Supporting Information

On the Mechanism, Reactivity and Selectivity of Ni-Catalyzed [4+4+2] Cycloadditions of Dienes and Alkynes

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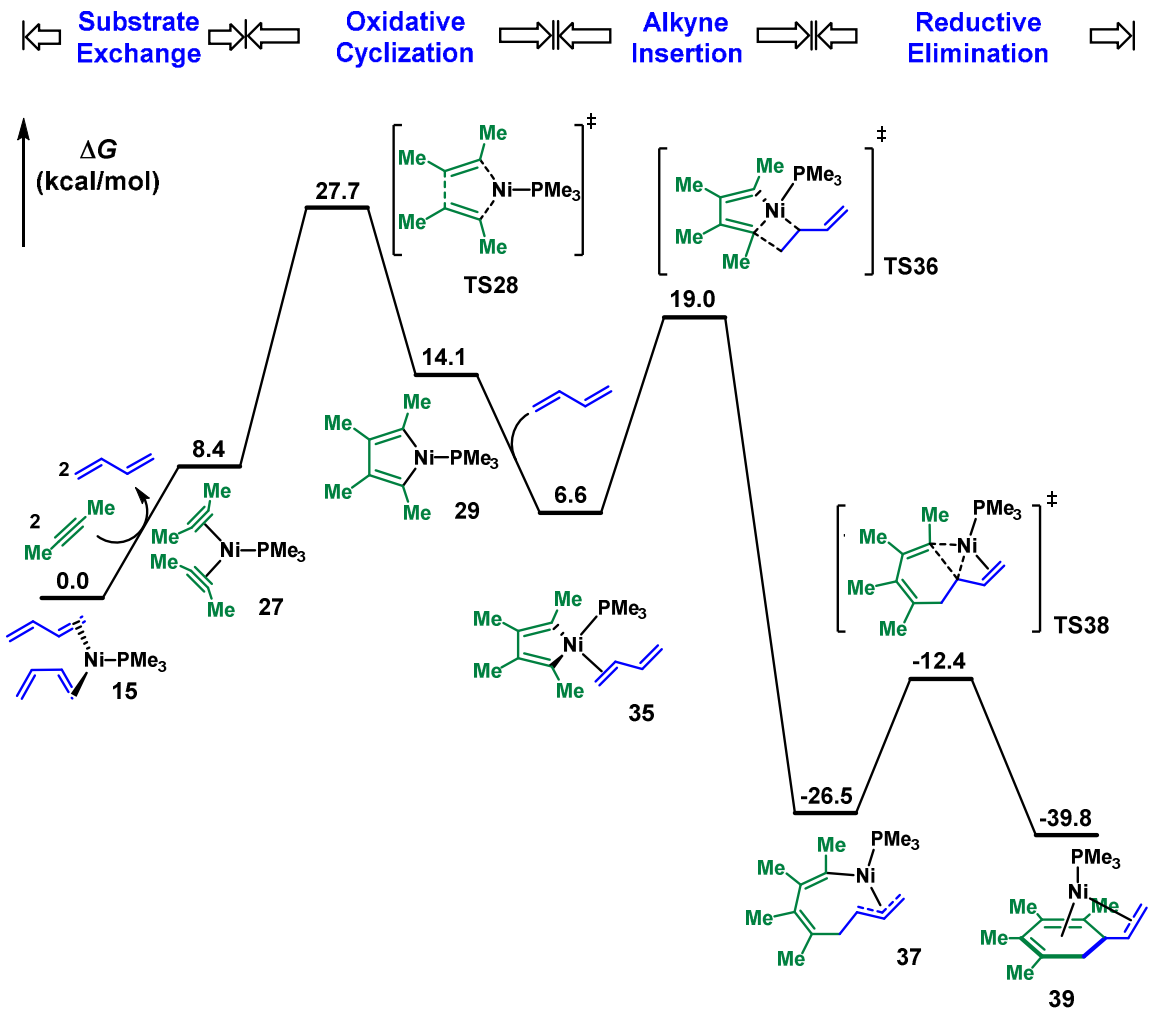

Figure S1. Free energy profile of [Ni(PMe_3)]-mediated [2+2+2] cycloaddition of two 2-butynes and one butadiene, Gibbs free energies are shown in kcal/mol.

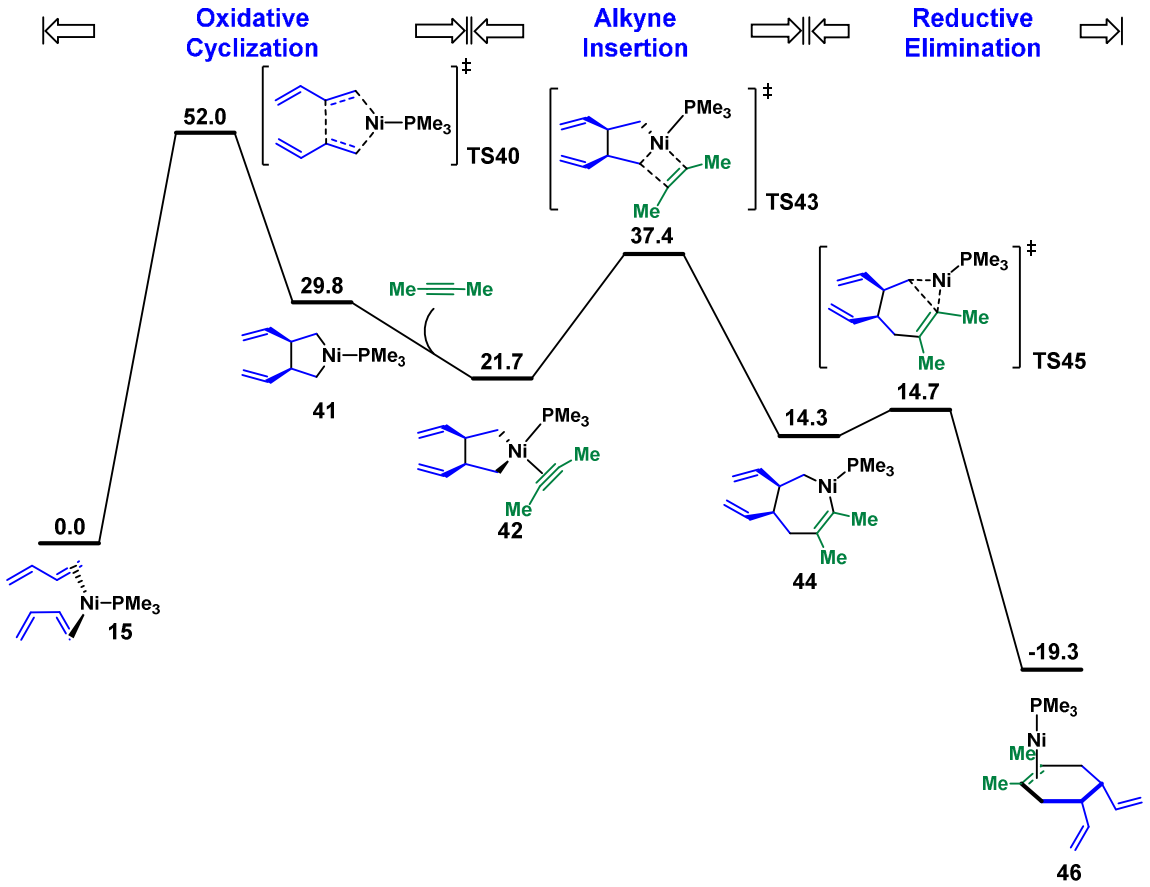

Figure S2. Free energy profile of [Ni(PMe_3)]-mediated [2+2+2] cycloaddition of two butadienes and one 2-butyne, Gibbs free energies are shown in kcal/mol.

Energies and Coordinates of DFT-Computed Stationary Points

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G-sol = -943.639156 Hartree

Ni	0.11876500	-0.19379700	-0.31646900
P	-2.04007100	-0.15567100	0.11284200
C	1.39618700	1.31546100	-0.88583600
C	0.07193400	1.60802900	-1.23271800
H	-0.26036700	1.45765400	-2.25919500
H	-0.49014800	2.35857600	-0.67959300
C	1.61858700	-1.62419900	-0.27491400
C	0.40823800	-2.06865400	0.29085500
H	1.80795300	-1.85016700	-1.32617800
C	2.08119000	1.86797700	0.29727400
C	1.67998300	2.90260800	1.05288300
C	-2.49631000	0.94889100	1.53303500
H	-1.99120200	0.60279700	2.44040000
H	-2.15605900	1.96847000	1.32831600
H	-3.57872500	0.95971200	1.70830400
C	-3.17185000	0.46806000	-1.21952700
H	-4.21506500	0.49887700	-0.88412900
H	-2.86494600	1.47284100	-1.52421900
H	-3.10111800	-0.18648300	-2.09458600
C	-2.91538500	-1.71996300	0.59272400
H	-2.42810200	-2.16078700	1.46792800
H	-3.97108600	-1.53893800	0.82527100
H	-2.85360300	-2.44457300	-0.22586500
H	-0.24055600	-2.73470200	-0.27512000
H	0.77931600	3.47164000	0.83437600
H	2.25874300	3.22741700	1.91299000
H	3.01390300	1.36982500	0.55373100
H	2.05313500	0.87671700	-1.63506800
C	2.81308500	-1.34125500	0.52149400
C	4.06906000	-1.29989000	0.04874800
H	2.64611000	-1.17748700	1.58768300
H	4.91729200	-1.10662100	0.69894300
H	4.28874500	-1.46828400	-1.00374900
H	0.33310900	-2.17750400	1.37416400

15-cc

G-sol = -943.636253 Hartree

Ni	0.13498500	-0.09414400	-0.49748500
P	-1.95156500	-0.14075000	0.19803200
C	1.35061200	1.51898100	-0.94260300
C	-0.01115800	1.84377200	-1.01562600
H	-0.49604600	1.89545800	-1.98992100
H	-0.46732400	2.47159300	-0.25173700
C	1.61196100	-1.50687100	-0.80992000
C	0.41982700	-2.06510300	-0.32280800
H	1.74780100	-1.47775900	-1.89239800
C	2.22249800	1.86868300	0.19327100
C	1.91987800	2.65081400	1.24124600
C	-2.18612000	0.67475000	1.84924500
H	-1.57528300	0.16014200	2.59772000
H	-1.84695100	1.71368200	1.79751100
H	-3.23515100	0.65500500	2.16782100
C	-3.23203600	0.72425700	-0.82998200
H	-4.22037400	0.69015400	-0.35704800
H	-2.94396600	1.76882900	-0.97937900
H	-3.29470500	0.24706100	-1.81362300
C	-2.79960900	-1.76528700	0.48798900
H	-2.22697400	-2.35813500	1.20757800
H	-3.81724500	-1.62666000	0.87045800
H	-2.84783600	-2.32927400	-0.44915400
H	-0.25488600	-2.57446400	-1.00908200
H	0.95393300	3.13832000	1.34816000
H	2.64379900	2.83699500	2.02912300
H	3.22053800	1.43651000	0.15697100
H	1.87105400	1.25845100	-1.86272000
C	2.85994700	-1.36268500	-0.04073600
C	3.13786500	-1.87639700	1.16673200
H	3.64139000	-0.79147100	-0.54323000
H	4.09853000	-1.70488600	1.64356500
H	2.42476200	-2.48425000	1.71795000
H	0.35682000	-2.40750000	0.70968800

15-tt

G-sol = -943.644353 Hartree

Ni	-0.07714800	0.03841600	0.01834300
P	2.12073800	0.02747900	0.00748400
C	-1.56602800	1.28960500	-0.66814000
C	-0.29990500	1.64144600	-1.16477600

H	0.21133600	2.51871100	-0.76884200
H	-0.02901400	1.37945400	-2.18716900
C	-0.22645400	-1.58893700	1.18216100
C	-1.50386600	-1.29813800	0.67244600
H	0.32710400	-2.44454200	0.79260000
H	0.01834600	-1.31871100	2.20840200
C	-2.18920100	1.99891900	0.45127600
C	-3.48519700	1.92442000	0.79710400
C	-2.08091700	-2.03634000	-0.45307600
C	-3.37509200	-2.02442000	-0.81316900
H	-3.73680200	-2.60211100	-1.65877300
H	-4.11409800	-1.44609800	-0.26302700
C	3.05524100	1.55437600	-0.48243000
H	2.74932300	1.86834400	-1.48516400
H	2.81944600	2.36809500	0.21142800
H	4.13875100	1.38809500	-0.47658400
C	2.99666000	-0.41224200	1.58351800
H	4.08431900	-0.44037000	1.44993400
H	2.75442500	0.32578500	2.35539700
H	2.65447800	-1.39065300	1.93349300
C	2.83795500	-1.21697600	-1.16863100
H	2.50442000	-0.99111100	-2.18657800
H	3.93406300	-1.21764500	-1.14484400
H	2.47487400	-2.21627100	-0.90871500
H	-1.38290100	-2.64967700	-1.02675600
H	-2.23226200	0.68651100	-1.28304400
H	-4.18942800	1.31210500	0.23812900
H	-3.88370800	2.48288400	1.63905400
H	-1.52677100	2.64363700	1.03247600
H	-2.20601200	-0.73455500	1.28502500

TS16 (Imaginary Frequency = -355.30)

G-sol = -943.617070 Hartree

Ni	0.00590100	0.10950700	-0.21548200
P	-2.12428900	-0.06368800	0.12212500
C	1.34098800	-1.65201800	-0.72261300
C	0.40671400	-1.77412300	0.33524900
H	0.77493700	-1.77327600	1.36332700
H	-0.43228200	-2.45292600	0.18168400
C	0.04721600	2.05711400	-0.66579100
C	1.40032700	1.64818700	-0.58478000
H	-0.35562600	2.32146700	-1.64287400
H	-0.38013900	2.63029000	0.15800600

C	2.73906400	-1.41236900	-0.65084400
C	3.46873900	-1.13245500	0.48772600
C	2.12566300	1.52220100	0.63207000
C	3.43939300	1.09128400	0.70467900
C	-3.00255600	-1.21792700	-1.03655900
H	-2.89192900	-0.85559800	-2.06371100
H	-2.55243800	-2.21372500	-0.97934300
H	-4.07010500	-1.29572800	-0.79927800
C	-2.65183800	-0.72370300	1.77429400
H	-3.74113000	-0.83094500	1.83840600
H	-2.18486800	-1.69717000	1.94949300
H	-2.31536200	-0.04096900	2.56123900
C	-3.20070200	1.44086400	-0.00551800
H	-3.10131400	1.88122900	-1.00235000
H	-4.25500600	1.20171300	0.17667800
H	-2.87583100	2.18849300	0.72503600
H	0.97118800	-1.90327200	-1.71874800
H	1.95296400	1.46928800	-1.50661400
H	4.07513900	1.17363000	-0.17099400
H	3.96201000	1.11648900	1.65683800
H	3.04526200	-1.32296900	1.46968100
H	4.55372400	-1.14820300	0.44506700
H	1.58339700	1.71057400	1.56018000
H	3.25846900	-1.35157200	-1.60760200

TS16-cc (Imaginary Frequency = -394.48)

G-sol = -943.598163 Hartree

Ni	-0.03764600	-0.16266200	-0.29295600
P	2.12342200	0.00254000	0.09702400
C	-1.39768200	-1.76533400	-0.53349600
C	-0.45368200	-1.91727000	0.52445200
H	0.31177500	-2.68580300	0.41149900
H	-0.78958900	-1.78675200	1.55523200
C	-0.59683100	1.53888200	-1.34070200
C	-0.82670100	1.88115000	-0.00496200
H	0.24304700	1.99422800	-1.86023600
H	-1.41561700	1.21221000	-1.97970200
C	-2.76305000	-1.36383900	-0.50739000
C	-3.51037500	-0.89375500	0.55301200
C	-1.99223600	1.72074700	0.80416500
C	-3.25531900	1.33971700	0.39488500
C	2.61839600	-0.07171700	1.88554100
H	2.17205900	0.77117900	2.42354900

H	2.23133600	-0.99475900	2.32781800
H	3.70702400	-0.03936300	2.01490500
C	3.17064800	-1.35271500	-0.62028900
H	4.22536300	-1.25251600	-0.33713300
H	2.79788600	-2.32117700	-0.27217500
H	3.09347600	-1.33493400	-1.71248400
C	3.07008100	1.50083700	-0.46774700
H	2.63795600	2.40244600	-0.02032900
H	4.13099300	1.44780600	-0.19542100
H	2.98953800	1.59511100	-1.55588400
H	-0.00335500	2.38467400	0.50421200
H	-3.51673600	1.35035800	-0.65830400
H	-4.08919300	1.46755500	1.07767200
H	-3.14258400	-0.97767700	1.57184500
H	-4.58806100	-0.81483000	0.44847000
H	-3.25205300	-1.35725900	-1.48330600
H	-1.84596200	1.90395400	1.86827000
H	-1.07404300	-2.14823200	-1.50590900

TS16-tt (Imaginary Frequency = -401.65)

G-sol = -943.614283 Hartree

Ni	0.06105400	0.03310700	-0.03632800
P	2.21094000	0.00972000	-0.00383600
C	-1.45648300	1.64015800	-0.40782800
C	-0.13847400	2.02095600	-0.05454100
H	0.02962300	2.41833100	0.95061200
H	0.47390600	2.49495000	-0.82030800
C	-0.06998000	-1.96803500	-0.00769900
C	-1.38929200	-1.63009900	0.38551300
H	0.07830300	-2.35378700	-1.02001800
H	0.57178600	-2.44135400	0.73652600
C	-2.57681500	1.52218900	0.43983400
C	-3.79913200	1.02834200	-0.00556300
C	-2.53624400	-1.54956600	-0.42982500
C	-3.76190200	-1.09724600	0.04984200
H	-4.65171800	-1.23152000	-0.56011100
H	-3.94244700	-1.14888800	1.12096800
C	3.15784500	1.54778300	-0.42394900
H	2.93761800	1.84592200	-1.45407200
H	2.84906000	2.36390900	0.23605900
H	4.23856600	1.39506900	-0.32273200
C	2.92456300	-0.40451800	1.65724800
H	4.01984800	-0.44295200	1.62878500
H	2.61338300	0.35008400	2.38663700

H	2.54042600	-1.37402300	1.98764100
C	3.05745400	-1.22554600	-1.09704200
H	2.80199900	-1.02279600	-2.14217500
H	4.14677300	-1.18350000	-0.98283000
H	2.71025900	-2.23328200	-0.85315800
H	-2.41639700	-1.73077100	-1.49908600
H	-1.65892300	1.50903300	-1.47379200
H	-4.01082400	1.07328000	-1.07131000
H	-4.67590900	1.13242900	0.62870400
H	-2.43316800	1.70838600	1.50528000
H	-1.56502700	-1.50784000	1.45716600

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G-sol = -943.648393 Hartree

Ni	-0.00134700	0.36487600	0.08985400
P	-2.09120500	-0.21191100	-0.00740100
C	1.51992100	-1.92183800	-0.46168000
C	0.62742100	-1.44488200	0.61367400
H	1.15529700	-1.28886400	1.56329000
H	-0.18424100	-2.16035100	0.79547700
C	-0.22226300	2.39302600	-0.18330100
C	1.09519100	1.99084700	-0.49062100
H	-0.83054900	2.83606300	-0.96779700
H	-0.46894400	2.72461400	0.82658800
C	2.82973600	-1.62834200	-0.60116700
C	3.57380600	-0.71095800	0.32215900
C	1.90436300	1.29200500	0.41700400
C	3.27718200	0.79673600	0.04390200
C	-2.44420300	-1.60655500	-1.17336900
H	-2.20257400	-1.29454500	-2.19443800
H	-1.81340500	-2.46381100	-0.92309100
H	-3.49723800	-1.90798400	-1.13173000
C	-2.79991100	-0.83577000	1.58607000
H	-3.83057100	-1.18653900	1.45854800
H	-2.18438900	-1.65626300	1.96503500
H	-2.78750800	-0.03116900	2.32841700
C	-3.37593800	1.02169600	-0.51751000
H	-3.14631100	1.39598700	-1.52004500
H	-4.38055600	0.58291500	-0.52172100
H	-3.36135700	1.87244200	0.17070500
H	1.06127400	-2.54840900	-1.23070100
H	3.45761900	0.98988400	-1.02184200
H	4.02094100	1.38796500	0.59852900
H	3.33260500	-0.92147300	1.37371100

H	4.65523300	-0.86162900	0.21579000
H	1.72637400	1.44065900	1.48548300
H	1.40207300	1.98472200	-1.53854800
H	3.37018500	-2.00786100	-1.46754000

17-cc

G-sol = -943.647476 Hartree

Ni	-0.10326000	-0.37682200	-0.35576400
P	1.97272600	0.18548200	0.08516100
C	-0.98395900	-2.18454800	-0.37095700
C	-0.09938200	-2.17699000	0.72390100
H	0.73134200	-2.87822100	0.72690200
H	-0.42538600	-1.84851300	1.70946100
C	-0.71490600	1.29924400	-1.20324900
C	-1.16290600	2.02835700	0.00050500
H	0.07903200	1.82593600	-1.74160000
H	-1.52799100	1.07667600	-1.90070700
C	-1.99510200	-1.21223000	-0.54606300
C	-2.90645300	-0.66988900	0.53469100
C	-2.31051000	1.82678500	0.68520800
C	-3.35418700	0.80431700	0.31775500
C	2.38556300	0.30639800	1.88787800
H	1.75370300	1.06898300	2.35434200
H	2.17368100	-0.65093700	2.37282500
H	3.43809100	0.56681200	2.04949000
C	3.26110900	-0.99833000	-0.52723600
H	4.27199200	-0.67736200	-0.25011100
H	3.07322300	-1.99166800	-0.10931200
H	3.19874100	-1.07188300	-1.61780800
C	2.63495100	1.79387300	-0.55273000
H	2.02317400	2.62003400	-0.17736900
H	3.67502800	1.95132200	-0.24517400
H	2.58098400	1.80545100	-1.64575700
H	-0.68756200	-2.75941300	-1.25001400
H	-0.47028300	2.76924100	0.40934600
H	-3.65883200	0.91307000	-0.73501500
H	-4.25743500	0.97675500	0.91510800
H	-2.44995600	-0.76502100	1.52733300
H	-3.81310400	-1.29623300	0.54979000
H	-2.49248200	2.41264300	1.58507200
H	-2.44086200	-1.18081200	-1.54102800

17-tt

G-sol = -943.624420 Hartree

Ni	0.10764200	0.05408000	-0.03844100
P	2.22444100	0.00853100	0.00491700
C	-1.52082900	1.72050100	-0.39020600
C	-0.16444400	2.02225600	0.02018600
H	-0.04823300	2.38392000	1.04881200
H	0.42321200	2.61309300	-0.68581200
C	-0.08069000	-1.93698600	-0.10296400
C	-1.43448100	-1.70869900	0.36311300
H	0.00697800	-2.27347400	-1.14294800
H	0.55164400	-2.52843700	0.56507400
C	-2.59590300	1.44708200	0.40840100
C	-3.79988600	0.74690100	-0.09299100
C	-2.55229600	-1.49186900	-0.39142500
C	-3.76415600	-0.84293300	0.15817400
H	-4.68500700	-1.23614000	-0.29056900
H	-3.82871800	-1.00403000	1.24165800
C	3.17089900	1.59079000	-0.15451200
H	2.95345200	2.05123000	-1.12306500
H	2.85514900	2.28752700	0.62753100
H	4.25073600	1.42140800	-0.07330800
C	2.92259200	-0.68784400	1.57317300
H	4.01757700	-0.73093500	1.53973600
H	2.61686200	-0.06261200	2.41802000
H	2.52650000	-1.69455600	1.73330200
C	3.03179200	-1.03947300	-1.28947800
H	2.78090500	-0.65114800	-2.28167700
H	4.12196200	-1.04748400	-1.17523600
H	2.65261200	-2.06234400	-1.21857500
H	-2.48984600	-1.61549100	-1.47472700
H	-1.67834600	1.60679000	-1.46741900
H	-3.91341400	0.90376400	-1.17305600
H	-4.71693400	1.10463400	0.39179100
H	-2.49911200	1.58058200	1.48796200
H	-1.55416500	-1.60685400	1.44629200

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G-sol = -1099.434370 Hartree

Ni	-0.29218100	-0.46132100	-0.31625000
P	-1.93953800	1.23266300	-0.03528500
C	1.56853200	1.62359100	0.15606600
C	0.99444400	0.88323000	-1.00441200
H	1.76294400	0.40096000	-1.60880000

H	0.42083700	1.56274400	-1.65161600
C	1.08667900	-1.88095000	-0.56285800
C	2.32465100	-1.50779900	0.14502700
H	0.62369300	-2.79428200	-0.16791800
H	1.25357700	-1.99585500	-1.64262600
C	2.84520000	1.76797900	0.57137500
C	4.12486700	1.27533900	-0.07426400
C	3.45796800	-1.08445800	-0.43763500
C	4.47707600	-0.21024900	0.23357500
C	-2.23705500	1.74205500	1.72694600
H	-2.59778000	0.88403200	2.30261300
H	-1.29888300	2.08491000	2.17454600
H	-2.97929900	2.54589400	1.79526300
C	-1.72204400	2.88597000	-0.84745500
H	-2.54551200	3.56247700	-0.59171500
H	-0.77692300	3.33911800	-0.53624200
H	-1.69191400	2.76017700	-1.93452200
C	-3.67360600	0.83216400	-0.56865000
H	-3.99973700	-0.09905800	-0.09655300
H	-4.37120600	1.63277300	-0.29722900
H	-3.70404100	0.69798800	-1.65501600
H	0.83161000	2.13376700	0.78576900
H	4.47291400	-0.36709700	1.32086600
H	5.49687300	-0.41534300	-0.12327000
H	4.06283800	1.38579800	-1.16586200
H	4.95317500	1.91859900	0.25562500
H	3.54435400	-1.16163400	-1.52444000
H	2.25504500	-1.41710100	1.23335800
H	2.99312500	2.33839500	1.49038000
C	-1.85862700	-2.02970600	-0.11295500
C	-1.45110700	-1.81237400	1.02290600
C	-1.02937400	-1.82381000	2.42892900
H	-1.66035700	-2.50277400	3.01646000
H	0.00862700	-2.16804700	2.50591300
H	-1.08094200	-0.82947800	2.88417400
C	-2.41294000	-2.51491600	-1.38101200
H	-1.61793900	-2.95212300	-1.99599600
H	-3.17336900	-3.28580900	-1.20254100
H	-2.87555900	-1.70839500	-1.95985300

TS19 (Imaginary Frequency = -313.06)

G-sol = -1099.411624 Hartree

Ni	0.49998800	0.26269100	-0.01780900

P	2.21036100	-1.11263000	-0.12229400
C	-1.74698300	-0.67250600	1.57094300
C	-0.71844200	-1.21590400	0.64420200
H	-1.15365300	-1.78733600	-0.18321700
H	-0.07707400	-1.90208900	1.22206600
C	-0.89100200	1.10815700	-1.40413200
C	-2.31007300	0.86934800	-1.10835700
H	-0.67730600	2.06141400	-1.88760400
H	-0.42478000	0.31485000	-2.00418700
C	-3.09303700	-0.76646200	1.52407900
C	-3.92709700	-1.49561500	0.49226400
C	-2.99120000	-0.24010900	-1.42547900
C	-4.27639800	-0.62797500	-0.75478900
C	2.95246900	-1.59367700	1.50590300
H	3.33726300	-0.70079500	2.00859000
H	2.17936700	-2.03341500	2.14328400
H	3.76845000	-2.31532200	1.38258300
C	1.88206000	-2.76199900	-0.89876300
H	2.76706200	-3.40774600	-0.86445700
H	1.05459700	-3.25428400	-0.38114000
H	1.58895100	-2.61478700	-1.94340800
C	3.70460800	-0.56846500	-1.07187700
H	4.10485700	0.34944500	-0.63328000
H	4.48538100	-1.33829600	-1.07275500
H	3.41872900	-0.35091200	-2.10602300
H	-1.33754000	-0.13157400	2.42956800
H	-4.82602700	0.26541800	-0.43010900
H	-4.93692300	-1.19703100	-1.42301700
H	-3.39920700	-2.39437600	0.14594900
H	-4.86209100	-1.84123100	0.95505900
H	-2.50359200	-1.01112300	-2.02484100
H	-2.81567400	1.61672700	-0.49785500
H	-3.65964300	-0.26572300	2.31087300
C	1.39462800	1.94972200	0.10804300
C	0.11927600	2.18300400	0.14714000
C	-0.89143300	3.19010300	0.57616500
H	-0.38799900	3.99355600	1.12953600
H	-1.41462700	3.64975900	-0.27216500
H	-1.64841800	2.74778100	1.23295400
C	2.66369600	2.68309900	0.38496000
H	3.23557600	2.83611100	-0.54068200
H	2.48683400	3.67494300	0.82662800
H	3.31597100	2.12580300	1.06890100

20

G-sol = -638.520879 Hartree

Ni	0.40760600	0.17256300	-0.12236600
C	-1.36496100	-1.60741800	1.07677000
C	-0.43499300	-1.61933900	-0.06516400
H	-0.93346300	-1.78755700	-1.02675700
H	0.35113700	-2.36742500	0.07321700
C	0.80828400	2.23905500	-0.37072800
C	-0.53580100	2.02198500	-0.05411200
H	1.43219400	2.82162800	0.30075400
H	1.15561600	2.18386100	-1.40157500
C	-2.64041700	-1.16551000	1.04805000
C	-3.26123700	-0.55870700	-0.17155000
C	-1.35633700	1.13742800	-0.78728300
C	-2.79706900	0.91540500	-0.39811300
H	-0.97047400	-1.96502000	2.03011000
H	-3.01486600	1.47913300	0.51859500
H	-3.43452600	1.34463200	-1.18460400
H	-3.02457600	-1.14031600	-1.07281700
H	-4.35439700	-0.55099800	-0.08281300
H	-1.12587700	0.99490600	-1.84660000
H	-0.89438900	2.33932900	0.92681100
H	-3.22930300	-1.16749900	1.96431900
C	2.22651800	-0.73173200	-0.47322200
C	2.32589500	-0.09817400	0.58681600
C	2.49898100	-1.60044400	-1.62979400
H	2.46579400	-1.03490100	-2.56815700
H	3.49377300	-2.05561100	-1.54221500
H	1.75817400	-2.40374400	-1.69894400
C	2.85227400	0.49083900	1.83062800
H	2.17496700	0.31659900	2.67380300
H	3.82487900	0.04756200	2.07976100
H	2.98554900	1.57335000	1.72956600

20-cc

G-sol =-638.521976 Hartree

Ni	-0.29693400	0.24404300	-0.14838200
C	0.38530200	2.15766000	-0.08571100
C	-0.18227600	1.95656100	1.17143500
H	-1.06578200	2.51861400	1.45981500
H	0.38031000	1.50635400	1.98646900
C	0.28439900	-1.30569000	-1.20932100
C	0.92436500	-1.96561400	-0.06107400
H	-0.56297700	-1.86971100	-1.60854500

H	0.96888200	-1.02581500	-2.01341600
C	1.39785500	1.30149000	-0.60792900
C	2.60026600	0.82646000	0.18553200
C	2.14785400	-1.67380900	0.44345600
C	3.06073200	-0.62576500	-0.12856800
H	-0.15692000	2.79187100	-0.78866200
H	0.33046400	-2.71468900	0.46617700
H	3.14356000	-0.73035800	-1.22068600
H	4.07280600	-0.75753000	0.27259700
H	2.41684000	0.91388500	1.26336300
H	3.44050600	1.50230600	-0.03937500
C	-2.05691400	-0.46335800	0.76829700
C	-2.33752300	-0.21285400	-0.40681400
C	-2.97105200	-0.04947100	-1.72279400
H	-2.43783400	-0.62752800	-2.48506000
H	-4.01258900	-0.39540500	-1.69275200
H	-2.97047200	0.99974000	-2.03921900
C	-2.09041000	-0.83844400	2.19065900
H	-1.92443700	0.03677400	2.82880400
H	-3.06247800	-1.27516600	2.45245600
H	-1.31162800	-1.57193000	2.42565900
H	1.60258300	1.41846800	-1.67257200
H	2.48775600	-2.19609500	1.33664100

20-tt

G-sol = -638.496597 Hartree

Ni	-0.55736000	0.00017700	-0.00092300
C	1.15851600	-1.56665100	-0.65530000
C	-0.18253400	-1.94780200	-0.26328800
H	-0.26439500	-2.49839500	0.67834500
H	-0.78614500	-2.39331300	-1.05492000
C	-0.18071000	1.94846200	0.25842800
C	1.15961100	1.56775400	0.65355600
H	-0.26055100	2.49653300	-0.68494100
H	-0.78515900	2.39680000	1.04784400
C	2.27044200	-1.50693000	0.13345700
C	3.48130700	-0.76087300	-0.26881900
C	2.27324200	1.50685100	-0.13273700
C	3.48211000	0.75897100	0.27233300
H	4.40183200	1.21262000	-0.11589800
H	3.56440000	0.71496100	1.36481100
H	2.21414100	1.86149800	-1.16338200
H	1.27595000	-1.22940600	-1.68889500
H	3.56604600	-0.71674800	-1.36109700

H	4.39942900	-1.21617600	0.12125700
C	-2.41321100	-0.59899200	0.19641700
C	-2.41348700	0.59872500	-0.19486100
C	-3.10550000	1.85732600	-0.55061000
H	-2.75223800	2.25762700	-1.50721300
H	-4.18610100	1.68308900	-0.62978900
H	-2.94261000	2.63167100	0.20704500
C	-3.10410000	-1.85729900	0.55438000
H	-4.18509000	-1.68432600	0.63091900
H	-2.93872000	-2.63382300	-0.20042100
H	-2.75233100	-2.25413200	1.51295600
H	2.20883400	-1.86196700	1.16381100
H	1.27466400	1.23127300	1.68768800

TS21 (Imaginary Frequency = -206.41)

G-sol = -638.505798 Hartree

Ni	-0.30890300	0.04072000	-0.04662500
C	1.75532400	1.63617900	0.80271300
C	0.74246200	1.66763000	-0.26913600
H	1.17121700	1.59271800	-1.27628900
H	0.12476200	2.56639700	-0.21484800
C	-1.07159700	-1.92356800	0.07434800
C	0.35531800	-1.81687600	0.34299800
H	-1.62826400	-2.41572300	0.86634900
H	-1.35517600	-2.27258400	-0.91836200
C	2.93605400	0.98303700	0.77015900
C	3.38160900	0.12100800	-0.37293100
C	1.28067800	-1.39695700	-0.59973300
C	2.75519200	-1.30941200	-0.31230200
H	1.50300500	2.17388400	1.71889800
H	2.96080400	-1.73049100	0.67977600
H	3.28154200	-1.94155600	-1.04136700
H	3.12578700	0.57340400	-1.33978400
H	4.47201000	0.00329300	-0.35971000
H	0.99367800	-1.38942500	-1.65241400
C	-2.38630000	-0.29946300	0.08966700
C	-1.97321100	0.88311500	-0.20034900
C	-3.64040700	-1.03973000	0.40552400
H	-4.49675900	-0.36725000	0.27327100
H	-3.78828700	-1.90992600	-0.24634700
H	-3.65337900	-1.40043800	1.44188800
C	-2.52567900	2.24531200	-0.42783600
H	-2.17156000	2.94030300	0.34264600
H	-2.19424900	2.64824600	-1.39193000

H	-3.62397700	2.25039100	-0.41258400
H	3.57929400	1.00614300	1.64915300
H	0.69217400	-1.96921000	1.36840600

TS21-cc (Imaginary Frequency = -232.20)

G-sol = -638.500007 Hartree

Ni	0.23797900	-0.07413900	-0.54177900
C	-0.05980800	-2.01225700	-0.70031200
C	1.02791400	-1.87128300	0.26885900
H	1.89121100	-2.48210900	0.02017000
H	0.76528400	-1.93947700	1.32345400
C	-0.94600900	1.37723800	-1.07458700
C	-1.55137200	1.86675200	0.18825400
H	-0.39510900	2.16486900	-1.59667200
H	-1.68401600	0.94501200	-1.76084100
C	-1.34561700	-1.50415800	-0.53634200
C	-2.14329300	-1.29142500	0.72690200
C	-2.49230300	1.25935200	0.93743500
C	-3.12036800	-0.08190800	0.64527100
H	0.21660500	-2.37680100	-1.68951400
H	-1.14972400	2.80457000	0.57768100
H	-3.58618700	-0.09320800	-0.35271600
H	-3.93394000	-0.25755200	1.35830300
H	-1.49850000	-1.19121400	1.60752000
H	-2.74803700	-2.20022100	0.87953400
C	2.14584400	-0.18939600	0.36800400
C	1.66821200	0.96913100	0.04885700
C	2.10899400	2.38998600	0.08067800
H	1.43443000	2.98950200	0.70340100
H	3.12809600	2.50383100	0.47579500
H	2.08026700	2.82625500	-0.92482300
C	3.42310500	-0.76295000	0.88771400
H	3.92847700	-1.38663000	0.13915400
H	4.10143700	0.05599400	1.15545300
H	3.26967400	-1.38229500	1.78063200
H	-2.80678900	1.74431500	1.86040100
H	-1.96838700	-1.54343500	-1.43150600

TS21-tt (Imaginary Frequency = -207.21)

G-sol = -638.487256 Hartree

Ni	-0.42196900	0.16991800	-0.06928200
C	1.53952200	1.64994400	0.34143500

C	0.22484600	2.01841100	-0.16788500
H	0.20211300	2.32336200	-1.22118200
H	-0.33395700	2.71894400	0.45565100
C	-0.66450900	-1.90933400	-0.02610500
C	0.72241200	-1.66587100	-0.42514100
H	-0.79143800	-2.28970400	0.98831400
H	-1.21195100	-2.50149200	-0.75488900
C	2.62356600	1.25933500	-0.37334800
C	3.61435300	0.32562700	0.22173400
C	1.77782900	-1.49721700	0.42497700
C	3.16231000	-1.18239500	-0.02433300
H	3.88163100	-1.82338500	0.50252200
H	3.25958500	-1.39121800	-1.09658600
H	1.60085100	-1.57025500	1.49927100
H	1.60303400	1.53514400	1.42785500
H	3.69579100	0.48340200	1.30481300
H	4.62128100	0.42040000	-0.20318400
C	-2.20307200	0.69066900	0.04533900
C	-2.34981400	-0.58328600	0.03402800
C	-3.39578800	-1.64114000	0.07186200
H	-3.22279900	-2.37364800	0.86959900
H	-4.37032100	-1.17031400	0.25002200
H	-3.45870400	-2.19538700	-0.87310300
C	-2.98933800	1.95033200	0.10706900
H	-4.06958300	1.75489300	0.13961000
H	-2.72075900	2.53512000	0.99467600
H	-2.78031500	2.58301300	-0.76316300
H	2.61031400	1.35457700	-1.46115500
H	0.92646100	-1.64160800	-1.49696800

22

G-sol = -638.552716 Hartree

Ni	-0.33221200	0.33632800	-0.24281500
C	-1.96315100	1.44551400	-0.85434600
C	-1.13239700	2.15060900	0.06341700
H	-1.33586400	2.12543400	1.13386500
H	-0.65536100	3.06450300	-0.27761400
C	1.71344800	-1.64620500	-0.62731400
C	0.20065600	-1.69514400	-0.53033200
H	2.00916300	-1.77098000	-1.67974600
H	2.15458500	-2.51036800	-0.10094500
C	-2.46907800	0.16989800	-0.61712800
C	-2.77761700	-0.48344400	0.71494600
C	-0.47639800	-1.54873700	0.66176400

C	-1.96821900	-1.79806800	0.83288100
H	-1.93852500	1.76665100	-1.89650300
H	-2.31200800	-2.48992700	0.05231300
H	-2.15990100	-2.28145700	1.79916700
H	-2.53383200	0.18063000	1.55181200
H	-3.85245800	-0.70621500	0.79202700
H	0.10046300	-1.41169000	1.57540600
C	2.30214800	-0.35126300	-0.07716600
C	1.48402300	0.67848000	0.23411100
C	3.81294100	-0.37821500	0.01426400
H	4.23941500	0.55510200	0.38847600
H	4.15214900	-1.19228400	0.67253400
H	4.26023800	-0.57375000	-0.97171900
C	1.96552400	1.98868200	0.80930400
H	1.79814600	2.81348300	0.10353600
H	1.40306500	2.24714800	1.71608800
H	3.03086100	1.99691600	1.07606100
H	-0.34802900	-2.06117700	-1.39831600
H	-2.86145300	-0.36184700	-1.48403100

22-cc

G-sol = -638.534675 Hartree

Ni	-0.50022100	0.27381500	-0.62562700
C	-2.15984200	1.29422800	-0.16580700
C	-2.54765100	0.37053700	-1.16272300
H	-2.84784900	0.75557300	-2.13511300
H	-3.01124300	-0.57434300	-0.89434300
C	1.90986200	-1.47987300	-0.37406400
C	0.50017800	-1.66812600	-0.90281900
H	2.61646400	-1.83229700	-1.13998100
H	2.08194400	-2.13662700	0.49548300
C	-1.53968200	0.84330500	1.02866600
C	-1.82605700	-0.50868700	1.67690400
C	-0.63944900	-1.80515400	-0.14514900
C	-0.77702300	-1.61864800	1.34726600
H	-2.08737600	2.35453700	-0.40893200
H	0.41661600	-1.93326200	-1.95713800
H	0.18655200	-1.34570700	1.78689800
H	-1.11223800	-2.55667500	1.81516700
H	-2.81464600	-0.86571500	1.35828700
H	-1.87102500	-0.38811800	2.76652800
C	1.20891200	0.85248800	0.01411400
C	2.22387000	-0.04138300	-0.01259300
C	3.68230700	0.21349300	0.30237600

H	4.32423900	-0.04997600	-0.55076200
H	3.88967300	1.25299000	0.56684000
H	4.01478100	-0.41419400	1.14303900
C	1.39354000	2.30432800	0.40761500
H	1.05621700	2.48324400	1.43900000
H	2.43425400	2.65054500	0.34799600
H	0.80006900	2.97303500	-0.22938900
H	-1.11571300	1.60350500	1.67862600
H	-1.52832900	-2.18239200	-0.64737400

22-tt

G-sol = -638.557829 Hartree

Ni	0.28029900	0.41128700	-0.06019000
C	1.82149200	1.64839700	0.44333900
C	0.69718100	2.36182600	-0.06153400
H	0.66195600	2.63390300	-1.11730900
H	0.16456100	3.03839800	0.59868600
C	-1.56044900	-1.87406500	0.08750500
C	-0.15744400	-1.67436900	-0.43231700
H	-1.52884800	-2.27670400	1.11309900
H	-2.05440600	-2.64981600	-0.51868700
C	2.38250700	0.63818300	-0.33177500
C	3.20010600	-0.51571200	0.19958200
C	0.96155000	-1.62762700	0.35680400
C	2.39478800	-1.78263000	-0.13418700
H	2.84557000	-2.68390100	0.30678200
H	2.38814000	-1.93061300	-1.22216900
H	0.82426100	-1.68765500	1.43956900
H	2.02523200	1.66472400	1.51494400
H	3.31942000	-0.42272500	1.28726100
H	4.20765200	-0.55772600	-0.23656100
C	-1.65031200	0.58080900	-0.03531300
C	-2.34576600	-0.58024900	0.04474300
C	-3.84566300	-0.76650500	0.14113400
H	-4.10513400	-1.36026600	1.03066000
H	-4.39814400	0.17336500	0.20289000
H	-4.23233900	-1.32461400	-0.72454400
C	-2.34861900	1.92380600	-0.07689400
H	-3.44167300	1.85858900	-0.15414900
H	-2.12381200	2.51551100	0.82141500
H	-2.00295900	2.52247300	-0.92942800
H	-0.02921100	-1.74913600	-1.51377200
H	2.33513100	0.72897300	-1.41987300

TS23 (Imaginary Frequency = -348.35)

G-sol = -638.502995 Hartree

Ni	-0.35914000	0.18608800	-0.55499800
C	-1.07265000	1.86370500	0.13338600
C	-0.01628900	1.41755900	1.07903500
H	-0.31420000	0.76078900	1.89599500
H	0.57851800	2.24520100	1.46671900
C	1.34381600	-1.89470100	0.29606200
C	-0.02122800	-1.83741300	-0.37630200
H	1.96556100	-2.66481200	-0.17941000
H	1.24387300	-2.21047400	1.34712000
C	-2.18385900	1.10497100	-0.30920500
C	-3.01063100	0.06533900	0.45834600
C	-1.12165400	-1.47167700	0.37697300
C	-2.59642800	-1.37041800	0.05758700
H	-0.85550000	2.78507200	-0.40967000
H	-2.78633000	-1.53378900	-1.00934000
H	-3.17489700	-2.11993300	0.62289800
H	-2.85453600	0.18197000	1.54071000
H	-4.08322000	0.22507100	0.28141000
H	-0.92860600	-1.33833300	1.44687500
C	2.09060100	-0.56339300	0.20476500
C	1.47724200	0.65755300	0.16570400
C	3.59224600	-0.72924200	0.06081100
H	3.86286500	-1.09073900	-0.94222900
H	4.15065200	0.19001500	0.24971000
H	3.94961800	-1.48982500	0.76885500
C	2.29154900	1.89731900	-0.17879600
H	1.64211700	2.69788400	-0.55070600
H	2.82992200	2.30288500	0.69096100
H	3.03136100	1.69941200	-0.96140200
H	-0.11931700	-2.24600800	-1.38284100
H	-2.71825600	1.55755400	-1.14590400

24

G-sol = -1099.500451 Hartree

Ni	-0.23036500	-0.18428200	0.54994700
C	-1.53552700	-0.69300100	1.99280800
C	-0.42655000	-1.56140700	2.08415300
H	-0.43040500	-2.53139200	1.59477800
H	0.22430300	-1.49140900	2.95035900
C	1.90749700	-1.51100400	-1.43011300

C	0.44071700	-1.30100500	-1.69585500
H	2.47533000	-1.28154600	-2.34614200
H	2.09106300	-2.58042700	-1.23641800
C	-2.30558000	-0.59916900	0.81079300
C	-2.71200500	-1.80505000	-0.03919300
C	-0.53272600	-2.10885100	-1.24186900
C	-2.01646500	-1.91965200	-1.41314200
H	-2.21849900	-1.02469600	-2.01478600
H	-2.44692800	-2.77573800	-1.95570000
H	-2.50822600	-2.72712800	0.52295600
H	-3.80026900	-1.78004800	-0.19191000
H	-0.23566600	-2.99470300	-0.67703100
C	1.70654300	-0.09550600	0.65448200
C	2.48890100	-0.69633100	-0.26737900
C	2.27080700	0.66242400	1.83940400
H	3.36716200	0.72191100	1.87341600
H	1.89610400	1.69680700	1.86803300
H	1.94166300	0.20517600	2.78274500
C	4.00701000	-0.74027200	-0.27653100
H	4.41311800	-0.28272400	-1.19184200
H	4.46409000	-0.23204000	0.57557800
H	4.36857700	-1.78006500	-0.26938900
P	-0.46114400	1.80796100	-0.39557500
C	-0.94406800	3.10160900	0.84263800
C	-1.76286200	2.06360300	-1.69695400
C	1.00228500	2.60007300	-1.20670600
H	-1.07009800	4.08665800	0.37811300
H	-1.88327200	2.81301000	1.32542900
H	-0.17258500	3.16718200	1.61597200
H	-1.81111800	3.10921600	-2.02304900
H	-1.54668200	1.43448200	-2.56670000
H	-2.73952900	1.76812800	-1.30209400
H	1.32231500	1.99371200	-2.05936300
H	0.76907100	3.61325700	-1.55397300
H	1.83517400	2.63825300	-0.50010700
H	-1.62048000	0.10870000	2.72799700
H	-3.01319400	0.22979500	0.77944100
H	0.16850200	-0.44264600	-2.31043100

24-cc

G-sol = -1099.493206 Hartree

Ni	-0.22914800	0.14393400	0.70934700
C	-0.56662400	1.62425800	2.02219700
C	0.79078400	1.24894600	2.10183600

H	1.15557600	0.77561200	3.00859100
H	1.54514700	1.74149800	1.49426800
C	1.92412600	-0.30083600	-1.47966200
C	2.46488100	1.06655700	-1.14761100
H	2.49245700	-0.70623100	-2.33164300
H	0.88424200	-0.21482000	-1.81658200
C	-1.14926300	2.05987900	0.81394900
C	-0.48907200	3.03407200	-0.17361200
C	1.79369300	2.22566900	-1.08405400
C	0.33934600	2.49385100	-1.38070900
H	3.52532100	1.08734600	-0.89089800
H	-0.15235500	1.61235300	-1.80026700
H	0.29793700	3.26879600	-2.16134800
H	0.15436100	3.72497000	0.38957700
H	-1.29640800	3.65100500	-0.58769100
C	1.10809700	-1.24591200	0.69792500
C	2.01312100	-1.28899300	-0.30345500
C	1.11317400	-2.20390600	1.87054500
H	1.84975000	-3.01558400	1.79656000
H	1.30674100	-1.67002400	2.81148600
H	0.12786200	-2.67726900	1.99617200
C	3.20181900	-2.22818700	-0.40631100
H	4.14325800	-1.66311500	-0.48338100
H	3.30007600	-2.90111400	0.44898100
H	3.14424700	-2.84928200	-1.31390900
P	-1.72635400	-0.90143000	-0.51254100
C	-3.22014900	-1.29823700	0.51253200
C	-1.30507100	-2.56074700	-1.21190400
C	-2.50323100	-0.07432400	-1.98163400
H	-3.97212600	-1.84879400	-0.06512400
H	-2.92021300	-1.90287900	1.37408300
H	-3.66476000	-0.37051400	0.88582600
H	-2.15949900	-3.00039600	-1.73915400
H	-0.46117400	-2.46485000	-1.90044400
H	-0.99573600	-3.22758100	-0.40245100
H	-1.75033600	0.08684800	-2.75962200
H	-3.31395100	-0.68256700	-2.39936400
H	-2.90206600	0.90057000	-1.68667100
H	-1.23829000	1.28343800	2.81243500
H	2.35476400	3.11340700	-0.78330100
H	-2.23715600	2.12793500	0.83006700

24-tt

G-sol = -1099.495613 Hartree

Ni	0.09494000	-0.17104000	0.57231500
C	0.95613400	-1.49783200	1.85835600
C	0.05669000	-0.68997600	2.56988600
H	0.37133600	0.26144600	2.99798100
H	-0.81627900	-1.14241500	3.03061900
C	-1.96313300	-1.58691300	-1.30385900
C	-0.48664000	-1.43788000	-1.55144700
H	-2.16692800	-2.58529100	-0.88316000
H	-2.48970800	-1.56493800	-2.27215800
C	1.99306600	-0.95149900	1.05711700
C	2.70468700	-1.87048000	0.06862900
C	0.47013200	-2.26825900	-1.09771000
C	1.95036600	-2.06318600	-1.28005900
H	2.39454700	-2.91950800	-1.80964300
H	2.10870300	-1.18202100	-1.91238700
H	0.16301500	-3.14069000	-0.51826200
H	0.67557700	-2.53899000	1.69736600
H	2.84647200	-2.86080200	0.52862700
H	3.71256800	-1.49799000	-0.15153600
C	-1.80663400	0.19860800	0.47520600
C	-2.56438800	-0.51286900	-0.39175700
C	-4.07311900	-0.42999300	-0.55234000
H	-4.53560000	-1.41642700	-0.39436500
H	-4.55028300	0.26517200	0.14167800
H	-4.34916700	-0.12332100	-1.57295900
C	-2.40036200	1.22900400	1.41438900
H	-3.46295200	1.44869700	1.24628600
H	-2.29493800	0.90871800	2.45998400
H	-1.86608700	2.18750700	1.34561700
P	0.78647700	1.69127000	-0.43710200
C	1.20407700	2.99054000	0.82139300
C	-0.41226700	2.59450000	-1.52336500
C	2.31650100	1.75219000	-1.49355200
H	1.50813400	3.93266600	0.34992600
H	0.33527300	3.17497800	1.46016400
H	2.02090400	2.63224500	1.45639800
H	-0.00601300	3.55337000	-1.86553400
H	-0.65125500	1.97711300	-2.39509700
H	-1.34263000	2.76615400	-0.97602700
H	2.17448000	1.14451000	-2.39303400
H	2.55738200	2.77724900	-1.80000800
H	3.16379000	1.33966100	-0.93701400
H	2.56562700	-0.11387700	1.45524100
H	-0.19210200	-0.59887900	-2.18233200

TS25 (Imaginary Frequency = -321.15)

G-sol = -1099.464305 Hartree

Ni	-0.19572500	-0.27612800	0.58349600
C	0.85424400	-1.15868100	1.97746500
C	1.75400600	-0.10586700	1.49168900
H	2.52833600	-0.40727700	0.79393000
H	2.16944800	0.48583900	2.30979700
C	2.14853600	1.01154200	-1.55612000
C	1.41465000	-0.28987700	-1.71623200
H	2.09568900	1.59289000	-2.48975900
H	3.22280700	0.81871500	-1.39303600
C	0.32299600	-2.24415600	1.25058400
C	1.05342200	-3.14623100	0.24312600
C	1.91567800	-1.49816800	-1.44076300
C	1.10101500	-2.74339200	-1.25583200
H	0.08090800	-2.59176700	-1.62956400
H	1.53580900	-3.58532000	-1.81486100
H	2.09241200	-3.28381700	0.58086100
H	0.59104000	-4.14032400	0.29819100
H	2.96984300	-1.57936000	-1.16237000
C	0.97988700	1.39519600	0.68197800
C	1.59689000	1.88859700	-0.42733900
C	0.48031000	2.33094200	1.77666100
H	1.28119000	2.94713900	2.21241400
H	-0.28793000	3.01680900	1.39884800
H	0.02754300	1.76588100	2.59926800
C	1.83662300	3.36439600	-0.66175100
H	1.28233400	3.72612600	-1.54146100
H	1.55271400	3.98929400	0.18812100
H	2.89982800	3.55711600	-0.87512500
P	-2.12081100	0.17429700	-0.29816700
C	-3.34570500	0.82886500	0.93668800
C	-3.09920800	-1.21708000	-1.04968500
C	-2.27372400	1.45657200	-1.63905500
H	-4.32211200	1.02603300	0.47757500
H	-3.47082600	0.10106700	1.74454900
H	-2.96392900	1.75691000	1.37373400
H	-4.08602600	-0.88932600	-1.39907100
H	-2.54649700	-1.63951100	-1.89558900
H	-3.22556200	-2.00876500	-0.30468100
H	-1.72058200	1.13095900	-2.52670500
H	-3.31720400	1.63948900	-1.92263500
H	-1.82561200	2.39362600	-1.29326400
H	0.36773900	-0.94490900	2.93316000
H	-0.44258900	-2.78762700	1.80399800

H	0.36598000	-0.20873500	-2.00017600

TS25-cc (Imaginary Frequency = -317.91)

G-sol = -1099.462448 Hartree

Ni	0.29988300	-0.32907900	0.69081300
C	-0.87704600	-1.12181200	2.03081900
C	-1.58898800	0.09425000	1.63063300
H	-1.86152400	0.71124100	2.48795800
H	-2.42381000	-0.04852900	0.95555400
C	-1.51150700	1.07987400	-1.56804400
C	-2.73529300	0.21151500	-1.39242800
H	-1.68175800	1.72723200	-2.44088700
H	-0.64662800	0.45038400	-1.81841600
C	-0.54318600	-2.20995500	1.20138000
C	-1.36393500	-2.84980400	0.07489200
C	-2.77146800	-1.12233000	-1.26026900
C	-1.61832200	-2.09097600	-1.26229800
H	-3.68225400	0.75201600	-1.34794900
H	-0.68944500	-1.60519300	-1.57484700
H	-1.83732000	-2.86017700	-2.01867400
H	-2.33894400	-3.16795800	0.47720700
H	-0.84285700	-3.77742600	-0.19257100
C	-0.64686500	1.47559400	0.78991500
C	-1.12927000	1.97442100	-0.38281800
C	-0.11438100	2.40145700	1.87576300
H	-0.88371400	3.07287000	2.28615500
H	0.28750300	1.82393000	2.71628300
H	0.70131700	3.03221900	1.50051500
C	-1.20659200	3.45620800	-0.68293700
H	-2.21192700	3.73148900	-1.03605000
H	-0.97830800	4.08397100	0.18185700
H	-0.51411000	3.74014000	-1.49145000
P	2.13843900	-0.15020400	-0.41691800
C	3.61147600	-0.10181500	0.71604800
C	2.47315300	1.34043900	-1.47781800
C	2.63703400	-1.51390000	-1.57762000
H	4.55181700	-0.02229900	0.15699900
H	3.52612600	0.75508100	1.39191200
H	3.63184300	-1.01146600	1.32406300
H	3.49048700	1.33585200	-1.88708100
H	1.75781300	1.37016200	-2.30614800
H	2.32968600	2.24673200	-0.88122400
H	1.91944900	-1.57710900	-2.40231500
H	3.63960900	-1.35357700	-1.99269300
H	2.61773200	-2.46757500	-1.04132500

H	-0.36524200	-1.08369000	2.99602800
H	0.09289800	-2.94499800	1.69526000
H	-3.75059600	-1.58504600	-1.11845100

TS25-tt (Imaginary Frequency = -333.21)

G-sol = -1099.457751 Hartree

Ni	-0.13146100	0.10914300	0.42536300
C	0.97087000	1.35414900	1.56549600
C	1.27249800	-0.01950500	1.98255000
H	0.60276900	-0.46587800	2.72067600
H	2.30991200	-0.15537600	2.29259400
C	2.48126000	0.12686500	-1.24827300
C	1.28484500	1.02436100	-1.46953700
H	3.27700700	0.69882200	-0.74351000
H	2.91074700	-0.17619300	-2.21503000
C	-0.29160000	1.95216200	1.37159900
C	-0.35009400	3.25137200	0.57097800
C	1.23062400	2.33854200	-1.19239100
C	-0.04391900	3.10043800	-0.96570100
H	0.00037200	4.10879700	-1.40109700
H	-0.88116300	2.57145000	-1.43614100
H	2.14428600	2.83755000	-0.86021400
H	1.82240600	1.86260300	1.12280100
H	0.35874200	3.98573600	0.98375400
H	-1.34397800	3.70630500	0.66518000
C	1.35541300	-1.27276100	0.62028600
C	2.17742600	-1.16624600	-0.46677800
C	2.90547200	-2.36078700	-1.05605400
H	3.97841400	-2.13779000	-1.16000200
H	2.81890700	-3.26767700	-0.45460500
H	2.54539900	-2.59306000	-2.06997700
C	1.11995600	-2.62221900	1.28322000
H	0.89646200	-3.40672600	0.55190200
H	1.98796800	-2.96122600	1.86849900
H	0.27134600	-2.57304100	1.97334600
P	-1.96282600	-0.76444600	-0.29416800
C	-1.96049100	-2.51389800	-0.92964400
C	-2.84108400	0.08584300	-1.69868700
C	-3.33858000	-0.85920200	0.95283200
H	-2.95515100	-2.83699200	-1.25963600
H	-1.26323500	-2.59270800	-1.77043400
H	-1.61029300	-3.18726600	-0.14115700
H	-3.77313700	-0.42399500	-1.97168000
H	-3.07012700	1.11777700	-1.41389200

H	-2.18752400	0.11682500	-2.57718400
H	-3.55645800	0.14532900	1.32937300
H	-4.25340700	-1.28852000	0.52617700
H	-3.01983700	-1.47445800	1.80066800
H	-1.11193100	1.76250300	2.06383400
H	0.38923600	0.52321900	-1.84125000

26

G-sol = -1099.490333 Hartree

Ni	-0.03665900	-0.60787500	-0.09766400
C	0.96344100	-0.59072700	1.67573200
C	2.10096700	0.36241800	1.30218700
H	2.82584100	-0.10606400	0.63957200
H	2.65367300	0.62950800	2.21791900
C	1.58845600	1.04479500	-1.82019200
C	0.84664600	-0.30519600	-1.89785900
H	1.36087000	1.63085200	-2.71771800
H	2.67133700	0.85385200	-1.86543300
C	0.70545300	-1.92655900	1.36320200
C	1.51388300	-2.95475600	0.56294500
C	1.49204900	-1.33997300	-1.21391900
C	1.23902100	-2.80716100	-0.96183600
H	0.20978000	-3.10552800	-1.19804100
H	1.91115000	-3.46533000	-1.53695700
H	2.59041300	-2.81549200	0.73371100
H	1.27184800	-3.96554700	0.91503100
H	2.48891600	-1.08237300	-0.85878900
C	1.53707300	1.67509000	0.70985300
C	1.30331600	1.95428600	-0.59942300
C	1.22686400	2.64668400	1.83571500
H	2.15797400	3.00417400	2.29976000
H	0.64784800	3.52237600	1.54153300
H	0.66599800	2.13952600	2.63275300
C	0.75887600	3.29332700	-1.06473700
H	-0.15426200	3.14676500	-1.65849100
H	0.52980100	4.00384400	-0.27015200
H	1.48194400	3.77744500	-1.73705500
P	-2.14305900	0.01269800	0.02018700
C	-2.76569100	0.75196900	1.61247700
C	-3.32853700	-1.40884300	-0.17352400
C	-2.87218000	1.21708800	-1.19726700
H	-3.84452900	0.94814200	1.58781400
H	-2.55016200	0.06823100	2.44064900
H	-2.24010100	1.69257000	1.80903400

H	-4.37355400	-1.09129500	-0.07130100
H	-3.19217100	-1.86669300	-1.15880400
H	-3.11273500	-2.17014600	0.58331200
H	-2.71538000	0.84237200	-2.21412000
H	-3.94586000	1.37641400	-1.03743100
H	-2.35468000	2.17804000	-1.11136000
H	0.31507100	-0.17582700	2.45034100
H	-0.12180000	-2.36127800	1.92681100
H	0.13727800	-0.45317200	-2.71092800

26-cc

G-sol = -1099.492686 Hartree

Ni	0.76408900	0.15427600	-0.74442500
C	-0.87647900	0.61883000	-1.76530100
C	-2.26971000	0.27560900	-1.25233600
H	-2.96282900	0.36093300	-2.10392500
H	-2.58126000	1.03336000	-0.53387900
C	-1.52008500	-0.36239100	1.58693300
C	-2.31920600	0.89114900	1.84500800
H	-1.33766700	-0.85857100	2.55180600
H	-0.52802100	-0.09612600	1.18514700
C	-0.15669000	1.78076700	-1.44528800
C	-0.57649100	2.90873000	-0.49744600
C	-1.93291700	2.15064900	1.60067700
C	-0.61145600	2.62292500	1.03855800
H	-3.31883400	0.73037700	2.25174100
H	0.19163200	1.91517700	1.27004300
H	-0.35672100	3.56062800	1.55127700
H	-1.55542000	3.30655500	-0.80604900
H	0.13668300	3.72728100	-0.65243100
C	-2.45458400	-1.11430200	-0.64417300
C	-2.16298600	-1.38916500	0.64594100
C	-3.01053700	-2.11856600	-1.62982500
H	-4.01791800	-1.82315000	-1.95773100
H	-2.38793700	-2.14006700	-2.53538000
H	-3.07019600	-3.14022000	-1.25010800
C	-2.37608800	-2.73483700	1.30490500
H	-3.02845100	-2.63019600	2.18399000
H	-2.82456600	-3.48617300	0.65271400
H	-1.42451700	-3.14196100	1.67739900
P	2.63795700	-0.49979000	0.14071700
C	4.00984400	-0.95749100	-1.02765000
C	2.61425300	-2.00051700	1.23968500
C	3.50204500	0.72680600	1.23541300

H	4.91879000	-1.26056000	-0.49340000
H	3.68114000	-1.78153000	-1.66906900
H	4.24000900	-0.10284800	-1.67151400
H	3.61467400	-2.24226700	1.61863700
H	1.94467300	-1.82555500	2.08780900
H	2.23128500	-2.85957900	0.67916400
H	2.85176500	0.98906100	2.07568000
H	4.44682500	0.32721600	1.62387400
H	3.70660000	1.64049100	0.66888900
H	-0.61564900	0.13399000	-2.71359300
H	0.57830200	2.10697200	-2.18643900
H	-2.64973200	2.94469600	1.81788600

26-tt

G-sol = -1099.481599 Hartree

Ni	0.06858200	-0.00973900	-0.24065600
C	1.79439400	-0.14236400	-1.29362800
C	1.59539900	1.29018500	-1.74159900
H	1.05139100	1.35450500	-2.69223700
H	2.55578000	1.81050100	-1.89779200
C	1.98818600	1.06726900	1.48728200
C	1.55274800	-0.37735400	1.67795800
H	2.93871100	1.09989800	0.94457400
H	2.15228100	1.59617200	2.43750600
C	1.03580400	-1.30599500	-1.50401700
C	1.53188600	-2.61923500	-0.88102200
C	2.23999600	-1.45279200	1.24936500
C	1.58891800	-2.68949000	0.69852900
H	2.12767800	-3.60823600	0.96884700
H	0.56528400	-2.77496400	1.08415200
H	3.28796100	-1.31898200	0.97234900
H	2.70150100	-0.26720700	-0.71701600
H	2.54182600	-2.84729000	-1.25590100
H	0.89447900	-3.44797200	-1.21436200
C	0.72508900	1.97591700	-0.66007600
C	0.85633600	1.81114000	0.72061400
C	-0.01958700	2.57495700	1.70222800
H	0.48783700	3.48525300	2.05900200
H	-0.98886600	2.87249600	1.29781500
H	-0.21456000	1.95981600	2.58933500
C	-0.22817600	2.99120800	-1.26564200
H	-0.82107000	2.53936500	-2.06962300
H	-0.91735000	3.45042700	-0.55541500
H	0.35425600	3.80558800	-1.72482200

P	-2.02827600	-0.49996600	0.07321900
C	-3.23317300	0.41855300	-1.00859500
C	-2.80380100	-0.21959300	1.74601800
C	-2.58987200	-2.24756200	-0.24008700
H	-4.27078000	0.12179400	-0.81228300
H	-3.13218600	1.49537700	-0.84037300
H	-3.00129500	0.21921400	-2.06002500
H	-3.86612500	-0.49256900	1.76378400
H	-2.27644200	-0.81646600	2.49867400
H	-2.70242100	0.83442200	2.02429000
H	-2.06282700	-2.92784900	0.43726400
H	-3.67065100	-2.37130500	-0.09663500
H	-2.33113700	-2.53153000	-1.26545300
H	0.37637000	-1.40327500	-2.36767800
H	0.51931500	-0.51405800	2.00815200

27

G-sol = -943.613322 Hartree

Ni	-0.42495900	0.02343200	-0.01877400
P	1.78794500	0.08896300	0.00124900
C	2.74103400	1.68496400	-0.01390200
H	3.82055100	1.49596700	0.02073100
H	2.51113000	2.24759600	-0.92379900
H	2.46293900	2.30074600	0.84559500
C	2.56568900	-0.70661200	1.48910300
H	2.20354100	-1.73161800	1.60279600
H	3.66020900	-0.71563900	1.42121400
H	2.27017300	-0.14812900	2.38338900
C	2.65520700	-0.76970900	-1.39904500
H	2.37593400	-0.28529700	-2.34058800
H	3.74471100	-0.72202400	-1.28493300
H	2.34829700	-1.81591100	-1.45543000
C	-0.83306000	1.94269200	0.04575700
C	-1.89555900	1.30887000	-0.21484700
C	-1.66933300	-1.47409600	0.21492400
C	-0.52909100	-1.94425000	-0.06696900
C	-3.34409500	1.32894400	-0.53043000
H	-3.57644000	0.72199000	-1.41319100
H	-3.94878200	0.94258900	0.29751700
H	-3.67619900	2.35685100	-0.73157100
C	-0.20674800	3.27259400	0.26719200
H	0.31391100	3.32505100	1.23095800
H	0.52866000	3.51402800	-0.50887500
H	-0.96802700	4.06479800	0.25916900

C	-3.08743700	-1.72992700	0.56489200
H	-3.24163400	-2.79761900	0.77449100
H	-3.39620900	-1.16564800	1.45252900
H	-3.76603900	-1.45163500	-0.24899000
C	0.26682300	-3.17677900	-0.31101800
H	-0.30217000	-4.07200000	-0.02490100
H	0.52562500	-3.27982900	-1.37278300
H	1.20891700	-3.19495300	0.24967000

27b

G-sol = -1697.699471 Hartree

Ni	0.03466800	-0.40268600	0.09725800
P	0.22633500	-2.56028200	0.61743200
C	-1.04394000	-3.14158600	1.82870000
H	-0.82622500	-4.16819400	2.14515000
H	-1.03370900	-2.49002600	2.70852200
H	-2.03186100	-3.10736800	1.36800700
C	0.12364700	-3.77534400	-0.76066500
H	0.92649900	-3.56084700	-1.47114000
H	0.22720100	-4.80146400	-0.38956100
H	-0.84651400	-3.65973600	-1.25087700
C	1.77066800	-3.03803200	1.51624800
H	1.90985000	-2.38043500	2.38063200
H	1.69875200	-4.07363700	1.86782600
H	2.62993500	-2.94179500	0.85156400
C	-1.87139800	-0.36252800	-0.12320800
C	-1.44529700	0.83879700	-0.09991700
C	1.42160200	0.98708800	0.16390600
C	1.92421600	-0.10150700	-0.24096800
C	-1.66582500	2.28146000	-0.10600400
O	-1.62686400	2.97926200	0.88970100
O	-1.88434000	2.73419000	-1.35205100
C	-3.06821500	-1.17869800	-0.33006600
O	-3.08084500	-2.37375000	-0.57340900
O	-4.18985200	-0.43266000	-0.24105500
C	1.42263100	2.42491900	0.41846900
O	1.26458900	3.26011400	-0.45030100
O	1.58887500	2.68976600	1.72287000
C	3.08350500	-0.78713900	-0.80679900
O	3.10572900	-1.94143500	-1.19896600
O	4.14873500	0.03859800	-0.86867200
C	-1.96658200	4.16639500	-1.47658800
H	-2.13658000	4.35189000	-2.53724200
H	-2.79446800	4.55701900	-0.87915600

H	-1.02744100	4.61844900	-1.15056800
C	-5.41850100	-1.14068200	-0.47393500
H	-6.20717600	-0.39751200	-0.35466400
H	-5.43402800	-1.56062500	-1.48339700
H	-5.53906700	-1.95060700	0.25067600
C	1.46150900	4.07834300	2.08658900
H	0.45642100	4.42833200	1.84218400
H	1.63135900	4.10829400	3.16281800
H	2.20579300	4.68236800	1.56130900
C	5.32920700	-0.52634400	-1.46382400
H	5.12851500	-0.83679000	-2.49268600
H	6.07301000	0.27021400	-1.44051100
H	5.67242800	-1.39160300	-0.89013300

27c

G-sol = -1172.568754 Hartree

Ni	-0.61231700	-0.05800400	-0.01536800
P	-2.80280000	-0.03908900	0.00014900
C	-3.77450500	-1.61568800	-0.10037800
H	-4.85204100	-1.41942100	-0.07047100
H	-3.53877100	-2.13954800	-1.03234100
H	-3.51246100	-2.27044000	0.73690900
C	-3.56015100	0.72345100	1.51090700
H	-3.17285700	1.73661400	1.65144600
H	-4.65353200	0.76198500	1.44162800
H	-3.27840000	0.13334000	2.38890800
C	-3.59436700	0.92742100	-1.36938100
H	-3.32642900	0.47440600	-2.32931200
H	-4.68641200	0.94736000	-1.27519800
H	-3.21424500	1.95290600	-1.36708100
C	-0.54536500	-1.99186900	-0.14137200
C	0.65035300	-1.61405000	-0.02062000
C	0.58706900	1.51340100	-0.00927300
C	-0.63125200	1.85050800	0.10894300
C	2.09943600	-2.02910400	0.02403000
C	2.58574200	-2.26626700	-1.42217900
C	2.21256300	-3.31733600	0.85614900
H	1.99312600	-3.03999800	-1.92200400
H	2.50667100	-1.34195700	-2.00359700
H	3.63603700	-2.57904800	-1.40042200
H	3.26052400	-3.63487500	0.89048400
H	1.87280500	-3.13269400	1.87957100
H	1.60907200	-4.12041100	0.42182600
C	1.96414900	2.09122900	-0.00326200

C	1.94832100	3.49049100	-0.64276600
C	2.51228700	2.14004000	1.43504800
H	1.30119300	4.16775100	-0.07667400
H	2.95943900	3.92022800	-0.65400800
H	1.58180500	3.43119200	-1.67142100
H	3.52897700	2.55693800	1.43782600
H	1.88305600	2.77633100	2.06521100
H	2.54141700	1.13455200	1.86213600
H	-1.29065900	-2.76034700	-0.23851100
H	-1.35319900	2.64594600	0.21085300
O	2.93879300	-1.08494000	0.66713100
H	2.92293600	-0.27506700	0.11382300
O	2.81623700	1.23909800	-0.81402500
H	3.70289100	1.63806700	-0.81144700

TS28 (Imaginary Frequency = -215.18)

G-sol = -943.582573 Hartree

Ni	0.13167400	0.02668400	-0.00620200
P	-1.99940200	0.04132700	-0.00234300
C	-2.79483800	-0.81710100	1.43639600
H	-3.88934600	-0.79006700	1.37224100
H	-2.46232800	-1.85927500	1.46754000
H	-2.47835700	-0.33428100	2.36638800
C	-2.87785400	1.67323100	0.02245900
H	-2.59451700	2.25277800	-0.86194500
H	-3.96757900	1.55172200	0.03688000
H	-2.56657000	2.23606500	0.90787200
C	-2.81570700	-0.79496800	-1.44014000
H	-2.47633300	-1.83366800	-1.49188000
H	-3.90912300	-0.77306400	-1.35915800
H	-2.51458700	-0.29683600	-2.36705400
C	0.94047600	1.71744100	0.21255500
C	1.92322500	0.93545200	-0.15520400
C	0.81937100	-1.71888300	-0.21742300
C	1.85251000	-1.00874700	0.15739400
C	3.22895700	1.15040500	-0.85734700
H	4.10092200	0.95642700	-0.22213900
H	3.31795100	0.50725400	-1.74124400
H	3.28885600	2.19558800	-1.18651800
C	0.77915900	3.19847500	0.29170700
H	-0.10841400	3.53309000	-0.25920400
H	0.63580400	3.51747800	1.33283200
H	1.65055600	3.74552900	-0.10126000
C	0.55214500	-3.18425700	-0.29668800

H	1.38272400	-3.79342700	0.09320300
H	-0.35482900	-3.45534500	0.25886100
H	0.38145200	-3.49282300	-1.33676000
C	3.13597700	-1.31776900	0.86610800
H	4.02279200	-1.18583200	0.23574400
H	3.26549400	-0.68316800	1.75119700
H	3.11905600	-2.36486200	1.19429200

TS28b (Imaginary Frequency = -165.46)

G-sol = -1697.676281 Hartree

Ni	-0.00977900	0.77728000	-0.02814900
P	0.05101200	2.93563800	-0.01816800
C	1.25073900	3.68570000	-1.20108100
H	1.31056400	4.77314100	-1.07694500
H	2.23501400	3.23235900	-1.05066400
H	0.93193500	3.46024300	-2.22393700
C	-1.53280500	3.80469300	-0.39008400
H	-2.32039100	3.41550200	0.26204500
H	-1.43874800	4.88860600	-0.25762600
H	-1.81943800	3.59631500	-1.42610100
C	0.54992900	3.64078700	1.61339200
H	1.53904700	3.26129300	1.88575200
H	0.57982600	4.73590000	1.58080400
H	-0.16302700	3.32274800	2.38008300
C	-1.75966900	0.07781700	-0.13450400
C	-0.99720600	-0.93551400	0.17203300
C	1.72943000	0.05383400	0.10630800
C	0.95923400	-0.94899900	-0.21330000
C	3.14692200	0.40127200	0.10351400
O	3.65918700	1.18492100	-0.67716900
O	3.81460600	-0.20351500	1.10591700
C	1.14749800	-2.22621700	-0.93616400
O	0.28492100	-2.86121000	-1.50629200
O	2.45165300	-2.57193000	-0.91938100
C	-1.19213800	-2.20474300	0.90659800
O	-0.33205200	-2.84118500	1.47925600
O	-2.49851000	-2.54224900	0.89688200
C	-3.16958900	0.44986700	-0.07219400
O	-3.63831700	1.20175800	0.76445900
O	-3.88066900	-0.09088400	-1.08163900
C	5.20877200	0.12953700	1.20240800
H	5.34133600	1.20802200	1.32638500
H	5.57387300	-0.40608200	2.07898900
H	5.74311800	-0.19348700	0.30490700

C	2.76629000	-3.78458700	-1.62155200
H	3.83997000	-3.92334300	-1.49197400
H	2.21434700	-4.62640600	-1.19538500
H	2.51529500	-3.69152500	-2.68177700
C	-2.81834300	-3.74633700	1.61145500
H	-3.89289100	-3.88086700	1.48476700
H	-2.27125100	-4.59508300	1.19281800
H	-2.56530900	-3.64411000	2.67034800
C	-5.27057800	0.27082800	-1.11364000
H	-5.78159000	-0.09118400	-0.21737200
H	-5.38625300	1.35653600	-1.17496200
H	-5.67425100	-0.21025200	-2.00486600

TS28c (Imaginary Frequency = -296.48)

G-sol = -1172.527761 Hartree

Ni	0.76131800	-0.04168100	0.00427300
P	2.92189300	-0.02818400	0.01068000
C	3.71506400	-0.81326500	-1.46841500
H	4.80910700	-0.75351700	-1.42432400
H	3.41608100	-1.86462600	-1.52648800
H	3.36184800	-0.31205800	-2.37453800
C	3.72037600	1.64399800	0.02509500
H	3.42653600	2.17819800	0.93436900
H	4.81427700	1.57840100	-0.01312600
H	3.36344400	2.21975600	-0.83432200
C	3.80377200	-0.86984000	1.40557300
H	3.50580900	-1.92248600	1.43893000
H	4.89366200	-0.80733600	1.30210300
H	3.50549000	-0.40709400	2.35152200
C	0.04762700	1.10650900	-1.31838900
C	-0.93512900	0.90848800	-0.48346500
C	-0.98724900	-0.86013900	0.43436800
C	-0.05915500	-1.11712300	1.32013200
C	-2.02846500	1.78263000	0.14201700
C	-2.42541300	2.85627800	-0.89278000
C	-1.48507800	2.43288000	1.42324200
H	-1.57531800	3.48638000	-1.17491900
H	-2.82018600	2.38419400	-1.79907500
H	-3.20805300	3.48978400	-0.46248500
H	-2.28442000	3.01734600	1.89273300
H	-1.15784200	1.66207200	2.12655900
H	-0.64020500	3.09179400	1.20071600
C	-2.10546100	-1.72223500	-0.13574600
C	-1.48582000	-2.93982700	-0.84581600

C	-3.04852700	-2.15718000	0.99924700
H	-0.90680000	-3.54545500	-0.14249400
H	-2.27374200	-3.57424900	-1.27620000
H	-0.82301900	-2.60781800	-1.65015500
H	-3.85453800	-2.78975000	0.60261300
H	-2.50657800	-2.73665800	1.75293700
H	-3.48277600	-1.27669300	1.47836300
H	0.24474800	1.86678000	-2.06404500
H	0.05552100	-1.88151300	2.08025500
O	-3.19488500	1.07469400	0.54211600
H	-3.38467400	0.43536600	-0.17365800
O	-2.86084800	-0.98239400	-1.12712500
H	-3.53704200	-1.58645100	-1.47542200

29

G-sol = -943.604302 Hartree

Ni	0.10542600	-0.44225000	-0.00013400
P	2.40171200	-0.04392800	0.00038500
C	3.35576100	-1.63748500	0.00147700
H	4.43691500	-1.45736900	0.00170500
H	3.09619100	-2.22571800	0.88785400
H	3.09674100	-2.22665500	-0.88445700
C	3.15935800	0.83624500	-1.44332500
H	2.76581000	1.85547900	-1.50057800
H	4.25206000	0.87791800	-1.36468700
H	2.88598100	0.31757800	-2.36763100
C	3.15841600	0.83775400	1.44357400
H	2.88468300	0.31995300	2.36822500
H	4.25114400	0.87963900	1.36545800
H	2.76461300	1.85695500	1.49962100
C	-1.59787000	-1.26340300	-0.00037900
C	-2.65074800	-0.41967400	0.00051200
C	-0.88369000	1.17664000	-0.00064100
C	-2.22383400	1.01103700	0.00034600
C	-4.11643900	-0.78582500	0.00098500
H	-4.63733100	-0.38296400	0.88147600
H	-4.63792500	-0.38287200	-0.87911400
H	-4.26725900	-1.86915800	0.00099300
C	-1.61920900	-2.76896500	-0.00147800
H	-1.10375300	-3.18113900	-0.88381500
H	-1.10186300	-3.18261600	0.87905600
H	-2.63491300	-3.19031300	-0.00070800
C	-0.10983200	2.46224200	-0.00227500
H	0.54167400	2.55118200	0.88031300

H	0.54028600	2.54951300	-0.88607300
H	-0.76365200	3.34531900	-0.00262200
C	-3.25753200	2.11455600	0.00106200
H	-3.91318500	2.04864400	-0.87855500
H	-3.91189600	2.04856500	0.88159600
H	-2.80821200	3.11123300	0.00075700

29b

G-sol = -1697.676288 Hartree

Ni	-0.12921200	0.99774600	-0.16134000
P	-1.13771600	2.86878000	0.07925500
C	-2.01283100	2.99569700	1.69447200
H	-2.52878100	3.95794600	1.79125600
H	-2.73653600	2.17704200	1.74840100
H	-1.29400400	2.88687800	2.51220900
C	-0.06456800	4.36792600	0.01493100
H	0.43867300	4.41682000	-0.95544300
H	-0.64896400	5.28285700	0.16722900
H	0.70310100	4.29559300	0.79102300
C	-2.46235800	3.21285200	-1.15439800
H	-3.22455800	2.43319400	-1.07032900
H	-2.92440700	4.19029200	-0.97484100
H	-2.04529200	3.19110100	-2.16560500
C	1.66210600	0.50105000	0.21437300
C	1.11425900	-0.70470200	-0.05326500
C	-1.41899600	-0.35825000	-0.28131400
C	-0.41531100	-1.13219100	0.14668500
C	-2.87486900	-0.49074800	-0.26261800
O	-3.60550500	0.15773600	0.47279100
O	-3.32951100	-1.32748700	-1.21308500
C	-0.51973600	-2.40634600	0.91782500
O	0.42303400	-2.97617100	1.42870700
O	-1.79441900	-2.83798400	1.00645700
C	1.83238300	-1.79225000	-0.80460200
O	1.28567600	-2.57941900	-1.54819900
O	3.15711400	-1.76896400	-0.57281200
C	3.03718800	0.95842300	0.00094700
O	3.45435100	1.40838300	-1.05061700
O	3.75788600	0.92063700	1.14342600
C	-4.75788100	-1.44552000	-1.30080700
H	-5.21768600	-0.46873000	-1.47558800
H	-4.94211400	-2.11316200	-2.14271600
H	-5.16393500	-1.86966400	-0.37842100
C	-1.97489500	-4.05554500	1.74557700

H	-3.04545400	-4.25969900	1.71219800
H	-1.41239400	-4.87052500	1.28255200
H	-1.63897300	-3.93127400	2.77861100
C	3.91928100	-2.74665700	-1.29746900
H	4.95365700	-2.59546300	-0.98787000
H	3.58350800	-3.75515500	-1.04281600
H	3.81365000	-2.59292500	-2.37469700
C	5.09371600	1.43222500	1.03757100
H	5.68341900	0.82838700	0.34207400
H	5.08624700	2.46840200	0.68722100
H	5.51058500	1.36986700	2.04346200

29c

G-sol = -1172.529612 Hartree

Ni	0.84635600	-0.04675700	0.02532200
P	2.98718100	-0.02074200	0.00326800
C	3.77411000	-0.84671300	-1.45495700
H	4.86793500	-0.77855600	-1.41805700
H	3.48104900	-1.90097000	-1.47820000
H	3.41251800	-0.37517000	-2.37348200
C	3.77108100	1.65711900	-0.03548600
H	3.47036200	2.21912500	0.85439200
H	4.86543400	1.59587200	-0.06716200
H	3.41500000	2.20094400	-0.91569100
C	3.86672700	-0.81554300	1.42538300
H	3.57441400	-1.86826100	1.48810000
H	4.95648800	-0.74838500	1.32339100
H	3.56022100	-0.32681600	2.35526900
C	-0.04070300	0.97549000	-1.27134900
C	-1.03040300	0.72334400	-0.40036600
C	-1.07708700	-0.68971700	0.38563300
C	-0.14862500	-1.00294800	1.30795600
C	-2.08388600	1.74481400	0.12209800
C	-2.45502900	2.74127900	-0.98957000
C	-1.51243700	2.46986000	1.34757300
H	-1.59745900	3.34295900	-1.30827700
H	-2.84641900	2.21043800	-1.86455200
H	-3.23303900	3.41492600	-0.61580400
H	-2.29038800	3.10519200	1.78615600
H	-1.19217900	1.74404600	2.10148200
H	-0.65484000	3.09029300	1.06935500
C	-2.14358900	-1.68601900	-0.12580900
C	-1.46464600	-2.84890300	-0.86585400
C	-3.00875600	-2.18334800	1.04243400

H	-0.81433500	-3.41181400	-0.18947900
H	-2.21643000	-3.54079500	-1.27166800
H	-0.85858100	-2.46607200	-1.69275700
H	-3.78122100	-2.87372400	0.67664200
H	-2.40503600	-2.71974400	1.78037400
H	-3.48905600	-1.33395200	1.53453800
H	0.02640000	1.82358300	-1.94623400
H	-0.18278100	-1.87369300	1.95975700
O	-3.26886600	1.10175300	0.58350300
H	-3.51602900	0.45679000	-0.10870900
O	-2.99352600	-0.99619600	-1.07809200
H	-3.63911600	-1.64263600	-1.40683500

30

G-sol = -1099.455206 Hartree

Ni	0.31903200	0.51944100	0.00428500
P	1.41826200	-1.50319800	0.01316300
C	0.32704100	-2.97491400	-0.23406200
H	0.87535200	-3.91881100	-0.13430000
H	-0.48171700	-2.93674700	0.50150800
H	-0.12844700	-2.92214600	-1.22702800
C	2.73256800	-1.78773700	-1.26677600
H	3.53488400	-1.05542000	-1.13248000
H	3.15600200	-2.79750300	-1.20399200
H	2.31003900	-1.64420400	-2.26649200
C	2.32788300	-1.96694600	1.56252200
H	1.63184500	-1.97706400	2.40703500
H	2.79506900	-2.95546300	1.47791100
H	3.10350600	-1.22320100	1.77104900
C	-1.08207700	0.10072800	-1.23722400
C	-2.27854900	-0.29192100	-0.74362700
C	-1.09617300	0.11580600	1.23491400
C	-2.28887300	-0.27936300	0.73172000
C	-3.49932000	-0.69117100	-1.54064000
H	-3.83176600	-1.70862700	-1.29002000
H	-4.35104500	-0.02733800	-1.33513600
H	-3.31724900	-0.66203500	-2.61877600
C	-0.66898600	0.28010500	-2.67094400
H	-0.50958500	1.33972300	-2.91720400
H	0.27846100	-0.22957900	-2.89910400
H	-1.42107700	-0.11074000	-3.37112700
C	-0.71580700	0.35582200	2.66995100
H	0.27079100	-0.06127500	2.91467000
H	-0.65579800	1.43060200	2.89586000

H	-1.43782400	-0.08756600	3.37085000
C	-3.52666900	-0.63958300	1.52092500
H	-4.35140900	0.05916400	1.31960000
H	-3.89794900	-1.64054000	1.26014800
H	-3.34629100	-0.62650000	2.59980400
C	1.69972500	1.91308600	-0.00678100
C	0.51497500	2.39634600	-0.01578000
C	-0.44049800	3.52926100	-0.03834400
H	-1.09437700	3.50071300	0.84098700
H	0.07494900	4.49913600	-0.05609500
H	-1.09202200	3.46639300	-0.91751200
C	3.16195000	2.19286900	-0.01116300
H	3.37902900	3.26989400	-0.04014800
H	3.64617700	1.77848800	0.88193100
H	3.65047700	1.72993400	-0.87749400

30b

G-sol = -2230.584413 Hartree

Ni	0.73768400	-0.10898400	-0.22140300
P	0.94111800	-1.05607500	-2.29722500
C	-0.67089700	-1.46035900	-3.09459900
H	-0.51903100	-1.85528200	-4.10533600
H	-1.21659100	-2.19330700	-2.49431600
H	-1.27729400	-0.55157800	-3.15290300
C	1.74854000	0.07750100	-3.50444000
H	2.77772300	0.25011100	-3.17769100
H	1.74765300	-0.36086800	-4.50940900
H	1.21242200	1.03026100	-3.51186200
C	1.91733600	-2.61181800	-2.42917300
H	1.54226300	-3.33988100	-1.70659000
H	1.86582700	-3.02156100	-3.44443400
H	2.95895800	-2.38514600	-2.18493400
C	-0.68199800	1.15281300	-0.37052700
C	-1.95300700	0.72306300	-0.15306300
C	-0.72158800	-1.19291900	0.33184200
C	-1.96953800	-0.66266500	0.30327000
C	2.60619700	0.08260900	0.28790400
C	1.84000700	0.69935600	1.10660400
C	-0.29102400	-2.50248500	0.83208700
O	0.82067400	-2.97880900	0.63604300
O	-1.23667500	-3.14025100	1.55882200
C	-0.22524200	2.45729100	-0.90813100
O	0.06457200	2.64830700	-2.07724600
O	-0.05390500	3.36479700	0.06709300

C	-3.20351400	1.46607100	-0.43966400
O	-4.30315900	0.94849400	-0.50172500
O	-2.99018000	2.78312200	-0.65759600
C	-3.22738000	-1.34265300	0.76846200
O	-3.78839100	-1.07918800	1.80695000
O	-3.64633500	-2.26679000	-0.11749000
C	-4.87558900	-2.92171800	0.23382200
H	-4.76612500	-3.45936500	1.17975400
H	-5.68024800	-2.18811700	0.32837800
H	-5.08097200	-3.61594900	-0.58182100
C	-0.86314800	-4.42706900	2.07380100
H	-0.63794600	-5.11978200	1.25778400
H	0.01417800	-4.34076000	2.72006400
H	-1.72650300	-4.77271900	2.64299600
C	-4.15674100	3.54362600	-1.00429500
H	-4.60350300	3.16360300	-1.92722300
H	-4.89855300	3.49312900	-0.20296400
H	-3.80728300	4.56731900	-1.14112100
C	0.53750800	4.61382800	-0.33145600
H	1.48258000	4.43852800	-0.85084300
H	-0.14189900	5.16281000	-0.98927900
H	0.70673800	5.16005200	0.59577000
C	1.67582200	1.64746300	2.21516100
O	2.20479900	2.73933500	2.24874900
O	0.85912800	1.15578800	3.16022200
C	3.96113000	-0.28087300	-0.11856400
O	4.37444700	-0.24989900	-1.26407500
O	4.69417100	-0.68546500	0.93541900
C	0.61382100	2.02984200	4.27602200
H	-0.05231900	1.47416200	4.93535100
H	1.54998000	2.27335400	4.78547300
H	0.13744400	2.95225900	3.93426000
C	6.03316100	-1.11211900	0.62592100
H	6.60930700	-0.28466800	0.20376200
H	6.45956700	-1.43298100	1.57624200
H	6.01539700	-1.93920800	-0.08867000

30c

G-sol = -1442.869189 Hartree

Ni	-0.84269700	-0.34925500	-0.03745100
P	-1.33230400	1.86424500	-0.34076300
C	0.12405300	2.98110600	-0.55275400
H	-0.18186600	4.02691300	-0.67093900
H	0.77850800	2.88842600	0.31840000

H	0.69695900	2.66613300	-1.42937700
C	-2.37546200	2.28174600	-1.81025900
H	-3.32901600	1.75759200	-1.70735100
H	-2.55036300	3.36153600	-1.89085900
H	-1.87917600	1.93412900	-2.72242600
C	-2.25586800	2.66919100	1.04419100
H	-1.67991800	2.57223200	1.97029900
H	-2.43700700	3.73282400	0.84759200
H	-3.20774100	2.14570900	1.16449900
C	0.66816900	-0.49907700	-1.16126900
C	1.93229300	-0.43342400	-0.68724100
C	0.59447100	-0.22741800	1.18303700
C	1.88748300	-0.24404200	0.79674900
C	-2.56411800	-1.25064500	0.16459700
C	-1.56658300	-2.05143000	0.24575700
C	3.05316900	0.01804300	1.77126300
C	3.34366500	1.53454300	1.83683100
C	2.74823900	-0.51821500	3.17610700
H	2.47911800	2.08524200	2.22573000
H	4.20260100	1.71727800	2.49349200
H	3.57994600	1.92272000	0.84048500
H	3.62450900	-0.35757600	3.81276000
H	1.89276700	-0.01150000	3.63279000
H	2.54064000	-1.59177400	3.13645800
C	3.15313900	-0.67177100	-1.57249700
C	3.69194100	-2.10446900	-1.38519100
C	2.86752200	-0.40681500	-3.05794800
H	3.92827600	-2.28734900	-0.33462700
H	2.94331500	-2.83363200	-1.71177400
H	4.59919900	-2.25732600	-1.98769500
H	2.48760400	0.60825300	-3.20501900
H	3.79447900	-0.51909800	-3.63592000
H	2.14407500	-1.11785300	-3.46728300
O	4.24697700	-0.66650600	1.38074400
H	4.49450600	-0.28601500	0.51336200
O	4.17747300	0.28514100	-1.16132300
H	4.95565900	0.12748700	-1.72213600
H	0.22844100	-0.10282000	2.20452100
H	0.39603400	-0.69547000	-2.20157500
C	-4.05128000	-1.15003200	0.21002300
C	-4.67241800	-1.99600900	-0.91717000
C	-4.56641400	-1.59996900	1.59003600
H	-4.31177200	-1.65170400	-1.89078900
H	-4.41453900	-3.05347000	-0.80201300
H	-5.76745600	-1.90869700	-0.90059800
H	-4.12856000	-0.98008700	2.37776100

H	-5.65975700	-1.50463400	1.63877900
H	-4.30796300	-2.64583500	1.78323700
H	-1.16610200	-3.04276000	0.39573300
O	-4.40703000	0.23674400	0.00533200
H	-5.37670100	0.28567200	0.04095400

TS31 (Imaginary Frequency = -282.32)

G-sol = -1099.437292 Hartree

Ni	0.26383900	0.26698600	-0.23783700
P	2.13360900	-0.73509900	0.37005900
C	1.94392700	-2.35983600	1.23642600
H	2.91103400	-2.78702100	1.52741800
H	1.32855200	-2.21765100	2.13039100
H	1.41884300	-3.06063400	0.58134700
C	3.35152100	-1.14813100	-0.96440500
H	3.65836500	-0.22815200	-1.47162000
H	4.23953400	-1.64932300	-0.56157500
H	2.87721400	-1.80062200	-1.70361000
C	3.19213200	0.20306600	1.56676800
H	2.61045700	0.42743200	2.46653600
H	4.08745900	-0.36179600	1.85323400
H	3.49267900	1.15292300	1.11502500
C	-0.77946100	-1.24854700	-0.82587700
C	-2.03271100	-1.30014000	-0.30173200
C	-1.33088700	0.68847900	0.86054800
C	-2.25968900	-0.30265600	0.75388100
C	-3.14634700	-2.24789400	-0.69860600
H	-3.47463700	-2.86725600	0.14779300
H	-4.03726200	-1.70951900	-1.05335000
H	-2.83868200	-2.93078000	-1.49515000
C	-0.28717500	-2.05584100	-1.99837400
H	0.21612700	-1.40136200	-2.72707100
H	0.46189800	-2.80664200	-1.70102700
H	-1.07875900	-2.59251400	-2.54081500
C	-1.18745900	1.65918300	2.00448700
H	-0.13363900	1.76387300	2.28873600
H	-1.53980800	2.67124300	1.75534500
H	-1.73015700	1.32109100	2.89554700
C	-3.43950700	-0.45334800	1.69161600
H	-4.38080100	-0.49241800	1.12685600
H	-3.38279100	-1.39019600	2.26394800
H	-3.52233300	0.37102300	2.40366500
C	0.58396900	2.13021700	-0.59167300
C	-0.68628800	1.86300900	-0.71682900

C	-1.96373800	2.33814800	-1.32024700
H	-2.60985400	2.81887600	-0.57528400
H	-1.75727100	3.06924700	-2.11325300
H	-2.52399900	1.50178700	-1.75163600
C	1.53065800	3.24949500	-0.86116000
H	1.08042200	4.05274000	-1.46335700
H	1.86939100	3.70141100	0.08221800
H	2.43270900	2.90390300	-1.38069600

TS31b (Imaginary Frequency = -204.78)

G-sol = -2230.571237 Hartree

Ni	-0.64300100	-0.63878300	-0.22601100
P	-1.36160600	-2.12752800	-1.75230500
C	-0.10374600	-2.54546000	-3.03041500
H	-0.52190100	-3.21509600	-3.79097900
H	0.24420300	-1.62612100	-3.51174400
H	0.74316400	-3.02567100	-2.53321800
C	-1.92736400	-3.76276100	-1.11780800
H	-2.74288000	-3.60213500	-0.40639900
H	-2.27988600	-4.39783300	-1.93872800
H	-1.09268600	-4.25786200	-0.61382600
C	-2.80014900	-1.50232100	-2.71725700
H	-2.57167900	-0.50111300	-3.09302200
H	-3.03391600	-2.17239800	-3.55234200
H	-3.66369100	-1.43348100	-2.05030600
C	1.15806900	-1.22129100	0.06376300
C	2.09395900	-0.23410800	-0.00720600
C	0.16556400	1.11788900	-0.42448300
C	1.52733500	1.05070200	-0.40994900
C	-2.26912700	0.09579900	0.49312500
C	-1.24278700	0.63719700	1.07135200
C	-0.60287700	2.08770700	-1.23334800
O	-1.59184300	1.79388300	-1.88528800
O	-0.08670100	3.33362700	-1.19904600
C	2.40703200	2.12988300	-0.99937100
O	2.75259700	2.13292200	-2.16128900
O	2.74601100	3.04758200	-0.08865800
C	1.38123100	-2.61513900	0.50371800
O	1.45285600	-3.57816900	-0.24337200
O	1.36117200	-2.72451600	1.84912200
C	3.55080700	-0.36184900	0.24955600
O	4.35178500	0.54847400	0.14178800
O	3.90927300	-1.61734500	0.60144500
C	-0.70464200	4.28373000	-2.08268000

H	-1.76636300	4.39079800	-1.84682500
H	-0.17573800	5.22193100	-1.91348600
H	-0.59648800	3.96468800	-3.12286800
C	3.69250200	4.02857000	-0.53850200
H	4.62576400	3.53927700	-0.82908700
H	3.29413900	4.58674700	-1.39022900
H	3.85349100	4.68909100	0.31385200
C	5.31030200	-1.81060200	0.83990100
H	5.88960500	-1.55992300	-0.05274100
H	5.64854500	-1.18500500	1.67055000
H	5.42166500	-2.86738900	1.08462900
C	1.50259700	-4.05761400	2.36509400
H	0.69489900	-4.70084500	2.00483800
H	2.46162000	-4.48468800	2.05996800
H	1.45578900	-3.95562100	3.44954600
C	-0.80088800	1.31499500	2.30908700
O	0.31545000	1.70892400	2.55875600
O	-1.84879900	1.41004300	3.15982500
C	-3.71200400	-0.08952600	0.54538500
O	-4.26218600	-1.17698200	0.48121200
O	-4.37230700	1.08081600	0.64155600
C	-1.54533100	2.02596200	4.42241900
H	-2.48266400	2.02143000	4.97926500
H	-0.77810700	1.45547700	4.95282000
H	-1.18927100	3.04897200	4.27380400
C	-5.80601600	0.97737400	0.64464200
H	-6.14735300	0.41621100	1.51869400
H	-6.16972000	2.00438000	0.68136400
H	-6.15768600	0.47611700	-0.26122700

TS31c (Imaginary Frequency = -232.11)

G-sol = -1442.857416 Hartree

Ni	-0.76513200	0.12538500	-0.12635200
P	-1.82425400	1.85606900	0.74875900
C	-0.77738600	3.23956000	1.38580000
H	-1.38880700	4.04314000	1.81299400
H	-0.09789800	2.85500300	2.15232800
H	-0.16637600	3.64164200	0.57307800
C	-3.00587100	2.72064900	-0.37813600
H	-3.75228800	1.98984500	-0.69994300
H	-3.49775800	3.56317100	0.12245400
H	-2.47133500	3.09268900	-1.25830800
C	-2.87693900	1.44499600	2.20981500
H	-2.25912200	0.98279500	2.98649500

H	-3.35874800	2.33952600	2.62250200
H	-3.63468300	0.72710600	1.88671300
C	0.80708500	1.05827500	-0.67239400
C	2.00480200	0.44780900	-0.51019400
C	0.55209700	-1.20461500	0.42439000
C	1.84150400	-0.79548000	0.30824000
C	-2.12699300	-1.19284500	-0.52236600
C	-0.96796800	-1.63035000	-0.89667200
H	0.71390700	1.92799600	-1.33053700
H	0.25410400	-1.98548100	1.11473600
C	3.28917300	0.89707500	-1.23788100
C	3.52282400	-0.00882300	-2.46795700
C	3.22205700	2.36342900	-1.68398700
H	2.68938600	0.06716100	-3.17567900
H	4.44783300	0.28887100	-2.97643400
H	3.61821900	-1.05612100	-2.16354400
H	4.19689800	2.64218000	-2.09638900
H	2.46218200	2.52784700	-2.45343600
H	3.01047900	3.01666100	-0.83145500
C	2.92840100	-1.45236700	1.17261100
C	3.39057400	-0.47896500	2.27526500
C	2.50167600	-2.78829800	1.79842200
H	2.56120200	-0.25454300	2.95444700
H	4.19951500	-0.92949300	2.86788000
H	3.75152300	0.45230800	1.83365900
H	3.36196100	-3.23521900	2.31402800
H	1.71185200	-2.66112500	2.54453800
H	2.15854800	-3.48943300	1.03237900
O	4.44638100	0.84662200	-0.39045800
H	4.57658800	-0.10019300	-0.18246600
O	4.05079900	-1.75049200	0.28789500
H	4.74005200	-2.16654000	0.83300600
C	-3.56979900	-1.54989300	-0.65265100
C	-3.93324700	-1.83598200	-2.12164900
C	-3.89281400	-2.76131300	0.24291600
H	-3.71536200	-0.96191700	-2.74213600
H	-3.36355300	-2.68782300	-2.50720500
H	-5.00189600	-2.07364000	-2.21674700
H	-3.64436500	-2.53854200	1.28480900
H	-4.96271600	-3.00441500	0.18532300
H	-3.32706500	-3.64432300	-0.07108800
O	-4.34274500	-0.41335100	-0.19432600
H	-5.27915700	-0.65130700	-0.29677700
H	-0.43614000	-2.36906400	-1.47907000

32

G-sol = -1099.462948 Hartree

Ni	-0.34164600	0.28831000	-0.26664800
C	0.18427800	2.05858700	-0.42174700
C	1.44850000	1.53621500	-0.37637000
C	1.95389000	-0.74799100	0.74706800
C	1.85129500	0.61292000	0.77405200
C	2.60281300	1.90599100	-1.29220600
H	3.45959900	2.28870000	-0.72028200
H	2.94921000	1.01237400	-1.82762400
H	2.32180400	2.65925900	-2.03470400
C	-0.25983300	3.30455800	-1.12399600
H	0.53240600	3.80721200	-1.69858900
H	-1.10378100	3.11270200	-1.79813800
H	-0.62057900	4.02794600	-0.37780800
C	2.48616400	-1.50838100	1.95894700
H	2.18459900	-2.55895200	1.91945500
H	3.58403100	-1.48786200	2.01089500
H	2.10938200	-1.09892500	2.90083600
C	2.24213300	1.42823000	1.99889600
H	2.89318100	0.88932100	2.69196600
H	2.76754700	2.34182200	1.69477200
H	1.34953700	1.75348200	2.55098500
C	0.27922200	-1.41225900	-0.90604000
C	1.52164300	-1.60970700	-0.40201300
C	2.53469900	-2.64410000	-0.86806300
H	2.76508600	-3.38429200	-0.08916700
H	2.18580400	-3.19587000	-1.74462400
H	3.48812300	-2.16692900	-1.13563500
C	-0.34664600	-2.22751500	-2.00779900
H	0.32404200	-2.96451500	-2.47137500
H	-1.22001600	-2.78565300	-1.63750500
H	-0.72147200	-1.57458500	-2.80877300
P	-2.30839400	-0.18552400	0.39366600
C	-3.54499000	-0.49442900	-0.94984600
H	-4.52763500	-0.75317200	-0.53775900
H	-3.64234300	0.40331600	-1.56813400
H	-3.19562800	-1.31069900	-1.58809700
C	-3.16706500	1.09615900	1.41693000
H	-3.22143400	2.02906600	0.84848700
H	-4.17846200	0.78313900	1.70365000
H	-2.57932600	1.28797900	2.31988800
C	-2.48536300	-1.69654300	1.44751200
H	-2.12109500	-2.56742500	0.89552700
H	-1.86802400	-1.58503700	2.34443200

H	-3.52700500	-1.86261700	1.74650600

32b

G-sol = -2230.599407 Hartree

Ni	-0.41515000	0.78067500	-0.48479700
C	-2.03778900	0.04805400	0.11227200
C	-1.32647700	-0.95627700	0.67949700
C	1.12780400	-1.30815200	-0.17984500
C	-0.21792600	-1.54450700	-0.18063100
C	1.37341500	1.06715700	0.16188300
C	1.82619200	-0.16667600	0.47986800
P	-0.92299900	2.65772300	-1.40748200
C	-1.13278900	4.03657100	-0.21238600
H	-1.32805500	4.97816900	-0.73869900
H	-1.97727400	3.78718400	0.43601000
H	-0.23635300	4.12864900	0.40606100
C	-2.48809400	2.67329400	-2.37931000
H	-3.32327300	2.47893600	-1.70207200
H	-2.63368100	3.64685100	-2.86148000
H	-2.46027600	1.89178000	-3.14418900
C	0.33793700	3.24294100	-2.62022300
H	1.31685900	3.30129700	-2.13730000
H	0.41081000	2.52254200	-3.44116100
H	0.06613700	4.22432000	-3.02592000
C	2.00671700	2.33412300	0.57402400
O	1.60566100	3.04719900	1.47615100
O	3.02597000	2.68384900	-0.24898100
C	3.02414600	-0.52928300	1.28133600
O	3.43194500	-1.67109500	1.39295100
O	3.60555600	0.53193400	1.87650200
C	2.05824200	-2.13188400	-1.04956200
O	2.89478400	-1.64708000	-1.77873100
O	1.86257900	-3.44979300	-0.87951600
C	-0.81288800	-2.57788300	-1.11143700
O	-1.62300900	-3.40866300	-0.76863900
O	-0.38813000	-2.42149700	-2.38602500
C	-1.51878900	-1.59131700	2.01713000
O	-0.75212200	-2.39701500	2.50208500
O	-2.62214800	-1.12893400	2.64398600
C	-3.33147500	0.62220000	0.50399400
O	-3.50242300	1.78277400	0.84655000
O	-4.34399500	-0.25150100	0.32749400
C	3.69029700	3.91187000	0.08831700
H	2.99003300	4.75197300	0.07751600
H	4.14013800	3.83952700	1.08205000

H	4.46111700	4.04415300	-0.67160200
C	4.76192700	0.23193800	2.67222200
H	4.51049900	-0.48775500	3.45551500
H	5.55880500	-0.18318000	2.04895500
H	5.07007300	1.18244000	3.10866600
C	2.76171400	-4.29809100	-1.61082700
H	2.65003100	-4.13892400	-2.68710400
H	3.79406300	-4.08663200	-1.32143700
H	2.48567800	-5.31678500	-1.33825800
C	-0.89829200	-3.38810200	-3.31912800
H	-0.58167000	-4.39518900	-3.03451100
H	-1.99041400	-3.35265100	-3.34569000
H	-0.47769500	-3.10989400	-4.28570700
C	-2.85340600	-1.67617600	3.95036100
H	-3.76630100	-1.19954500	4.30890700
H	-2.98084100	-2.76058300	3.89390900
H	-2.01521100	-1.44994200	4.61494400
C	-5.65432500	0.25342300	0.62237400
H	-5.73267300	0.51622300	1.68092600
H	-5.87499000	1.13941200	0.02002800
H	-6.34052000	-0.55790300	0.37799900

32c

G-sol = -1442.890672 Hartree

Ni	0.87728400	0.28192400	0.27163700
C	1.68289900	-1.34762200	-0.19244200
C	0.55828800	-2.02255400	-0.56424900
C	-1.64496800	-0.56817900	-0.63664900
C	-0.70419500	-1.44850500	-1.08148300
C	-0.65152000	0.91904800	1.09251500
C	-1.67782000	0.12439800	0.70093900
P	1.80211600	2.13795600	-0.11101600
C	2.03394800	3.18554500	1.39358800
H	2.47889300	4.15496700	1.14107000
H	2.68605100	2.66737500	2.10356100
H	1.06497400	3.34551100	1.87425200
C	3.48846600	2.16573400	-0.87081800
H	4.19070600	1.63087700	-0.22471900
H	3.84607800	3.19212100	-1.01720300
H	3.45831300	1.65325100	-1.83688000
C	0.85031600	3.24374900	-1.24470400
H	-0.14288200	3.41549300	-0.82157500
H	0.72866100	2.75113300	-2.21422100
H	1.36131000	4.20260400	-1.39157700

C	-2.84190100	-0.22118900	1.68118200
C	-3.41017600	1.03506700	2.36687300
C	-2.31309800	-1.21914700	2.72425500
H	-2.66227800	1.55383300	2.97494200
H	-4.23891100	0.74066700	3.01991800
H	-3.78727800	1.73913100	1.61709100
H	-3.13078400	-1.52420600	3.38751300
H	-1.51201800	-0.77277400	3.32093600
H	-1.92128300	-2.11231600	2.22722200
C	-2.75223700	-0.21180200	-1.67104100
C	-3.57503000	-1.43701300	-2.10906000
C	-2.13296700	0.49987900	-2.88734600
H	-4.00385500	-1.93111400	-1.23444100
H	-2.96002300	-2.16261700	-2.64933600
H	-4.38472800	-1.12754400	-2.78455600
H	-1.59436400	1.39585100	-2.56448500
H	-2.91996300	0.80227300	-3.59316000
H	-1.43671500	-0.15079600	-3.42374800
C	2.96840600	-2.09165000	0.09662500
C	3.52031900	-1.70129300	1.47980300
C	3.99988200	-1.78221300	-1.00719000
H	3.72146800	-0.62618100	1.53876500
H	4.45960300	-2.23401500	1.68727900
H	2.79584300	-1.96011300	2.25823700
H	4.94100500	-2.31499800	-0.81020500
H	4.22466600	-0.71297700	-1.06253500
H	3.61438200	-2.10861900	-1.97817500
H	-0.72287700	1.46288500	2.03866300
H	-0.92647800	-1.88104500	-2.06118900
H	0.58849100	-3.11561000	-0.62190800
O	-3.91211700	-0.90798800	1.03246600
H	-4.22466900	-0.29458400	0.33999400
O	-3.64885600	0.74255400	-1.04157000
H	-4.30435800	0.99570900	-1.71148300
O	2.70805300	-3.51129700	0.08793800
H	3.54902000	-3.95705800	0.27588100

TS33 (Imaginary Frequency = -171.92)

G-sol = -1099.448535 Hartree

Ni	0.37447000	-0.64712600	-0.27689900
C	-1.08684200	-1.90281700	-0.28460100
C	-2.16307600	-1.09593300	-0.01624300
C	-1.46075300	1.31681400	0.54993500
C	-2.04836500	0.12546700	0.85288800

C	-3.59055000	-1.32303800	-0.50185700
H	-4.32512400	-1.16582600	0.29852700
H	-3.83458000	-0.59704600	-1.29078200
H	-3.74871800	-2.32352700	-0.91160300
C	-1.22283100	-3.21754800	-1.02121400
H	-2.25109900	-3.56756700	-1.19915600
H	-0.72342000	-3.16270800	-1.99929500
H	-0.70323600	-4.00963100	-0.46625200
C	-1.47739100	2.44356100	1.57943400
H	-0.76147600	3.22890100	1.31740000
H	-2.46504800	2.91943200	1.66652900
H	-1.21526900	2.08036100	2.57993500
C	-2.71372900	-0.04633400	2.21623100
H	-3.39882600	0.77296100	2.46844900
H	-3.27389800	-0.98330800	2.26853800
H	-1.95532800	-0.08706300	3.01103600
C	0.23265700	0.95269300	-1.21604500
C	-0.81023200	1.67230800	-0.75566700
C	-1.41953900	2.87131700	-1.46576900
H	-1.43180200	3.75945800	-0.82025300
H	-0.88193300	3.13884600	-2.37904300
H	-2.46443600	2.66750600	-1.73777700
C	1.02527800	1.18514800	-2.47516800
H	0.56411800	1.92598200	-3.14091500
H	2.04286100	1.54081300	-2.25662100
H	1.13496800	0.25518900	-3.04818500
P	2.34275400	-0.21206800	0.46709500
C	3.75205500	-0.68945300	-0.63397000
H	4.71672400	-0.50701900	-0.14630000
H	3.67094500	-1.75198800	-0.88239000
H	3.70834500	-0.11791300	-1.56525500
C	2.71067800	-1.17222700	2.00612600
H	2.58499300	-2.23989600	1.80372800
H	3.73076700	-0.98598200	2.36342600
H	1.99797400	-0.89235400	2.78790600
C	2.78489900	1.51298600	0.96907600
H	2.72684400	2.17452600	0.10043100
H	2.06241600	1.86861000	1.70980800
H	3.79321500	1.56210900	1.39592300

TS33b (Imaginary Frequency = -55.10)

G-sol = -2230.566709 Hartree

Ni	-0.52878300	-0.46020300	-0.84258600
C	-1.30497300	-0.82776600	0.77909000

C	-0.16881300	-0.90154300	1.50262200
C	1.69568500	-0.30896900	-0.07727800
C	0.93856000	-1.27744100	0.56323900
C	0.07602800	1.32857500	-0.49473500
C	1.31073000	1.13265900	0.00945000
P	-2.18812400	-0.40210300	-2.22325800
C	-3.12267500	1.16504800	-2.41056100
H	-3.89304400	1.06091100	-3.18289800
H	-3.58241600	1.40696800	-1.44999900
H	-2.42746100	1.96016600	-2.68993500
C	-3.48753700	-1.70363600	-2.12217900
H	-4.06183100	-1.55532900	-1.20524100
H	-4.16093700	-1.64346200	-2.98498300
H	-3.01906500	-2.69164500	-2.09600900
C	-1.42367100	-0.67497800	-3.88476100
H	-0.68382500	0.10694500	-4.07945600
H	-0.91581500	-1.64402800	-3.91109800
H	-2.18910800	-0.65221200	-4.66924600
C	-0.60446400	2.62611200	-0.58916400
O	-1.29961100	3.10441900	0.28566700
O	-0.43946900	3.20954300	-1.81119600
C	2.32922800	2.08074600	0.51647400
O	3.48649000	1.75900200	0.71966600
O	1.85583500	3.33150600	0.68422200
C	2.88613800	-0.61976900	-0.95073100
O	2.99730500	-0.23024700	-2.09409400
O	3.81004100	-1.33208800	-0.29034700
C	1.13551400	-2.75078100	0.35096500
O	0.93982700	-3.59156900	1.19886000
O	1.54327800	-3.04177600	-0.91061400
C	0.16529100	-0.34824000	2.83321400
O	1.29984900	-0.28471800	3.26824400
O	-0.92044200	0.10028900	3.49974100
C	-2.70789500	-0.64632900	1.18323000
O	-3.51398800	0.08056400	0.61841700
O	-3.04778700	-1.46035100	2.20239400
C	-1.05424600	4.49984200	-1.94738100
H	-2.13810000	4.43330700	-1.81373700
H	-0.65112800	5.19650100	-1.20754100
H	-0.81192900	4.83377500	-2.95730000
C	2.81520300	4.29366700	1.14524100
H	3.25122000	3.97509100	2.09571700
H	3.61623300	4.41983500	0.41116200
H	2.25883500	5.22312000	1.26993700
C	5.02252200	-1.58423300	-1.01832900
H	4.81534100	-2.17483800	-1.91526600

H	5.49044500	-0.64028500	-1.30839300
H	5.66389700	-2.13595200	-0.33104900
C	1.83420300	-4.42732100	-1.15144200
H	2.63279400	-4.76981200	-0.48797700
H	0.94443800	-5.03947200	-0.98204300
H	2.14859300	-4.48279600	-2.19403500
C	-0.64991900	0.66688700	4.78880100
H	-1.61974900	0.97367200	5.18209600
H	-0.18473000	-0.07356700	5.44564700
H	0.01600500	1.52930500	4.69751100
C	-4.40805200	-1.35973100	2.64713800
H	-4.61634900	-0.35163700	3.01577500
H	-5.10191700	-1.59070600	1.83352400
H	-4.50436400	-2.09000900	3.45103500

TS33c (Imaginary Frequency = -143.02)

G-sol = -1442.885663 Hartree

Ni	1.09972900	0.37525700	0.20252800
C	1.80632800	-1.34881500	-0.26963800
C	0.72456200	-2.06302200	-0.70637200
C	-1.52622300	-0.71314200	-0.65376900
C	-0.57542700	-1.55573800	-1.15305700
C	-0.45338700	0.66691300	1.11171800
C	-1.50889600	-0.06703800	0.70174800
P	1.36091200	2.46596800	-0.11023100
C	1.32093600	3.55850500	1.38050900
H	1.54806500	4.59760500	1.11684900
H	2.05467300	3.20808900	2.11305700
H	0.32955400	3.51477500	1.84032600
C	2.99615900	2.88205900	-0.86880700
H	3.80107800	2.55006400	-0.20594500
H	3.09568100	3.95977700	-1.04548400
H	3.09798500	2.34724100	-1.81775100
C	0.16445400	3.28162000	-1.25549900
H	-0.84960100	3.15801500	-0.86545300
H	0.21655300	2.79773200	-2.23546100
H	0.38772400	4.34843600	-1.37122000
C	-2.63677700	-0.40873200	1.73160200
C	-3.17116700	0.85227400	2.43691000
C	-2.07261400	-1.40957900	2.75301600
H	-2.39513000	1.37455800	3.00596000
H	-3.96872400	0.56329600	3.13003100
H	-3.58344700	1.55199500	1.70148100
H	-2.86662100	-1.71205700	3.44541300

H	-1.24788000	-0.96949400	3.32134700
H	-1.70335200	-2.30231300	2.23880400
C	-2.70810700	-0.41211400	-1.61883200
C	-3.53206900	-1.66678300	-1.96296200
C	-2.19529000	0.26768700	-2.90131800
H	-3.88358100	-2.14855900	-1.04846200
H	-2.93609300	-2.38977300	-2.52770600
H	-4.39545500	-1.39560900	-2.58674800
H	-1.66038300	1.18881700	-2.65285100
H	-3.03779100	0.52307200	-3.56014600
H	-1.52015000	-0.38401800	-3.46243800
C	3.08815200	-2.08741200	0.06159100
C	3.45496900	-1.86840800	1.54191900
C	4.22125300	-1.58481000	-0.85457200
H	3.57959800	-0.80384200	1.76722300
H	4.39650100	-2.38124800	1.78707600
H	2.66420900	-2.26822800	2.18448600
H	5.16339600	-2.10348100	-0.62509100
H	4.38449400	-0.50965200	-0.72803200
H	3.96744900	-1.77696500	-1.90207400
H	-0.45066900	1.15883900	2.08688900
H	-0.85132000	-2.01803700	-2.10497100
H	0.82415800	-3.14504000	-0.84725900
O	-3.73548000	-1.08799300	1.13009300
H	-4.07379100	-0.47385500	0.44995500
O	-3.57626300	0.55122300	-0.95947600
H	-4.28280000	0.76772300	-1.58940500
O	2.91791600	-3.50488000	-0.16277500
H	3.75905500	-3.93216900	0.06243200

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G-sol = -1099.576286 Hartree

C	1.40778000	1.30876900	-0.57156600
C	1.42742100	0.15920000	-1.41923000
C	1.41107100	-1.14698200	-0.84664700
C	1.42977800	-1.30653600	0.57285500
C	1.41218800	-0.15736200	1.41719900
C	1.42557700	1.15180600	0.84574700
C	1.41772200	-0.31583900	2.92647900
H	1.05911000	0.58486100	3.42692200
H	0.76974900	-1.13525100	3.24726800
H	2.42719800	-0.52243300	3.31190300
C	1.52641400	2.36045500	1.76063400
H	0.61635200	2.50854700	2.35387200

H	2.35881300	2.24756400	2.46568700
H	1.70543500	3.28112400	1.20468500
C	1.40666100	2.69552800	-1.18839600
H	0.75775400	3.38032500	-0.63667200
H	2.41429800	3.13667900	-1.20531000
H	1.04438700	2.67822800	-2.21732300
C	1.53112100	0.34775000	-2.92320600
H	0.62255900	0.78853700	-3.35015400
H	2.36439200	1.01468000	-3.17552700
H	1.71075000	-0.59347100	-3.44345600
C	1.41716000	-2.37510500	-1.73823800
H	2.42790900	-2.61002800	-2.10354500
H	1.05136200	-3.25678500	-1.20995700
H	0.77522000	-2.24175900	-2.61236400
C	1.53448000	-2.70290300	1.16218000
H	0.62423200	-3.29130000	0.99666700
H	2.36557400	-3.25641100	0.70879000
H	1.71695100	-2.68280800	2.23695800
Ni	-0.25134300	-0.00154300	-0.00051300
P	-2.34167500	-0.00238400	0.00050500
C	-3.23161400	-0.77669100	1.44784400
H	-4.32321200	-0.72460600	1.34369100
H	-2.93281800	-1.82634400	1.53804900
H	-2.93760300	-0.26396100	2.36982400
C	-3.23042000	1.63862900	-0.05204400
H	-2.93094800	2.18419900	-0.95312700
H	-4.32210000	1.52325300	-0.05114300
H	-2.93535200	2.23764700	0.81594000
C	-3.23115900	-0.86904200	-1.39366600
H	-4.32270500	-0.80810200	-1.29433900
H	-2.93536100	-0.42047400	-2.34791500
H	-2.93428500	-1.92300200	-1.41233000

34b

G-sol = -2230.695801 Hartree

C	0.00509900	1.45779000	-0.60069000
C	-1.24181400	0.77454900	-0.68914400
C	-1.26403900	-0.64209500	-0.82394400
C	-0.04603100	-1.37491700	-0.85592000
C	1.20013900	-0.69147400	-0.76274900
C	1.22473100	0.73172700	-0.65791800
Ni	-0.06385700	-0.10075000	0.88469400
P	-0.15105200	-0.14662300	3.02312000
C	0.75933700	-1.49834200	3.91194500

H	0.64697800	-1.42275500	5.00056900
H	0.38016600	-2.46952000	3.57801500
H	1.82262100	-1.44514800	3.65682900
C	0.49868900	1.36174300	3.88444500
H	-0.03623500	2.24195900	3.51427900
H	0.38705600	1.29576800	4.97372200
H	1.55716200	1.49039500	3.63663100
C	-1.84009800	-0.29840700	3.77609800
H	-1.80437500	-0.28530000	4.87248700
H	-2.46351400	0.53065600	3.42660300
H	-2.30330000	-1.23174800	3.44070500
C	0.00536500	2.95377300	-0.39386000
O	-0.50264600	3.50715700	0.55551000
O	0.63298100	3.58020700	-1.40130600
C	2.51727100	1.49680000	-0.59811000
O	2.78035200	2.34856200	0.22292600
O	3.33497500	1.14546200	-1.60935300
C	-2.50319600	1.58810100	-0.70763900
O	-2.64823500	2.58395900	-1.38279400
O	-3.44684500	1.08579300	0.11070000
C	-2.56076800	-1.40461800	-0.92298300
O	-2.88842300	-2.30030700	-0.17770300
O	-3.29018800	-0.97621700	-1.96824700
C	2.46959600	-1.48990400	-0.84926300
O	2.67817900	-2.33968900	-1.68789300
O	3.34431900	-1.16011600	0.12176900
C	-0.10335900	-2.86421700	-1.07128000
O	-0.68671800	-3.37421000	-2.00206000
O	0.55352900	-3.54289800	-0.11618900
C	4.60197600	-1.85343000	0.06765900
H	5.18402300	-1.46497000	0.90346800
H	4.44668300	-2.93005700	0.17262500
H	5.10622500	-1.65669200	-0.88231000
C	4.60035600	1.82672400	-1.63997800
H	5.12298100	1.42945600	-2.51016800
H	4.44848000	2.90431800	-1.73937300
H	5.16303800	1.62816900	-0.72378300
C	0.63398800	-4.96321000	-0.32800900
H	1.15120900	-5.35794400	0.54665000
H	-0.36715100	-5.39183400	-0.41283800
H	1.20058900	-5.17204200	-1.23925000
C	-4.53301500	-1.67087500	-2.17129400
H	-4.97652300	-1.21857400	-3.05836400
H	-4.34659300	-2.73544400	-2.33103100
H	-5.18596800	-1.54519000	-1.30327000
C	-4.69976100	1.79166900	0.10107000

H	-5.33498700	1.26343700	0.81209200
H	-4.55151700	2.82927600	0.40952900
H	-5.13854200	1.77354500	-0.90016100
C	0.73487800	5.00839800	-1.26245700
H	1.22330600	5.35437300	-2.17359500
H	-0.25929800	5.45014800	-1.16419400
H	1.33494900	5.25571600	-0.38283200

34c

G-sol = -1443.006086 Hartree

C	1.36078900	-0.39440800	-0.88969600
C	0.39090700	-0.37836900	-1.93913800
C	-0.91440400	-0.88251700	-1.79635400
C	-1.33219600	-1.41102200	-0.55619200
C	-0.37120800	-1.46749100	0.47727200
C	0.97809600	-1.02621600	0.35162600
Ni	-0.46983400	0.58382900	-0.22145600
P	-1.12010000	2.47170300	0.43809400
C	-2.47592600	2.54295800	1.71704800
H	-2.72812700	3.57335800	1.99933000
H	-3.37269600	2.05179100	1.32516000
H	-2.15969600	1.99412400	2.61009400
C	0.12036700	3.60238300	1.24915700
H	0.95129900	3.78556100	0.56065200
H	-0.32394200	4.56251600	1.54146900
H	0.52737100	3.11276300	2.13985100
C	-1.83285900	3.65225700	-0.81995500
H	-2.15281400	4.59924000	-0.36633200
H	-1.08259700	3.86311300	-1.58943000
H	-2.69322800	3.18456900	-1.31034900
H	-0.69653900	-1.88491000	1.41926400
H	0.64848200	0.05364900	-2.89611900
H	-1.59330900	-0.82506100	-2.64102100
C	1.84377700	-1.32534400	1.61829000
C	1.36172500	-0.46910800	2.80903000
C	1.75747000	-2.82672900	1.96332600
H	1.50079100	0.59368800	2.58422200
H	0.30305300	-0.62730500	3.03642400
H	1.95700900	-0.72224000	3.69348400
H	2.05713300	-3.43187300	1.10139900
H	2.45574400	-3.02874300	2.78171900
H	0.75721400	-3.13507800	2.27646500
C	2.74310900	0.19903800	-1.24061100
C	3.77068900	-0.91367900	-1.53088600

C	2.70653400	1.17202200	-2.43415600
H	3.43762500	-1.51808700	-2.38174100
H	4.74311500	-0.47529500	-1.79572300
H	3.89495500	-1.55742200	-0.65934600
H	3.67917600	1.67569400	-2.50277300
H	2.55164400	0.66184700	-3.38942400
H	1.93310200	1.93314000	-2.29917400
C	-2.72741200	-2.00382900	-0.36483100
C	-3.82835300	-1.09785300	-0.93972400
C	-2.77939700	-3.40472000	-1.00920700
H	-3.74600800	-0.98318600	-2.02537600
H	-4.81443800	-1.53401300	-0.73191400
H	-3.77531500	-0.10753000	-0.47936400
H	-3.77029700	-3.85712300	-0.86636900
H	-2.58527200	-3.35698100	-2.08612000
H	-2.03016800	-4.05721000	-0.55025100
O	3.23759200	-1.11530200	1.44617600
H	3.34871800	-0.20181500	1.10954600
O	3.16907200	1.00194900	-0.10102100
H	4.04418300	1.36381000	-0.32122300
O	-2.92549500	-2.13361000	1.05136100
H	-3.78890600	-2.55628500	1.18021300

35

G-sol = -1099.458022 Hartree

Ni	0.14390100	-0.40112900	-0.39699700
P	1.12367300	1.49654200	0.50351300
C	-0.08394100	2.80215000	1.01117300
H	0.40346200	3.64071200	1.52206600
H	-0.61280900	3.17432900	0.12848100
H	-0.82764300	2.35142200	1.67535300
C	2.04481600	1.18045300	2.07866800
H	2.85710900	0.47469300	1.87863600
H	2.46053500	2.10390700	2.49843800
H	1.36880600	0.73029500	2.81262000
C	2.37359600	2.47493500	-0.45894600
H	1.93048700	2.81784000	-1.39968900
H	2.73263600	3.34744000	0.10011700
H	3.22619300	1.83146700	-0.69791400
C	-1.13785500	-1.04253500	0.86388200
C	-2.42651700	-0.65164200	0.73523000
C	-1.44693400	0.34599500	-1.13050200
C	-2.61652900	0.16788700	-0.47679700
C	-3.57236800	-0.99868100	1.65659700

H	-4.08214500	-0.09868000	2.02828500
H	-4.33635300	-1.59860300	1.14171200
H	-3.24149600	-1.57339800	2.52670600
C	-0.51761800	-1.91829200	1.91647600
H	-0.36350800	-2.94809000	1.56072000
H	0.46841200	-1.55047500	2.23531200
H	-1.14054900	-1.97639300	2.82044400
C	-1.17912900	1.03312000	-2.43914100
H	-0.47913400	1.87690300	-2.34146200
H	-0.73566300	0.34677300	-3.17614200
H	-2.10014000	1.43125700	-2.88726800
C	-3.97398800	0.69025100	-0.88420500
H	-4.69218800	-0.12825700	-1.03270300
H	-4.40374100	1.34529300	-0.11300300
H	-3.93442100	1.26427800	-1.81465700
C	1.82220400	-1.46713000	-1.23813500
C	0.57448000	-2.08919800	-1.41362000
H	0.30120700	-2.95446300	-0.81333400
H	0.05052000	-2.01007200	-2.36342600
H	2.20955400	-0.83213500	-2.03594400
C	2.79149100	-1.87677800	-0.22358500
C	4.07857000	-1.48945400	-0.15500000
H	2.42033500	-2.57994000	0.52465300
H	4.74347800	-1.85951900	0.61948000
H	4.51107300	-0.80957500	-0.88682900

TS36

G-sol = -1099.438285 Hartree

Ni	-0.05083600	0.04983500	-0.15713900
P	-1.79188900	-1.17191100	0.47293000
C	-1.46158100	-2.75823700	1.36526500
H	-2.38389300	-3.18833700	1.77271900
H	-1.00017100	-3.47978300	0.68587900
H	-0.75897700	-2.56758600	2.18204200
C	-2.79087800	-0.23668100	1.71732800
H	-3.14208600	0.69507400	1.26305400
H	-3.64984800	-0.82252000	2.06521700
H	-2.16007800	0.01191700	2.57704200
C	-3.07990900	-1.68066100	-0.75806000
H	-2.63067700	-2.33270400	-1.51412700
H	-3.90859300	-2.21339200	-0.27715600
H	-3.47281100	-0.79108900	-1.25951000
C	1.42057800	1.21701600	0.45449400
C	2.62545900	0.57355900	0.39592100

C	1.36725400	-1.21928500	-0.48297300
C	2.62021100	-0.70228800	-0.31764600
C	3.86515600	1.04712400	1.12119500
H	4.17766200	0.33684900	1.90061600
H	4.71295100	1.13822900	0.42812000
H	3.72353600	2.02324000	1.59305100
C	1.08122500	2.27957700	1.47416000
H	1.33321100	3.30242800	1.14880300
H	0.00341000	2.28077800	1.68505600
H	1.59046100	2.09858300	2.42780200
C	1.07034500	-2.48587200	-1.24921400
H	0.19065900	-2.35451100	-1.89758500
H	1.89304800	-2.81999100	-1.89752800
H	0.83325400	-3.32410300	-0.57733300
C	3.92792900	-1.32929000	-0.75656200
H	4.49347500	-0.66299100	-1.42376900
H	4.58184200	-1.53814200	0.10164200
H	3.77918700	-2.27497400	-1.28433900
C	-0.99475500	1.57144300	-1.20091300
C	0.42169000	1.84965300	-1.18584300
H	0.71164000	2.85629500	-0.89247900
H	1.02328500	1.46298600	-2.00578500
H	-1.37247900	0.97381300	-2.03278300
C	-1.96322100	2.49163400	-0.61370200
C	-3.28114100	2.54994500	-0.88789700
H	-1.56230500	3.20085900	0.11375900
H	-3.93110200	3.27577800	-0.40861200
H	-3.74301200	1.89075500	-1.62116900

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G-sol = -1099.510749 Hartree

Ni	0.52856100	-0.60246100	-0.45829500
P	2.31709100	0.25676800	0.48515600
C	2.27133400	2.03889300	0.98320500
H	3.20183400	2.34068100	1.47777200
H	2.10988100	2.66818900	0.10410500
H	1.43046400	2.19897300	1.66434600
C	2.80567300	-0.54107000	2.08587900
H	3.02471900	-1.59901800	1.91577600
H	3.68455700	-0.05742400	2.52800900
H	1.97204700	-0.47650500	2.79258300
C	3.89766500	0.16716800	-0.48011500
H	3.78511400	0.72074300	-1.41767200
H	4.74053400	0.58692200	0.08121900

H	4.11656500	-0.87653700	-0.72646800
C	-2.67723200	-0.56239800	0.40365600
C	-2.19564100	0.66987300	0.68297700
C	-0.35612400	1.03318200	-0.96639400
C	-1.48466300	1.47939000	-0.36670800
C	-2.40205400	1.36895800	2.01592000
H	-1.49459100	1.91615700	2.30249700
H	-3.21262400	2.10950000	1.97097700
H	-2.64107800	0.67926100	2.82925200
C	-3.47724400	-1.42262300	1.35602900
H	-4.48801700	-1.59493900	0.95728700
H	-3.02641900	-2.41897500	1.47238100
H	-3.59106900	-0.99245500	2.35340100
C	0.30049900	1.74994700	-2.13311000
H	1.36928200	1.93676400	-1.95498200
H	0.26031400	1.11808600	-3.03271000
H	-0.15289300	2.71328700	-2.40211100
C	-2.19065200	2.79634400	-0.67102900
H	-3.21904700	2.61959200	-1.01951900
H	-2.27335300	3.42638300	0.22507000
H	-1.68199200	3.38952900	-1.43424300
C	-1.02678300	-1.65743500	-1.21605700
C	-2.45183400	-1.18838900	-0.97167600
H	-3.15039500	-2.02880900	-1.10851300
H	-2.69270000	-0.45597500	-1.75035900
H	-0.73496800	-1.73966900	-2.26640400
C	-0.30749400	-2.43084900	-0.27466500
C	1.07858900	-2.62478400	-0.40214200
H	-0.75355000	-2.59777300	0.70672300
H	1.62135600	-3.11638600	0.40116900
H	1.53572700	-2.70946300	-1.38929200

TS38

G-sol = -1099.488256 Hartree

Ni	0.64193800	-0.73678900	-0.11523500
P	2.47547200	0.27759900	0.40281200
C	2.81130700	2.03324100	-0.11458400
H	3.72000700	2.43319000	0.35122800
H	2.92240300	2.08146500	-1.20269900
H	1.95906700	2.66102800	0.16475500
C	2.68014200	0.42205200	2.24387900
H	2.65488100	-0.57697100	2.68965400
H	3.62369900	0.91274000	2.51203900
H	1.84790500	0.99851600	2.66023600

C	4.07837200	-0.53172000	-0.07209600
H	4.15718900	-0.57609800	-1.16338400
H	4.94640800	0.00874000	0.32464200
H	4.08843600	-1.55778000	0.30799900
C	-2.92718600	-0.28324700	0.45984100
C	-2.26243000	0.88290600	0.60391500
C	-0.54683000	0.48000300	-1.14899700
C	-1.40558300	1.33624600	-0.53378300
C	-2.38475300	1.81235700	1.79055600
H	-1.39160200	2.04606400	2.19833600
H	-2.84047900	2.77121500	1.50946200
H	-2.98340100	1.39127400	2.60126600
C	-3.90870400	-0.87975400	1.43493900
H	-4.87128100	-1.07261300	0.93908600
H	-3.55829400	-1.85305700	1.80864900
H	-4.10633200	-0.24383500	2.30084500
C	0.11004500	0.81100400	-2.47993100
H	0.62985300	-0.06044700	-2.89275300
H	-0.61482500	1.14537100	-3.23717200
H	0.86054300	1.60455100	-2.37263500
C	-1.64067800	2.76103600	-1.00213300
H	-2.71003200	2.95616700	-1.17000000
H	-1.30820300	3.49231400	-0.25185500
H	-1.10934100	2.98525400	-1.93018200
C	-1.19650800	-1.37945200	-1.04091100
C	-2.67721500	-1.09088600	-0.81341200
H	-3.22145200	-2.04431900	-0.76515200
H	-3.07244600	-0.54041600	-1.67905800
H	-0.96331600	-1.63812400	-2.07611800
C	-0.58708100	-2.25809700	-0.04025600
C	0.70689400	-2.80032800	-0.11807500
H	-1.10439300	-2.32322100	0.91869900
H	1.06487400	-3.41406200	0.70520800
H	1.17505300	-3.01300200	-1.08039300

39

G-sol = -1099.531903 Hartree

Ni	-0.47185500	-0.50343100	-0.17789600
P	-2.49653200	0.33737100	-0.24615200
C	-3.12637700	1.53653900	1.03468200
H	-4.15140200	1.86569000	0.82326700
H	-3.10330700	1.06545900	2.02300900
H	-2.47262300	2.41418300	1.06852700
C	-2.86841500	1.30143200	-1.79382800

H	-2.70831700	0.66285200	-2.66818700
H	-3.90056500	1.67294400	-1.80476800
H	-2.18432300	2.15303300	-1.86917800
C	-3.89577000	-0.88593800	-0.25322400
H	-3.88629200	-1.45736500	0.68087900
H	-4.87120700	-0.39529200	-0.35867000
H	-3.75515600	-1.59000900	-1.07885200
C	2.87133400	0.63035600	-0.52042500
C	1.84313700	1.22644500	0.13363700
C	1.07010200	-0.94536200	1.10496400
C	1.00095600	0.45467100	1.10102500
C	1.50957100	2.69692700	-0.02486200
H	0.43052500	2.83392000	-0.16633600
H	1.78993900	3.28140600	0.86201300
H	2.00779700	3.14836500	-0.88462600
C	3.84742900	1.31343700	-1.44468100
H	4.87905900	1.08368100	-1.13950200
H	3.74685300	0.94181500	-2.47585000
H	3.75171300	2.40077600	-1.47101800
C	0.58997100	-1.82483500	2.23890800
H	0.25175300	-2.79688600	1.86189200
H	1.41123700	-2.02737100	2.94573400
H	-0.23338900	-1.38838200	2.81032500
C	0.48338100	1.22798500	2.30434300
H	1.31046600	1.52248100	2.97062600
H	-0.03068300	2.14815300	2.01275700
H	-0.22012900	0.64262100	2.89977000
C	1.86907000	-1.63980600	-0.00546600
C	3.14121100	-0.85194500	-0.32137300
H	3.61087000	-1.26663200	-1.22523900
H	3.87597500	-0.98786900	0.49038700
H	2.13357600	-2.66564300	0.28623400
C	0.88202600	-1.60398600	-1.16897800
C	-0.34109600	-2.27366900	-1.24230600
H	1.19409800	-1.02641300	-2.04144700
H	-0.87552400	-2.30334800	-2.18879300
H	-0.60021400	-3.07015500	-0.54409500

TS40

G-sol = -943.556297 Hartree

Ni	-0.31717600	-0.42252100	-0.10238300
P	-2.39096000	-0.05105700	-0.01079700
C	1.97201300	-0.80222300	0.19049900
C	1.09361000	-1.48648700	-0.92711900

H	1.16854600	-2.57064600	-0.81547100
H	1.45444900	-1.20706500	-1.92387900
C	1.62207300	0.74849400	0.61936500
C	0.17356600	0.89887700	1.13983600
H	2.32684100	0.94220000	1.44023400
C	3.42658900	-0.85456300	-0.19234600
C	4.37157000	-1.51126900	0.48591600
C	-3.40956700	-1.27439400	-0.95077600
H	-3.08507700	-1.28315000	-1.99551100
H	-3.24212200	-2.27443100	-0.53941600
H	-4.47857700	-1.03430200	-0.90089400
C	-3.18650900	-0.06623000	1.65866200
H	-4.26886700	0.08969000	1.58689300
H	-2.99670700	-1.02898100	2.14313400
H	-2.74967600	0.72074100	2.28023400
C	-2.94370800	1.56414300	-0.72140900
H	-2.62343400	1.63049100	-1.76562400
H	-4.03393400	1.66653500	-0.67472300
H	-2.48057400	2.38665100	-0.16883700
H	0.05874500	0.54273900	2.17241500
H	4.14861400	-2.05156400	1.40451300
H	5.40233200	-1.54454200	0.14183200
H	3.68962100	-0.32792500	-1.10912900
H	1.84746300	-1.37218500	1.12148800
C	1.89685000	1.71810100	-0.50062400
C	2.83193700	2.67016800	-0.48251800
H	1.26294800	1.61397700	-1.38395300
H	2.97651700	3.34738300	-1.32055300
H	3.49196300	2.80555200	0.37229700
H	-0.21429700	1.91757200	1.04673100

41

G-sol = -943.5916073 Hartree

Ni	-0.50808000	0.61492800	-0.51677500
P	-2.56832600	-0.10219300	0.16664000
C	2.36531200	0.71874100	-0.55658900
C	1.11277700	1.34257500	-1.21308100
H	1.09352500	1.08466100	-2.28665400
H	1.09424900	2.44253800	-1.12687100
C	1.98437800	-0.78214700	-0.42916400
C	0.56088100	-0.80345300	0.16759700
H	1.91910700	-1.17020900	-1.45590200
C	2.66880300	1.37153200	0.76714100
C	3.83852300	1.91775700	1.10827100

C	-3.99458900	1.06093500	-0.07192600
H	-3.80732100	1.99042300	0.47578700
H	-4.09692500	1.30789900	-1.13388200
H	-4.93688000	0.62658300	0.28110400
C	-3.19441800	-1.64793100	-0.63995300
H	-4.16532300	-1.95557000	-0.23474700
H	-3.29061900	-1.48456600	-1.71802200
H	-2.47042900	-2.45415600	-0.48572600
C	-2.70911600	-0.52153800	1.96503400
H	-2.48811200	0.36708800	2.56460400
H	-3.70893700	-0.88941600	2.22293900
H	-1.96986700	-1.28877000	2.21543000
H	0.06193500	-1.76933600	-0.00087300
H	4.68950600	1.91514200	0.42934000
H	3.99203500	2.39079900	2.07539100
H	1.84420100	1.40880900	1.48165900
H	3.26015800	0.81973700	-1.18944300
C	2.95082800	-1.64591400	0.33580900
C	3.49869400	-2.77640100	-0.11767500
H	3.19520600	-1.30458800	1.34308100
H	4.17878500	-3.37064000	0.48795700
H	3.29009100	-3.14979000	-1.11926800
H	0.57429300	-0.60665400	1.25139800

42

G-sol = -1099.440172 Hartree

Ni	0.34699100	-0.31836900	-0.21119500
P	1.99885300	1.17772900	0.41705900
C	-2.52709000	-0.77404200	-0.43515700
C	-1.16492900	-1.35083900	-0.86478400
H	-1.06057500	-1.24508500	-1.96000200
H	-1.07138500	-2.42030000	-0.62812400
C	-2.33374400	0.75306800	-0.61408700
C	-0.98414500	1.08598200	0.06008000
H	-2.22008900	0.92231400	-1.69545300
C	-2.85949100	-1.16983800	0.98015100
C	-3.94850600	-1.84248900	1.36138300
C	3.71093400	0.57108400	0.80528200
H	3.67469000	-0.10723800	1.66407600
H	4.10982000	0.00922800	-0.04473200
H	4.39233600	1.39740500	1.03773100
C	2.35600900	2.47444700	-0.86133200
H	3.08541400	3.21231200	-0.50710300
H	2.74524200	1.99969600	-1.76832800

H	1.42613800	2.98766800	-1.12378600
C	1.64593800	2.21658300	1.91075500
H	1.55052700	1.57065700	2.78993800
H	2.43922900	2.95050700	2.09345000
H	0.69614700	2.74041000	1.77348300
H	-0.65156600	2.09006200	-0.24539500
H	-4.71005600	-2.14713300	0.64550700
H	-4.12397700	-2.11423300	2.39984400
H	-2.12392200	-0.89053600	1.73701300
H	-3.34802900	-1.12856100	-1.07896500
C	-3.47039600	1.61138300	-0.12790700
C	-4.11818100	2.52561800	-0.85500200
H	-3.75911700	1.46462900	0.91476100
H	-4.91973400	3.13150800	-0.43895600
H	-3.87135600	2.70173200	-1.90121400
H	-1.10780900	1.12316800	1.15575000
C	1.49920500	-2.14511900	0.15386000
C	1.78211700	-1.80316700	-0.98932400
C	2.23687400	-1.62419000	-2.37282800
H	2.92097000	-2.43148800	-2.66371300
H	1.38624100	-1.63043000	-3.06337300
H	2.76243600	-0.67107000	-2.50571700
C	1.25941700	-2.77073400	1.45843400
H	1.56097500	-2.11273300	2.28179800
H	0.19330700	-2.99152100	1.58336500
H	1.82152200	-3.70903400	1.54856700

TS43

G-sol = -1099.415056 Hartree

Ni	-0.51218900	0.30241700	-0.07789400
P	-2.20944300	-1.05280200	0.10200200
C	2.38938300	0.24505400	-0.65567700
C	1.11866800	0.95130400	-1.15286200
H	0.60556900	0.35352400	-1.92523100
H	1.34573400	1.90680900	-1.62545600
C	1.96446700	-1.21194700	-0.33662000
C	0.70683500	-1.14145200	0.54853900
H	1.67537900	-1.65996900	-1.30040800
C	3.03100400	0.94435800	0.51676500
C	4.26004400	1.46507900	0.51595400
C	-3.92559900	-0.47285800	-0.29036900
H	-4.21825700	0.32189200	0.40106500
H	-3.95047400	-0.06412400	-1.30526100
H	-4.65042400	-1.29213400	-0.21754800

C	-2.10479600	-2.54282400	-0.99493700
H	-2.94144600	-3.22859000	-0.81746000
H	-2.12633300	-2.22118400	-2.04136600
H	-1.16234100	-3.06761600	-0.81953100
C	-2.46008700	-1.80307600	1.77623700
H	-2.69617000	-1.01148000	2.49469400
H	-3.27728500	-2.53364900	1.76884800
H	-1.53980300	-2.29483000	2.10199400
H	0.30406500	-2.15633400	0.66850500
H	4.89913100	1.41885900	-0.36407800
H	4.67792600	1.95358100	1.39283800
H	2.42896700	1.00979800	1.42293900
H	3.12698500	0.24367700	-1.47466400
C	3.06084400	-2.06280000	0.24888700
C	3.49571400	-3.21882400	-0.25937100
H	3.50107600	-1.69507600	1.17702000
H	4.27052100	-3.80629400	0.22721600
H	3.09100200	-3.62442000	-1.18573400
H	0.96941100	-0.80269400	1.56565700
C	-1.37309400	2.01934700	-0.21153000
C	-0.11913100	2.27604700	-0.05026500
C	0.79301000	3.37248500	0.38811300
H	0.19585500	4.27993400	0.55012900
H	1.29848000	3.13009400	1.32901200
H	1.57432900	3.60618000	-0.34296600
C	-2.65442000	2.78160900	-0.14940400
H	-3.27409400	2.60680400	-1.03768800
H	-3.25536800	2.47706300	0.71693600
H	-2.48655000	3.86552400	-0.06923100

44

G-sol = -1099.451889 Hartree

Ni	-0.75803100	0.48714500	-0.59558000
P	-2.87753000	0.43277300	0.25275700
C	2.44815500	-0.04313100	0.81613100
C	1.26811700	-0.89354400	1.38164000
H	0.54347700	-0.20188300	1.83456100
H	1.66672000	-1.50733800	2.20017500
C	1.94291400	1.24837300	0.08784200
C	0.98927200	0.98462400	-1.09650400
H	1.38948400	1.81656400	0.85190400
C	3.37424600	-0.87928600	-0.03240300
C	4.65739700	-1.12367600	0.24394000
C	-4.23289300	-0.40508400	-0.69635000

H	-4.36179600	0.08628900	-1.66602800
H	-3.95997000	-1.44881500	-0.87948900
H	-5.18419700	-0.37724600	-0.15204800
C	-2.96394900	-0.43401900	1.88557100
H	-3.99068000	-0.49612600	2.26447000
H	-2.55258700	-1.44170100	1.77382200
H	-2.34472400	0.10016200	2.61303300
C	-3.65881400	2.07192500	0.63994800
H	-3.78171100	2.64979800	-0.28203300
H	-4.63916300	1.95301400	1.11561700
H	-3.00717600	2.64091400	1.31116700
H	0.68382700	1.96332300	-1.53507900
H	5.14102000	-0.71305500	1.12868800
H	5.27598200	-1.74125200	-0.40299100
H	2.93485700	-1.31359900	-0.92984600
H	3.02754400	0.31395100	1.67951500
C	3.10344800	2.11402400	-0.34629400
C	3.35757200	3.34329500	0.10882600
H	3.76012100	1.67889900	-1.10048200
H	4.19867100	3.92912200	-0.25394800
H	2.73103100	3.81360200	0.86573200
H	1.48115700	0.41978500	-1.89745800
C	-0.22097700	-1.29576400	-0.58798200
C	0.58115200	-1.80254600	0.36649600
C	0.94627100	-3.26941800	0.50920400
H	0.46960000	-3.91426500	-0.23363000
H	2.03381300	-3.40580800	0.42371400
H	0.66634300	-3.64539600	1.50428300
C	-0.76857500	-2.04589800	-1.78084600
H	-1.83848300	-1.86001000	-1.93994800
H	-0.26161900	-1.71682400	-2.69872600
H	-0.63373400	-3.13299400	-1.70541200

TS45

G-sol = -1099.451348 Hartree

Ni	-0.90931200	0.31261900	-0.46287800
P	-2.94733600	0.32315100	0.27172100
C	2.51483800	0.11677300	0.89970800
C	1.48051500	-0.91431400	1.42931200
H	0.69179300	-0.36504600	1.96351500
H	1.97612600	-1.55448800	2.16947400
C	1.78398800	1.21723900	0.06550700
C	0.89636800	0.65566700	-1.05982700
H	1.12614400	1.73829100	0.77575500

C	3.63147300	-0.56665600	0.14971900
C	4.92036100	-0.52902400	0.49450900
C	-4.13115700	-0.78379400	-0.63345400
H	-4.19478400	-0.47386200	-1.68117500
H	-3.75831300	-1.81251600	-0.60693700
H	-5.13338200	-0.75495100	-0.18896500
C	-3.18822000	-0.25157500	2.02023600
H	-4.24881800	-0.27659300	2.29841300
H	-2.76276700	-1.25368100	2.13156200
H	-2.65576300	0.41847400	2.70266200
C	-3.89718700	1.92192300	0.29052600
H	-3.96112000	2.32171300	-0.72651200
H	-4.91124100	1.78963100	0.68720800
H	-3.36722800	2.65475500	0.90755600
H	0.27418600	1.48607800	-1.49815400
H	5.26402400	0.02823000	1.36426200
H	5.68262900	-1.05269700	-0.07723000
H	3.33647900	-1.13939900	-0.72977500
H	2.95949300	0.63020900	1.76380000
C	2.74665200	2.24164400	-0.48704100
C	2.76060800	3.53389200	-0.15334200
H	3.47149200	1.87009100	-1.21205300
H	3.47198700	4.23121500	-0.58856600
H	2.05939200	3.94530900	0.57113700
H	1.47332200	0.25143300	-1.89545600
C	0.18373200	-1.20381900	-0.68889300
C	0.89407500	-1.76984800	0.31694300
C	1.23590000	-3.24186900	0.39186500
H	0.83260800	-3.82348200	-0.44113100
H	2.32596300	-3.39347400	0.41828400
H	0.84443800	-3.68414100	1.31980300
C	-0.19878800	-1.93169700	-1.96907000
H	-1.19578800	-2.38476100	-1.89291500
H	-0.23770100	-1.23570000	-2.81407000
H	0.50867000	-2.72849000	-2.23590300

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G-sol = -1099.505543 Hartree

Ni	1.01751200	-0.43491900	-0.01586200
P	2.97389600	0.45437000	-0.21834600
C	-2.57158400	0.11204500	-0.92272700
C	-1.49077600	-0.89493500	-1.37891100
H	-0.82756300	-0.39885200	-2.10512100
H	-1.97847200	-1.70838800	-1.93552600

C	-1.93090800	1.11094000	0.08539700
C	-1.42749400	0.35396700	1.33042600
H	-1.05621400	1.54731900	-0.41890500
C	-3.77289900	-0.60995000	-0.36019100
C	-5.02795100	-0.45523500	-0.78736300
C	3.84209200	0.83402100	1.37859700
H	3.24677100	1.54626800	1.95831400
H	3.93970000	-0.08300500	1.96756000
H	4.83839400	1.25841300	1.20376300
C	4.25818600	-0.56708700	-1.09146100
H	5.22947400	-0.05812600	-1.11953600
H	4.37101000	-1.52707500	-0.57833600
H	3.93281000	-0.76910000	-2.11693300
C	3.15744100	2.07648300	-1.10958800
H	2.54423700	2.83629300	-0.61481400
H	4.20070900	2.41537900	-1.12872700
H	2.79758200	1.97151100	-2.13816000
H	-0.82341400	1.03687900	1.94330600
H	-5.27718100	0.23724000	-1.58947800
H	-5.85437600	-1.01407400	-0.35522400
H	-3.57548800	-1.32124400	0.44289500
H	-2.90494000	0.68563300	-1.79753000
C	-2.86481600	2.23048300	0.46131600
C	-2.62758300	3.52687700	0.25273400
H	-3.80025800	1.93001300	0.93521500
H	-3.33835300	4.29502300	0.54710200
H	-1.71112900	3.87177900	-0.22364500
H	-2.29133600	0.08308900	1.96305300
C	-0.62755500	-0.91015200	1.03382500
C	-0.66360500	-1.50594500	-0.24118400
C	-0.27959800	-2.95367600	-0.50050500
H	0.42796700	-3.35579200	0.22832400
H	-1.17308900	-3.59978200	-0.49073300
H	0.17490300	-3.05980200	-1.49434200
C	-0.25417600	-1.66415300	2.29973700
H	0.22455200	-0.99173000	3.02244700
H	-1.15583700	-2.06914700	2.78917400
H	0.42813800	-2.49863600	2.12457600