

Quantitative characterization of group electrophilicity and nucleophilicity for intramolecular Diels-Alder reactions

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Supporting Information

S1: Cartesian coordinates and total energies of reactants

S2: Cartesian coordinates, total energies and imaginary frequencies for transition state structures

Complete reference 9.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M.W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision C.02; Gaussian: Wallingford, CT, **2004**.

Table S1: Cartesian coordinates and total energies of reactants

Compound 1

C	1.24189200	1.14265100	-0.05177100
H	1.46041600	1.10888000	-1.12033000
C	1.90161200	0.29441200	0.76901200
H	1.69210800	0.35783300	1.83824500
C	2.90902800	-0.70495700	0.38675000
H	3.13957500	-1.44605400	1.15130500
C	3.58004400	-0.76074300	-0.77415100
H	3.45726000	-0.01760100	-1.55837500
H	4.31273300	-1.53953400	-0.96084800
C	0.26919500	2.20264700	0.40916600
H	0.31680700	3.05534400	-0.27889500
H	0.57496100	2.57849400	1.39244000
C	-1.20052600	1.72933700	0.52599600
H	-1.24950500	0.96696300	1.31494800
H	-1.80422200	2.56748200	0.88923300
C	-1.81579400	1.18000000	-0.78791200
H	-2.62387200	1.82979600	-1.14127800
H	-1.07967600	1.17813700	-1.60012100
C	-2.43349300	-0.21555500	-0.64401000
H	-2.84612300	-0.58138200	-1.58996700
H	-3.24135800	-0.20504500	0.09085800
C	-0.27329500	-1.33745100	-0.65610900
H	0.00598700	-0.72887000	-1.50503000
H	0.42720800	-2.07407500	-0.27945800
N	-1.45486600	-1.24366400	-0.15873000
C	-1.89771700	-2.10104300	0.95497700
H	-2.09798100	-1.47369500	1.82805800
H	-2.81860900	-2.61070600	0.65949200
H	-1.12732700	-2.83609600	1.18914200

Total energy (a.u.): -446.361054

Compound 2

C	3.23669000	-0.51522100	-1.22963800
H	3.39537400	-1.56164700	-1.46764500
H	3.62264700	0.23562000	-1.90803100
C	2.57940200	-0.17333800	-0.12187200
C	1.98458800	-1.08917700	0.90977600
H	2.29901400	-0.75413000	1.90302800
C	0.44211000	-1.18508900	0.87734800
H	0.01269400	-0.18707900	1.01299200
H	0.13038800	-1.77464400	1.75015700
C	-0.11664900	-1.83518800	-0.39334600
H	0.31055200	-2.84192000	-0.50728000
H	0.20219300	-1.26467500	-1.27661200
C	-1.65627300	-1.94879600	-0.39678200
H	-1.95082900	-2.54335400	-1.27515300
H	-1.98794500	-2.51376400	0.48487000
C	-2.36034400	-0.62153700	-0.44608400
H	-2.11731000	0.01674000	-1.29783000
C	-3.23487900	-0.17393100	0.46859700
H	-3.42727300	-0.79325600	1.34647500
C	-3.95644800	1.10420000	0.41681200
H	-4.22742300	1.52896900	1.38401300
C	-4.31821000	1.76360000	-0.69187400
H	-4.12434100	1.36744100	-1.68568800

H	-4.82912900	2.72057900	-0.63996300
H	2.41521300	-2.08481100	0.74870000
N	2.42029000	1.28535800	0.14144800
O	2.80226100	2.08589400	-0.70924600
O	1.91451800	1.60151700	1.21927100

Total energy (a.u.): -595.139648

Compound 3

C	4.18437700	0.27537400	0.86046100
H	4.55780800	1.29329800	0.82559000
H	4.53229600	-0.37805000	1.65102400
C	3.31676200	-0.15040500	-0.05714800
C	2.74174400	0.62998600	-1.20507400
H	2.83666500	0.03583500	-2.11920700
C	1.26350100	1.04595800	-1.02952200
H	0.64846700	0.15063800	-0.89204000
H	0.93537000	1.50119700	-1.97362900
C	1.02493500	2.03622000	0.11602500
H	1.64655200	2.93009500	-0.03697100
H	1.35279900	1.59398500	1.06694600
C	-0.44783100	2.47938300	0.24710000
H	-0.49796600	3.27188200	1.00935100
H	-0.78429500	2.93297200	-0.69469500
C	-1.38053100	1.36668700	0.63730800
H	-1.14130700	0.84573000	1.56592100
C	-2.45454100	0.98469000	-0.06564600
C	-3.40415800	-0.07672900	0.31321600
C	-3.67095100	-0.46928700	1.57162800
H	-3.19147800	0.03291400	2.40250800
H	-4.35405400	-1.27418000	1.81097700
H	3.36079500	1.52628400	-1.33206800
N	2.86749700	-1.56779200	0.05000900
O	3.22711900	-2.23114700	1.02018200
O	2.15805800	-1.99437200	-0.86210900
H	-2.67143200	1.46135300	-1.02111800
O	-3.99291600	-0.58628000	-0.81393700
C	-4.96837100	-1.59968500	-0.64205500
H	-5.33234800	-1.84449200	-1.64176900
H	-4.53523600	-2.49699400	-0.18063900
H	-5.80282100	-1.24668600	-0.02108700

Total energy (a.u.): -709.666358

Compound 4

C	-0.70938500	0.15028000	2.10242800
H	-1.13279700	1.05392000	2.53158600
C	-1.17630300	-1.06187300	2.43835500
H	-1.98258500	-1.17890000	3.15582100
H	-0.75518500	-1.96163600	2.00154800
C	0.38963300	0.32520800	1.14267900
O	0.96629600	-0.69988800	0.71283700
C	0.83331500	1.72368600	0.79602900
H	1.13840800	2.17858800	1.75129100
H	1.71933800	1.67460100	0.16585000
C	-0.24002400	2.63479600	0.15509700
H	-1.06243200	2.81546200	0.85986800
H	0.23687700	3.60751000	-0.01367200
C	-0.80788800	2.09922400	-1.17875400
H	0.01552800	1.76578400	-1.81874100

H	-1.30461800	2.93672300	-1.68959600
C	-1.79317800	0.98297400	-0.97410200
H	-2.70711200	1.25039400	-0.43978100
C	-1.62106400	-0.28549300	-1.38872300
H	-0.71579100	-0.52404900	-1.94293100
C	-2.52977800	-1.40619800	-1.13471400
H	-2.38089800	-2.27706200	-1.77241500
C	-3.47682800	-1.47388200	-0.18456800
H	-3.66336300	-0.65773500	0.50843700
H	-4.10578900	-2.35286600	-0.07866300
B	2.17464200	-0.77109800	-0.41913300
F	3.20347100	-0.04561600	0.11904400
F	1.61405400	-0.18572000	-1.53567200
F	2.39201300	-2.10293800	-0.52425900

Total energy (a.u.): -789.227514

Compound 5

C	2.21558400	1.00692600	-0.57081500
H	2.33296000	0.68539700	-1.60460000
C	2.31267900	2.29867800	-0.23972100
H	2.50845600	3.07146900	-0.97722900
H	2.19683400	2.60214000	0.79732600
C	1.96042500	-0.04428100	0.46479800
C	1.81432300	-1.47744000	-0.03389500
H	2.68525200	-1.71848800	-0.66150700
H	1.81883400	-2.14149300	0.83445100
C	0.55378500	-1.75523200	-0.87216000
H	0.46560800	-1.05721900	-1.71280700
H	0.62546000	-2.76571900	-1.28646500
C	-1.39127000	-0.62726100	0.00262300
C	-2.26749300	-0.37558500	1.00108500
H	-2.41145400	-0.98538600	1.88427800
C	-2.99726900	0.85170400	0.67464700
H	-3.75264700	1.29170000	1.31800600
C	-2.58335600	1.34282000	-0.51150700
H	-2.91300100	2.25221900	-0.99907600
C	-1.50726200	0.44161800	-1.06798300
H	-0.57070100	0.99435700	-1.22629600
H	-1.78694100	0.00362900	-2.03755500
O	1.89549600	0.22718900	1.65198500
O	-0.62793800	-1.75272600	-0.07835400

Total energy (a.u.): 538.652648

Compound 6

C	0.89154300	1.66780800	-0.72757900
H	1.32156500	1.38828000	-1.68749600
C	0.02498000	2.68139300	-0.63315400
H	-0.28016500	3.26336300	-1.49815600
H	-0.39744300	2.94496100	0.33241400
C	1.31167400	0.89069800	0.48034100
O	0.94213800	1.20222700	1.60175300
C	2.28252500	-0.26572400	0.26191500
H	3.21531900	0.16968600	-0.12913800
H	2.50773100	-0.68403200	1.24837600
C	1.83657400	-1.38229300	-0.70391600
H	1.65064100	-0.97008100	-1.70495000
H	2.67997900	-2.07533800	-0.81600100
C	0.59913200	-2.18602400	-0.24297000
H	0.73387600	-2.49632700	0.80147000

H	0.56222800	-3.10818500	-0.84237200
C	-0.70410300	-1.45290500	-0.39755400
H	-0.98403800	-1.19099500	-1.41929700
C	-1.53246800	-1.12569200	0.60704600
H	-1.26280600	-1.43087200	1.61873600
C	-2.79751600	-0.39286800	0.48018300
H	-3.52111100	-0.56979400	1.27645200
C	-3.12033700	0.47330800	-0.49072100
H	-2.42368700	0.73554900	-1.28240400
H	-4.09123000	0.95975900	-0.51320000

Total energy (a.u.): -464.648751

Compound 7

C	1.45109700	1.28625400	-0.88231600
H	1.57749100	0.83779600	-1.86602600
C	1.01243600	2.54203300	-0.75276200
H	0.77154000	3.16236600	-1.61113200
H	0.88555000	2.97169300	0.23698800
C	1.78103700	0.45026100	0.31365500
C	2.15459100	-1.00669700	0.06007700
H	3.07724900	-1.00185100	-0.54091300
H	2.40114300	-1.44801000	1.03139000
C	1.11134900	-1.87541800	-0.67269600
H	0.88420400	-1.45000000	-1.65885900
H	1.57543000	-2.85107600	-0.86584900
C	-0.20450300	-2.10833900	0.10714700
H	0.04149200	-2.42652600	1.12855300
H	-0.72176900	-2.95733800	-0.36426800
C	-1.13563900	-0.93092100	0.16443600
C	-1.46790600	-0.18078500	1.24033200
H	-1.07873000	-0.31133800	2.24509000
C	-2.42224900	0.86174400	0.85093100
H	-2.83736200	1.59617400	1.53370100
C	-2.68950500	0.75318500	-0.46685700
H	-3.35571400	1.37630700	-1.05261900
C	-1.90041700	-0.39893200	-1.03175700
H	-1.23111200	-0.07160100	-1.84158300
H	-2.55264400	-1.16945800	-1.47170300
O	1.80268500	0.92357000	1.43951000

Total energy (a.u.): -502.762979

Compound 8

C	1.87414700	1.65458400	-0.58567700
H	2.48450300	1.38267200	-1.44485100
C	1.04641300	2.70322100	-0.63594500
H	0.95169500	3.32295500	-1.52302300
H	0.44091200	2.95738400	0.22943700
C	1.99942900	0.82428900	0.65278600
O	1.42291700	1.12602400	1.68608200
C	2.93163500	-0.38157200	0.59226600
H	3.94634800	0.00386200	0.40744300
H	2.93192000	-0.83490200	1.58888700
C	2.62304400	-1.44776600	-0.47959500
H	2.66267700	-1.00344900	-1.48346100
H	3.43138100	-2.18904300	-0.44700000
C	1.27571500	-2.18228200	-0.29778100

H	1.18044100	-2.52164500	0.74164300
H	1.30536400	-3.08767900	-0.92266600
C	0.07188600	-1.36901800	-0.68537500
H	0.03198600	-1.04368400	-1.72575300
C	-0.93152400	-1.04241900	0.13957400
H	-0.92166300	-1.39832700	1.16865000
C	-2.10944500	-0.23092100	-0.21090900
C	-2.15562500	0.69234600	-1.18884800
H	-1.26370400	0.90684600	-1.76324700
H	-3.04768000	1.25543400	-1.43175300
O	-3.14623200	-0.54301000	0.62796500
C	-4.34948000	0.19084700	0.48467500
H	-5.02348600	-0.17483900	1.26176800
H	-4.17663100	1.26673500	0.62167800
H	-4.80472000	0.02571100	-0.50115300

Total energy (a.u.): -579.175438

Compound 9

C	1.36649200	1.28929200	-0.85241200
H	1.40112100	0.85733700	-1.85030700
C	0.97460900	2.55314100	-0.66564300
H	0.68685100	3.19663200	-1.49188500
H	0.93621900	2.96631200	0.33845700
C	1.76166000	0.42097400	0.29826300
O	1.84282300	0.85737600	1.43663600
C	2.11806000	-1.02903000	-0.01665700
H	2.99940500	-1.01152000	-0.67603200
H	2.42431000	-1.49525500	0.92568100
C	1.02479800	-1.87275300	-0.70294700
H	0.74894400	-1.43593800	-1.67014000
H	1.45474200	-2.85782200	-0.92297900
C	-0.25577500	-2.07842200	0.13669300
H	0.01211600	-2.38647000	1.15420500
H	-0.82481900	-2.90880700	-0.30401200
C	-1.14153300	-0.88013300	0.23263100
C	-1.56056100	-0.08805500	1.26119400
H	-1.26560500	-0.18466700	2.29672800
C	-2.43022600	0.90165500	0.69573400
H	-2.94425500	1.69758300	1.21659300
C	-2.47995400	0.64026500	-0.63811100
H	-2.99248000	1.09737500	-1.47097900
O	-1.70556800	-0.44192200	-0.94136100

Total energy (a.u.): -538.686596

Compound 10

C	1.21682500	1.20708700	-0.80133200
H	1.11595000	0.66248400	-1.73315800
C	0.99653600	2.52446200	-0.76882100
H	0.71633100	3.07639100	-1.66131100
H	1.09748900	3.07521900	0.16139900
C	1.62398700	0.49491900	0.44671500
O	1.85919800	1.07629800	1.48215400
C	1.33930000	-1.73312800	-0.61368000
H	1.39888300	-1.26788500	-1.60270700
H	2.04525000	-2.56870800	-0.60146500
C	-0.07796900	-2.25108900	-0.32308800
H	-0.07649900	-2.69756400	0.67794400
H	-0.27284700	-3.06223000	-1.04125200

C	-1.15074100	-1.20416000	-0.42398500
H	-1.34661600	-0.80086600	-1.41848000
C	-1.87399300	-0.75568200	0.61460300
H	-1.70708600	-1.20887000	1.59282000
C	-2.90938900	0.28354900	0.55907500
H	-3.70238800	0.19584700	1.30226500
C	-2.94070500	1.31873100	-0.29071400
H	-2.14531900	1.49465800	-1.01007100
H	-3.75517400	2.03713700	-0.27644500
O	1.80191600	-0.85676700	0.42007400

Total energy (a.u.): -618.483535

Compound 11

C	-1.75553600	-0.95415100	0.05320900
C	-1.04040700	-1.86094700	-0.63068400
H	-1.49539800	-2.50071900	-1.38024100
H	0.02461000	-1.97809400	-0.45183000
C	-1.18142500	-0.03370700	1.11362200
C	-1.24543600	1.46526200	0.74097300
H	-2.29801100	1.72332400	0.56676500
H	-0.93253400	2.05089000	1.61625600
C	-0.42258400	1.89022200	-0.48856500
H	-0.54274300	1.14824500	-1.28816000
H	-0.84581100	2.82674300	-0.87424900
C	1.08943600	2.14226900	-0.25890900
H	1.19795800	2.93725100	0.49296400
H	1.50234100	2.53926700	-1.19540400
C	1.89999100	0.94489100	0.16081600
H	1.88203400	0.68299400	1.21904000
C	2.64051200	0.19693600	-0.67407300
H	2.70567900	0.50483200	-1.71909200
C	3.40588700	-1.00541500	-0.31954700
H	4.23052000	-1.24641700	-0.99093600
C	3.17572400	-1.82630900	0.71559100
H	2.34912300	-1.67239400	1.40540500
H	3.81312800	-2.68396300	0.90881200
C	-3.16305700	-0.81400000	-0.21711400
N	-4.30223200	-0.66796700	-0.40503100
H	-1.74244900	-0.18148200	2.04609800
H	-0.15144300	-0.34501500	1.30788300

Total energy (a.u.): -482.878138

Compound 12

C	-1.68135600	-0.85528200	0.03645900
C	-1.02707000	-1.76290100	-0.68518800
H	-1.51788900	-2.37641600	-1.43247800
H	0.03938800	-1.90304900	-0.53253500
C	-1.09532100	0.03867600	1.09509000
C	-1.07988400	1.54179500	0.73313300
H	-2.11673500	1.85661300	0.56549800
H	-0.73151500	2.10140800	1.61230000
C	-0.23854400	1.92791300	-0.49680800
H	-0.38402600	1.18366700	-1.28974500
H	-0.62511800	2.87679100	-0.89103100
C	1.28060900	2.12755800	-0.26292200
H	1.41333500	2.92363100	0.48447200

H	1.71258000	2.50327900	-1.19967300
C	2.04771000	0.90706000	0.17013000
H	1.98625300	0.63378800	1.22382000
C	2.80329900	0.15349000	-0.64585800
H	2.91331400	0.47162500	-1.68406700
C	3.53239100	-1.06676600	-0.27639400
H	4.38842900	-1.30662100	-0.90795600
C	3.23548300	-1.90407300	0.72780400
H	2.37257000	-1.75311900	1.37224400
H	3.84944900	-2.77492000	0.93756400
H	-1.66820900	-0.09080900	2.02267500
H	-0.07999700	-0.31890800	1.29345600
Cl	-3.42445500	-0.62775200	-0.23218900

Total energy (a.u.): -850.233059

Compound 13

C	0.00373000	-0.00402100	0.01528200
H	-0.01596300	-0.00267700	1.10786600
C	1.18523500	-0.00606300	-0.60577500
H	2.12229700	0.00031900	-0.05459900
H	1.25876000	0.00120100	-1.69172200
C	-1.34212900	0.01792100	-0.65935000
C	-2.30952200	-1.06921300	-0.14205200
H	-2.41263800	-0.94190900	0.94523900
H	-3.30792200	-0.88214600	-0.56185100
C	-1.91291300	-2.53042000	-0.42279400
H	-0.84993500	-2.67687800	-0.18993700
H	-2.46673300	-3.17199000	0.27542300
C	-2.21712000	-3.05008400	-1.84974000
H	-3.26747900	-2.83255300	-2.08736000
H	-2.13366100	-4.14771500	-1.82143700
C	-1.34723300	-2.53205000	-2.95878900
C	-1.71519200	-1.81069800	-4.04369200
H	-2.72358900	-1.47321400	-4.26553800
C	-0.54712500	-1.54792800	-4.89270700
H	-0.57884500	-0.98436500	-5.81994900
C	0.54420100	-2.11473300	-4.33814900
H	1.55683800	-2.09857300	-4.72488200
H	-1.81198800	0.99530500	-0.46701000
H	-1.21758000	-0.06179200	-1.74412300
C	0.14102100	-2.79885400	-3.05747100
H	0.68912500	-2.40358500	-2.18971700
H	0.35453800	-3.87890600	-3.08301600

Total energy (a.u.): -428.749379

Compound 14

C	-0.28828500	2.38439900	0.44062500
H	0.55002700	2.23782700	-0.23621600
H	-0.12776300	3.06224100	1.27550600
C	-1.45608800	1.76592400	0.25831500
H	-2.26462400	1.94750100	0.97058100
C	-1.80619800	0.85098400	-0.88675500
H	-0.92187400	0.67364600	-1.51063800
C	-2.45645100	-0.48954600	-0.46955000
H	-3.08435700	-0.84208300	-1.29855900
H	-3.14707900	-0.29798900	0.36515200
C	-1.51752000	-1.64873200	-0.08539200
H	-0.96330500	-1.97752600	-0.97312100
H	-2.15626200	-2.49925300	0.18633700

C	-0.54284100	-1.38852000	1.08175500
H	-1.01168800	-0.70018600	1.79901200
H	-0.40325200	-2.32485800	1.64597200
C	0.83294900	-0.86033900	0.75498200
H	1.37273600	-0.45608100	1.61220100
C	1.47228400	-0.89022800	-0.42479500
H	0.98695700	-1.34492000	-1.28753000
C	2.82424300	-0.36973300	-0.67112500
H	3.36291600	-0.84332400	-1.49318300
C	3.43086900	0.62600900	-0.00964000
H	2.93483700	1.17469300	0.78722100
H	4.44630800	0.92740100	-0.25009700
H	-2.53134500	1.38160400	-1.52315600

Total energy (a.u.): -390.628125

Compound 15

C	-1.93851500	-0.83864300	-0.30696000
C	-1.42650600	-1.68184900	-1.20899800
H	-2.04972700	-2.10971400	-1.98731200
H	-0.37205000	-1.93363200	-1.19590100
C	-1.13939700	-0.18541900	0.79548500
C	-1.02887800	1.35064500	0.63809100
H	-2.04350200	1.75425800	0.53592100
H	-0.62336200	1.77572600	1.56694800
C	-0.18488300	1.82252000	-0.56209900
H	-0.33201500	1.13362000	-1.40327600
H	-0.56077400	2.79843200	-0.89576900
C	1.33156700	1.99281600	-0.29814800
H	1.45823000	2.76829500	0.47327900
H	1.79503400	2.38635300	-1.21211700
C	2.06917800	0.75556100	0.13485800
H	1.86365700	0.38991500	1.14136000
C	2.94813600	0.08204300	-0.62513400
H	3.11835500	0.42783300	-1.64634900
C	3.70044200	-1.11352600	-0.22303800
H	3.98835300	-1.78007800	-1.03703800
C	4.07392000	-1.43629200	1.02279200
H	3.86668700	-0.78926800	1.87172700
H	4.61086000	-2.35694900	1.23185300
H	-1.59354300	-0.40721700	1.77126100
H	-0.14686000	-0.64344200	0.80936000
O	-3.26008800	-0.45887400	-0.44887000
C	-4.06957000	-0.46978300	0.72060500
H	-3.77148000	0.29771800	1.44684100
H	-5.08698200	-0.25651600	0.38449900
H	-4.05314200	-1.45277400	1.21095400

Total energy (a.u.): -505.154338

Compound 16

C	-2.06360500	-1.06772800	-0.15598300
H	-1.33791500	-1.18316200	-0.96111600
C	-3.18027700	-1.79723900	-0.18420100
H	-3.38788600	-2.49889400	-0.98818900
H	-3.93118800	-1.72536000	0.60104700
C	-1.71075100	-0.07444900	0.91951000
C	-1.72337700	1.39839800	0.44549400
H	-2.74324700	1.63502600	0.11429200
H	-1.52504800	2.04427700	1.31336000
C	-0.75676100	1.78243700	-0.68941200

H	-0.88120200	1.10348400	-1.54124600
H	-1.04616900	2.77683800	-1.05361400
C	0.74154900	1.86141500	-0.31782400
H	0.87116400	2.50042200	0.56460400
H	1.26599200	2.36659700	-1.14248500
C	1.42478900	0.56230800	-0.04011000
C	2.18092900	0.09621000	0.99618000
H	2.41740100	0.63613400	1.90298800
C	2.59281500	-1.23392700	0.64665700
H	3.20167100	-1.90813700	1.23303800
C	2.05929100	-1.48246000	-0.57814800
H	2.08153800	-2.32907100	-1.24717400
O	1.34694000	-0.40001300	-1.01547800
H	-2.42646200	-0.17094200	1.74646000
H	-0.72177900	-0.31690000	1.32888300

Total energy (a.u.): -464.671727

Compound 17

C	-2.05991100	-1.11655000	-0.02152000
H	-1.21573900	-1.36109500	-0.66652500
C	-3.16135500	-1.86597000	-0.08904500
H	-3.24096500	-2.70885000	-0.77071300
H	-4.02703000	-1.66946100	0.54130400
C	-1.88211000	0.06700500	0.89369700
C	-1.81496500	1.42596900	0.16161200
H	-2.73979900	1.56899800	-0.41450600
H	-1.77345200	2.23250700	0.90449800
C	-0.64656100	1.60977100	-0.80441000
H	-0.60963500	0.82482900	-1.56367800
H	-0.73255000	2.57303200	-1.31441800
C	1.34689600	0.56341100	0.03536200
C	2.19728200	0.18819400	1.03317300
H	2.38072700	0.72828500	1.94970000
C	2.77991800	-1.05210300	0.59781400
H	3.50318000	-1.65211300	1.13299300
C	2.23867800	-1.33935900	-0.61277900
H	2.33797000	-2.15246300	-1.31399600
O	1.35415200	-0.34494400	-0.98125900
H	-2.71669300	0.10348700	1.60498300
H	-0.96748900	-0.06076300	1.48836600
O	0.62262800	1.68136900	-0.11142000

Total energy (a.u.): -500.563140

Compound 18

C	4.22260300	1.98443700	0.61764100
H	4.35816600	1.77635700	1.67740800
H	4.09871000	3.02798000	0.34054500
C	4.21791600	1.00824200	-0.29228700
H	4.08388100	1.26826600	-1.34455300
C	4.41478700	-0.45547200	-0.00111900
H	4.54561600	-0.59939500	1.07993400
C	3.30230400	-1.39775800	-0.51287200
H	3.65253900	-2.42674400	-0.36075800
H	3.19079800	-1.27687900	-1.60018400
C	1.92659200	-1.24881700	0.16541800
H	2.06866900	-1.09466000	1.24507100

H	1.37465500	-2.19205500	0.06324200
C	1.04657100	-0.11426100	-0.40423100
H	1.58616000	0.83625800	-0.30746300
H	0.88137500	-0.28412800	-1.47602600
C	-0.27300400	-0.00440400	0.30194000
H	-0.22725900	0.25260800	1.36175900
C	-1.46834200	-0.19842100	-0.27490900
H	-1.53174400	-0.39285700	-1.34080700
C	-2.74249700	-0.13930900	0.44367400
C	-2.98802200	-0.42015300	1.72789400
H	-2.19067600	-0.77363100	2.37178200
H	-3.98108800	-0.30425900	2.14232100
H	5.35716900	-0.77636800	-0.47119700
N	-3.91772300	0.27538200	-0.38375300
O	-5.01424200	0.37291500	0.16136800
O	-3.71030200	0.49550200	-1.57657900

Total energy (a.u.): -595.136695

Compound 19

C	-2.41704300	-0.84529700	0.32638500
C	-1.75208700	-1.84432500	-0.27241800
H	-2.23405200	-2.62458500	-0.84895400
H	-0.67371300	-1.89461400	-0.18111700
C	-1.76612200	0.24809600	1.13486200
C	-1.91358900	1.65114000	0.50107200
H	-2.98285500	1.82623800	0.33766400
H	-1.58975200	2.40540300	1.23191700
C	-1.15895000	1.85631900	-0.82737200
H	-1.17384200	0.92306600	-1.40455800
H	-1.69859500	2.59900900	-1.42908600
C	0.30133400	2.35863400	-0.70793600
H	0.28471200	3.33962800	-0.20858500
H	0.69069700	2.53121900	-1.71952600
C	1.24677400	1.45671700	0.03540100
H	1.09491200	1.37240000	1.11183200
C	2.24581300	0.76322600	-0.53203300
H	2.36466400	0.82515600	-1.61576000
C	3.20369700	-0.11518100	0.15805900
C	3.55286000	-0.04150300	1.45632400
H	3.16143700	0.72184200	2.12184900
H	4.25813700	-0.75915700	1.86377800
H	-2.23663200	0.26564300	2.12726600
H	-0.71296900	-0.00760900	1.28029300
O	-3.77195100	-0.66175500	0.29193200
C	-4.54434700	-1.59293200	-0.44834300
H	-4.43751100	-2.60799100	-0.04374300
H	-5.58319400	-1.27020200	-0.35595500
H	-4.25280900	-1.59876900	-1.50694100
C	3.86127600	-1.16577300	-0.68240000
O	4.64502800	-1.99834800	-0.27333000
H	3.57905500	-1.14058200	-1.75879800

Total energy (a.u.): -618.483535

Compound 20

C	-2.69448800	-0.75533000	0.52428800
C	-1.91086700	-1.77112100	0.92089700
H	-1.92955700	-2.75471100	0.46742900
H	-1.24962800	-1.63466500	1.76876100
C	-2.73385500	0.59688200	1.19705000

C	-2.75065200	1.80768300	0.24257800
H	-3.66514500	1.75145600	-0.35823400
H	-2.83961900	2.71420300	0.85716400
C	-1.56051500	1.97558800	-0.71697000
H	-1.47409100	1.09536100	-1.36606100
H	-1.80123500	2.81606700	-1.38024700
C	-0.18449400	2.27442700	-0.05937200
H	-0.35268600	2.85122500	0.86327500
H	0.39958000	2.92180200	-0.72422500
C	0.63095200	1.05152400	0.25092300
H	0.19513100	0.32918700	0.93872500
C	1.83429300	0.79440000	-0.28297500
H	2.31265500	1.52360900	-0.92956200
C	2.57903800	-0.44252000	-0.03869000
C	2.09133600	-1.66492300	0.19917000
H	1.01954900	-1.83233300	0.19411000
H	2.75377000	-2.49862000	0.39440200
H	-3.64992100	0.64556100	1.80346600
H	-1.89867400	0.66058600	1.90259700
O	-3.59153000	-0.80723900	-0.50177900
C	-3.71106700	-2.02838000	-1.21647400
H	-4.03576100	-2.84293400	-0.55637400
H	-4.46510600	-1.85746600	-1.98679600
H	-2.75907700	-2.30616500	-1.68698800
N	4.06638700	-0.30932800	-0.08528400
O	4.75366300	-1.30392900	0.13407700
O	4.51749400	0.80538800	-0.34817300

Total energy (a.u.): -709.663357

Compound 21

C	-2.33687400	-0.69439200	0.54346000
C	-1.58412700	-1.72947600	0.94913900
H	-1.64714000	-2.72120500	0.51792800
H	-0.89983600	-1.59897600	1.77938600
C	-2.31194300	0.67453400	1.18185300
C	-2.28258700	1.85886800	0.19476900
H	-3.19817400	1.82135300	-0.40577500
H	-2.33653600	2.78480200	0.78402300
C	-1.08500300	1.95279900	-0.76508000
H	-1.03090800	1.05144800	-1.38820400
H	-1.29056800	2.78223200	-1.45361100
C	0.29914800	2.21548700	-0.10846600
H	0.14746300	2.80091100	0.81163900
H	0.90177300	2.84380800	-0.77529100
C	1.07846800	0.97004400	0.20704100
H	0.61713100	0.25807500	0.88898000
C	2.27946900	0.67975600	-0.31308300
H	2.77584000	1.40347900	-0.95825500
C	3.02293300	-0.57251400	-0.05854100
C	2.46157700	-1.77434100	0.17862700
H	1.38281400	-1.89513200	0.15972200
H	3.06587400	-2.65053100	0.38755400
H	-3.22027100	0.77920100	1.79271600
H	-1.46862500	0.71984900	1.87920900
O	-3.25569800	-0.73638100	-0.46418200
C	-3.43546500	-1.96865000	-1.14609800
H	-3.77678900	-2.75440600	-0.45994000
H	-4.19831700	-1.78771300	-1.90542300
H	-2.50455700	-2.29374500	-1.62836300
C	4.46098900	-0.47015300	-0.09308000
N	5.61812800	-0.35773900	-0.13372600

Total energy (a.u.): -597.404498

Compound 22

C	-0.06239000	-1.36326700	-0.15958300
H	0.11653500	-1.24376100	0.90612200
H	0.67157200	-1.91925200	-0.72999700
C	-1.17154900	-0.89413900	-0.75898700
H	-1.31877600	-1.05166700	-1.82692500
C	-3.23018600	0.52084300	-0.88895900
H	-4.22907900	0.21886500	-0.53985000
H	-3.16776500	0.21855100	-1.94159200
C	-3.13542600	2.05303000	-0.77991200
H	-3.15460900	2.34141000	0.28056000
H	-4.05473200	2.46142100	-1.22357400
C	-1.92670100	2.73252000	-1.46711000
C	-0.59575500	2.52203300	-0.79634800
H	-0.14423100	1.53598700	-0.89086200
C	0.05202000	3.47430600	-0.10436000
H	-0.39574900	4.46867400	-0.05371700
C	1.33937400	3.32851500	0.58836300
H	1.83468800	4.26647200	0.84144400
C	1.94158500	2.18330600	0.94030200
H	1.49871500	1.20912700	0.74620500
H	2.90910800	2.18842700	1.43415100
N	-2.22420800	-0.23407200	-0.16124800
H	-2.09745400	0.02002800	0.81060300
H	-2.13298900	3.80972400	-1.51312600
H	-1.87840100	2.38096400	-2.50930100

Total energy (a.u.): -406.668408

Compound 23

C	-3.10059500	-1.18211300	-0.20871200
C	-2.26671800	-1.91232900	-0.95791700
H	-2.62558800	-2.53524900	-1.77384800
H	-1.19350900	-1.91565900	-0.78257200
C	-2.59612300	-0.32188800	0.93269900
C	-2.73930800	1.20241500	0.70066000
H	-3.79657000	1.42475700	0.50953400
H	-2.49443700	1.72507800	1.63606600
C	-1.89240300	1.77793500	-0.45228200
H	-1.82709000	1.04152800	-1.26285100
H	-2.40960900	2.65115300	-0.86992100
C	-0.46566200	2.25201500	-0.07653100
H	-0.55707200	3.04654000	0.67917500
H	-0.01249200	2.71182700	-0.96360400
C	0.45994400	1.19172400	0.44969900
H	0.25602000	0.81649300	1.45259600
C	1.51548300	0.70862700	-0.22365100
H	1.77610800	1.12205600	-1.19284300
C	2.38690700	-0.35646400	0.27584700
C	2.08204900	-1.36398700	1.10075300
H	1.06747900	-1.48814800	1.46237700
H	2.83769400	-2.07168600	1.41654100
H	-3.15510400	-0.57731500	1.84543800
H	-1.54734300	-0.56925900	1.12993700
N	3.79613900	-0.30790800	-0.22421100
O	4.59047900	-1.15468300	0.17660500
O	4.07463700	0.58849400	-1.01980400
C	-4.59147600	-1.18677800	-0.44960000
H	-5.13359400	-1.50832700	0.45047400

H	-4.96703100	-0.18547300	-0.69813800
H	-4.86434800	-1.85838500	-1.26908300

Total energy (a.u.): -634.452954

Compound 24

C	-1.83805900	-2.35535500	0.81064800
H	-1.83198700	-2.02510300	1.84427700
H	-1.60306200	-3.39224300	0.60001700
C	-2.12285500	-1.52787900	-0.18836300
H	-2.14584200	-1.79095700	-1.23930900
C	-2.71380500	0.61596900	-0.98697300
C	-3.07654800	2.00839700	-0.51285200
H	-2.76927100	2.14018500	0.52790000
H	-4.17327300	2.06388300	-0.53211100
C	-2.50788500	3.10586400	-1.42168900
H	-2.77317300	2.86828800	-2.46090000
H	-3.02329100	4.05025700	-1.19332900
C	-1.02238100	3.33596700	-1.33101200
H	-0.64327700	4.11680400	-1.99107500
C	-0.14771200	2.68324400	-0.55002200
H	-0.49495200	1.85723700	0.07029400
C	1.29328900	2.96238500	-0.47396600
H	1.92269500	2.10723300	-0.22505800
C	1.87953700	4.15286400	-0.65646800
H	1.30312500	5.05350200	-0.85361500
H	2.95848700	4.26619200	-0.60511400
O	-2.42386800	-0.20045900	0.07552000
O	-2.70618900	0.24805100	-2.13764500

Total energy (a.u.): -500.572784

Compound 25

C	-1.75526200	-0.68901000	-0.28048400
C	-1.07248000	-1.59782400	-0.97191900
H	-1.54416700	-2.18618800	-1.75175100
H	-0.02180600	-1.76943300	-0.76610000
C	-1.22362900	0.20088800	0.80854900
C	-1.25976600	1.70555500	0.45004000
H	-2.29341700	1.96371000	0.18954900
H	-1.02436200	2.28502900	1.35328900
C	-0.33346000	2.13844300	-0.70313200
H	-0.30522100	1.35090900	-1.46672700
H	-0.76823800	3.02122400	-1.18925200
C	1.11522100	2.51794400	-0.30778400
H	1.06669300	3.36178100	0.39730100
H	1.62817400	2.88992900	-1.20383100
C	1.93785500	1.42004800	0.30755800
H	1.66517700	1.11331000	1.31763400
C	2.96678400	0.80788500	-0.29890100
H	3.20854800	1.10169300	-1.32248100
C	3.80884700	-0.25986800	0.26329300
C	3.99140800	-0.52229400	1.57124800
H	3.53458100	0.07387200	2.35530100
H	4.62453300	-1.35282600	1.86752100
H	-1.81960700	0.03541800	1.71342700
H	-0.20260400	-0.12073100	1.03418500
C	4.54558400	-1.10909100	-0.72636900
O	5.24980300	-2.05742700	-0.44517100
H	4.40662300	-0.80776000	-1.78890600
O	-3.09173800	-0.44477900	-0.66405000

C	-4.09394600	-0.78506900	0.20129600
O	-3.91235200	-1.31181000	1.27257500
C	-5.43407300	-0.41137200	-0.38567800
H	-5.57041500	-0.90029700	-1.35562600
H	-6.22630500	-0.71423700	0.29951600
H	-5.48239000	0.66931600	-0.55618100

Total energy (a.u.): -731.835050

Compound 26

C	-0.57045500	-1.41217400	-0.11544400
H	-0.45044200	-1.40310200	0.96277800
H	-0.05192400	-2.17283000	-0.68698300
C	-1.31688800	-0.50332800	-0.74233900
H	-1.44299600	-0.50262300	-1.82634400
C	-2.92943300	1.22141900	-0.84061500
H	-3.78095500	0.55942500	-1.05938500
H	-2.49457200	1.53523600	-1.80302000
C	-3.41276000	2.44080200	-0.06420400
H	-3.82868400	2.11923700	0.89817400
H	-4.25575800	2.84663500	-0.63891200
C	-2.38484300	3.57062800	0.14023400
H	-1.77864700	3.67284100	-0.77499800
H	-2.93396200	4.52214000	0.21085700
C	-1.45848500	3.50669400	1.32845000
H	-0.83977400	4.39730800	1.45089900
C	-1.34304500	2.53108800	2.24100300
H	-1.97089200	1.64726800	2.15967100
C	-0.41663800	2.55171700	3.38200000
H	-0.74554000	1.99373500	4.26002400
C	0.77704000	3.15829900	3.42869700
H	1.18899100	3.68300000	2.57007100
H	1.38764100	3.13853900	4.32688700
O	-1.95329600	0.50692300	-0.08521100

Total energy (a.u.): -426.527671

Compound 27

C	-1.20876000	-2.15706600	-0.33568900
H	-1.33538500	-2.40418000	0.71620700
H	-0.44894200	-2.70012100	-0.88515600
C	-1.97646000	-1.24855000	-0.95587900
H	-1.81812900	-1.01213900	-2.00544600
C	-3.42487600	0.76034600	-0.87730300
H	-4.43265800	0.97549200	-0.50507900
H	-3.47817500	0.72733300	-1.96931800
C	-2.48271200	1.90956400	-0.46472800
H	-2.23085200	1.82486800	0.59853700
H	-3.01116400	2.86827700	-0.58085500
C	-1.22051000	1.99876900	-1.32601600
C	-0.00849200	2.67216700	-0.81228700
H	0.80104300	2.70600000	-1.53828100
C	0.13699800	3.23485200	0.40490400
H	-0.70841200	3.23278100	1.09099800
C	1.34436000	3.89277200	0.90889700
H	1.19053200	4.58264200	1.73792100
C	2.59372700	3.69262500	0.46456900
H	2.81976300	2.98063200	-0.32476400
H	3.43545500	4.22815300	0.89308600
O	-1.21628400	1.55477600	-2.46899400
N	-3.05158100	-0.56249700	-0.39921900

H	-3.13194900	-0.67435000	0.60624800
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Total energy (a.u.): -480.686362

Compound 28

C	-1.90714500	-2.65900900	-0.59542400
H	-2.19436100	-2.98106800	0.40029600
H	-1.35090200	-3.34703800	-1.22088700
C	-2.22056300	-1.44926300	-1.05944100
H	-1.93124200	-1.10111800	-2.04858000
C	-3.21836100	0.71845400	-0.89122600
H	-4.22379600	0.98085100	-0.54706700
H	-3.22940700	0.65166100	-1.98446300
C	-2.22887900	1.79071800	-0.43515700
H	-2.07399100	1.69334000	0.64485200
H	-2.67137900	2.78494400	-0.59881200
C	-0.89506200	1.75489700	-1.18560600
C	0.27809100	2.46925200	-0.64112200
H	1.16648800	2.37393000	-1.26174400
C	0.30795300	3.18489200	0.50193000
H	-0.58543600	3.21969600	1.12341800
C	1.45751600	3.92692900	1.02292500
H	1.42897600	4.14651400	2.08948100
C	2.49803600	4.37211400	0.30342700
H	2.56146700	4.22889000	-0.77202300
H	3.31650300	4.91016100	0.77191000
O	-2.92616600	-0.54990900	-0.30938700
O	-0.79674100	1.17144200	-2.25948200

Total energy (a.u.): -500.548240

Compound 29

C	0.24692400	0.42604200	0.14703600
C	0.12880700	0.26168300	1.51085100
C	1.26733900	-0.47388300	1.94512900
C	2.03782600	-0.73018300	0.83065600
N	1.41179100	-0.18250400	-0.26736400
H	-0.40242600	0.91117600	-0.56845300
H	-0.68796200	0.61924800	2.12347300
H	1.49102100	-0.78985400	2.95541400
H	2.97285500	-1.26231200	0.72223100
C	1.93928400	-0.18272800	-1.62620800
H	2.26913900	-1.19985300	-1.86881600
H	1.10938000	0.04995500	-2.30039900
C	3.10561300	0.79589400	-1.84069200
H	3.92795000	0.51122000	-1.17179900
H	3.47054800	0.66277900	-2.86775300
C	2.76842500	2.28450700	-1.60481500
H	2.39682800	2.39753300	-0.57651000
H	3.69787100	2.86364900	-1.66828800
C	1.76262500	2.84974900	-2.56922800
H	0.74902900	2.45070800	-2.51463800
C	2.02885500	3.79056700	-3.48913400
H	3.05432300	4.15482600	-3.57457700
C	1.06332800	4.37505800	-4.42879600
H	1.48327100	4.73254100	-5.36984600
C	-0.25226800	4.52342100	-4.22273700
H	-0.90030300	4.94688200	-4.98456100
H	-0.72302900	4.23930300	-3.28467200

Total energy (a.u.): -556.923545

Compound **30**

C	-0.15695100	-0.20451900	0.56991800
C	-0.16871200	-1.03934500	1.65059500
C	1.12271900	-1.66215100	1.73441100
C	1.87887200	-1.18685400	0.70030800
N	1.09956100	-0.28338100	-0.02826600
H	-0.90393200	0.44709400	0.14605800
H	-1.00564200	-1.19804900	2.31725100
H	1.44844900	-2.37981800	2.47555900
H	2.89586600	-1.40642100	0.41790300
C	1.45110700	0.46709000	-1.17019800
C	2.87324000	0.32671300	-1.68324300
H	3.21619200	-0.71039500	-1.61130900
H	2.84505700	0.60202200	-2.74046600
C	3.86941400	1.25749100	-0.93430100
H	3.84859800	1.00374000	0.13557600
H	4.88007700	1.03178800	-1.29455200
C	3.57473100	2.71894300	-1.12541800
H	2.59568600	3.06581600	-0.79746500
C	4.43173300	3.59863300	-1.66570200
H	5.42760800	3.24987300	-1.94584000
C	4.16428300	5.02405600	-1.89841600
H	5.03811900	5.67627700	-1.87734900
C	2.96633400	5.56691300	-2.15339400
H	2.84965900	6.63755400	-2.29449900
H	2.06805000	4.96076800	-2.24125500
O	0.64105300	1.21840900	-1.67943000

Total energy (a.u.): -556.923545

Table S2: Cartesian coordinates, total energies and imaginary frequencies for transition state structures.

TS1.

C	-0.74939400	1.62195800	-0.28395000
H	-0.56596200	1.65463800	-1.37587300
C	0.27921000	1.77551300	0.59063300
H	0.07919000	1.97622100	1.65965700
C	1.63296600	1.59211200	0.20341900
H	2.41693100	1.87903600	0.93268300
C	1.99645900	0.92658600	-0.96518600
H	1.29933300	0.94222200	-1.82684200
H	3.06241100	0.95644400	-1.26643500
C	-2.13525600	1.30529100	0.11366900
H	-2.85633400	1.67468200	-0.66498100
H	-2.41171100	1.79286500	1.08690400
C	-2.26313500	-0.21056300	0.25754200
H	-1.84692600	-0.51888800	1.25208200
H	-3.36037900	-0.45291900	0.27561900
C	-1.59577300	-0.99485600	-0.85724500
H	-2.35393600	-1.69933600	-1.30326100
H	-1.27285200	-0.31909900	-1.69098900
C	-0.42756100	-1.88331400	-0.43005100
H	-0.07964500	-2.44361000	-1.34828200
H	-0.81696200	-2.64664200	0.30714400
C	1.84415600	-0.93446800	-0.53579100
H	1.86788600	-1.27251100	-1.59742100
H	2.81164500	-0.98100700	0.01694800
N	0.73299700	-1.25156800	0.17796600
C	0.81405500	-1.22301100	1.62012400
H	-0.18153800	-1.46060700	2.07832400
H	1.56724700	-1.97468700	1.98416300
H	1.13626400	-0.19731400	1.95581500

Total energy (a.u.): -446.329952

Imaginary frequency (cm^{-1}): 279i

TS2

C	-0.27833800	-0.17052000	0.25437400
H	-0.94930100	-0.62050600	0.98082500
H	0.76845400	-0.42495500	0.34611200
C	-0.59773600	1.10815100	-0.19921500
C	-1.75588300	1.92746700	0.34361600
H	-1.39141600	2.44864600	1.24206300
C	-2.47294300	2.99235900	-0.51746300
H	-1.74995800	3.75829200	-0.80465400
H	-3.19665500	3.47733700	0.15152100
C	-3.23646500	2.52066100	-1.76300600

H	-3.78063300	3.38219000	-2.17006800
H	-4.00353000	1.78510000	-1.47570300
C	-2.36726100	1.91665600	-2.87973500
H	-2.99969900	1.74586800	-3.76598900
H	-1.58740000	2.62554400	-3.18737200
C	-1.74964500	0.61766600	-2.45558700
H	-2.35293100	0.04176600	-1.75827300
C	-0.64181200	0.02191300	-2.99461000
H	-0.09597600	0.52873000	-3.78783900
C	-0.03617500	-1.10626600	-2.38873900
H	0.95214300	-1.39205500	-2.73986900
C	-0.52449400	-1.68964700	-1.22731800
H	-1.59243800	-1.70631300	-1.03509900
H	0.01918100	-2.52022800	-0.78500500
H	-2.49704600	1.20202100	0.70578900
N	0.49942000	1.80022900	-0.83330100
O	1.47815500	1.12701800	-1.19976600
O	0.42158000	3.02804600	-1.00174500

Total energy (a.u.): -595.109207

Imaginary frequency (cm^{-1}): 415i

TS3

C	-0.08077000	-0.35717100	-0.03344200
H	-0.08785300	-0.39357700	1.05277500
H	0.88979800	-0.46005500	-0.49988400
C	-0.99406000	0.50611600	-0.64205800
C	-1.95686400	1.40730800	0.10731900
H	-1.44213500	2.36246000	0.29357500
C	-3.33776800	1.77301400	-0.48870100
H	-3.18383100	2.25377400	-1.45716000
H	-3.75539900	2.53974700	0.17787400
C	-4.39617200	0.66746700	-0.62865900
H	-5.34536700	1.14780700	-0.89839800
H	-4.56722000	0.18760200	0.34753700
C	-4.09713900	-0.42777900	-1.66953100
H	-4.98424500	-1.07525400	-1.75923600
H	-3.93396700	0.01447200	-2.66075600
C	-2.91617400	-1.25809700	-1.26703100
H	-2.79379600	-1.36091100	-0.19238700
C	-2.10313700	-1.97513200	-2.08431100
C	-0.89448500	-2.57314600	-1.60845400
C	-0.47015200	-2.41969800	-0.28569700
H	-1.23713800	-2.40438800	0.47792700
H	0.45721500	-2.87893400	0.03892600
H	-2.10258500	0.95277800	1.09696900
N	-0.69679400	0.80865400	-2.00772100
O	0.07604200	0.04501300	-2.62122400
O	-1.21988000	1.80502000	-2.53863900
H	-2.24329000	-1.96757700	-3.16217400
O	-0.15467800	-3.13055300	-2.59147400
C	1.13710800	-3.64070800	-2.28747000
H	1.51303900	-4.06518500	-3.21941000
H	1.80857800	-2.84058200	-1.95686600
H	1.08840300	-4.42442500	-1.52060400

Total energy (a.u.): -709.635612

Imaginary frequency (cm^{-1}): 397i

TS4

C	0.05447300	0.12448700	0.02716400
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H	0.06656100	0.08535700	1.11189500
C	1.24686700	0.09623400	-0.69175100
H	2.17892200	0.28771200	-0.16775800
H	1.22158100	0.39199300	-1.73406300
C	-1.21422800	0.18261700	-0.62376500
O	-1.22989600	0.30119600	-1.89488600
C	-2.48816400	0.15690600	0.19811200
H	-2.49560200	1.07283300	0.80648900
H	-3.34342000	0.21647700	-0.47207700
C	-2.61263900	-1.06001000	1.13997700
H	-1.90967900	-0.96903100	1.97846000
H	-3.61713500	-1.05604200	1.57868300
C	-2.36499400	-2.40526700	0.41726900
H	-3.05085400	-2.50316800	-0.42936000
H	-2.57424500	-3.21952000	1.12648900
C	-0.94615300	-2.48806100	-0.05407300
H	-0.18604700	-2.44065000	0.72348100
C	-0.56573000	-2.66244700	-1.35799000
H	-1.34403700	-2.79834500	-2.10283200
C	0.74688100	-2.41411600	-1.83207900
H	0.88363300	-2.42979300	-2.91152500
C	1.78929300	-1.92652600	-1.05538600
H	1.82691700	-2.14167600	0.00784700
H	2.76007300	-1.77416800	-1.51947000
B	-2.49986300	0.12320500	-2.84026900
F	-2.99603000	-1.14717900	-2.54560800
F	-3.39464600	1.11681900	-2.50937800
F	-1.98357800	0.22353700	-4.09733700

Total energy (a.u.): -789.216893

Imaginary frequency (cm⁻¹): 342i

TS5

C	0.33652400	0.24590900	0.19425000
H	0.23099700	0.06717900	1.26030300
C	1.54040500	-0.10679000	-0.42004400
H	2.42572700	-0.22734200	0.19983400
H	1.73455000	0.28706000	-1.41256500
C	-0.79896600	0.85431200	-0.48589300
C	-2.13784700	0.75713100	0.27345900
H	-2.18232100	1.55584600	1.02885600
H	-2.93598300	0.94669400	-0.45031700
C	-2.36353700	-0.57760500	0.99933900
H	-1.71050400	-0.67617800	1.87557700
H	-3.39758500	-0.66139300	1.34370200
C	-0.94445100	-1.85221500	-0.42444100
C	-0.73744900	-1.85142000	-1.80111000
H	-1.49645500	-1.60682600	-2.53375700
C	0.62567400	-2.04956300	-2.04941200
H	1.09119300	-1.99473100	-3.02789200
C	1.32644900	-2.11441900	-0.82523900
H	2.34372000	-2.48871100	-0.75648800
C	0.28384900	-2.46023800	0.22846200
H	0.50406600	-2.14472100	1.24818400
H	0.15984800	-3.55543700	0.23098200
O	-0.74660700	1.36974100	-1.60053900
O	-2.17775600	-1.71355800	0.12977200

Total energy (a.u.): -538.624349

Imaginary frequency (cm⁻¹): 413i

TS6 cis-boat

C	0.22237500	-1.10618000	-0.86712100
H	-0.23283100	-0.90402800	-1.83253900
C	1.59024100	-1.36072200	-0.77676700
H	2.13517600	-1.60581900	-1.68512300
H	1.92793300	-1.86464300	0.12324000
C	-0.63551700	-1.23481000	0.31247500
O	-0.19471400	-1.60959400	1.39964600
C	-2.11830900	-0.87773300	0.15805400
H	-2.62265400	-1.71019000	-0.35485700
H	-2.53252200	-0.83142400	1.17093700
C	-2.40501400	0.42616900	-0.60951500
H	-2.19462300	0.29275100	-1.67880700
H	-3.47535100	0.65767200	-0.53833100
C	-1.58639100	1.62943500	-0.08659100
H	-1.81741400	1.79400700	0.97370300
H	-1.90710200	2.53046000	-0.63045500
C	-0.10780400	1.42163000	-0.25751100
H	0.25801200	1.40764600	-1.28022100
C	0.79035800	1.41722200	0.78470300
H	0.40922100	1.61102100	1.78606800
C	2.11290300	0.94467400	0.67851900
H	2.66804400	0.80902800	1.60432200
C	2.63118100	0.38695800	-0.49021000
H	2.32016700	0.78341900	-1.45229700
H	3.65752000	0.02699100	-0.47901600

Total energy (a.u.): -464.626425
Imaginary frequency (cm⁻¹): 430i

TS6 trans-boat

C	-0.09444300	-0.94415300	0.88700000
H	0.13560400	-0.31677500	1.74074900
C	-1.36457900	-1.50753200	0.76702300
H	-2.01880900	-1.50120900	1.63305600
H	-1.45284100	-2.37572000	0.11893900
C	0.97961800	-1.25988500	-0.05618600
O	0.82760100	-2.05351100	-0.98589700
C	2.30949100	-0.51281100	0.11167200
H	2.90567200	-1.04631000	0.86714400
H	2.84521100	-0.61548800	-0.83842400
C	2.19451800	0.96405400	0.53046100
H	1.83363200	1.03252200	1.56376800
H	3.19462300	1.41597400	0.52741100
C	1.25837500	1.81176100	-0.37034300
H	1.72498500	1.91966700	-1.35961800
H	1.17670800	2.81840000	0.05922100
C	-0.10678500	1.19962800	-0.53083800
H	-0.18353000	0.42619300	-1.28692100
C	-1.27401300	1.68982000	0.01368600
H	-1.23429000	2.60844300	0.59948800
C	-2.47605400	0.95413300	0.01141700
H	-3.30858900	1.34627200	0.59318300
C	-2.55518700	-0.35525900	-0.46489300
H	-1.95355900	-0.65200800	-1.31983000
H	-3.51127600	-0.87040600	-0.40498100

Total energy (a.u.): -464.623827
Imaginary frequency (cm⁻¹): 449i

TS6 cis-chair

C	0.41057400	-1.17214400	-0.90123900
H	0.06758900	-1.03160900	-1.92273700
C	1.76476000	-1.33605200	-0.62104800
H	2.44666900	-1.56265400	-1.43664200
H	2.00808700	-1.78538800	0.33647600
C	-0.58397500	-1.29707600	0.16422800
O	-0.27022400	-1.56943500	1.32477900
C	-2.04105400	-0.99044300	-0.18569200
H	-2.22944900	-1.12732500	-1.25874200
H	-2.67496000	-1.69331400	0.36530700
C	-2.40574700	0.45030100	0.23114000
H	-3.48347700	0.61421400	0.10442000
H	-2.19098400	0.55786800	1.30139000
C	-1.63760600	1.52336900	-0.57081500
H	-1.92981200	2.51559400	-0.19485400
H	-1.95677100	1.48559400	-1.61955700
C	-0.13601800	1.37302500	-0.49815800
H	0.39864400	1.32304200	-1.44043300
C	0.58001200	1.47112700	0.67167300
H	0.04112900	1.69824300	1.59052000
C	1.92421500	1.06574200	0.80000600
H	2.33101400	1.00395900	1.80716000
C	2.65424400	0.49966800	-0.24276800
H	2.47546000	0.83252000	-1.26096500
H	3.68221300	0.19963300	-0.05352700

Total energy (a.u.): -464.625510
Imaginary frequency (cm⁻¹): 428i

TS6 trans-chair

C	-0.19571500	-1.01046800	0.88765500
H	-0.08685800	-0.45931300	1.81622100
C	-1.41665700	-1.60169700	0.57374100
H	-2.16513400	-1.70308500	1.35261200
H	-1.40325900	-2.39066900	-0.17370800
C	1.00835200	-1.22590000	0.08237300
O	1.01025400	-1.89825700	-0.95009000
C	2.26331400	-0.46513300	0.51265200
H	2.25171700	-0.26409900	1.59142800
H	3.13483400	-1.08825900	0.28714600
C	2.37812900	0.86457900	-0.26859600
H	3.32293100	1.35972100	-0.01371400
H	2.42530400	0.62287400	-1.33830300
C	1.21076900	1.83815500	-0.01963100
H	1.36633600	2.72438100	-0.65637100
H	1.22652100	2.20310300	1.01633600
C	-0.13072500	1.23331400	-0.33348700
H	-0.13913500	0.56072200	-1.18642100
C	-1.34138500	1.65242400	0.17215700
H	-1.35885400	2.48256400	0.87863700
C	-2.53081500	0.91920700	-0.01682300
H	-3.41100400	1.23606100	0.54029700
C	-2.55643400	-0.32333800	-0.64559800
H	-1.87551700	-0.53044400	-1.46582400
H	-3.50291000	-0.85435700	-0.71427600

Total energy (a.u.): -464.625855
Imaginary frequency (cm⁻¹): 442i

TS7

C	0.30841400	0.16940100	0.29515100
H	0.13893700	-0.06099500	1.34152600
C	1.56883400	-0.07848200	-0.25529900
H	2.41463900	-0.19524800	0.41863100
H	1.80474500	0.40435200	-1.19828300
C	-0.79482600	0.75547600	-0.45695300
C	-2.18495600	0.64975500	0.19298800
H	-2.32425800	1.51876700	0.85304200
H	-2.91765700	0.75540200	-0.61512700
C	-2.43536600	-0.63373500	1.00756400
H	-1.82649700	-0.62540200	1.91962900
H	-3.47942400	-0.64789200	1.34640700
C	-2.15638000	-1.94420400	0.22576900
H	-2.91806700	-2.04822100	-0.55824400
H	-2.29413200	-2.79239500	0.91070800
C	-0.79776900	-2.00746500	-0.42094400
C	-0.56605700	-1.87564500	-1.78864000
H	-1.33022700	-1.64380700	-2.52302800
C	0.80884200	-1.93430600	-2.05125800
H	1.26692500	-1.77321300	-3.02137900
C	1.50732300	-2.03000100	-0.82888500
H	2.55043500	-2.33179400	-0.77973800
C	0.48741400	-2.53524000	0.18258700
H	0.67629600	-2.27007500	1.22428100
H	0.47705600	-3.63696700	0.11689400
O	-0.65580900	1.27319800	-1.56517900

Total energy (a.u.): -502.734803
Imaginary frequency (cm⁻¹): 418i

TS8

C	0.06730000	-0.10506900	-0.13150400
H	0.09188000	0.02007900	0.94765200
C	1.25128700	-0.33202300	-0.84119000
H	2.19562600	-0.07546900	-0.36601300
H	1.20633500	-0.13682400	-1.90899600
C	-1.20318800	0.00654500	-0.83242000
O	-1.28219300	-0.02029100	-2.06437600
C	-2.47662900	0.13281700	0.01651700
H	-2.51970300	1.14679200	0.44083500
H	-3.32017400	0.03946700	-0.67580600
C	-2.60063300	-0.88720600	1.16484700
H	-1.88841500	-0.64530800	1.96477000
H	-3.59911600	-0.80394900	1.61303400
C	-2.36645600	-2.35113900	0.72132900
H	-3.08483900	-2.61902900	-0.06355000
H	-2.56624900	-3.00848300	1.58077700
C	-0.96443400	-2.56318300	0.22586200
H	-0.17714800	-2.41949600	0.95931700
C	-0.65837300	-3.01900900	-1.02490100
H	-1.46112500	-3.27898300	-1.71101700
C	0.63638000	-2.93920100	-1.60140100
C	1.70422800	-2.30559400	-0.94758300
H	1.75267700	-2.43423100	0.12743500
H	2.68211200	-2.30082700	-1.41874400
O	0.66269100	-3.31215800	-2.90818600
C	1.87933900	-3.20994400	-3.63404000
H	1.66730200	-3.61418200	-4.62517500
H	2.20246800	-2.16671000	-3.73213800
H	2.67889000	-3.79648800	-3.16278800

Total energy (a.u.): -579.151379
Imaginary frequency (cm^{-1}): 419*i*

TS9

C	0.29515100	0.11682300	0.22506000
H	0.11641500	-0.15149700	1.26033600
C	1.55407900	-0.22913400	-0.32061700
H	2.37400500	-0.36361900	0.38330700
H	1.84995400	0.28442600	-1.23219900
C	-0.74597000	0.87391700	-0.45412100
O	-0.58359400	1.48546900	-1.50853400
C	-2.14466800	0.78660300	0.19289200
H	-2.28913800	1.67292000	0.82714600
H	-2.87024200	0.87859300	-0.62397700
C	-2.40797800	-0.47568700	1.03817500
H	-1.82240700	-0.43287100	1.96327000
H	-3.45915000	-0.48975900	1.35214900
C	-2.10202900	-1.81596800	0.31312900
H	-2.91321100	-2.02900500	-0.39421000
H	-2.09465800	-2.63277300	1.04428900
C	-0.81344600	-1.82975900	-0.45860900
C	-0.64502300	-1.70151500	-1.86219900
H	-1.41351200	-1.37980200	-2.55204000
C	0.68571900	-1.90636600	-2.12362800
H	1.20573300	-1.77447300	-3.06335500
C	1.31247700	-2.06707500	-0.84148000
H	2.24546400	-2.59223400	-0.66764800
O	0.30688300	-2.42870500	0.05495400

Total energy (a.u.): -538.644225
Imaginary frequency (cm^{-1}): 454*i*

TS10

C	0.11315300	0.16817100	0.07358400
H	-0.24443400	-0.13732900	1.05030100
C	1.45318800	-0.00403800	-0.25928600
H	2.15842700	-0.24620700	0.53092500
H	1.84410500	0.60097600	-1.07000900
C	-0.74833100	0.99465100	-0.78191800
O	-0.34559200	1.67060400	-1.70728700
C	-2.71996400	-0.08229700	0.15232800
H	-2.32060300	-0.23146300	1.16392500
H	-3.77077400	0.20387100	0.25115800
C	-2.59465400	-1.37698300	-0.67775800
H	-3.08028600	-1.21096700	-1.64611200
H	-3.15392500	-2.16492300	-0.15286100
C	-1.16039900	-1.77362400	-0.87613300
H	-0.66036900	-2.21317500	-0.01847500
C	-0.53838000	-1.79789100	-2.10673500
H	-1.13300000	-1.55477000	-2.98604700
C	0.85845600	-1.87120400	-2.26295300
H	1.26045700	-1.68731700	-3.25711800
C	1.73565400	-1.86953100	-1.18201800
H	1.45716900	-2.37674800	-0.26330800
H	2.80566800	-1.86844800	-1.37580800
O	-2.09952000	1.02157500	-0.50038200

Total energy (a.u.): -500.536109
Imaginary frequency (cm^{-1}): 454*i*

TS11

C	0.05609100	0.03665400	-0.14892300
H	0.19976400	0.08381300	0.92806700
H	0.97157900	0.03372900	-0.72851000
C	-1.07511000	0.67030800	-0.68100000
C	-2.10189200	1.37733500	0.20419000
H	-1.65713600	2.32193700	0.55162700
C	-3.45407200	1.70909800	-0.45530100
H	-3.26816800	2.25049500	-1.39225300
H	-3.97833200	2.41338800	0.20323100
C	-4.39526500	0.52413000	-0.72911000
H	-5.34209100	0.92014300	-1.11732200
H	-4.63945300	0.03054300	0.22373100
C	-3.86310700	-0.53298600	-1.71148200
H	-4.65112800	-1.28508700	-1.87757900
H	-3.66139500	-0.07998700	-2.69142200
C	-2.62378700	-1.21110300	-1.20033200
H	-2.55900700	-1.29186900	-0.11872700
C	-1.74875300	-1.95627000	-1.95823400
H	-1.91983400	-2.04071400	-3.03012000
C	-0.51626200	-2.40588400	-1.44386800
H	0.20875400	-2.80831700	-2.14902100
C	-0.08953900	-2.09413800	-0.15813300
H	-0.80875000	-2.03796600	0.65306200
H	0.90527800	-2.39905100	0.15781900
H	-2.25952800	0.77188200	1.10762700
C	-1.01017300	1.09066400	-2.04724400
N	-0.97567500	1.45121900	-3.15662800

Total energy (a.u.): -482.847031

Imaginary frequency (cm^{-1}): 472i

TS12

C	0.12893700	0.27828100	0.27839000
C	0.21948800	-0.23360100	1.57268100
H	1.15597200	-0.72491300	1.83062100
H	-0.23413800	0.32646400	2.38160100
C	1.28057300	0.35273000	-0.69740300
C	0.95559900	0.63993300	-2.18443000
H	0.85084200	1.72339600	-2.31493800
H	1.84308200	0.35105000	-2.76387700
C	-0.29332800	-0.02728100	-2.78529400
H	-1.18250800	0.53847600	-2.49029000
H	-0.22796000	0.04394300	-3.87899500
C	-0.52012000	-1.50113800	-2.39515500
H	0.33396200	-2.10782100	-2.72561500
H	-1.39525100	-1.86764600	-2.94861400
C	-0.74031000	-1.69340000	-0.91291000
H	0.09533300	-2.11395700	-0.36558200
C	-1.98247800	-1.69846300	-0.30891400
H	-2.85905400	-1.46759500	-0.91368500
C	-2.12896700	-1.76813800	1.08622700
H	-3.09377100	-1.50749400	1.51660500
C	-1.02137400	-1.89413300	1.92452700
H	-0.21065000	-2.55122000	1.62354000
H	-1.17154800	-1.86212000	3.00148400
H	1.98715500	1.12883100	-0.36366500
H	1.82374200	-0.59726800	-0.60692700
Cl	-1.11181600	1.55313500	0.09732600

Total energy (a.u.): -850.186912

Imaginary frequency (cm^{-1}): 526i

TS13

C	0.22260100	-0.01501200	0.32039400
H	0.04693100	-0.34137800	1.34372200
C	1.52484500	-0.15821900	-0.14898400
H	2.31603300	-0.44883300	0.53666800
H	1.86107800	0.42148400	-1.00440200
C	-0.76732200	1.01074600	-0.18381000
C	-2.25913100	0.56529600	-0.18628900
H	-2.88766500	1.42416800	0.07894200
H	-2.55786300	0.27884900	-1.20334000
C	-2.57143600	-0.60725500	0.75829100
H	-2.13180300	-0.41605300	1.74548000
H	-3.65488300	-0.67147200	0.91949700
C	-2.08344300	-1.97353200	0.20546600
H	-2.83825800	-2.33092600	-0.50904900
H	-2.06238600	-2.70728400	1.02175000
C	-0.74153100	-1.93158900	-0.49504000
C	-0.57945300	-1.72952000	-1.87391300
H	-1.36945300	-1.41250200	-2.54859200
C	0.77009700	-1.87219700	-2.22634200
H	1.18983600	-1.66224000	-3.20507000
C	1.50793000	-2.14293600	-1.06713400
H	2.55135100	-2.44440900	-1.06910100
H	-0.67353600	1.90284400	0.45651400
H	-0.47600000	1.33697000	-1.18985500
C	0.51526000	-2.65079100	-0.04371200
H	0.79427200	-2.51351200	1.00370200
H	0.37574300	-3.73286100	-0.21429600

Total energy (a.u.): -464.616733

Imaginary frequency (cm^{-1}): 488i

TS14-cis

C	-1.37557500	1.66792600	-0.28755400
H	-1.74431400	2.01032200	0.67611000
H	-1.84967000	2.14449500	-1.14162000
C	-0.04688400	1.26516600	-0.39784100
H	0.38551100	1.29104600	-1.39677100
C	0.93686200	1.32061300	0.75187900
H	0.51372800	0.77994400	1.60792200
C	2.34331000	0.77211500	0.40474200
H	2.85846400	0.51983400	1.34130600
H	2.93642200	1.57381000	-0.05615700
C	2.38309300	-0.44327400	-0.54206900
H	3.40106900	-0.85456800	-0.53901900
H	2.19889600	-0.11529500	-1.57400200
C	1.38218800	-1.56123200	-0.20109400
H	1.60105900	-2.43059300	-0.84076900
H	1.54076000	-1.89287500	0.83454800
C	-0.05837100	-1.14559100	-0.38205600
H	-0.37537900	-0.96315800	-1.40470500
C	-1.01218800	-1.38077800	0.59214800
H	-0.68253700	-1.84496700	1.52229900
C	-2.30960500	-0.84453700	0.55974900
H	-2.91083100	-0.91146900	1.46506400
C	-2.71867600	0.01576100	-0.45273300
H	-2.37517900	-0.14740500	-1.46945500
H	-3.69930100	0.48306900	-0.39071200
H	1.05638500	2.36079700	1.09494500

Total energy (a.u.): -390.593814
Imaginary frequency (cm⁻¹): 529i

TS14-trans

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.08569600
C	1.22431300	0.00000000	-0.64397500
H	1.25767400	-0.27714000	-1.69789800
C	2.37463000	0.56471800	-0.06775900
H	3.23955400	0.72610400	-0.70952900
C	2.34347000	1.18296700	1.17597900
H	1.71097300	0.79106300	1.96564000
H	3.22916000	1.70082800	1.53756600
C	-1.28032400	-0.49833400	-0.62228700
H	-1.51675900	-1.48023200	-0.18087900
H	-1.14086700	-0.66766200	-1.69765500
C	-2.49726200	0.42734300	-0.38715000
H	-2.49870000	1.24265700	-1.12306600
H	-3.41405200	-0.14734100	-0.56720900
C	-2.51682700	1.01778000	1.03164600
H	-3.53570300	1.32874100	1.29277200
H	-2.25572300	0.22545300	1.74727200
C	-1.57589500	2.23780400	1.21744400
H	-1.31904000	2.33807900	2.28047100
H	-2.15328800	3.14259000	0.96821600
C	-0.30797100	2.29260000	0.38376600
H	-0.46216600	2.39629600	-0.68624800
C	0.89168000	2.78134000	0.89685500
H	0.92886500	3.08805700	1.94077600
H	1.57002400	3.32058000	0.24536500

Total energy (a.u.): -390.593413
Imaginary frequency (cm⁻¹): 524i

TS15

C	0.03378100	-0.06075800	-0.04909600
H	0.12438800	-0.07721400	1.03345600
H	0.97093900	-0.06729800	-0.59322400
C	-1.06371800	0.57978200	-0.61806200
C	-2.05293100	1.36621300	0.23296700
H	-1.56285400	2.29721700	0.56236600
C	-3.37764500	1.75111000	-0.44580500
H	-3.15665900	2.25042600	-1.39780700
H	-3.87822900	2.49534900	0.18747500
C	-4.34656600	0.58987600	-0.69910100
H	-5.28697400	0.99282600	-1.09763300
H	-4.60046900	0.11482400	0.26086500
C	-3.81315100	-0.47883400	-1.66265600
H	-4.60391300	-1.22946800	-1.82471000
H	-3.61046300	-0.02870000	-2.64347700
C	-2.56700300	-1.16087100	-1.15876300
H	-2.55437900	-1.36653900	-0.09081700
C	-1.73025800	-1.89302500	-1.97956400
H	-1.91581000	-1.87900000	-3.05295200
C	-0.51702600	-2.43777700	-1.52558500
H	0.19105500	-2.80048300	-2.26890000
C	-0.08185300	-2.25063800	-0.22240300
H	-0.79521500	-2.22726400	0.59457800
H	0.91297700	-2.58123000	0.06753400

H	-2.25008100	0.80094700	1.15409700
O	-0.93925600	1.00760100	-1.94741200
C	-0.15588400	2.18189200	-2.12537800
H	0.86124700	2.05584500	-1.72911000
H	-0.10178800	2.35768100	-3.20332600
H	-0.61190500	3.06070200	-1.64650600

Total energy (a.u.): -505.113400
Imaginary frequency (cm⁻¹): 523i

TS16

C	0.17400600	-0.07404900	0.09598600
H	0.11427300	-0.54681800	1.07564000
C	1.43885500	-0.15414600	-0.50674800
H	2.27830100	-0.52508100	0.07504100
H	1.71431100	0.55314700	-1.28600000
C	-0.81857500	1.05713700	-0.08429500
C	-2.30910000	0.61530900	-0.01380300
H	-2.90456400	1.42082200	0.43271400
H	-2.70743600	0.47820800	-1.02799400
C	-2.53106300	-0.68376500	0.78168500
H	-2.03862600	-0.59985200	1.75856100
H	-3.59967200	-0.80957800	0.99257500
C	-2.02603200	-1.95291100	0.03854100
H	-2.83943600	-2.34405100	-0.58674600
H	-1.77911400	-2.73965800	0.75975400
C	-0.82110600	-1.70468600	-0.83390400
C	-0.81892900	-1.30638300	-2.20253600
H	-1.64380800	-0.82910100	-2.71530700
C	0.46065000	-1.50148700	-2.67098500
H	0.87873600	-1.19852600	-3.62234500
C	1.19559500	-2.00273000	-1.56626800
H	2.15333500	-2.50794500	-1.58198500
O	0.30437700	-2.48758900	-0.63992400
H	-0.63691800	1.80043800	0.70751800
H	-0.62835400	1.57615000	-1.03197000

Total energy (a.u.): -428.703803
Imaginary frequency (cm⁻¹): 560i

TS17

C	0.24900400	0.01063300	0.12726200
H	0.22426300	-0.22928400	1.19009600
C	1.51172600	-0.13579700	-0.46082900
H	2.37578900	-0.31689900	0.17177000
H	1.73876800	0.36122900	-1.40130300
C	-0.82238900	0.99897500	-0.28499900
C	-2.26545300	0.46148900	-0.04976700
H	-2.90734600	1.25843700	0.34599300
H	-2.71936500	0.14822800	-0.99775600
C	-2.34311200	-0.72172000	0.91777900
H	-1.86219500	-0.48375400	1.87567400
H	-3.38516800	-0.98048000	1.12365800
C	-0.67377700	-1.81245400	-0.39644700
C	-0.67624900	-1.79478700	-1.82231900
H	-1.51377600	-1.49549400	-2.43715800
C	0.62181300	-2.04645200	-2.20597700
H	1.05396200	-1.96909800	-3.19556200
C	1.34817800	-2.23985800	-1.00513800
H	2.32386200	-2.69060100	-0.87973800

O	0.45956900	-2.49212200	0.01114600
H	-0.68684600	1.92790200	0.28864700
H	-0.69606900	1.27262100	-1.33913800
O	-1.77477400	-1.94187200	0.38844800

Total energy (a.u.): -500.508168
Imaginary frequency (cm⁻¹): 564i

TS18

C	0.00807500	0.02529900	0.07614300
H	-0.03440400	0.05719200	1.16185800
H	1.00938600	0.01578600	-0.34542200
C	-1.02214400	-0.58201900	-0.62295700
H	-0.81860800	-0.91990800	-1.63870300
C	-2.22310600	-1.20248100	0.05221600
H	-2.56603200	-0.55202600	0.86827200
C	-3.39926400	-1.56889200	-0.87403100
H	-4.07610100	-2.22747800	-0.31519000
H	-3.01631000	-2.17187700	-1.71156200
C	-4.22544300	-0.39866800	-1.42972000
H	-4.64233200	0.17922500	-0.59383900
H	-5.08546100	-0.80761300	-1.97562600
C	-3.45563500	0.54619200	-2.37273400
H	-3.07196400	-0.02981500	-3.22447000
H	-4.15722200	1.28046800	-2.79590700
C	-2.30868300	1.26024800	-1.69583200
H	-1.37345800	1.30860000	-2.24383700
C	-2.47148200	2.04266600	-0.58169400
H	-3.45528000	2.17385400	-0.14215500
C	-1.37372100	2.51638800	0.17165600
C	-0.05678000	2.18847000	-0.09942200
H	0.24672400	2.09865000	-1.13468900
H	0.71215200	2.49611000	0.59860600
H	-1.88333200	-2.13101900	0.53981500
N	-1.67050100	3.10164100	1.48364200
O	-0.74237000	3.23858900	2.28679300
O	-2.83443000	3.44429400	1.71269600

Total energy (a.u.): -595.106764
Imaginary frequency (cm⁻¹): 438i

TS19

C	-0.01196300	-0.32396100	-0.05114000
C	-0.09209700	-0.23121600	1.34712600
H	0.81573500	-0.43992900	1.90438900
H	-0.97557200	-0.69486900	1.77788300
C	-1.12308100	-0.84841600	-0.92789100
C	-1.14115000	-0.42964500	-2.41956000
H	-0.35270000	-0.98519100	-2.94057100
H	-2.09179100	-0.79983800	-2.82754800
C	-0.97532800	1.05656300	-2.78363900
H	0.07452500	1.34079100	-2.65217000
H	-1.19520600	1.15524100	-3.85559100
C	-1.83917500	2.07151900	-1.99829900
H	-2.90353700	1.82137600	-2.10470100
H	-1.70198800	3.05866600	-2.46066600
C	-1.44257100	2.11516300	-0.54700400
H	-2.03697300	1.52100900	0.13964100
C	-0.38317400	2.81669200	-0.06229800
H	0.15611200	3.47931700	-0.74367200

C	0.20503200	2.59780400	1.22402200
C	-0.30925200	1.61189000	2.09068200
H	-1.38903800	1.52454400	2.17243300
H	0.21391800	1.49420400	3.03625800
H	-1.05268700	-1.94954500	-0.91534000
H	-2.07672200	-0.61439700	-0.44505100
O	1.13850900	-0.14489000	-0.71964300
C	2.38442200	-0.05409900	-0.00909600
H	2.61065700	-1.01652900	0.46607000
H	3.13342800	0.15990200	-0.77242900
H	2.38357700	0.73862800	0.74145400
C	1.52410600	3.14309000	1.48221400
O	2.30519100	2.75274500	2.35085000
H	1.82611100	3.96988900	0.79796000

Total energy (a.u.): -618.450552
Imaginary frequency (cm⁻¹): 403i

TS20

C	0.00705100	-0.34658000	-0.04528800
C	-0.05708300	-0.24987400	1.35515700
H	0.86442300	-0.43364300	1.89914600
H	-0.92371600	-0.73308000	1.79867700
C	-1.12518300	-0.84841400	-0.90805000
C	-1.15439200	-0.42916800	-2.39976600
H	-0.37878400	-0.99552900	-2.92822300
H	-2.11377500	-0.78910900	-2.79590800
C	-0.97374600	1.05327700	-2.77391200
H	0.07681200	1.33145000	-2.63710400
H	-1.18298200	1.14161900	-3.84865700
C	-1.83799600	2.08688000	-2.01287500
H	-2.90331500	1.84736700	-2.13025100
H	-1.68188200	3.06668700	-2.48327900
C	-1.46196800	2.14143000	-0.55677500
H	-2.07404700	1.55861700	0.12498200
C	-0.38984700	2.81929900	-0.07381800
H	0.18615400	3.46664600	-0.73023400
C	0.15977400	2.58139300	1.22405000
C	-0.33102900	1.57884500	2.07626100
H	-1.41221700	1.49188400	2.12233200
H	0.16425300	1.47226100	3.03460600
H	-1.07298400	-1.95032700	-0.89506800
H	-2.06780100	-0.59937100	-0.41134100
O	1.13980500	-0.15760600	-0.72964000
C	2.39839900	-0.02337900	-0.04459200
H	2.66430200	-0.97855600	0.42326300
H	3.12213300	0.21832300	-0.82302000
H	2.38389300	0.76576600	0.71081200
N	1.46472300	3.10131100	1.48364200
O	2.17680800	2.52015700	2.33415200
O	1.85119600	4.09371300	0.84673300

Total energy (a.u.): -709.632173
Imaginary frequency (cm⁻¹): 386i

TS21

C	-0.01949800	-0.31450100	-0.08829100
C	-0.04636700	-0.21863400	1.31842200
H	0.89002000	-0.42304900	1.82967200

H	-0.89198800	-0.72664600	1.77617300
C	-1.15501300	-0.86750400	-0.91507900
C	-1.21206300	-0.46993000	-2.41306500
H	-0.47859400	-1.07660100	-2.95643400
H	-2.19795500	-0.78659800	-2.78015300
C	-0.96836200	0.99941000	-2.79949700
H	0.10067500	1.21847000	-2.70832900
H	-1.22049500	1.10581000	-3.86324600
C	-1.74181400	2.06948400	-1.99603100
H	-2.82292800	1.90035700	-2.09369800
H	-1.53523800	3.04758500	-2.45099300
C	-1.34153000	2.07816800	-0.54500100
H	-1.97391300	1.51622100	0.13319900
C	-0.29192900	2.78491200	-0.03517600
H	0.27345100	3.44098900	-0.69644700
C	0.21562200	2.58418900	1.28596500
C	-0.33188400	1.56566600	2.10209100
H	-1.41549000	1.48387200	2.11633500
H	0.10545700	1.43224100	3.08894400
H	-1.08500700	-1.96785500	-0.88270200
H	-2.09454600	-0.62170000	-0.41015800
O	1.11273300	-0.18410600	-0.80642900
C	2.38146800	-0.01124200	-0.16179600
H	2.62106900	-0.88851500	0.45158900
H	3.10514800	0.07031800	-0.97380100
H	2.41693200	0.89388800	0.44808900
C	1.49061800	3.11592600	1.61764900
N	2.55360200	3.52306400	1.88374800

Total energy (a.u.): -597.366975
Imaginary frequency (cm⁻¹): 425i

TS22

C	-0.22595700	0.12915300	0.23265100
H	-0.63093100	0.68443500	1.07489200
H	0.84800100	0.23075200	0.10997500
C	-0.77380500	-1.12689400	-0.04131300
H	-0.16442400	-1.88010700	-0.53329700
C	-2.53591900	-2.83077000	0.08038000
H	-3.20104700	-3.22836100	0.85636500
H	-1.76160100	-3.59322200	-0.08317700
C	-3.33741600	-2.63559000	-1.21968100
H	-4.15038600	-1.91943700	-1.03930800
H	-3.82078100	-3.59478300	-1.45086800
C	-2.50765200	-2.18270700	-2.44001400
C	-1.86918700	-0.82378900	-2.24331500
H	-0.83301100	-0.71671400	-2.54645100
C	-2.60640600	0.30349800	-1.94616900
H	-3.69294600	0.21084900	-1.89866400
C	-2.04431100	1.50626700	-1.47465200
H	-2.71457600	2.26255600	-1.07013200
C	-0.67848300	1.60415500	-1.22046000
H	0.02412500	1.13258800	-1.90095200
H	-0.28842000	2.51143900	-0.76234800
N	-1.86328200	-1.65961800	0.64528900
H	-2.50734000	-0.94618000	0.97473800
H	-3.15652100	-2.19213100	-3.33039800
H	-1.72721700	-2.93115100	-2.63458600

Total energy (a.u.): -406.628673
Imaginary frequency (cm⁻¹): 511i

TS23

C	0.00705100	-0.34658000	-0.04528800
C	-0.05708300	-0.24987400	1.35515700
H	0.86442300	-0.43364300	1.89914600
H	-0.92371600	-0.73308000	1.79867700
C	-1.12518300	-0.84841400	-0.90805000
C	-1.15439200	-0.42916800	-2.39976600
H	-0.37878400	-0.99552900	-2.92822300
H	-2.11377500	-0.78910900	-2.79590800
C	-0.97374600	1.05327700	-2.77391200
H	0.07681200	1.33145000	-2.63710400
H	-1.18298200	1.14161900	-3.84865700
C	-1.83799600	2.08688000	-2.01287500
H	-2.90331500	1.84736700	-2.13025100
H	-1.68188200	3.06668700	-2.48327900
C	-1.46196800	2.14143000	-0.55677500
H	-2.07404700	1.55861700	0.12498200
C	-0.38984700	2.81929900	-0.07381800
H	0.18615400	3.46664600	-0.73023400
C	0.15977400	2.58139300	1.22405000
C	-0.33102900	1.57884500	2.07626100
H	-1.41221700	1.49188400	2.12233200
H	0.16425300	1.47226100	3.03460600
H	-1.07298400	-1.95032700	-0.89506800
H	-2.06780100	-0.59937100	-0.41134100
O	1.13980500	-0.15760600	-0.72964000
C	2.39839900	-0.02337900	-0.04459200
H	2.66430200	-0.97855600	0.42326300
H	3.12213300	0.21832300	-0.82302000
H	2.38389300	0.76576600	0.71081200
N	1.46472300	3.10131100	1.48364200
O	2.17680800	2.52015700	2.33415200
O	1.85119600	4.09371300	0.84673300

Total energy (a.u.): -634.452950

Imaginary frequency (cm^{-1}): 428i

TS24

C	0.14672200	-0.05930900	-0.48195300
H	0.65273600	0.12388400	0.45753000
H	0.55895100	0.41446100	-1.36509000
C	-0.60968600	-1.20361300	-0.63211400
H	-0.70377100	-1.68728200	-1.60058300
C	-1.54705900	-3.06114800	0.67234300
C	-2.94422600	-3.01973300	0.04444900
H	-3.60657700	-2.84766900	0.90242500
H	-3.15536100	-4.04543100	-0.27489300
C	-3.27873700	-2.02472900	-1.07882300
H	-2.86288400	-2.38377600	-2.02826300
H	-4.36955100	-2.01701900	-1.21804400
C	-2.74759500	-0.63886300	-0.80046400
H	-2.48224000	-0.05384200	-1.67645900
C	-2.94718300	0.02823300	0.39655400
H	-3.48307300	-0.47450700	1.20034700
C	-2.22612300	1.19242500	0.73093700
H	-2.25777200	1.52344500	1.76751500
C	-1.29037700	1.75333700	-0.11319300
H	-1.39861200	1.69250800	-1.18953400
H	-0.65663700	2.56463100	0.23521800

O	-0.62001600	-2.07857600	0.45969900
O	-1.26328400	-3.93398000	1.45592900

Total energy (a.u.): -500.517606
Imaginary frequency (cm^{-1}): 517*i*

TS25

C	-0.01690300	-0.09745800	0.12442800
C	-0.08123900	-0.00317600	1.50925400
H	0.86411100	-0.03171700	2.04132600
H	-0.90214200	-0.52199700	1.99700400
C	-0.98791600	-0.83454000	-0.76076400
C	-0.94948900	-0.51698500	-2.27835500
H	-0.13693000	-1.09927500	-2.73005400
H	-1.87632100	-0.92047900	-2.70736300
C	-0.77651200	0.94721700	-2.71900000
H	0.26841400	1.24568300	-2.58211000
H	-0.97871300	0.99978600	-3.79699000
C	-1.65774600	1.98937500	-1.99677800
H	-2.71843200	1.74250000	-2.13788900
H	-1.49508800	2.96295600	-2.47824200
C	-1.33643600	2.08301800	-0.52763600
H	-1.99997100	1.54957700	0.14376000
C	-0.37772900	2.89846100	0.00785400
H	0.19754200	3.54153800	-0.66102100
C	0.05321500	2.80856100	1.35915700
C	-0.51114300	1.87335000	2.23531400
H	-1.57948400	1.68726500	2.19018600
H	-0.08320700	1.81766800	3.23276900
H	-0.79420100	-1.91161700	-0.65260300
H	-1.99426300	-0.66940400	-0.35794800
C	1.29277800	3.49307000	1.74669500
O	1.88938100	3.33514400	2.80171700
H	1.68076100	4.20719100	0.98420900
O	1.22323100	0.25511500	-0.43346100
C	2.12481100	-0.74169000	-0.70657300
O	1.90163500	-1.91395600	-0.52364400
C	3.39826300	-0.15122400	-1.25948400
H	3.81728600	0.56907900	-0.54961300
H	4.11515200	-0.95068100	-1.44850200
H	3.19052800	0.38927700	-2.18901400

Total energy (a.u.): -731.799745
Imaginary frequency (cm^{-1}): 457*i*

TS26

C	-0.18388600	0.00722000	0.27028900
H	-0.59486700	0.46110200	1.16511200
H	0.88378800	0.12782700	0.12279000
C	-0.77056400	-1.15928000	-0.19721500
H	-0.18544200	-1.88719300	-0.76024100
C	-2.44289700	-2.82741800	-0.14311700
H	-3.07276200	-3.26918000	0.63512300
H	-1.64981100	-3.55454600	-0.38579100
C	-3.27964200	-2.52857700	-1.38833300
H	-4.09253600	-1.84700600	-1.11035900
H	-3.75090700	-3.47065600	-1.70047300
C	-2.47751900	-1.94091900	-2.56597800
H	-1.69988500	-2.65876300	-2.86103600
H	-3.14133200	-1.84259300	-3.43864400

C	-1.83596600	-0.61209200	-2.22044500
H	-0.82731500	-0.44920900	-2.58773300
C	-2.57971600	0.47806200	-1.80696800
H	-3.66068800	0.36654800	-1.72060100
C	-2.00615000	1.63053500	-1.24033200
H	-2.66857400	2.33779300	-0.74450300
C	-0.63987800	1.72761700	-1.02477800
H	0.05554800	1.29799100	-1.73809800
H	-0.23953000	2.57628600	-0.47441100
O	-1.85553000	-1.67697300	0.46699700

Total energy (a.u.): -426.491024

Imaginary frequency (cm^{-1}): 539i

TS27

C	-0.19724600	0.00243800	0.11778500
H	-0.56999300	0.43848000	1.03855600
H	0.86113600	0.14014200	-0.07792600
C	-0.75702600	-1.20014700	-0.28912000
H	-0.22218900	-1.90803800	-0.91862100
C	-2.45881600	-2.84522900	-0.20692100
H	-3.09520800	-3.24052400	0.58818400
H	-1.67719800	-3.58275200	-0.43529800
C	-3.28910800	-2.57862400	-1.48554600
H	-4.11278600	-1.90103000	-1.24239900
H	-3.70000500	-3.53655400	-1.81918900
C	-2.36105700	-2.03376200	-2.56684500
C	-1.98300000	-0.62902600	-2.43096200
H	-1.04965100	-0.37042200	-2.92472100
C	-2.74912200	0.36133100	-1.82852300
H	-3.80232300	0.17097300	-1.63271000
C	-2.19203300	1.51354200	-1.25750100
H	-2.84357000	2.16849700	-0.68345400
C	-0.81083800	1.64281900	-1.11602000
H	-0.15097900	1.27537400	-1.89433900
H	-0.41038700	2.49047700	-0.56419200
O	-1.86023400	-1.66884300	0.34608600
O	-1.79282800	-2.80446300	-3.34033500

Total energy (a.u.): -480.655006

Imaginary frequency (cm^{-1}): 426i

TS28

C	-0.20637100	0.10887200	0.25176100
H	-0.57329900	0.69055600	1.09391500
H	0.86718600	0.16274800	0.10094300
C	-0.81162500	-1.12181100	-0.00301600
H	-0.29615600	-1.88552600	-0.57706300
C	-2.72694300	-2.67278800	0.04007200
H	-3.44432200	-2.98316400	0.80623200
H	-2.01720400	-3.49581400	-0.10072500
C	-3.46781400	-2.45288700	-1.31729700
H	-4.24721600	-1.69460100	-1.19041100
H	-3.94207900	-3.40256400	-1.58313700
C	-2.44219300	-2.09908900	-2.38985300
C	-2.00422700	-0.71453900	-2.43253300
H	-1.02814700	-0.56831500	-2.88889900
C	-2.69494100	0.36708500	-1.90456900
H	-3.76619400	0.27038600	-1.73236500
C	-2.07896000	1.52739500	-1.40574500

H	-2.70436800	2.27666400	-0.92489300
C	-0.69687300	1.57603900	-1.21192000
H	-0.03754500	1.08436400	-1.91874000
H	-0.25912000	2.45674700	-0.74635400
O	-1.86325000	-3.00562900	-2.99718300
N	-1.98492700	-1.53396100	0.56202500
H	-2.53191400	-0.81169800	1.01636900

Total energy (a.u.): -500.512183

Imaginary frequency (cm^{-1}): 411*i*

TS29

C	-0.09414800	-0.03371100	0.03038500
C	-0.22625300	-0.13556100	1.47244200
C	1.02933200	-0.58696400	1.97239600
C	1.86599000	-0.76101600	0.90010800
N	1.18189700	-0.59507600	-0.28551200
H	-0.91754400	-0.37601500	-0.59216000
H	-1.17762300	-0.27814100	1.96495600
H	1.29335400	-0.73946200	3.01055500
H	2.91617900	-1.02724900	0.88278800
C	1.85554000	-0.28637900	-1.54521600
H	2.63702100	0.47351400	-1.37868100
H	2.35078900	-1.19104600	-1.91979400
C	0.85264100	0.25261200	-2.56495700
H	1.34544400	0.33511800	-3.54068100
H	0.04020100	-0.47391800	-2.69046000
C	0.30752000	1.63638300	-2.14475400
H	1.07281000	2.38508100	-2.38646200
H	-0.56598000	1.87941100	-2.76214600
C	-0.03876000	1.77033800	-0.65264400
H	-1.10144400	1.93313900	-0.46762000
C	0.83404000	2.53565100	0.16486600
H	1.80319400	2.82799700	-0.23695000
C	0.59359300	2.69922300	1.53170000
H	1.39802500	3.10415800	2.14506300
C	-0.51864200	2.17696800	2.16601700
H	-0.60913100	2.22181100	3.24825700
H	-1.45176400	2.02990700	1.63365800

Total energy (a.u.): -482.836296

Imaginary frequency (cm^{-1}): 505*i*

TS30

C	-0.09810700	-0.06857900	-0.03972600
C	-0.01699800	-0.40373300	1.27571200
C	1.31051100	-0.08906500	1.75111900
C	2.01685100	0.47474600	0.64088900
N	1.14866600	0.37652700	-0.48423000
H	-0.92502100	-0.08805800	-0.73412900
H	-0.82740500	-0.80303200	1.87142800
H	1.80880300	-0.62160100	2.54982700
H	3.06366600	0.25324100	0.46831200
C	1.38299300	1.00696300	-1.70282200
C	2.69196900	1.77259700	-1.73094600
H	3.53079500	1.09187400	-1.54066500
H	2.81544900	2.17956200	-2.73688500
C	2.69504300	2.92634800	-0.68057300
H	3.69486300	3.37650200	-0.68015300
H	2.00456000	3.69732800	-1.04152500

C	2.28901200	2.52659600	0.73524400
H	3.11224500	2.37927000	1.43226500
C	1.08782400	3.03655900	1.26080200
H	0.44001200	3.60854500	0.59804500
C	0.56659700	2.62217100	2.48991900
H	-0.45793200	2.90392900	2.72670500
C	1.18794500	1.66474900	3.27391700
H	0.69080900	1.27406500	4.15814000
H	2.26803400	1.56574500	3.27996800
O	0.57076000	0.98012100	-2.61340900

Total energy (a.u.): -556.874278

Imaginary frequency (cm^{-1}): 542i