938500
Mg	7.19932200	-4.08394800	-0.68580000
Cl	2.89455600	-3.34694800	-1.56126500
Cl	8.96177300	-4.17904700	-2.08127200
Cl	-15.12498200	0.13410400	0.05152400
Mg	-12.97515000	-0.23929500	0.46582100
Cl	-11.39091900	-0.56178200	-1.16140100
Mg	-7.32871000	-0.74131300	0.10061600
Cl	-9.28701000	-0.75524400	1.65445100
Cl	-5.36050700	-0.75930700	-1.33125300
Mg	-1.59439900	-1.16040000	-0.09469100
Cl	-3.41025000	-1.13066000	1.52230600
Cl	0.22450700	-1.32258800	-1.71100600
Mg	4.28594200	-1.55812300	-0.14501400
Mg	10.30373900	-2.62605600	-0.72487900
Cl	2.24026900	-1.43875400	1.19802400
Cl	6.46269700	-2.17095900	-1.88849900
Cl	8.46574000	-2.85945400	1.05763600
Cl	12.42103700	-3.11347200	-0.24118500
Cl	-11.90437200	1.78885400	1.37076800
Mg	-10.03347300	1.08871800	0.21920000
Cl	-6.37388800	0.96765200	1.60422800
Cl	-8.24565000	1.24713700	-1.20773700
Mg	-4.34811500	0.89049500	0.41745700
Cl	-0.34588900	0.66816200	1.24977200
Cl	-2.49282100	0.95831700	-1.27585900
Mg	1.47190800	0.42036900	-0.46085300
Cl	5.58534000	-0.58724900	1.10051200
Cl	3.58374400	0.38157900	-1.47878100
Mg	7.55571100	-0.96512200	-0.02341300
Cl	9.61853500	-0.43242300	-1.04922900
Ti	-1.30934600	2.93001200	-0.03744800
Cl	-3.26899700	2.83296400	1.39876800
Cl	0.75694900	2.59471400	-1.29859800
C	-1.81139000	4.25815800	-1.52089800
C	-0.70316900	5.04613900	1.34112300
H	-2.67593400	4.63427700	-0.91678600
H	-2.23624800	3.60925000	-2.31266400
C	-0.98748500	5.40834200	-2.13660400
C	0.02700100	3.93907400	1.69965000
H	-0.34395500	5.63912600	0.48892200
H	-0.23404400	3.35768300	2.59202300
H	0.99145100	3.72657700	1.22918700
C	-1.83144700	5.64486300	2.12530900
H	-2.69976900	5.88788800	1.49109900
H	-2.16213000	4.99348300	2.94693100
H	-1.47998700	6.59972700	2.55947400
C	-0.61299300	5.09154200	-3.59385100
C	-1.73327100	6.75235400	-2.03783400
H	-0.03323300	5.51392400	-1.57859900
H	0.03115300	5.88117800	-4.01588200
H	-0.07371900	4.13420000	-3.66761100
H	-1.51955400	5.02335200	-4.22050400

H	-1.12954300	7.57287400	-2.46170300
H	-2.68559700	6.71137200	-2.59417300
H	-1.96899300	7.01356600	-0.99129600
S	8.42771000	2.89579800	0.60927400
C	6.79385600	3.26553900	-1.62069200
C	9.45777300	1.88576900	2.98636700
C	9.66196700	3.22269600	3.39258100
C	10.38904300	3.49480400	4.55520100
C	10.91707600	2.44149800	5.31837500
C	10.71274800	1.10986300	4.92175900
C	9.98388100	0.82832100	3.76449200
C	6.11244000	2.80566300	-2.77178300
C	5.58301200	3.72324100	-3.68178400
C	5.72566000	5.10179600	-3.45559500
C	6.39697600	5.56413800	-2.31233600
C	6.92874800	4.65319500	-1.39492300
H	9.23868700	4.04800100	2.81353600
H	10.54068000	4.53085700	4.86998400
H	11.48843000	2.65939800	6.22553000
H	11.12683800	0.28965400	5.51441500
H	9.81921300	-0.20119200	3.43733400
H	6.00790300	1.73002500	-2.92951200
H	5.05778000	3.36213500	-4.57012500
H	5.31175100	5.81861700	-4.17111300
H	6.50271900	6.63772200	-2.13374700
H	7.43471100	5.02314100	-0.49897900

Dibenzoyl sulfide (TS 1,2-si)

C	7.33913500	2.21055500	-0.74544900
C	8.70448300	1.51506700	1.73772200
O	8.35131800	0.35414300	1.53540300
O	7.08442500	1.01537400	-0.86911700
Cl	-12.40101500	-2.58460300	1.33991300
Mg	-10.41131200	-2.44563200	0.12915700
Cl	-6.35631100	-2.74735300	1.33058300
Mg	-4.57175100	-2.85991600	-0.04323300
Cl	-8.60311900	-2.56018200	-1.21328700
Cl	-2.79483600	-2.97177700	-1.42710700
Cl	-0.69586100	-3.14931100	1.18687600
Mg	1.08105300	-3.26107200	-0.19700000
Cl	5.41930900	-3.99240200	0.73170600
Mg	7.19622300	-4.10426300	-0.65216800
Cl	2.89172700	-3.37575500	-1.53602800
Cl	8.95879000	-4.21495000	-2.04634400
Cl	-15.12710900	0.12705500	0.03700800
Mg	-12.97741100	-0.24235200	0.45555600
Cl	-11.39309700	-0.58288600	-1.16790400
Mg	-7.33105700	-0.74970300	0.09640600
Cl	-9.28951700	-0.74626900	1.65009900
Cl	-5.36266500	-0.78374800	-1.33499800
Mg	-1.59696700	-1.17227300	-0.09364600
Cl	-3.41284200	-1.12455600	1.52262100
Cl	0.22219700	-1.35246700	-1.70806900
Mg	4.28343000	-1.57197000	-0.13913100
Mg	10.30100500	-2.64764700	-0.70676300
Cl	2.23786200	-1.43750900	1.20223500
Cl	6.46019200	-2.20427000	-1.87565100
Cl	8.46277100	-2.86121600	1.07799400

Cl	12.41813400	-3.13030300	-0.21758600
Cl	-11.90622000	1.79524300	1.33852900
Mg	-10.03538000	1.08217800	0.19482600
Cl	-6.37596100	0.97524800	1.58146800
Cl	-8.24737600	1.22464700	-1.23356500
Mg	-4.35023300	0.88484000	0.39587400
Cl	-0.34771000	0.67047700	1.23097800
Cl	-2.49428500	0.93367600	-1.29820000
Mg	1.46920400	0.40339500	-0.47661200
Cl	5.58292900	-0.58796900	1.09589100
Cl	3.58183900	0.35334300	-1.49396500
Mg	7.55331900	-0.97851400	-0.02366200
Cl	9.61637700	-0.45749800	-1.05499300
Ti	-1.24244500	2.83663800	0.00577700
Cl	-3.36269500	2.89719800	1.28845800
Cl	0.69711500	2.52985300	-1.42033600
C	-1.71792500	4.70909800	-0.89448500
C	-0.51059000	5.02257200	1.09426000
H	-2.61115200	5.22808600	-0.50676100
H	-2.13342900	3.77837000	-1.41813500
C	-0.97321300	5.54380800	-1.94427900
C	-0.13404500	3.79946000	1.66860800
H	0.21136700	5.49486400	0.41860200
H	-0.63680200	3.44361000	2.57540600
H	0.87042200	3.40797400	1.47520300
C	-1.50689000	5.92967200	1.76967600
H	-1.94126400	6.67900700	1.09368000
H	-2.31856600	5.35767100	2.24383700
H	-0.96980100	6.47419100	2.56785400
C	-1.58116000	5.28475300	-3.34070000
C	-0.99844200	7.04942200	-1.62958600
H	0.08077600	5.20779200	-1.98142700
H	-1.05422900	5.87823900	-4.10649100
H	-1.49997200	4.22177600	-3.62202100
H	-2.64726200	5.56985200	-3.36809300
H	-0.47617400	7.61305400	-2.41987600
H	-2.03639600	7.42388500	-1.58389600
H	-0.50797100	7.29635500	-0.67433900
S	8.43132400	2.88872200	0.56405400
C	6.81606600	3.23161200	-1.68431400
C	9.44557800	1.90721100	2.96020100
C	9.65076400	3.24898400	3.34964600
C	10.36963400	3.53486100	4.51405500
C	10.88833300	2.49058500	5.29580600
C	10.68301100	1.15424100	4.91588200
C	9.96245900	0.85900600	3.75682900
C	6.12143000	2.75636200	-2.82111600
C	5.60464400	3.66096200	-3.75121400
C	5.77401400	5.04174300	-3.55990600
C	6.45904700	5.51949900	-2.43119100
C	6.97760400	4.62164600	-1.49351200
H	9.23466800	4.06760700	2.75609900
H	10.52209700	4.57468500	4.81572300
H	11.45316600	2.71923600	6.20439200
H	11.08978900	0.34101700	5.52304100
H	9.79717100	-0.17443100	3.44260000
H	5.99646400	1.67932400	-2.95205800
H	5.06888800	3.28775800	-4.62821100

H	5.37088000	5.74833700	-4.29159600
H	6.58659300	6.59495700	-2.28015300
H	7.49572300	5.00439200	-0.60996400

Dibenzoyl sulfide (Reactant 1,2-re)

Cl	-12.10095700	-2.16998300	1.82406500
Mg	-10.38233400	-2.33874500	0.37403700
Cl	-6.32643900	-2.72811300	1.44626700
Mg	-4.60355100	-2.92582500	0.00497500
Cl	-8.63863900	-2.50955100	-1.04568500
Cl	-2.88857400	-3.12295400	-1.44589300
Cl	-0.69061700	-3.30151700	1.08519200
Mg	1.02432200	-3.49854100	-0.36564600
Cl	5.51306000	-3.76705400	0.94312300
Mg	7.22787400	-3.96418100	-0.50769700
Cl	2.77467800	-3.69852500	-1.77323300
Cl	8.92809200	-4.15995600	-1.96846400
Cl	-15.04799900	0.32420500	0.45014900
Mg	-12.88908800	-0.08070900	0.77857900
Cl	-11.38593600	-0.47747000	-0.90821500
Mg	-7.29323400	-0.73101400	0.20313500
Cl	-9.18436600	-0.63158700	1.83361800
Cl	-5.38948000	-0.85902200	-1.30496500
Mg	-1.58513700	-1.32915200	-0.20792500
Cl	-3.33200500	-1.18527900	1.47762900
Cl	0.16023900	-1.60258500	-1.88929400
Mg	4.27696600	-1.90208000	-0.47401300
Mg	10.37024800	-2.60678500	-0.72028900
Cl	2.28834700	-1.67237000	0.93689900
Cl	6.48520900	-1.92483700	-1.75902800
Cl	8.60091100	-2.72335800	1.14204000
Cl	12.49031700	-3.14403100	-0.30499400
Cl	-11.73832400	1.97695300	1.56399400
Mg	-9.93714100	1.18176000	0.36320600
Cl	-6.23045100	1.00646100	1.59953800
Cl	-8.20846300	1.23624800	-1.14232100
Mg	-4.25570300	0.82333800	0.33864900
Cl	-0.22858600	0.51527000	1.00947800
Cl	-2.47821200	0.76698400	-1.43456400
Mg	1.50754700	0.14843900	-0.76097200
Cl	5.79500800	-0.15624400	1.20867300
Cl	3.58208500	0.01441800	-1.84609100
Mg	7.68847800	-0.69592900	0.01995500
Cl	9.72638800	-0.33615300	-1.07432600
Ti	-1.21361300	2.75204900	-0.39424000
Cl	-3.06649900	2.79487000	1.16862100
Cl	0.86291000	2.33277800	-1.64077400
C	-1.78062100	3.89541400	-2.02858500
C	-0.53960700	4.98126300	0.87688100
H	-1.08809100	4.74812000	-2.17310100
H	-1.55791200	3.18342000	-2.85026800
C	-3.25917600	4.34121900	-2.11431800
C	0.16021800	3.85525500	1.22978600
C	0.00626200	6.07519800	0.01066300
H	-0.20853300	3.19895300	2.02800000
H	1.18875700	3.69695500	0.89071500
H	-1.51061600	5.16573300	1.35463700
C	-3.55955000	5.57832600	-1.25608200

C	-3.64855100	4.59558300	-3.58542900
H	-3.90101200	3.51300400	-1.75008800
H	-4.62267800	5.86065300	-1.33243000
H	-3.33811100	5.40296300	-0.19131800
H	-2.96422900	6.44382000	-1.59871300
H	-4.70767800	4.89557700	-3.66549500
H	-3.03218000	5.40375500	-4.01618600
H	-3.50217500	3.69341800	-4.20111600
H	0.34194300	6.90249200	0.66433400
H	0.87193000	5.74089500	-0.58205900
H	-0.75832900	6.49486200	-0.66027000
C	8.82191400	1.74299600	1.87513200
C	7.35153900	2.51236300	-0.53741500
O	7.32255800	1.32535400	-0.84713600
O	8.67998800	0.57368800	1.52792400
S	8.02593700	3.16269800	1.03589700
C	9.62403100	2.11804000	3.06544300
C	6.76591600	3.56899000	-1.39993300
C	10.02719200	1.06658900	3.92075800
C	10.78569600	1.34530300	5.05944800
C	11.15323000	2.66842100	5.35415200
C	10.76238900	3.71523000	4.50478300
C	10.00108700	3.44545900	3.36334900
C	7.11887000	4.93230300	-1.30337900
C	6.52231700	5.86813600	-2.15478300
C	5.56883000	5.45464700	-3.09854400
C	5.21631000	4.09882000	-3.19866400
C	5.81525800	3.15453200	-2.36070600
H	9.73109500	0.04396500	3.67438200
H	11.09303700	0.52944900	5.71942600
H	11.74997100	2.88385100	6.24546800
H	11.05887800	4.74370400	4.72827300
H	9.71944900	4.26335300	2.69458600
H	7.87763200	5.25601100	-0.58556900
H	6.80884600	6.92140200	-2.08824500
H	5.10445000	6.19048600	-3.76204500
H	4.47287500	3.77489100	-3.93247500
H	5.54570600	2.09710300	-2.41955200

Dibenzoyl sulfide (TS 1,2-re)

Cl	-12.13773900	-2.14453600	1.80181700
Mg	-10.41566000	-2.34346400	0.35973600
Cl	-6.36309200	-2.71791400	1.44971000
Mg	-4.63677700	-2.94562700	0.01690500
Cl	-8.66859000	-2.54389000	-1.05194100
Cl	-2.91841800	-3.17292600	-1.42545900
Cl	-0.72720200	-3.30604800	1.11425400
Mg	0.99115500	-3.53324400	-0.32810500
Cl	5.47613200	-3.78293600	0.99717000
Mg	7.19436300	-4.01023400	-0.44516900
Cl	2.74481000	-3.76261800	-1.72707100
Cl	8.89802600	-4.23635000	-1.89751800
Cl	-15.07762800	0.32700800	0.37275900
Mg	-12.92015500	-0.07457200	0.71446500
Cl	-11.41327200	-0.50569000	-0.96052700
Mg	-7.32378600	-0.74366900	0.16607000
Cl	-9.21894900	-0.61033800	1.78943800
Cl	-5.41616300	-0.90330300	-1.33443300

Mg	-1.61566300	-1.35753000	-0.21862800
Cl	-3.36649700	-1.17897800	1.45922100
Cl	0.13371800	-1.66560700	-1.89004000
Mg	4.24637900	-1.94372400	-0.45862500
Mg	10.33924100	-2.66157600	-0.67560100
Cl	2.25448600	-1.68423700	0.94247900
Cl	6.45786800	-1.99419800	-1.73725400
Cl	8.56497900	-2.73995900	1.18403900
Cl	12.45745700	-3.19374400	-0.24461100
Cl	-11.76841300	1.99614300	1.46329100
Mg	-9.96532200	1.17555900	0.28261700
Cl	-6.26205500	1.01875300	1.53167900
Cl	-8.23272200	1.19876200	-1.21920300
Mg	-4.28493100	0.80902000	0.27977900
Cl	-0.25908300	0.50786100	0.96674900
Cl	-2.50227900	0.71591900	-1.48780600
Mg	1.48058900	0.10475100	-0.79203300
Cl	5.76265100	-0.16810000	1.19422900
Cl	3.55780500	-0.05288400	-1.86894300
Mg	7.65836700	-0.73312400	0.02096700
Cl	9.69959100	-0.39724100	-1.07473300
Ti	-1.13372900	2.62955000	-0.34842600
Cl	-3.18894500	2.82086900	1.04238500
Cl	0.73227000	2.19176900	-1.83409300
C	-1.57335000	4.45868800	-1.34971300
C	-0.22163000	4.83369600	0.52338400
H	-0.80925800	4.79377000	-2.07272800
H	-2.01658400	3.50754400	-1.81051100
C	-2.71864700	5.46966700	-1.21249900
C	0.03878300	3.65080200	1.23162200
C	0.88637300	5.55313900	-0.20414800
H	-0.57007300	3.38715000	2.10346100
H	1.04256400	3.21325300	1.18343200
H	-1.07621600	5.43507900	0.85273300
C	-2.23710800	6.93002900	-1.24918700
C	-3.75396500	5.23219600	-2.33487300
H	-3.23399200	5.28612000	-0.25077000
H	-3.09825300	7.61525000	-1.18864700
H	-1.56293500	7.18181300	-0.41527500
H	-1.70577400	7.14562500	-2.19332300
H	-4.58957900	5.94584300	-2.24340300
H	-3.29927400	5.36870300	-3.33145200
H	-4.17482900	4.21381800	-2.28804200
H	1.46031800	6.12562200	0.54728400
H	1.57863400	4.84396200	-0.68391200
H	0.52363700	6.26673600	-0.95663900
C	8.78110500	1.74041000	1.83589200
C	7.32236500	2.46450100	-0.59745600
O	7.29742100	1.27212300	-0.88631300
O	8.64573600	0.56522300	1.50668200
S	7.98345200	3.14323600	0.96916600
C	9.57534000	2.13800300	3.02393600
C	6.74259100	3.50425000	-1.48464000
C	9.97821300	1.10185500	3.89792100
C	10.72904400	1.40172400	5.03629200
C	11.08914100	2.73092600	5.31219900
C	10.69862500	3.76256300	4.44430100
C	9.94499700	3.47161500	3.30296500

C	7.08378800	4.87151800	-1.40318400
C	6.49421100	5.79004000	-2.27803800
C	5.55983500	5.35522200	-3.23127800
C	5.21922800	3.99528600	-3.31678200
C	5.81088200	3.06838500	-2.45451900
H	9.68786600	0.07418900	3.66612900
H	11.03610900	0.59771100	5.71075500
H	11.67984700	2.96298500	6.20335500
H	10.98941700	4.79569400	4.65330700
H	9.66366400	4.27763400	2.61980700
H	7.82831600	5.21194100	-0.67824700
H	6.77190500	6.84632000	-2.22271400
H	5.10182100	6.07738200	-3.91397600
H	4.49186200	3.65439800	-4.05902500
H	5.55113400	2.00797000	-2.50249900

Dibenzoyl sulfide (Reactant 2,1-sj)

C	7.30541000	2.23661400	-0.67878600
C	8.69262900	1.47055400	1.77115100
O	8.32341400	0.31852400	1.54702700
O	7.05042000	1.04554100	-0.83724800
Cl	-12.44111600	-2.54340600	1.30930800
Mg	-10.45274200	-2.38017600	0.09945500
Cl	-6.39703200	-2.72646000	1.28637500
Mg	-4.61496200	-2.80976600	-0.09264900
Cl	-8.64693200	-2.46646500	-1.24837100
Cl	-2.84040400	-2.89218900	-1.48174300
Cl	-0.73826600	-3.14378100	1.12355900
Mg	1.03629200	-3.22610400	-0.26553200
Cl	5.37332000	-3.99571500	0.63732400
Mg	7.14777700	-4.07813700	-0.75176900
Cl	2.84450700	-3.31259000	-1.60986500
Cl	8.90792500	-4.15904900	-2.15100700
Cl	-15.15980000	0.21005700	0.08061300
Mg	-13.01076600	-0.17735800	0.48623900
Cl	-11.43004800	-0.48150700	-1.14793400
Mg	-7.36678000	-0.69447300	0.10531400
Cl	-9.32286000	-0.72425000	1.66165500
Cl	-5.40062600	-0.69845300	-1.32956700
Mg	-1.63445400	-1.13155000	-0.10443200
Cl	-3.44768900	-1.11913100	1.51530100
Cl	0.18172700	-1.27648200	-1.72586700
Mg	4.24446300	-1.54993800	-0.16936800
Mg	10.25748300	-2.63107700	-0.77387300
Cl	2.20142100	-1.44291800	1.17813900
Cl	6.41650800	-2.14490300	-1.92501100
Cl	8.42120000	-2.88411600	1.00774200
Cl	12.37363200	-3.13335500	-0.30052100
Cl	-11.93126400	1.83328300	1.41940000
Mg	-10.06461800	1.14348500	0.25487300
Cl	-6.40356200	0.98853000	1.63264300
Cl	-8.27825200	1.31638000	-1.17220500
Mg	-4.37983900	0.92167100	0.44194600
Cl	-0.37687100	0.67242700	1.26501100
Cl	-2.52628800	1.00767900	-1.25324800
Mg	1.43657600	0.44302000	-0.45171700
Cl	5.54916200	-0.60234600	1.08841200
Cl	3.54748400	0.41184000	-1.47337200

Mg	7.51655100	-0.97070900	-0.04391300
Cl	9.57990400	-0.43045600	-1.06474800
Ti	-1.31628900	2.95237400	-0.00884400
Cl	-3.28482400	2.83799100	1.45968500
Cl	0.75604900	2.65180900	-1.22235500
C	-1.82707400	4.25027600	-1.51028900
C	-0.78047800	4.89038000	1.32307400
H	-2.70123400	4.57985100	-0.88914400
H	-2.23404400	3.61541000	-2.32121600
C	-1.03880900	5.44408300	-2.08254700
C	-0.04481300	3.93537400	1.98389300
H	-0.29062300	5.58059800	0.62684200
H	-0.55719000	3.31737700	2.73561500
C	1.44592600	3.79747200	1.91725500
C	-0.61097400	5.16866800	-3.53337500
C	-1.84563300	6.75238400	-1.98131500
H	-0.10835000	5.58149700	-1.49343800
H	0.00962700	5.99241800	-3.92440600
H	-0.02930200	4.23639300	-3.60884100
H	-1.49608600	5.07300500	-4.18660400
H	-1.26820500	7.60539300	-2.37708400
H	-2.78143000	6.67975700	-2.56191100
H	-2.11644700	6.98347900	-0.93653200
S	8.41858200	2.87398600	0.63389200
C	6.76931700	3.28667000	-1.57694000
C	9.45572400	1.82594200	2.99122300
C	9.67715400	3.15588800	3.41121800
C	10.41781700	3.40691400	4.56996500
C	10.94247100	2.33934500	5.31551400
C	10.72105200	1.01460300	4.90521200
C	9.97845100	0.75407100	3.75177500
C	6.08159600	2.84822400	-2.73270500
C	5.55256600	3.78253400	-3.62578400
C	5.70168300	5.15670300	-3.37789400
C	6.37913200	5.59778300	-2.22980900
C	6.91072900	4.66999100	-1.32931300
H	9.25702600	3.99218100	2.84578100
H	10.58303100	4.43757300	4.89543000
H	11.52469500	2.54074100	6.21955800
H	11.13273000	0.18337300	5.48402000
H	9.80075400	-0.26978000	3.41384700
H	5.97241400	1.77569800	-2.90765100
H	5.02285200	3.43798200	-4.51803100
H	5.28822500	5.88665100	-4.08026300
H	6.49008800	6.66792500	-2.03449000
H	7.42182800	5.02328400	-0.42956100
H	-1.80718700	5.12553800	1.61841400
H	1.87434300	4.23130000	2.84069400
H	1.76348700	2.74286800	1.89523200
H	1.87729900	4.32628100	1.05477100

Dibenzoyl sulfide (TS 2,1-si)

C	7.31297700	2.21810900	-0.73906900
C	8.68934300	1.50120000	1.73161000
O	8.32553600	0.34409200	1.52605200
O	7.05582800	1.02442100	-0.87218100
Cl	-12.43630700	-2.53290800	1.33387300
Mg	-10.44746700	-2.39192000	0.12199000

Cl	-6.39212100	-2.71325800	1.31714000
Mg	-4.60938400	-2.82211600	-0.05924000
Cl	-8.64100300	-2.50314900	-1.22312900
Cl	-2.83415500	-2.93028800	-1.44570700
Cl	-0.73307100	-3.13071700	1.16487800
Mg	1.04215800	-3.23878900	-0.22158900
Cl	5.37916500	-3.98868700	0.69780500
Mg	7.15429300	-4.09685800	-0.68866200
Cl	2.85102500	-3.35014700	-1.56321100
Cl	8.91511500	-4.20372200	-2.08530700
Cl	-15.15582600	0.19505100	0.05131800
Mg	-13.00678100	-0.18339700	0.46526200
Cl	-11.42516800	-0.51806000	-1.16206700
Mg	-7.36236200	-0.70482700	0.09684200
Cl	-9.31913100	-0.70571600	1.65260000
Cl	-5.39555600	-0.73535200	-1.33682600
Mg	-1.62972100	-1.14290200	-0.10192900
Cl	-3.44369600	-1.10031100	1.51646200
Cl	0.18726800	-1.31801200	-1.71947600
Mg	4.24943600	-1.55943500	-0.15621100
Mg	10.26327600	-2.64889000	-0.73717400
Cl	2.20573000	-1.42760700	1.18808600
Cl	6.42257700	-2.18688900	-1.89914000
Cl	8.42631400	-2.86861100	1.04815700
Cl	12.37946400	-3.14089500	-0.25332500
Cl	-11.92871900	1.84535000	1.36011500
Mg	-10.06119700	1.13427500	0.20987800
Cl	-6.40068800	1.00769300	1.59199400
Cl	-8.27427200	1.28065100	-1.21946500
Mg	-4.37639200	0.91902000	0.40369800
Cl	-0.37367100	0.68768900	1.23317300
Cl	-2.52211600	0.97341000	-1.29201300
Mg	1.44066900	0.42628800	-0.47802800
Cl	5.55308500	-0.58719100	1.08371700
Cl	3.55205600	0.37657900	-1.49796000
Mg	7.52117300	-0.97622000	-0.04045200
Cl	9.58471500	-0.45461000	-1.07055900
Ti	-1.24297000	2.85452100	0.01741600
Cl	-3.36091900	2.90320500	1.32979600
Cl	0.65906900	2.54241200	-1.44351500
C	-1.75782900	4.71777500	-0.85752000
C	-0.70047900	4.97974700	1.16539800
H	-2.69550000	5.17701800	-0.49998500
H	-2.08912600	3.78481600	-1.43707400
C	-0.99220800	5.63888900	-1.81574100
C	-0.14676100	3.85275500	1.77837800
H	-0.04267200	5.67246100	0.63249900
H	-0.73786700	3.37568400	2.57264600
C	1.34912500	3.61179100	1.80462200
C	-1.42367000	5.35824800	-3.27166600
C	-1.20456500	7.12372400	-1.47393400
H	0.08735600	5.40365600	-1.74553300
H	-0.88324700	6.02134300	-3.96772200
H	-1.20729300	4.31614300	-3.55891200
H	-2.50428000	5.53838500	-3.40638500
H	-0.62241500	7.76436300	-2.15618100
H	-2.26866400	7.39724400	-1.58307200
H	-0.90097500	7.37308700	-0.44429800

S	8.41827900	2.88253000	0.56637700
C	6.78365200	3.24869400	-1.66384400
C	9.44202300	1.88166000	2.95057200
C	9.66163800	3.21995800	3.34418300
C	10.39162100	3.49464400	4.50434000
C	10.90711400	2.44255600	5.27772800
C	10.68746200	1.10966100	4.89371200
C	9.95579900	0.82560000	3.73884900
C	6.09057300	2.78514700	-2.80645500
C	5.56752600	3.69950300	-3.72345000
C	5.72867600	5.07851500	-3.51294300
C	6.41185100	5.54461000	-2.37822000
C	6.93699400	4.63689800	-1.45373900
H	9.24844600	4.04470100	2.75710200
H	10.55546300	4.53180400	4.80919100
H	11.48075200	2.66243200	6.18295400
H	11.09188500	0.29039300	5.49427700
H	9.77953100	-0.20501800	3.42135500
H	5.97211000	1.70928800	-2.95235100
H	5.03338000	3.33537400	-4.60522800
H	5.32060900	5.79278900	-4.23436400
H	6.53276500	6.61862100	-2.21217400
H	7.45312100	5.01014100	-0.56497800
H	-1.65206600	5.38424700	1.51800500
H	1.78254900	4.13036700	2.67970500
H	1.59871000	2.54512700	1.91748900
H	1.84599200	3.99819300	0.90138900

Dibenzoyl sulfide (Reactant 2,1-re)

C	7.31728400	2.24823900	-0.70638500
C	8.70343200	1.50755800	1.75197100
O	8.34131800	0.35173600	1.53558000
O	7.06891600	1.05468800	-0.85639300
Cl	-12.41781400	-2.54519900	1.31130300
Mg	-10.42901000	-2.38938900	0.10117800
Cl	-6.37343400	-2.71880100	1.29334700
Mg	-4.59047300	-2.81133000	-0.08388300
Cl	-8.62229400	-2.48458900	-1.24483200
Cl	-2.81495300	-2.90307400	-1.47123900
Cl	-0.71391600	-3.12850200	1.13734500
Mg	1.06148400	-3.22013500	-0.24992700
Cl	5.39929100	-3.97490600	0.66200000
Mg	7.17467200	-4.06664900	-0.72532800
Cl	2.87068000	-3.31550900	-1.59249400
Cl	8.93574600	-4.15699600	-2.12282100
Cl	-15.14017100	0.19306500	0.05703900
Mg	-12.99075600	-0.18735700	0.46723900
Cl	-11.40862100	-0.50327200	-1.16332600
Mg	-7.34574900	-0.69875600	0.09399300
Cl	-9.30265700	-0.71805500	1.64945500
Cl	-5.37893200	-0.71211600	-1.33964600
Mg	-1.61234600	-1.12855200	-0.10888500
Cl	-3.42678200	-1.10482300	1.50987700
Cl	0.20472000	-1.28474600	-1.72774400
Mg	4.26696800	-1.53815000	-0.16675000
Mg	10.28208400	-2.61487900	-0.75836000
Cl	2.22255100	-1.42257700	1.17885800
Cl	6.44099800	-2.14492600	-1.91585500

Cl	8.44518600	-2.85524600	1.02437400
Cl	12.39875800	-3.10961700	-0.27945000
Cl	-11.91498700	1.83309400	1.38336900
Mg	-10.04658100	1.13611100	0.22596500
Cl	-6.38608100	0.99908500	1.60706700
Cl	-8.25967600	1.29936100	-1.20157400
Mg	-4.36115300	0.92465100	0.41800400
Cl	-0.35924000	0.68950200	1.24555800
Cl	-2.50785600	0.99917300	-1.27629600
Mg	1.45751300	0.44803700	-0.46834200
Cl	5.56947600	-0.57744300	1.08346800
Cl	3.56763600	0.41109900	-1.48825100
Mg	7.53809700	-0.95256100	-0.04449100
Cl	9.60117100	-0.41797100	-1.06886300
Ti	-1.31204800	2.95687500	-0.03966700
Cl	-3.29332800	2.87507500	1.40302700
Cl	0.84898600	2.71102600	-1.14221200
C	-1.82964700	4.20996500	-1.57954600
C	-0.70426100	4.87610800	1.24278100
H	-2.63631800	4.59573300	-0.89803900
H	-2.32942100	3.56865600	-2.33112800
C	-1.06704700	5.35407500	-2.26810300
C	0.02844400	3.98998100	1.99206300
H	-0.26115200	5.33644000	0.35116200
C	-0.36094800	3.49062800	3.34816500
H	1.01860700	3.69425000	1.61989800
C	-0.55752400	4.90873100	-3.64870300
C	-1.94163700	6.61788700	-2.38551600
H	-0.17605500	5.62262500	-1.66305900
H	0.04378900	5.70371400	-4.12049700
H	0.06575100	4.00435600	-3.57442900
H	-1.40655800	4.68553700	-4.31846200
H	-1.38672200	7.43753900	-2.87332500
H	-2.84246100	6.41378300	-2.98948600
H	-2.27323000	6.97621800	-1.39585100
S	8.42357300	2.90119100	0.60474700
C	6.77896800	3.28876100	-1.61392400
C	9.46229200	1.87569400	2.97109600
C	9.67530000	3.20972100	3.38233800
C	10.41195900	3.47294400	4.54096400
C	10.94094000	2.41359100	5.29508500
C	10.72788200	1.08482100	4.89348400
C	9.98934500	0.81214600	3.74022300
C	6.09952700	2.83827300	-2.76993500
C	5.56861600	3.76328600	-3.67144700
C	5.70728000	5.13995400	-3.43158600
C	6.37624300	5.59293300	-2.28322300
C	6.90990500	4.67452200	-1.37443200
H	9.25165000	4.03969100	2.81025700
H	10.57057200	4.50677000	4.85961100
H	11.51999300	2.62454400	6.19899400
H	11.14289000	0.25993100	5.47895800
H	9.81804100	-0.21500900	3.40908300
H	5.99808900	1.76393300	-2.93825000
H	5.04522900	3.40957100	-4.56384000
H	5.29186200	5.86262800	-4.14029000
H	6.47834700	6.66499700	-2.09380400
H	7.41363600	5.03691300	-0.47415800

H	-1.63586500	5.31069400	1.62013700
H	0.34348500	3.91030700	4.09066800
H	-1.38148300	3.79246200	3.62524600
H	-0.27758600	2.39467700	3.42145300

Dibenzoyl sulfide (TS 2,1-re)

C	7.33355800	2.22221300	-0.76774900
C	8.70270300	1.53053300	1.71422300
O	8.34598000	0.36993300	1.51600600
O	7.07835100	1.02690100	-0.88949600
Cl	-12.40921500	-2.54775700	1.33586000
Mg	-10.41989800	-2.41351600	0.12399500
Cl	-6.36469000	-2.71680200	1.32432000
Mg	-4.58090200	-2.83421500	-0.04999400
Cl	-8.61239800	-2.53298300	-1.21902400
Cl	-2.80461800	-2.95104300	-1.43440600
Cl	-0.70477000	-3.12485200	1.17908000
Mg	1.07151500	-3.24158000	-0.20533100
Cl	5.40936200	-3.97526700	0.72313400
Mg	7.18554600	-4.09209400	-0.66127800
Cl	2.88141500	-3.36114200	-1.54485200
Cl	8.94742700	-4.20773000	-2.05588600
Cl	-15.13308800	0.16382600	0.02806700
Mg	-12.98358800	-0.20695000	0.44656700
Cl	-11.40034300	-0.55271500	-1.17684900
Mg	-7.33796900	-0.72086700	0.08607000
Cl	-9.29569100	-0.71197200	1.64060300
Cl	-5.37022500	-0.76009900	-1.34609800
Mg	-1.60439000	-1.14979700	-0.10545400
Cl	-3.41943900	-1.09660900	1.51141700
Cl	0.21392400	-1.33548400	-1.72033100
Mg	4.27557600	-1.55565300	-0.15259400
Mg	10.29181900	-2.63871800	-0.72047700
Cl	2.23079700	-1.41604500	1.18928300
Cl	6.45097100	-2.19408100	-1.88871200
Cl	8.45417400	-2.84642900	1.06558800
Cl	12.40863300	-3.12250200	-0.23111000
Cl	-11.90990900	1.83151700	1.32444100
Mg	-10.04034000	1.11403300	0.18153400
Cl	-6.38045100	1.00636800	1.56689300
Cl	-8.25281300	1.25139300	-1.24795200
Mg	-4.35525900	0.91122800	0.38062500
Cl	-0.35262000	0.69467600	1.21447800
Cl	-2.50004400	0.95442500	-1.31438000
Mg	1.46326400	0.42188300	-0.49330300
Cl	5.57662200	-0.57023000	1.07964000
Cl	3.57537000	0.36733000	-1.51149800
Mg	7.54613400	-0.96526400	-0.03993200
Cl	9.60932200	-0.44869900	-1.07328500
Ti	-1.24708700	2.85771500	0.00821600
Cl	-3.37045300	2.92478900	1.27574100
Cl	0.69172600	2.55217200	-1.43091800
C	-1.73618000	4.72548500	-0.88194800
C	-0.30901900	4.96928800	0.85436900
H	-2.61431800	5.20384700	-0.41332600
H	-2.14050800	3.79023700	-1.40896600
C	-1.09920000	5.61749100	-1.95037000
C	-0.05123300	3.86436900	1.67488900

H	0.43698300	5.27508200	0.11638100
C	-0.64971900	3.69390500	3.05482100
H	0.89407300	3.33728800	1.48414200
C	-1.83885500	5.42830100	-3.29325000
C	-1.10657200	7.10220900	-1.54704600
H	-0.05273400	5.28957300	-2.10540400
H	-1.38918600	6.06775500	-4.07096600
H	-1.78201100	4.38333100	-3.64032200
H	-2.90334200	5.70551500	-3.20357400
H	-0.65642200	7.71705100	-2.34332200
H	-2.14084900	7.45773600	-1.39454500
H	-0.54292700	7.29670700	-0.62119200
S	8.43033600	2.90148400	0.53734200
C	6.80809900	3.24242500	-1.70607400
C	9.44763100	1.92414300	2.93387700
C	9.65730500	3.26647100	3.31904200
C	10.37980100	3.55371100	4.48087000
C	10.89767300	2.51027100	5.26428400
C	10.68790300	1.17340500	4.88863300
C	9.96373100	0.87682400	3.73218500
C	6.11538800	2.76615200	-2.84364000
C	5.59628100	3.67008600	-3.77307700
C	5.76119200	5.05120500	-3.58021100
C	6.44411900	5.52996500	-2.45065100
C	6.96515700	4.63277100	-1.51370900
H	9.24196700	4.08454300	2.72420200
H	10.53579400	4.59397500	4.77919800
H	11.46539100	2.73999500	6.17080000
H	11.09410900	0.36082300	5.49703300
H	9.79505500	-0.15705600	3.42122700
H	5.99391900	1.68885700	-2.97576700
H	5.06214700	3.29615200	-4.65074900
H	5.35611700	5.75728500	-4.31132300
H	6.56790800	6.60566700	-2.29827500
H	7.48121600	5.01612500	-0.62922700
H	-1.00084800	5.74455300	1.19830800
H	0.06841600	4.06828900	3.80750700
H	-1.58668400	4.26025800	3.16498600
H	-0.85663800	2.64006300	3.29571700

Diisobutyl phthalate (Reactant 1,2-si)

C	8.83016600	2.69502500	1.22497100
C	9.67386000	3.58375800	1.92449700
C	10.18542000	4.74008500	1.32659700
C	9.84502000	5.04196300	0.00400500
C	8.99838000	4.18295200	-0.70189300
C	8.48192400	3.00439000	-0.12339400
C	7.55443100	2.17711300	-0.95691000
O	7.43913200	2.62671400	-2.21006200
C	6.60567500	1.81895900	-3.11028600
C	6.72595800	2.39866100	-4.51756700
C	8.45602900	1.45812000	1.99883900
O	8.47331200	0.28986000	1.59201400
O	8.20116800	1.75680000	3.27816400
C	7.94601400	0.62205000	4.17533200
C	7.55124100	1.17627400	5.54128800
H	9.94118700	3.34434800	2.95551300
H	10.84653500	5.39844400	1.89699300

H	10.23313500	5.94228000	-0.48011900
H	8.71885500	4.41831400	-1.72978100
H	5.57073100	1.84821200	-2.73060400
H	6.96706100	0.77869500	-3.05877300
H	8.87034700	0.01907700	4.22836100
H	7.15045000	0.00630000	3.72751000
C	8.65903700	2.04347400	6.15753900
C	7.17922200	-0.00161400	6.45746900
C	8.16415900	2.30526600	-5.05267700
C	6.16846800	3.82885400	-4.60266500
H	6.08352200	1.74205300	-5.13669500
H	6.65047900	1.80197100	5.39335100
H	9.57700500	1.45110200	6.31920700
H	8.34379600	2.44400700	7.13468200
H	8.91253800	2.89715200	5.50910000
H	6.85265900	0.36498700	7.44361300
H	8.04533500	-0.66648700	6.61980900
H	6.36229500	-0.60714200	6.03221100
H	8.54080400	1.26999300	-5.01689300
H	8.84894900	2.92997200	-4.45581200
H	8.21552800	2.65186800	-6.09735300
H	6.76004900	4.52152000	-3.98091300
H	5.12159700	3.87562000	-4.25875300
H	6.20143300	4.19968400	-5.63976200
O	6.92521400	1.18810800	-0.55761600
Cl	-12.46381900	-2.28594700	1.18667900
Mg	-10.66089400	-2.30714600	-0.16763200
Cl	-6.69186400	-2.74976600	1.13123200
Mg	-4.88237900	-2.81672300	-0.21273000
Cl	-8.83477900	-2.33248900	-1.49040100
Cl	-3.08038900	-2.88218800	-1.56663100
Cl	-1.03782700	-3.24814000	1.07205600
Mg	0.76445400	-3.31364500	-0.28183800
Cl	5.06978900	-4.17755800	0.68529500
Mg	6.87101700	-4.24327900	-0.66808600
Cl	2.59923600	-3.38533600	-1.59079500
Cl	8.65964800	-4.30679900	-2.03313500
Cl	-15.37100800	0.27763300	-0.14403300
Mg	-13.22780700	-0.12533500	0.27691900
Cl	-11.62198200	-0.35625000	-1.34482400
Mg	-7.60664200	-0.66685300	-0.00400500
Cl	-9.59544500	-0.71596200	1.50970400
Cl	-5.61054100	-0.65578700	-1.39764500
Mg	-1.87851900	-1.18477500	-0.10917200
Cl	-3.72486500	-1.19566000	1.47226400
Cl	-0.03039100	-1.30597900	-1.69655700
Mg	3.99413700	-1.69176100	-0.06529300
Mg	10.00277800	-2.84364100	-0.57926300
Cl	1.92511700	-1.59485300	1.24165700
Cl	6.19501100	-2.26444000	-1.79419900
Cl	8.12446100	-3.12656500	1.14871300
Cl	12.10016600	-3.39319800	-0.07955300
Cl	-12.17248500	1.87234100	1.29989200
Mg	-10.29626800	1.17957300	0.14050500
Cl	-6.63127100	0.95065500	1.60075900
Cl	-8.48854600	1.35857600	-1.25834300
Mg	-4.59916200	0.86627300	0.42464200
Cl	-0.62550400	0.58185400	1.31863300

Cl	-2.72406800	0.99225300	-1.25284400
Mg	1.23474400	0.30816400	-0.32858700
Cl	5.48801000	-0.29563100	1.55097600
Cl	3.38185400	0.33489800	-1.30528100
Mg	7.40640300	-0.78535300	0.09637300
Cl	9.41379900	-0.30691100	-1.29532700
Ti	-1.51637600	2.89447700	0.06006900
Cl	-3.50186500	2.77965800	1.46192900
Cl	0.56870900	2.51746100	-1.15350000
C	-1.94764500	4.27071500	-1.39951200
C	-0.89883500	4.96116000	1.50257200
H	-2.81074100	4.65841500	-0.79964600
H	-2.37994400	3.65824800	-2.21583500
C	-1.07574400	5.40873600	-1.96949600
C	-0.20001200	3.83077100	1.85066900
H	-0.50644600	5.56844800	0.67549300
H	-0.49535800	3.23389100	2.72184800
H	0.77129000	3.60961800	1.39857800
C	-2.03400400	5.56284200	2.27471500
H	-2.88249500	5.83809800	1.62693500
H	-2.39599700	4.89824800	3.07214600
H	-1.67492400	6.49999100	2.74009600
C	-0.66809300	5.10696500	-3.42095800
C	-1.78749800	6.77091100	-1.86739000
H	-0.13571000	5.47825300	-1.38264500
H	0.01157200	5.88390700	-3.80923400
H	-0.15554300	4.13528000	-3.49686900
H	-1.55763300	5.07733600	-4.07449900
H	-1.15007100	7.58126200	-2.26025200
H	-2.72483000	6.76537100	-2.45006500
H	-2.04470500	7.02093100	-0.82315300

Diisobutyl phthalate (TS 1,2-sj)

C	8.83587900	2.70038900	1.16374900
C	9.68304500	3.59812600	1.84737600
C	10.19779300	4.74249300	1.22949500
C	9.85711000	5.02304600	-0.09771900
C	9.00674700	4.15513300	-0.78807600
C	8.48703700	2.98823400	-0.18923500
C	7.55586700	2.15003700	-1.00754500
O	7.43762700	2.58070100	-2.26709800
C	6.60130300	1.75969800	-3.15259200
C	6.71216400	2.32266500	-4.56744700
C	8.45897900	1.47756600	1.95847700
O	8.47326700	0.30263000	1.57124500
O	8.20561400	1.79828900	3.23270200
C	7.94882600	0.67931800	4.14913500
C	7.55988100	1.25739200	5.50686000
H	9.95061500	3.37525300	2.88203100
H	10.86169700	5.40816700	1.78802900
H	10.24791300	5.91361100	-0.59746100
H	8.72685300	4.37409000	-1.81948500
H	5.56835100	1.79062200	-2.76766600
H	6.96575800	0.72103800	-3.09014200
H	8.87106200	0.07384200	4.20946300
H	7.14979700	0.05924600	3.71358300
C	8.67335400	2.12891100	6.10653600
C	7.18403800	0.09634100	6.44273000

C	8.14763200	2.22749700	-5.10949400
C	6.14973200	3.75004100	-4.66624800
H	6.06838400	1.65680600	-5.17517000
H	6.66184500	1.88507000	5.35088700
H	9.58908200	1.53489400	6.27467600
H	8.36277700	2.54592600	7.07824300
H	8.92877300	2.97127100	5.44419500
H	6.86141700	0.48056200	7.42345100
H	8.04708500	-0.57026500	6.61412000
H	6.36312700	-0.51188900	6.02914700
H	8.52814000	1.19408600	-5.06272900
H	8.83359300	2.86221500	-4.52465400
H	8.19177500	2.56090200	-6.15879100
H	6.74182500	4.45147100	-4.05488600
H	5.10422400	3.79723400	-4.31823300
H	6.17692800	4.10921800	-5.70760200
O	6.92594500	1.16836200	-0.59169600
Cl	-12.46513700	-2.27499900	1.21588900
Mg	-10.66264500	-2.31978200	-0.13839400
Cl	-6.69318400	-2.74024600	1.16674400
Mg	-4.88418900	-2.83056400	-0.17641800
Cl	-8.83688900	-2.36821200	-1.46108900
Cl	-3.08256500	-2.91964800	-1.52960200
Cl	-1.03915600	-3.24004700	1.11444500
Mg	0.76256900	-3.32913100	-0.23874000
Cl	5.06817200	-4.17649700	0.74190800
Mg	6.86900000	-4.26578900	-0.61067500
Cl	2.59701000	-3.42356600	-1.54676500
Cl	8.65724800	-4.35308700	-1.97502700
Cl	-15.37248300	0.26539000	-0.15805500
Mg	-13.22915200	-0.13042400	0.26910600
Cl	-11.62390900	-0.38954900	-1.34892200
Mg	-7.60824200	-0.67710100	-0.00421500
Cl	-9.59648900	-0.69989100	1.51079600
Cl	-5.61295300	-0.69022700	-1.39825900
Mg	-1.87985400	-1.19737800	-0.10218100
Cl	-3.72600000	-1.18068000	1.47986200
Cl	-0.03247000	-1.34623900	-1.68773400
Mg	3.99252900	-1.70398700	-0.05131900
Mg	10.00094200	-2.86507400	-0.54706400
Cl	1.92368400	-1.58434300	1.25454800
Cl	6.19283400	-2.30666400	-1.77065800
Cl	8.12314000	-3.11794300	1.18614700
Cl	12.09836400	-3.40606200	-0.03863000
Cl	-12.17342500	1.88458100	1.25697100
Mg	-10.29760200	1.17168100	0.10922300
Cl	-6.63218800	0.96775600	1.57200600
Cl	-8.49031200	1.32634000	-1.29309800
Mg	-4.59878600	0.86242000	0.39711300
Cl	-0.62784400	0.59366900	1.29431800
Cl	-2.72623300	0.95954200	-1.28311100
Mg	1.23387400	0.29182500	-0.34826300
Cl	5.48704200	-0.28017800	1.54009800
Cl	3.38002000	0.30088300	-1.32600300
Mg	7.40493100	-0.79516000	0.09364400
Cl	9.41188900	-0.34105900	-1.30684000
Ti	-1.45135600	2.79778600	0.09048100
Cl	-3.59670400	2.85731100	1.33301900

Cl	0.51604800	2.45331900	-1.28774800
C	-1.86241500	4.69576800	-0.78411000
C	-0.70078700	4.94599300	1.23526600
H	-2.75002600	5.23411900	-0.40977600
H	-2.29167400	3.78552200	-1.33200900
C	-1.06838100	5.52451700	-1.80218300
C	-0.36421800	3.70511000	1.79657600
H	0.04834100	5.41513400	0.58774000
H	-0.89648500	3.34528600	2.68475500
H	0.63701600	3.29697200	1.62167900
C	-1.69344000	5.86264200	1.90350400
H	-2.09169700	6.63623300	1.23242700
H	-2.53070100	5.30054300	2.34405900
H	-1.16513900	6.37759400	2.72674800
C	-1.65512500	5.31172600	-3.21536300
C	-1.04976200	7.02396900	-1.45912100
H	-0.02572500	5.15358700	-1.82456400
H	-1.09163700	5.90005300	-3.95869700
H	-1.60394200	4.25174900	-3.51460700
H	-2.71012800	5.63362000	-3.25992300
H	-0.49131800	7.58381400	-2.22698600
H	-2.07530900	7.43280600	-1.42840600
H	-0.57217600	7.23625300	-0.48906000

Diisobutyl phthalate (Reactant 1,2-re)

Cl	-12.37486600	-2.09873400	1.62994100
Mg	-10.64460700	-2.27101200	0.19423700
Cl	-6.60527600	-2.73283200	1.29972900
Mg	-4.87120900	-2.93424400	-0.12763500
Cl	-8.88960200	-2.44612300	-1.21095200
Cl	-3.14501400	-3.13481600	-1.56460400
Cl	-0.97473400	-3.38048600	0.98467800
Mg	0.75144900	-3.58095900	-0.45227200
Cl	5.22292600	-3.93143000	0.89562900
Mg	6.94897500	-4.13200400	-0.54130400
Cl	2.51258800	-3.78550500	-1.84568700
Cl	8.66057800	-4.33087700	-1.98831700
Cl	-15.27313700	0.45614600	0.26381100
Mg	-13.12342400	0.01616200	0.60713200
Cl	-11.60946200	-0.37764900	-1.07065900
Mg	-7.53180800	-0.70476900	0.07626800
Cl	-9.43730500	-0.60193500	1.68972900
Cl	-5.61512100	-0.83816100	-1.41517800
Mg	-1.82897100	-1.37740600	-0.28834000
Cl	-3.59002800	-1.23301700	1.38210700
Cl	-0.07106300	-1.65143200	-1.95670300
Mg	4.02697100	-2.02911500	-0.50632400
Mg	10.11207800	-2.81608000	-0.70390400
Cl	2.02793900	-1.79161000	0.88855700
Cl	6.24710100	-2.06501400	-1.76995000
Cl	8.32295900	-2.93462700	1.13875500
Cl	12.22013200	-3.38916400	-0.27617400
Cl	-11.95179900	2.04596300	1.43315800
Mg	-10.15018900	1.24265700	0.23842500
Cl	-6.45864000	0.99737000	1.50772300
Cl	-8.40621200	1.29423400	-1.24945400
Mg	-4.47478700	0.80475000	0.26361300
Cl	-0.45842500	0.43010800	0.96860000

Cl	-2.68041600	0.74839100	-1.49357500
Mg	1.28947500	0.06402100	-0.79042200
Cl	5.55254100	-0.32907200	1.21566500
Cl	3.37246600	-0.08365800	-1.85725100
Mg	7.45014800	-0.87796900	0.03816000
Cl	9.50338200	-0.53198900	-1.03158000
Ti	-1.36304300	2.63140300	-0.32599600
Cl	-3.31292100	2.73769600	1.15142400
Cl	0.62295800	2.21476900	-1.71872300
C	-1.85128800	4.35067000	-1.32874600
C	-0.10252600	4.73497500	0.94691400
H	-1.02981000	4.67480400	-1.99418100
H	-2.36353100	3.50081700	-1.89095000
C	-2.86952300	5.47119700	-1.05555600
C	-0.01691200	3.52981100	1.58107600
C	1.01465900	5.35107700	0.16036400
H	-0.76640600	3.21501600	2.31439300
H	0.90339400	2.93954800	1.51770800
H	-0.99269500	5.35240800	1.12203400
C	-2.22010800	6.86263400	-1.13805700
C	-4.05873000	5.37911500	-2.03370400
H	-3.27806300	5.33481200	-0.03564700
H	-2.95869400	7.64830600	-0.90890800
H	-1.38293000	6.98117400	-0.43172400
H	-1.83200300	7.05275800	-2.15435500
H	-4.79497200	6.17462700	-1.82888400
H	-3.72058200	5.48946300	-3.07863400
H	-4.57848000	4.41047400	-1.94372900
H	1.45582600	6.16843400	0.76067900
H	1.80710800	4.62204900	-0.06477700
H	0.66592900	5.80223200	-0.78093700
C	9.09036000	2.58536900	1.15669900
C	10.14905800	3.29475300	1.75954200
C	10.82542700	4.31476100	1.08279800
C	10.42475100	4.66933700	-0.21028200
C	9.34987000	4.00457800	-0.80698200
C	8.67333900	2.95220700	-0.15304900
C	7.53818800	2.31492900	-0.89729600
O	6.98164400	3.17461900	-1.77236000
C	5.94784200	2.62016900	-2.64950800
C	5.23669100	3.77949900	-3.34571400
C	8.52606700	1.46976300	1.99234000
O	8.38051700	0.29614200	1.64894500
O	8.28395800	1.88499900	3.24612100
C	7.80875300	0.85280700	4.17521800
C	7.48639700	1.52494700	5.50683700
H	10.44846800	3.02226400	2.77407600
H	11.65919500	4.82935000	1.56853200
H	10.94210200	5.46418300	-0.75460800
H	9.02032800	4.28932500	-1.80759300
H	5.25806700	2.01395300	-2.04224200
H	6.44772400	1.95036900	-3.37098300
H	8.60584600	0.09504800	4.28149200
H	6.92936200	0.36598400	3.72337000
C	8.72169200	2.19420200	6.12740000
C	6.87481100	0.47751500	6.45217300
C	6.19608800	4.61919900	-4.20421400
C	4.45774500	4.64496300	-2.34131300

H	4.50535000	3.29063800	-4.01856400
H	6.72460200	2.30273900	5.30689900
H	9.50293100	1.44532400	6.34786400
H	8.46257000	2.69524400	7.07424300
H	9.15291600	2.94872300	5.45069700
H	6.59821700	0.93888600	7.41363700
H	7.59533100	-0.33105500	6.66612300
H	5.96967500	0.01811600	6.02218000
H	6.73118600	3.99575000	-4.93982900
H	6.94806900	5.12264300	-3.57437300
H	5.64728100	5.39802500	-4.75796600
H	5.14114900	5.10524900	-1.60839100
H	3.71745900	4.04052800	-1.78979200
H	3.91776100	5.45534200	-2.85785600
O	7.13710800	1.15486800	-0.78548500

Diisobutyl phthalate (TS 1,2-re)

Cl	-12.37023600	-2.11412400	1.63037800
Mg	-10.64049600	-2.28125800	0.19344000
Cl	-6.60048500	-2.74448900	1.29585200
Mg	-4.86691600	-2.94077900	-0.13284000
Cl	-8.88599700	-2.45130400	-1.21300100
Cl	-3.14123300	-3.13620600	-1.57111900
Cl	-0.96977100	-3.38852000	0.97650600
Mg	0.75590700	-3.58384800	-0.46176500
Cl	5.22811200	-3.93625500	0.88321100
Mg	6.95365500	-4.13168300	-0.55503900
Cl	2.51655900	-3.78336100	-1.85652200
Cl	8.66474600	-4.32538600	-2.00335800
Cl	-15.27028600	0.44348300	0.27315700
Mg	-13.12022200	0.00348700	0.61425500
Cl	-11.60677600	-0.38455200	-1.06534600
Mg	-7.52848600	-0.71319500	0.07889300
Cl	-9.43335800	-0.61611900	1.69344800
Cl	-5.61233200	-0.84119600	-1.41375700
Mg	-1.82549600	-1.38202000	-0.29011800
Cl	-3.58590700	-1.24349700	1.38148600
Cl	-0.06814400	-1.65019200	-1.96003400
Mg	4.03067000	-2.03029500	-0.51251000
Mg	10.11606600	-2.81377500	-0.71499500
Cl	2.03211900	-1.79793700	0.88391300
Cl	6.25028900	-2.06133500	-1.77716200
Cl	8.32777500	-2.93871800	1.12804500
Cl	12.22457000	-3.38714400	-0.28987200
Cl	-11.94921200	2.03134700	1.44590100
Mg	-10.14772200	1.23249600	0.24800300
Cl	-6.45551400	0.98518900	1.51503000
Cl	-8.40439200	1.28938000	-1.24044100
Mg	-4.47220100	0.79717000	0.26950600
Cl	-0.45523600	0.42230200	0.97166900
Cl	-2.67840900	0.74700700	-1.48859000
Mg	1.29203800	0.06244100	-0.78916200
Cl	5.55615700	-0.33472100	1.21395600
Cl	3.37468400	-0.08110700	-1.85728800
Mg	7.45353100	-0.87917000	0.03401200
Cl	9.50615300	-0.52899600	-1.03553700
Ti	-1.29614400	2.60454100	-0.26438000
Cl	-3.36459100	2.76945100	1.11045200

Cl	0.58574700	2.20745300	-1.74179400
C	-1.69629800	4.47913200	-1.19441500
C	-0.37085700	4.75823200	0.71743100
H	-0.91543100	4.83101800	-1.89088100
H	-2.14811800	3.55526600	-1.70023800
C	-2.82709200	5.50193800	-1.03006300
C	-0.13525900	3.54288300	1.37686000
C	0.75643900	5.50011800	0.04417800
H	-0.76222000	3.24774600	2.22538500
H	0.86345100	3.09446500	1.32543100
H	-1.22686100	5.35238000	1.05610200
C	-2.32413600	6.95536900	-1.00814900
C	-3.85658900	5.32090800	-2.16833200
H	-3.35388200	5.29178200	-0.08016100
H	-3.17635300	7.65021400	-0.93285000
H	-1.65721100	7.16692700	-0.15734100
H	-1.77825500	7.19756900	-1.93734600
H	-4.68196900	6.04363000	-2.05753900
H	-3.39191900	5.48576600	-3.15595700
H	-4.29287800	4.30793000	-2.16055400
H	1.31184200	6.04301800	0.83080800
H	1.46114600	4.80914100	-0.44394000
H	0.41624200	6.24283800	-0.69043200
C	9.10634100	2.57325100	1.16467300
C	10.17302100	3.27403800	1.76334300
C	10.84956300	4.29395300	1.08660700
C	10.44084300	4.65749900	-0.20149800
C	9.35796200	4.00152800	-0.79348800
C	8.68156900	2.94892800	-0.13991400
C	7.53817500	2.32089300	-0.87912100
O	6.97027000	3.19274600	-1.73503400
C	5.92410100	2.65001800	-2.60432900
C	5.19964900	3.81806000	-3.27145000
C	8.54006000	1.45745000	1.99851000
O	8.38415200	0.28659300	1.65027400
O	8.30752100	1.86838300	3.25547200
C	7.82860000	0.83542700	4.18185900
C	7.50940900	1.50503200	5.51549700
H	10.47828700	2.99505200	2.77436800
H	11.68965200	4.80173500	1.56858500
H	10.95811800	5.45263600	-0.74546600
H	9.02197400	4.29342900	-1.78993300
H	5.24514100	2.03298600	-1.99578900
H	6.41321400	1.99218600	-3.34395900
H	8.62282700	0.07429500	4.28561400
H	6.94710300	0.35328400	3.72909500
C	8.74735400	2.16823800	6.13725000
C	6.89452600	0.45720400	6.45825700
C	6.14350600	4.67293700	-4.13224500
C	4.43499300	4.66709300	-2.24225500
H	4.45867300	3.33768200	-3.93992300
H	6.75026200	2.28603000	5.31802400
H	9.52589500	1.41602000	6.35589500
H	8.49026000	2.66807400	7.08527900
H	9.18120000	2.92268400	5.46215100
H	6.61977200	0.91704300	7.42097700
H	7.61236900	-0.35434900	6.66992300
H	5.98767400	0.00202700	6.02739500

H	6.66774000	4.06183700	-4.88581800
H	6.90463800	5.16780500	-3.50665300
H	5.58462800	5.45917800	-4.66501900
H	5.12885400	5.12404600	-1.51717800
H	3.71046800	4.05141600	-1.68200000
H	3.88002800	5.47954400	-2.73941500
O	7.13981500	1.15883400	-0.77968200