Supporting information

Mechanistic Insights into Base-Free Nickel-Catalyzed Suzuki-Miyaura Cross-Coupling of Acid Fluoride and the origin of chemoselectivity: A DFT Study

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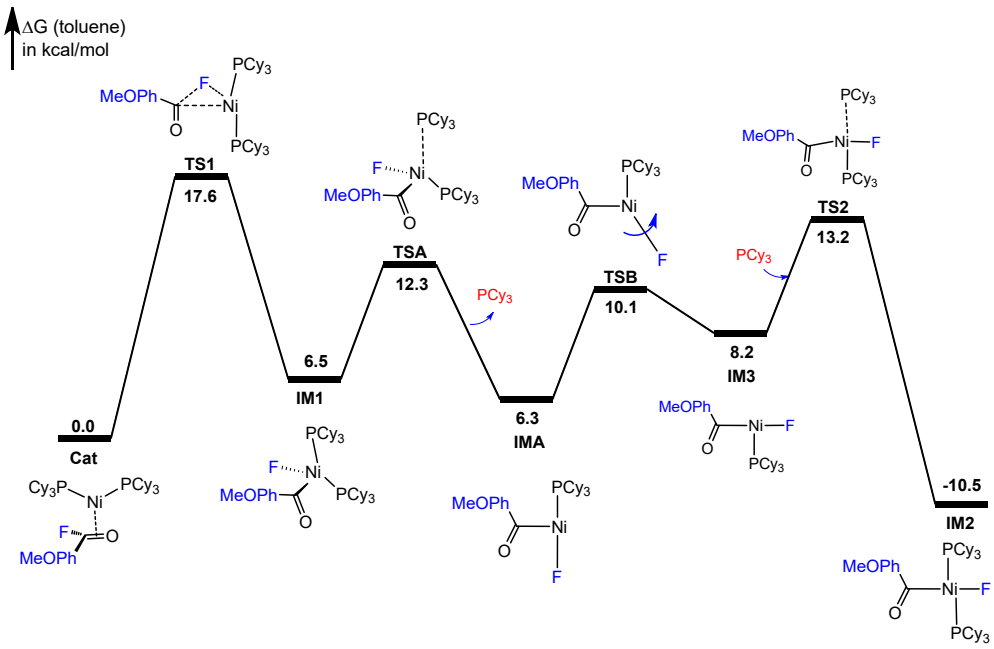


Figure S.1 Free energy profile for the conversion of **IM1** to **IM2**. Free energies are relative to **Cat** and PCy_3 and mass balanced.

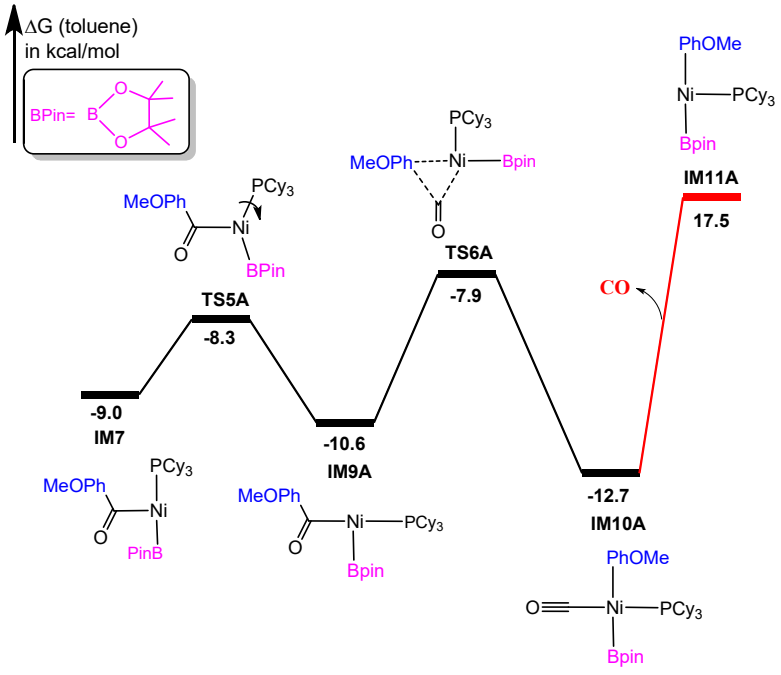


Figure S.2 Free energy profile for the dissociation of CO and PCy_3 ligand.

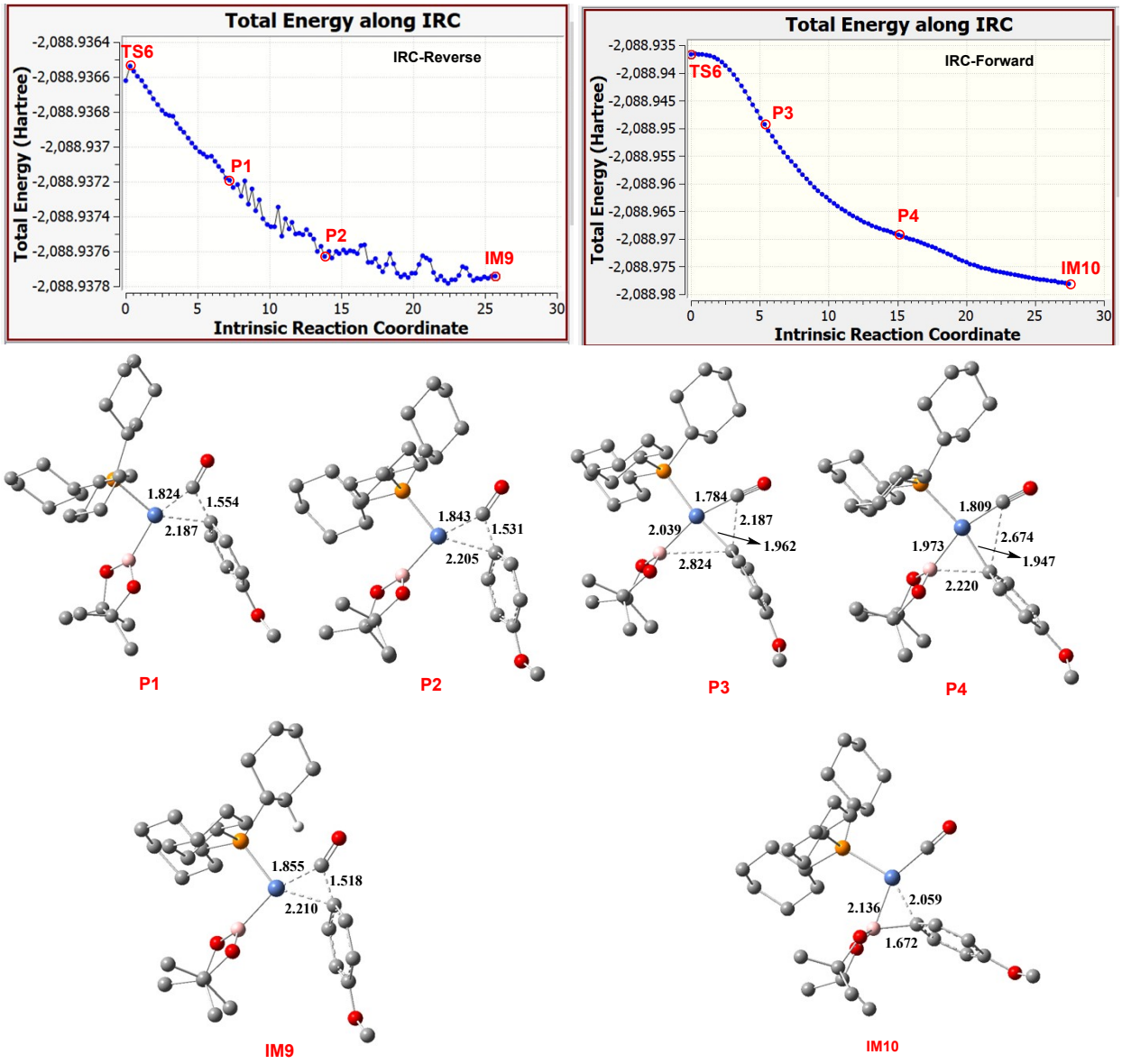
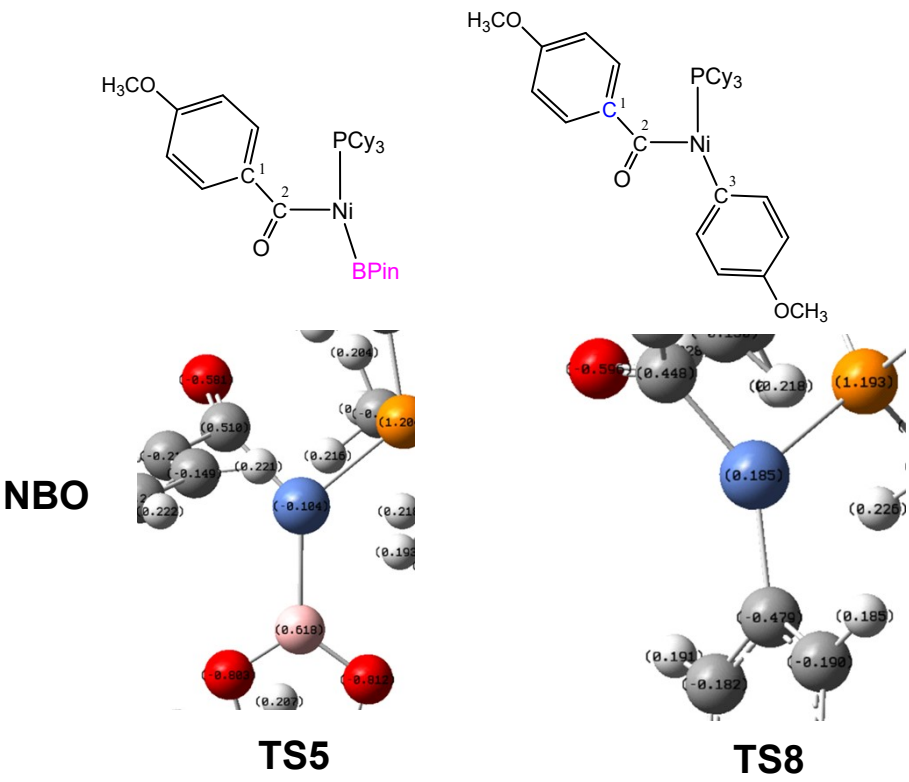


Figure S.3 IRC results to show that TS6 connects to IM9 and IM10 correctly. Values are key bond lengths in angstroms, Trivial H atoms are omitted for clarity.



	NBO charge	**ΔG(Kcal/mol)**	**Selected Angle(degree)**
TS5	Ni = -0.104 B= 0.618	23.4 relative to **IM2**	B-Ni-P = 126.9^0
TS8	Ni = 0.185 C^3 = -0.479	25.4 relative to **IM10**	C^3-Ni-P = 123.0^0

Figure S.4. Selected bond angles, dihedral angles, activation barriers ($\Delta G^{\ddagger}$), and NBO charges for **TS5** and **TS8**.

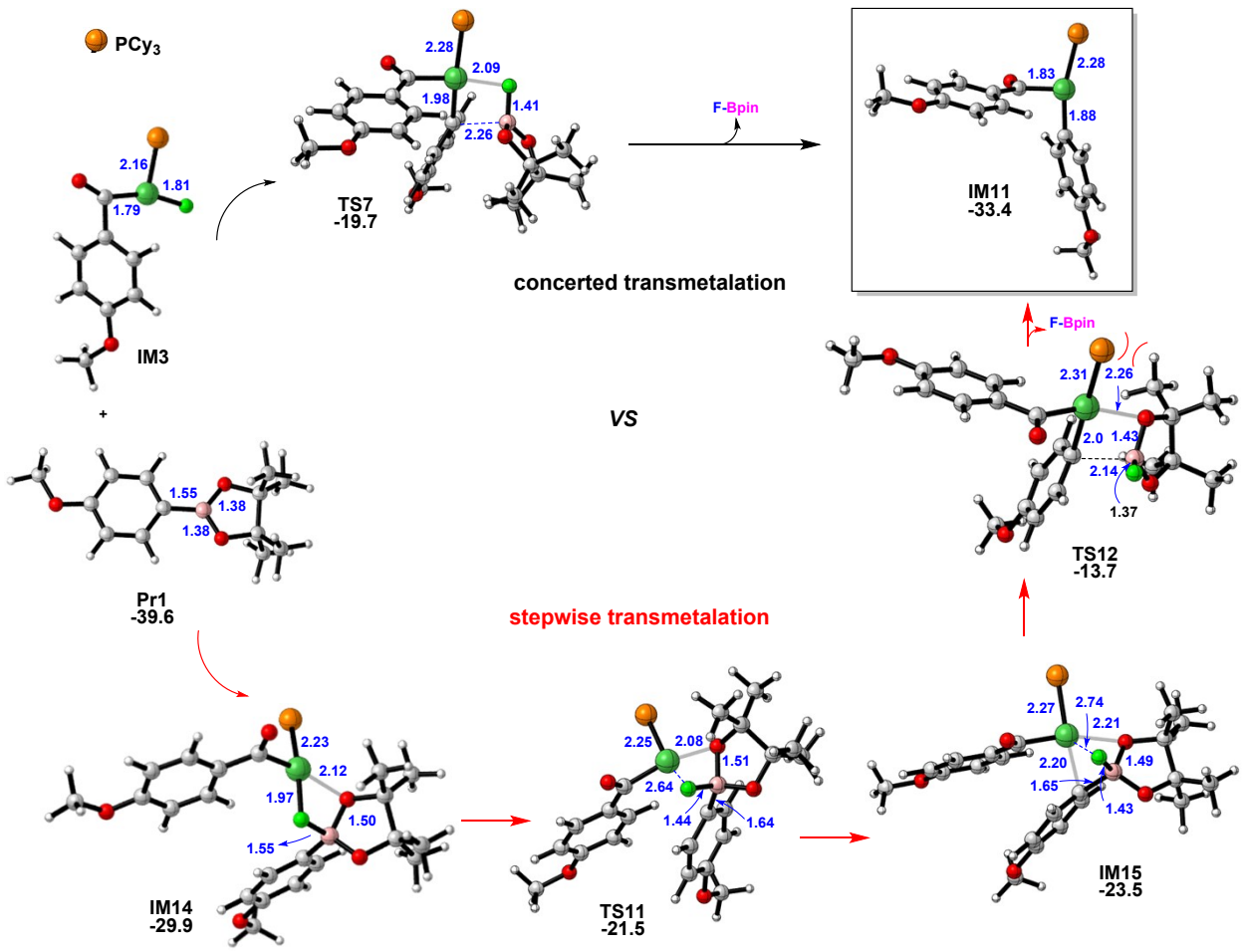


Figure S.5. Comparisons of the structures and barriers for concerted and stepwise transmetalation, along with key bond lengths (blue values) in angstroms and barriers in kcal/mol (black values). Trivial groups and H atoms are omitted for clarity

Table S.1: Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K and 1 atm for the Optimized Structures [BSI= 6-31G(d,p), BSII=6-311++G(d,p)]

Cat

B3LYP/BSI SCF energy: -2824.776282 a.u.
M06/BSII SCF energy in solution: -2823.835246 a.u.
M06/BSII free energy in solution: -2822.815689 a.u.

C	-3.21344800	0.17915900	-1.38059900
H	-2.88895900	-0.87075900	-1.42101700
C	-2.74225800	0.84762000	-2.69125700
H	-3.05712500	1.89730500	-2.68914000
H	-1.64746700	0.85262300	-2.75012500
C	-3.34297800	0.16632800	-3.93247600
H	-2.96061400	-0.86004500	-4.00874500
H	-3.01133900	0.69027000	-4.83727600
C	-4.87638100	0.13221800	-3.86766700
H	-5.26385700	1.15938300	-3.92705300
H	-5.28364400	-0.40435000	-4.73301800
C	-5.36036400	-0.51375900	-2.56244400
H	-5.07812600	-1.57645700	-2.55723200
H	-6.45535900	-0.48429600	-2.50464900
C	-4.75755200	0.17459200	-1.32384700
H	-5.11644900	-0.33074100	-0.42199400
H	-5.12990400	1.20405800	-1.27289400
C	-3.27572800	0.15228600	1.57502600
H	-4.31281100	0.48917000	1.44513100
C	-3.27446300	-1.39167100	1.58495500
H	-3.66113600	-1.79025800	0.63991900
H	-2.23749700	-1.73845500	1.67217300
C	-4.09815400	-1.95889300	2.75372000
H	-5.15573000	-1.69159100	2.61524300
H	-4.05113500	-3.05489200	2.74229100
C	-3.61020200	-1.41453500	4.10291200
H	-4.23966200	-1.79275500	4.91747800
H	-2.59307100	-1.78453300	4.29468500
C	-3.59715700	0.12002700	4.10323400
H	-3.19748200	0.49835200	5.05165100
H	-4.63065200	0.48916800	4.03094000
C	-2.77252300	0.68674800	2.93473800
H	-1.71640200	0.41840300	3.06319200
H	-2.81304800	1.77998700	2.96084500
C	-2.53562900	2.69142100	0.28195400
H	-2.05435700	2.86997000	1.25205100
C	-3.98100600	3.22210300	0.36386100

H	-4.47349900	3.11250200	-0.61137900
H	-4.57752100	2.64989500	1.08293300
C	-3.99509100	4.71147800	0.75711500
H	-5.02875600	5.07811500	0.78749900
H	-3.59618000	4.81612200	1.77588800
C	-3.15415000	5.56171000	-0.20603300
H	-3.13647300	6.60655700	0.12690700
H	-3.63040900	5.55856100	-1.19746700
C	-1.72510000	5.01393200	-0.33234000
H	-1.20061700	5.12549600	0.62615500
H	-1.15940400	5.59806200	-1.06877100
C	-1.72139300	3.52809900	-0.73096900
H	-0.69579300	3.15493300	-0.77701000
H	-2.15142000	3.43480700	-1.73534800
C	2.43024900	-1.22502400	-1.15496100
H	3.09338100	-0.71250600	-0.44441300
C	2.19305600	-0.21647500	-2.30156800
H	1.51013000	-0.64030200	-3.04660600
H	1.71106000	0.68202300	-1.90242200
C	3.51443600	0.15760800	-2.99374600
H	4.14685900	0.70789300	-2.28504300
H	3.31429000	0.84210800	-3.82712600
C	4.26489100	-1.08517900	-3.49438900
H	3.67958300	-1.56819900	-4.29061800
H	5.22261800	-0.79724500	-3.94461800
C	4.49433000	-2.09144300	-2.35800700
H	5.17373700	-1.64950700	-1.61551800
H	4.99092900	-2.99288100	-2.73810400
C	3.17479400	-2.47598000	-1.66425000
H	3.37922700	-3.16813800	-0.83994300
H	2.54420600	-3.01945700	-2.37940800
C	1.56735000	-2.53578300	1.35207300
H	1.83811000	-3.51217700	0.93050900
C	2.83203400	-1.96996500	2.02932600
H	3.64083800	-1.84893600	1.30093100
H	2.60773000	-0.98020700	2.43398500
C	3.31255100	-2.89291400	3.16447000
H	3.62483700	-3.85988400	2.74293000
H	4.20192300	-2.45901900	3.63778700
C	2.21501000	-3.12815700	4.21078700
H	2.56732800	-3.81821300	4.98716100
H	1.98642600	-2.17800700	4.71292800
C	0.93929100	-3.67021000	3.55284400
H	0.14040800	-3.77894200	4.29684200
H	1.13462900	-4.67739100	3.15628100
C	0.46377700	-2.75760100	2.40988300

H	0.17286700	-1.78179300	2.81972400
H	-0.43513800	-3.18674300	1.95137200
C	-0.23432400	-2.76420800	-0.95822400
H	-1.18460200	-2.62738500	-0.42167500
C	0.12797500	-4.26404500	-0.85002900
H	0.24630400	-4.56355300	0.19443600
H	1.08949000	-4.45582700	-1.34247500
C	-0.95218300	-5.15598900	-1.49003700
H	-0.65149900	-6.20800900	-1.41323800
H	-1.88441100	-5.05682900	-0.91534700
C	-1.22072700	-4.77941500	-2.95146900
H	-0.32305200	-4.98637500	-3.55154600
H	-2.02352500	-5.40062800	-3.36632400
C	-1.57626000	-3.29242000	-3.07024000
H	-2.53932200	-3.11014400	-2.57210300
H	-1.71309600	-3.01552900	-4.12280600
C	-0.49499900	-2.40032200	-2.43633600
H	0.43210400	-2.52584800	-3.00833000
H	-0.77628000	-1.34652700	-2.52836200
F	1.63068500	0.93228100	2.73928300
Ni	0.00459300	0.45054700	0.49875800
P	-2.26324400	0.82640400	0.12918000
P	0.89925500	-1.49371200	-0.08315800
O	0.27771600	2.11661400	1.33047400
C	1.38076100	1.45531200	1.43776500
C	3.77272500	3.42136900	-0.75059200
C	2.60932700	2.91211700	-0.19254800
C	5.02666100	3.01963600	-0.26287500
C	2.65410500	1.98458800	0.86514600
C	3.91003500	1.60265900	1.34998500
C	5.09040800	2.10625500	0.79468600
H	3.97048800	0.91665300	2.18628000
H	6.04327700	1.79041700	1.20348600
H	1.64371100	3.24106700	-0.56066800
H	3.73995600	4.14384900	-1.56008800
O	6.11225100	3.57989600	-0.87796500
C	7.40139600	3.22157400	-0.41196400
H	7.58985600	2.14544600	-0.52398000
H	8.11158900	3.77488800	-1.02893900
H	7.54569800	3.49985500	0.64032600

1a

B3LYP/BSI SCF energy: -559.35997 a.u.
M06/BSII SCF energy in solution: -559.186136 a.u.
M06/BSII free energy in solution: -559.0858 a.u.

F	-3.05303400	-1.30085400	-0.00024800

O	-3.38258900	0.89499000	0.00069500
C	-2.59989900	-0.01125900	0.00030700
C	0.85583100	1.44286200	-0.00029500
C	-0.52207700	1.32906400	-0.00003200
C	1.65815100	0.28607900	-0.00042600
C	-1.13240600	0.06038100	-0.00006000
C	-0.32961100	-1.08665000	-0.00025800
C	1.05900400	-0.98301900	-0.00046200
H	-0.79661300	-2.06464700	-0.00039000
H	1.66036000	-1.88378200	-0.00072600
H	-1.15186100	2.21236300	0.00017800
H	1.34567600	2.41063600	-0.00036500
O	2.99619200	0.50392300	-0.00082900
C	3.87186100	-0.61733700	0.00115700
H	3.73319200	-1.23660100	-0.89333300
H	4.88212100	-0.20680300	0.00238600
H	3.73048600	-1.23549900	0.89596700

TS1

B3LYP/BSI SCF energy: -2824.749181 a.u.
M06/BSII SCF energy in solution: -2823.804255 a.u.
M06/BSII free energy in solution: -2822.787616 a.u.

C	3.45868500	0.17588000	-1.19520600
H	3.30403700	1.22517900	-0.90040600
C	2.90218100	0.04565400	-2.63197600
H	3.03160300	-0.98131800	-2.98873800
H	1.82354100	0.23435700	-2.64093800
C	3.62904200	0.99808400	-3.59620200
H	3.41999100	2.03859500	-3.30949500
H	3.23545700	0.86927400	-4.61174300
C	5.14710800	0.76529000	-3.57984600
H	5.36218100	-0.23430000	-3.98371200
H	5.65187100	1.48253700	-4.23829600
C	5.71129600	0.86268200	-2.15482500
H	5.60885100	1.89611500	-1.79339600
H	6.78515400	0.63872300	-2.15331600
C	4.97909800	-0.08465400	-1.18677800
H	5.39207500	0.02755900	-0.17787600
H	5.17088500	-1.12120600	-1.49065600
C	3.21976400	-0.28483800	1.72090400
H	4.24875100	-0.66706400	1.69639800
C	3.30094300	1.23445300	1.97327800
H	3.85687400	1.73430300	1.17243200
H	2.28776100	1.65668500	1.96729100
C	3.96453800	1.54902000	3.32581000
H	5.01189600	1.21595900	3.29917800

H	3.98772800	2.63439700	3.48327000
C	3.24120700	0.85420800	4.48751800
H	3.75825800	1.05535100	5.43352000
H	2.23094100	1.27642600	4.58761400
C	3.13431100	-0.65751800	4.24557400
H	2.56355300	-1.13400700	5.05177000
H	4.14030800	-1.10052900	4.27319000
C	2.47938500	-0.97283800	2.89023900
H	1.43594000	-0.63139400	2.89664000
H	2.44189100	-2.05693000	2.74369400
C	2.74584400	-2.60128600	-0.02760200
H	1.94532100	-2.98671000	0.61772800
C	4.08874900	-3.14238400	0.50951800
H	4.91445900	-2.80043400	-0.12707100
H	4.29773300	-2.77103600	1.51761500
C	4.08213600	-4.68324600	0.53956300
H	5.05072500	-5.04938900	0.90284000
H	3.32865500	-5.02036000	1.26553200
C	3.76163400	-5.28557900	-0.83561500
H	3.71123800	-6.37926000	-0.76744700
H	4.58262500	-5.05390500	-1.53004500
C	2.45129600	-4.71742800	-1.39657900
H	1.60830000	-5.04803100	-0.77477900
H	2.26697800	-5.10830200	-2.40466600
C	2.46987400	-3.18029100	-1.43318400
H	1.51910200	-2.80648400	-1.82098000
H	3.26355800	-2.85959200	-2.12122200
C	-2.44005400	1.56416800	-1.21668800
H	-3.15163300	0.79849500	-0.87757800
C	-2.01169700	1.13861900	-2.64092900
H	-1.28532900	1.85312600	-3.04554100
H	-1.51233800	0.16590600	-2.60814000
C	-3.22429900	1.08406800	-3.58786100
H	-3.90377000	0.28669300	-3.25608900
H	-2.89267300	0.81146100	-4.59723100
C	-3.99042900	2.41417700	-3.61792100
H	-3.35104700	3.19183900	-4.06051000
H	-4.87320400	2.33315800	-4.26387900
C	-4.40309900	2.84610600	-2.20393900
H	-5.13372000	2.12875700	-1.80390200
H	-4.90584800	3.82084600	-2.23173700
C	-3.19119900	2.91075800	-1.25655800
H	-3.52277700	3.20610400	-0.25486300
H	-2.51398900	3.69930800	-1.60890700
C	-1.96264800	1.74105300	1.69300600
H	-2.31006700	2.78117800	1.64462000

C	-3.19889000	0.85200300	1.92561600
H	-3.92286400	0.96780100	1.11256700
H	-2.89529100	-0.19948800	1.92005100
C	-3.88834400	1.17889200	3.26144200
H	-4.29320500	2.20067500	3.22116300
H	-4.74565300	0.50994500	3.40296100
C	-2.92095100	1.06620600	4.44689700
H	-3.42369200	1.34774700	5.38005700
H	-2.61055400	0.01797600	4.56188000
C	-1.67756200	1.93817300	4.22480800
H	-0.96446400	1.80633400	5.04804200
H	-1.97135300	2.99788000	4.23457500
C	-0.99233700	1.61305000	2.88696500
H	-0.60707500	0.58516900	2.91343400
H	-0.12186500	2.26601500	2.75348100
C	0.08203600	2.90192200	-0.06393900
H	0.92893100	2.58685600	0.56099900
C	-0.40759900	4.25660400	0.49788400
H	-0.76473000	4.15176700	1.52635000
H	-1.25586600	4.62431400	-0.09123600
C	0.71757400	5.30884100	0.46928600
H	0.33756200	6.26461300	0.85048800
H	1.51709600	4.99608700	1.15623900
C	1.30399300	5.48902800	-0.93709300
H	0.53641800	5.91706000	-1.59771000
H	2.13252600	6.20715400	-0.91615500
C	1.77065300	4.14576100	-1.51339300
H	2.62269600	3.77516800	-0.92546200
H	2.13359900	4.27610200	-2.54035600
C	0.64120800	3.10205600	-1.48826900
H	-0.16257200	3.44827000	-2.14928900
H	0.99486100	2.15052200	-1.89644000
F	-0.35108600	-2.48700300	0.64617600
Ni	0.04209800	-0.51739900	-0.05429600
P	2.40464400	-0.73634700	0.07879000
P	-1.06016200	1.37952500	0.06619400
O	-0.63771700	-1.99040400	-1.68374000
C	-1.20282200	-1.81974600	-0.59421500
C	-4.87443000	-2.47531600	-1.20767900
C	-3.52647400	-2.15761100	-1.39113000
C	-5.33121100	-2.83720600	0.06513100
C	-2.62374800	-2.17335800	-0.32227100
C	-3.09274000	-2.55411500	0.94675800
C	-4.42705200	-2.88152000	1.13887400
H	-2.39101300	-2.61242800	1.76956800
H	-4.79615000	-3.19024900	2.11174800

H	-3.16179700	-1.91055800	-2.38240700
H	-5.54504000	-2.45416900	-2.05864000
O	-6.62052300	-3.17290700	0.36210200
C	-7.57208900	-3.17762900	-0.68944600
H	-8.52016500	-3.47388000	-0.23762500
H	-7.68362400	-2.18311100	-1.14099300
H	-7.30614300	-3.89781400	-1.47399100

IM1

B3LYP/BSI SCF energy: -2824.772796 a.u.
M06/BSII SCF energy in solution: -2823.82448 a.u.
M06/BSII free energy in solution: -2822.805361 a.u.

C	3.60018500	-0.30644800	-0.10102100
H	3.39166900	0.62818600	0.43605100
C	3.82340200	0.06330200	-1.58516400
H	4.03571200	-0.84870200	-2.15540700
H	2.91062000	0.48975700	-2.01795800
C	5.00315300	1.03246700	-1.77079300
H	4.76823800	1.99386200	-1.29392600
H	5.14517700	1.24083000	-2.83827400
C	6.29188000	0.46647100	-1.15945500
H	6.59284200	-0.43074600	-1.71908900
H	7.11278200	1.18669000	-1.26001100
C	6.08338100	0.09570100	0.31499900
H	5.89348500	1.01081500	0.89403600
H	6.99619500	-0.34910600	0.73005200
C	4.90354700	-0.87649400	0.50438200
H	4.77908400	-1.07819600	1.57301200
H	5.15150600	-1.83365500	0.03240600
C	2.19506400	-1.99044300	1.87068600
H	3.21447400	-2.39307900	1.93596000
C	2.06632500	-0.85401300	2.91001200
H	2.78218400	-0.04966600	2.69908300
H	1.06336400	-0.41350600	2.82189300
C	2.26966900	-1.35786200	4.34852100
H	3.30528100	-1.70796200	4.46674700
H	2.13963300	-0.52813400	5.05451800
C	1.30604600	-2.50446800	4.68074500
H	1.49385900	-2.87924400	5.69427800
H	0.27497400	-2.12305000	4.67267900
C	1.43283600	-3.63857200	3.65475800
H	0.71039400	-4.43387500	3.87474700
H	2.43105400	-4.09212600	3.74449900
C	1.22417700	-3.14060700	2.21427400
H	0.19345400	-2.80707600	2.06349000

H	1.36966000	-3.97613900	1.52254500
C	2.05034300	-2.80392900	-0.98593700
H	1.23212700	-3.38530000	-0.54962100
C	3.33054000	-3.65973900	-0.96084600
H	4.16041900	-3.11257500	-1.42661600
H	3.63696700	-3.88042100	0.06836200
C	3.12082100	-4.97680000	-1.73115900
H	4.04728900	-5.56474300	-1.72471500
H	2.36302100	-5.57877200	-1.21042200
C	2.65908200	-4.71866100	-3.17278300
H	2.47268400	-5.66941200	-3.68713400
H	3.46843000	-4.21924300	-3.72555700
C	1.40322300	-3.83561500	-3.20721800
H	0.56150200	-4.37918000	-2.75688500
H	1.11766600	-3.62039600	-4.24410200
C	1.60835100	-2.51798500	-2.43943700
H	0.67870600	-1.94162000	-2.43999500
H	2.36319300	-1.91751300	-2.96230600
C	-0.89269800	2.75483000	-1.54069700
H	-1.84629600	2.31265800	-1.85526900
C	0.09320600	2.44528200	-2.69001900
H	1.08983300	2.83761600	-2.45779600
H	0.17688200	1.36214600	-2.80931400
C	-0.39660400	3.07733100	-4.00429100
H	-1.33327400	2.58858800	-4.30411700
H	0.32826100	2.87803300	-4.80292400
C	-0.62817400	4.58860700	-3.86097500
H	0.33403500	5.08717300	-3.67328700
H	-1.01686400	5.00678900	-4.79738400
C	-1.58884600	4.89921200	-2.70400900
H	-2.58560100	4.50348900	-2.94480800
H	-1.70464900	5.98324900	-2.58182200
C	-1.10825100	4.27391300	-1.38121700
H	-1.83442900	4.48595600	-0.58865200
H	-0.17037500	4.75815200	-1.08148800
C	-2.05202200	2.17751600	1.12086500
H	-1.92409700	3.22028700	1.43490800
C	-3.42763700	2.09922900	0.42584200
H	-3.46383500	2.77227600	-0.43686100
H	-3.60540200	1.08941300	0.04730600
C	-4.55827800	2.47092200	1.40331400
H	-4.45069900	3.52392200	1.70272900
H	-5.52397500	2.38960300	0.89037100
C	-4.54243200	1.58402200	2.65525300
H	-5.33669100	1.88768800	3.34793000
H	-4.75555600	0.54650200	2.36457500

C	-3.17642100	1.64412400	3.35240700
H	-3.15472200	0.96519400	4.21356400
H	-3.01558300	2.65694400	3.75031800
C	-2.03462600	1.28880100	2.38487500
H	-2.12916700	0.24052000	2.07684200
H	-1.07184900	1.37221400	2.90424800
C	0.85778300	2.61162300	1.00395300
H	1.22028400	1.78998100	1.63731900
C	0.47910800	3.78240800	1.94218800
H	-0.30422400	3.48758300	2.64470700
H	0.07721200	4.61633900	1.35186800
C	1.69138600	4.27670300	2.75333300
H	1.38650000	5.11878100	3.38642200
H	2.01477200	3.47713800	3.43513800
C	2.86527700	4.67753500	1.85383000
H	2.58217700	5.55424200	1.25394700
H	3.72781500	4.97881500	2.46001100
C	3.24314500	3.52436500	0.91674400
H	3.63983600	2.69038900	1.51309000
H	4.04779200	3.83102000	0.23740100
C	2.03195100	3.04329500	0.09875700
H	1.70994100	3.86717400	-0.54838300
H	2.32497200	2.22675300	-0.56511500
F	-0.58350700	-2.28050800	-0.02136700
Ni	-0.35439300	-0.47272900	-0.25171900
P	1.98123300	-1.28295200	0.12927800
P	-0.55862100	1.77253300	0.02964800
O	-1.82014000	-0.14346300	-2.43294400
C	-1.94100200	-0.55720700	-1.28347100
C	-5.52594300	-1.79637300	-1.40947300
C	-4.30207000	-1.22446300	-1.75214400
C	-5.66936300	-2.41263900	-0.15802000
C	-3.21086000	-1.24547500	-0.87198400
C	-3.37017200	-1.87405000	0.37602600
C	-4.58149900	-2.44982000	0.73017500
H	-2.51538400	-1.94061000	1.03714700
H	-4.71255900	-2.95016400	1.68445800
H	-4.17405000	-0.74519100	-2.71775200
H	-6.35035800	-1.75899500	-2.11225800
O	-6.81462600	-3.00300000	0.28636500
C	-7.94108500	-3.02508900	-0.57607000
H	-8.72718000	-3.55078400	-0.03163600
H	-8.28662500	-2.01181300	-0.81848600
H	-7.72638100	-3.56223600	-1.50863400

IM2
B3LYP/BSI SCF energy: -2824.802371 a.u.
M06/BSII SCF energy in solution: -2823.851263 a.u.
M06/BSII free energy in solution: -2822.832367 a.u.

C	-2.76879400	-2.20034500	-0.79369000
H	-2.21165600	-2.91756600	-0.17766700
C	-2.18839900	-2.33114600	-2.21897600
H	-2.67004900	-1.61734500	-2.89649300
H	-1.12372600	-2.08157900	-2.20853100
C	-2.39448200	-3.75470800	-2.76206100
H	-1.81120200	-4.45937200	-2.15274300
H	-2.00066600	-3.82284000	-3.78336900
C	-3.87478100	-4.16256100	-2.73341200
H	-4.43784900	-3.52783100	-3.43292900
H	-3.99532500	-5.19488200	-3.08371300
C	-4.46751700	-4.00848000	-1.32538800
H	-3.98451500	-4.72761900	-0.64876100
H	-5.53665300	-4.25428600	-1.33085900
C	-4.26181200	-2.58572200	-0.77191300
H	-4.67006300	-2.52355700	0.24330200
H	-4.83680600	-1.87977800	-1.38560700
C	-2.85484900	-0.82214400	1.83742100
H	-3.95208700	-0.78972800	1.81332800
C	-2.44921800	-2.16723200	2.47824900
H	-2.86457500	-3.00131300	1.90321500
H	-1.36216100	-2.27557800	2.42822000
C	-2.95075700	-2.26369100	3.92949700
H	-4.05072800	-2.28443400	3.93674900
H	-2.62070500	-3.21363900	4.36720400
C	-2.46869300	-1.08628400	4.78764100
H	-2.87210400	-1.16204400	5.80475200
H	-1.37399100	-1.13071800	4.87995100
C	-2.86529700	0.25358000	4.15329000
H	-2.47156700	1.09053700	4.74306300
H	-3.96049000	0.35209300	4.16598900
C	-2.36148600	0.35656400	2.70498700
H	-1.26355700	0.34858000	2.70491700
H	-2.66690600	1.31655400	2.27237600
C	-3.34528800	0.84180100	-0.56627200
H	-2.77629700	1.71308800	-0.21072500
C	-4.77620400	0.96778600	0.00332300
H	-5.38124100	0.11044400	-0.31834500
H	-4.76933600	0.95441900	1.09705600
C	-5.45053400	2.27095600	-0.46507100

H	-6.47176200	2.31931800	-0.06737300
H	-4.90806600	3.12507100	-0.03509300
C	-5.46213800	2.40012500	-1.99357400
H	-5.89913200	3.36133800	-2.29044000
H	-6.10911200	1.61886700	-2.41812700
C	-4.04760300	2.25002500	-2.56779900
H	-3.42605200	3.09655400	-2.24394600
H	-4.07408900	2.28448700	-3.66371300
C	-3.38726500	0.93819600	-2.11004800
H	-2.38219700	0.86055700	-2.53074300
H	-3.97166900	0.09788500	-2.50670800
C	3.34532700	0.84169500	-0.56626200
H	2.77638000	1.71299600	-0.21068000
C	3.38726600	0.93812900	-2.11003700
H	3.97163000	0.09780800	-2.50673500
H	2.38218400	0.86053600	-2.53070600
C	4.04763800	2.24994700	-2.56777000
H	3.42612600	3.09649000	-2.24387600
H	4.07409500	2.28443900	-3.66368300
C	5.46219500	2.39998100	-1.99358000
H	6.10912800	1.61871200	-2.41817300
H	5.89921400	3.36118600	-2.29043200
C	5.45062800	2.27077000	-0.46508000
H	4.90820500	3.12489400	-0.03506400
H	6.47186900	2.31908400	-0.06741000
C	4.77626300	0.96761200	0.00329800
H	4.76942500	0.95421700	1.09703100
H	5.38126100	0.11025700	-0.31840900
C	2.85483000	-0.82224600	1.83742600
H	3.95207000	-0.78989800	1.81333500
C	2.36153700	0.35649500	2.70498600
H	2.66701900	1.31646500	2.27237300
H	1.26360700	0.34858000	2.70491300
C	2.86533700	0.25348500	4.15329100
H	3.96053600	0.35192900	4.16599400
H	2.47165700	1.09046800	4.74306100
C	2.46864700	-1.08635200	4.78764600
H	2.87204900	-1.16213400	5.80475800
H	1.37394100	-1.13071800	4.87995200
C	2.95063900	-2.26379300	3.92950700
H	2.62052500	-3.21371800	4.36721600
H	4.05060800	-2.28460600	3.93676300
C	2.44911200	-2.16730600	2.47825700
H	1.36204900	-2.27558500	2.42822400
H	2.86441800	-3.00141600	1.90322700
C	2.76873300	-2.20043600	-0.79369200

H	2.21163100	-2.91764600	-0.17762100
C	4.26175100	-2.58581900	-0.77200700
H	4.67006900	-2.52363900	0.24318000
H	4.83670800	-1.87988700	-1.38575000
C	4.46741400	-4.00858700	-1.32547300
H	5.53655000	-4.25439500	-1.33101100
H	3.98445700	-4.72771400	-0.64880200
C	3.87458300	-4.16269000	-2.73345400
H	4.43760600	-3.52797400	-3.43302000
H	3.99510100	-5.19501700	-3.08374600
C	2.39428400	-3.75483200	-2.76201100
H	1.81104300	-4.45948300	-2.15264000
H	2.00039800	-3.82298200	-3.78329000
C	2.18824300	-2.33126000	-2.21893800
H	2.66985200	-1.61747400	-2.89650000
H	1.12357200	-2.08168800	-2.20842800
F	-0.00002900	-2.16158900	0.68442100
Ni	0.00000200	-0.45368200	-0.09271700
P	-2.27747400	-0.59789600	0.05299600
P	2.27746900	-0.59797200	0.05300000
O	0.00003100	0.89558900	-2.37432500
C	0.00003100	1.08338700	-1.15204000
C	0.00007900	4.89365900	-1.14670900
C	0.00005800	3.56688600	-1.57100100
C	0.00010200	5.17800500	0.22838900
C	0.00005700	2.50611700	-0.65399000
C	0.00008200	2.81007000	0.71658800
C	0.00010400	4.12615600	1.15924000
H	0.00008400	1.99455600	1.43340100
H	0.00012200	4.37239300	2.21641500
H	0.00003900	3.32201700	-2.62891400
H	0.00007800	5.69191900	-1.88001200
O	0.00012300	6.43340900	0.75699500
C	0.00012200	7.54140300	-0.13087800
H	0.00014100	8.43182300	0.49955500
H	0.89383400	7.54987300	-0.76763600
H	-0.89361100	7.54989200	-0.76760800

TS2

B3LYP/BSI SCF energy: -2824.769908 a.u.
M06/BSII SCF energy in solution: -2823.808627 a.u.
M06/BSII free energy in solution: -2822.794671 a.u.

C	-3.27111600	-1.46247300	-1.08533800
H	-2.43686700	-2.12690800	-0.82075600
C	-3.03195700	-1.08105300	-2.56321200
H	-3.84302200	-0.42779900	-2.91445500

H	-2.09848900	-0.51929300	-2.66571500
C	-2.98688900	-2.33537900	-3.45067200
H	-2.11614100	-2.93739300	-3.15877600
H	-2.83622000	-2.04761200	-4.49904100
C	-4.26627300	-3.17362000	-3.30984700
H	-5.11666500	-2.60503200	-3.71473500
H	-4.19308300	-4.09069900	-3.90796200
C	-4.54916100	-3.51873900	-1.84019100
H	-3.76251500	-4.19157900	-1.47032000
H	-5.49647800	-4.06631100	-1.75245700
C	-4.58539000	-2.25979300	-0.95349000
H	-4.76794800	-2.55620000	0.08505700
H	-5.43748200	-1.63677700	-1.25238700
C	-3.60433100	-0.64848600	1.72963100
H	-4.65374000	-0.94962800	1.59929700
C	-2.80513100	-1.88527100	2.19456000
H	-2.85822700	-2.68439500	1.44825000
H	-1.74407000	-1.60938900	2.26686700
C	-3.29284500	-2.41452300	3.55363600
H	-4.31993800	-2.79219000	3.44717200
H	-2.67982600	-3.27098600	3.86182000
C	-3.26700600	-1.32368300	4.63293100
H	-3.66744000	-1.70996600	5.57841100
H	-2.22454200	-1.03465800	4.83116000
C	-4.05406300	-0.08593100	4.18306600
H	-3.98287000	0.70775900	4.93735700
H	-5.11967800	-0.34493400	4.10429200
C	-3.56300800	0.44046600	2.82373800
H	-2.53219700	0.80947700	2.92726100
H	-4.17291000	1.30307000	2.53558600
C	-4.10616900	1.41215000	-0.30578800
H	-3.97842900	2.04193200	0.58826300
C	-5.61430400	1.12191500	-0.44279900
H	-5.79103700	0.52634900	-1.34752300
H	-5.97764400	0.52452200	0.40145600
C	-6.42479900	2.42772800	-0.54629000
H	-7.49150400	2.20001100	-0.66690900
H	-6.32990700	2.98553700	0.39665700
C	-5.93233800	3.30630100	-1.70579800
H	-6.48967600	4.25104300	-1.73093100
H	-6.14206800	2.79575100	-2.65675800
C	-4.42356300	3.57600300	-1.60307700
H	-4.22686900	4.19606600	-0.71608700
H	-4.08242600	4.15617900	-2.46971000
C	-3.61736400	2.27020700	-1.49428000
H	-2.54921900	2.48563700	-1.39385300

H	-3.72728900	1.70697200	-2.42890300
C	3.75863300	0.24968800	0.17096100
H	3.27947300	1.08458300	0.69788900
C	4.18572900	0.79068700	-1.21109000
H	4.68415200	-0.00691400	-1.77595100
H	3.30714900	1.08891600	-1.79275800
C	5.15502300	1.97674400	-1.06955000
H	4.63078200	2.81404200	-0.58900200
H	5.45804300	2.32583200	-2.06397400
C	6.38774200	1.59754600	-0.23712800
H	6.97269200	0.84160400	-0.78049800
H	7.04442200	2.46616400	-0.10833900
C	5.97904900	1.03264100	1.12959700
H	5.50171900	1.82664000	1.72137800
H	6.86464100	0.71491800	1.69322500
C	5.00221600	-0.15054300	0.99578200
H	4.71812300	-0.48974500	1.99665100
H	5.51818400	-0.98942100	0.51493300
C	2.27774400	-1.76651200	1.76567900
H	3.30159300	-2.08134900	2.01115800
C	1.83712800	-0.71810500	2.81099200
H	2.49564000	0.15840000	2.78520300
H	0.83021700	-0.36483300	2.55118600
C	1.82373900	-1.30612900	4.23211800
H	2.85120800	-1.56594500	4.52518600
H	1.48047700	-0.54530900	4.94360800
C	0.93957300	-2.55735500	4.31551800
H	0.98661300	-2.98968600	5.32224500
H	-0.10709100	-2.27080400	4.14640600
C	1.35453900	-3.59810700	3.26703100
H	0.67896200	-4.46121100	3.29918900
H	2.35619600	-3.97887300	3.51534900
C	1.37221200	-3.01507100	1.84301500
H	0.35910600	-2.75437600	1.51844100
H	1.72261400	-3.78474300	1.14849000
C	2.83644200	-2.44052500	-1.06727000
H	2.01323600	-3.13135100	-0.84972100
C	4.17373200	-3.14087700	-0.75671500
H	4.25840300	-3.37992800	0.30967100
H	5.00838300	-2.46961200	-0.99740800
C	4.32219100	-4.42762100	-1.58953200
H	5.28900400	-4.89928600	-1.37475400
H	3.54813800	-5.14439200	-1.28154400
C	4.18409800	-4.14556300	-3.09243100
H	5.03076700	-3.52573700	-3.42187200
H	4.24523600	-5.08174300	-3.66025200

C	2.86991000	-3.41549000	-3.40456800
H	2.02200500	-4.07902900	-3.18668700
H	2.81219900	-3.17565700	-4.47303800
C	2.71765300	-2.12765400	-2.57590800
H	3.49146600	-1.41329400	-2.88251800
H	1.74742400	-1.66589900	-2.78017500
F	-0.15092400	-2.05037900	-0.87376800
Ni	0.42774900	-0.32371000	-0.72087400
P	-2.91872600	-0.01445300	0.08020300
P	2.35388800	-1.00635500	0.04777000
O	-0.23202200	1.34820800	-2.03519700
C	0.48840300	1.45634400	-1.03143000
C	1.78273600	4.15980700	1.27348500
C	1.79003200	5.27325500	0.41534500
C	1.36613500	5.13401600	-0.91631000
C	0.93977100	3.89006900	-1.37295300
C	0.94994000	2.76692400	-0.53246700
C	1.37435400	2.92273300	0.79823200
H	2.09809400	4.29902700	2.30227500
H	1.35051500	2.06457900	1.46254700
H	0.59310800	3.77205800	-2.39491000
H	1.35947400	5.98229600	-1.59040400
O	2.22029500	6.43728900	0.96842000
C	2.23541500	7.60898400	0.16347000
H	2.60466200	8.40889200	0.80647200
H	2.90628800	7.49815800	-0.69744100
H	1.23025500	7.86566300	-0.19280400

IM3

B3LYP/BSI SCF energy: -1777.559055 a.u.
M06/BSII SCF energy in solution: -1776.998246 a.u.
M06/BSII free energy in solution: -1776.444338 a.u.

C	2.02261100	-0.37557600	1.66651000
H	1.71903100	0.45438400	2.31654100
C	1.38607700	-1.63969500	2.28767300
H	1.59547400	-2.51840700	1.66533200
H	0.30169800	-1.50822400	2.33166100
C	1.93790900	-1.88111400	3.70313400
H	1.60744000	-1.06174500	4.35628400
H	1.50498400	-2.80060800	4.11491700
C	3.47121100	-1.95912600	3.72024200
H	3.79734500	-2.84822000	3.16099000
H	3.83546400	-2.08736800	4.74663400
C	4.09882200	-0.70862900	3.08839000
H	3.87213700	0.16699800	3.71270500
H	5.19161100	-0.79860800	3.06091300

C	3.56263500	-0.46510900	1.66596800
H	4.01047900	0.44606100	1.25150200
H	3.88343100	-1.29435000	1.02248500
C	1.82765100	1.88379700	-0.26902600
H	2.91978800	1.83458300	-0.38710200
C	1.51669700	2.82940600	0.91345500
H	2.00986100	2.47933000	1.82596000
H	0.44007300	2.80837000	1.12279900
C	1.97130700	4.26950400	0.61830300
H	3.06844800	4.29670900	0.54746500
H	1.69878400	4.91576100	1.46098500
C	1.37054200	4.80797400	-0.68655500
H	1.74320400	5.81903900	-0.88941900
H	0.28004200	4.89154700	-0.57675300
C	1.68927700	3.87458300	-1.86146700
H	1.21770500	4.23878400	-2.78194100
H	2.77350300	3.87672500	-2.04461800
C	1.22220600	2.43725300	-1.57947500
H	0.12736600	2.42338300	-1.49550200
H	1.47307300	1.79266100	-2.42872500
C	1.84355000	-0.88015200	-1.40043700
H	1.13315800	-0.58761900	-2.18555900
C	3.27314600	-0.59992500	-1.91196500
H	3.42148500	0.46891100	-2.09697400
H	4.01136100	-0.89343000	-1.15577700
C	3.54256800	-1.38300700	-3.21051800
H	4.56925600	-1.19502800	-3.54759100
H	2.87884800	-1.00355600	-3.99979500
C	3.30499200	-2.88920800	-3.03124800
H	4.05144500	-3.29158700	-2.33104300
H	3.45778900	-3.41188600	-3.98300700
C	1.89731100	-3.17037500	-2.48635800
H	1.14596000	-2.87692700	-3.23107500
H	1.76494700	-4.24475000	-2.31024700
C	1.63076400	-2.39490000	-1.18626000
H	2.31144800	-2.75933600	-0.40589800
H	0.60984700	-2.58790700	-0.84146000
F	-0.95601800	0.61942600	2.05128400
Ni	-0.91257300	0.12622400	0.30908200
P	1.22834800	0.13276800	0.04723400
O	-1.15402200	-0.86069200	-2.37737000
C	-1.48538800	-0.38043000	-1.31161900
C	-5.06850800	-1.29634200	-0.34626000
C	-3.77121900	-1.36938300	-0.83866800
C	-5.54587300	-0.08076900	0.17718000
C	-2.92884200	-0.24373000	-0.83579500

C	-3.42127100	0.96680400	-0.30763800
C	-4.71595800	1.04873700	0.19078700
H	-2.79577800	1.85607000	-0.30936200
H	-5.10755400	1.97634600	0.59407300
H	-3.39985500	-2.30346000	-1.25046900
H	-5.70019300	-2.17629300	-0.37359500
O	-6.79472500	0.09883300	0.68125400
C	-7.68392800	-1.00917200	0.71285800
H	-7.28671100	-1.82763300	1.32582400
H	-8.60646900	-0.63909100	1.16192300
H	-7.89869700	-1.38387200	-0.29577400

TS3

B3LYP/BSI SCF energy: -1777.55348 a.u.
M06/BSII SCF energy in solution: -1776.993191 a.u.
M06/BSII free energy in solution: -1776.440968 a.u.

C	1.97816700	-0.45791200	1.63736800
H	1.47985400	0.21839700	2.34397700
C	1.49313100	-1.87787900	2.00702100
H	1.91111400	-2.61810200	1.31367700
H	0.40308300	-1.92789100	1.91712200
C	1.91702700	-2.23784500	3.44124500
H	1.39437100	-1.57428600	4.14370400
H	1.59401000	-3.25889800	3.67674700
C	3.43345900	-2.09799600	3.64059700
H	3.95138300	-2.84337900	3.01971900
H	3.70305800	-2.31803600	4.68036600
C	3.91995000	-0.69413900	3.25239100
H	3.49516600	0.04286300	3.94816700
H	5.01008600	-0.62536600	3.35136400
C	3.50323100	-0.32759700	1.81670900
H	3.83982300	0.68821500	1.57876200
H	4.01434200	-1.00133300	1.11661400
C	1.67143500	2.00444300	-0.02633300
H	2.76004400	2.10007000	-0.14544600
C	1.26550300	2.73884800	1.27229200
H	1.82975800	2.33893000	2.12161700
H	0.20940600	2.53848300	1.48379600
C	1.53270600	4.25066100	1.17159000
H	2.61663700	4.42756400	1.10788500
H	1.19231000	4.73963000	2.09201100
C	0.85147900	4.87922900	-0.05076500
H	1.09053900	5.94757800	-0.11467900
H	-0.23898300	4.80624800	0.06399400
C	1.27313300	4.16009800	-1.33850200
H	0.75222600	4.58350300	-2.20571300

H	2.34733300	4.32027200	-1.51086800
C	0.98974500	2.65168000	-1.25437300
H	-0.09453000	2.49382600	-1.17555500
H	1.31130300	2.16227800	-2.18128400
C	2.14539300	-0.55418400	-1.47746800
H	1.49089100	-0.21294200	-2.29316300
C	3.57176000	-0.05472600	-1.79351100
H	3.60481100	1.03904100	-1.82429300
H	4.26231100	-0.36782300	-1.00095000
C	4.06081200	-0.61456600	-3.14208000
H	5.08468700	-0.27137300	-3.33334200
H	3.43777300	-0.20036100	-3.94733700
C	3.99205700	-2.14742900	-3.18733500
H	4.71016400	-2.56289200	-2.46564900
H	4.29822800	-2.51126200	-4.17525300
C	2.58279200	-2.65147100	-2.84469100
H	1.87921800	-2.34275700	-3.62983000
H	2.56409600	-3.74751700	-2.82248400
C	2.09948000	-2.09770000	-1.49456400
H	2.74568800	-2.48971400	-0.69878800
H	1.08469600	-2.45245500	-1.28697700
F	-1.05457400	0.66595100	1.65686600
Ni	-0.93570000	-0.13115800	0.02818300
P	1.26888900	0.16932600	0.02214200
O	-1.43783300	-1.37327300	-2.51075000
C	-1.37867800	-0.87976200	-1.44471900
C	-4.80306400	-1.71056500	0.53446300
C	-3.44575400	-1.67705100	0.25046300
C	-5.62540700	-0.63418300	0.16087800
C	-2.87317100	-0.56874400	-0.39965600
C	-3.70636600	0.48970400	-0.78058000
C	-5.07381700	0.47066200	-0.50259000
H	-3.28994600	1.34853800	-1.30083800
H	-5.69211100	1.30827400	-0.80306500
H	-5.25678900	-2.55554400	1.04248300
H	-2.82256400	-2.51914200	0.54005600
O	-6.94294100	-0.76487900	0.47759900
C	-7.83064700	0.28716000	0.12938400
H	-7.86193500	0.44729700	-0.95589700
H	-8.81717900	-0.02589100	0.47433300
H	-7.55689000	1.22772500	0.62376500

IM4

B3LYP/BSI SCF energy: -1777.558657 a.u.
M06/BSII SCF energy in solution: -1776.995537 a.u.
M06/BSII free energy in solution: -1776.444407 a.u.

C	-1.81179000	-1.00127800	-1.45511700
H	-1.21277800	-0.57446100	-2.26883600
C	-1.31707100	-2.45639900	-1.29495400
H	-1.83769900	-2.94948400	-0.46490100
H	-0.24885700	-2.45744500	-1.05633000
C	-1.56646500	-3.25594400	-2.58553500
H	-0.94512900	-2.83720800	-3.38893600
H	-1.23997100	-4.29344600	-2.44636200
C	-3.04286300	-3.21315800	-3.00704300
H	-3.65042800	-3.73686100	-2.25470600
H	-3.18496500	-3.75237100	-3.95107500
C	-3.54390600	-1.76806200	-3.14110500
H	-3.02091500	-1.27723500	-3.97365100
H	-4.61173000	-1.75436700	-3.39092900
C	-3.30044600	-0.96325400	-1.85167100
H	-3.64534600	0.06849100	-1.98591000
H	-3.90655500	-1.39558600	-1.04490800
C	-1.67528700	1.86659800	-0.62186700
H	-2.76941400	1.96640000	-0.64496100
C	-1.14303400	2.17474100	-2.04035600
H	-1.60872000	1.50501400	-2.77098300
H	-0.06805300	1.96979300	-2.07938500
C	-1.43546600	3.63107800	-2.43979400
H	-2.52246400	3.77519200	-2.52823400
H	-1.01485400	3.82498100	-3.43350100
C	-0.87783300	4.63229600	-1.41950000
H	-1.13059800	5.65808400	-1.71310300
H	0.21905400	4.56793600	-1.41133500
C	-1.41185100	4.33346600	-0.01244900
H	-0.97333400	5.02069100	0.72085800
H	-2.49788400	4.50432600	0.00956300
C	-1.11737700	2.88282200	0.40160800
H	-0.03011800	2.74380300	0.47610700
H	-1.52818700	2.69464800	1.40090200
C	-2.35769800	-0.11944600	1.48533600
H	-1.81896500	0.49195900	2.22547200
C	-3.81368500	0.39586200	1.45370900
H	-3.85005000	1.44044100	1.12750400
H	-4.39887400	-0.18069100	0.72716400
C	-4.46785500	0.27277200	2.84279100
H	-5.50773200	0.61684100	2.79113200
H	-3.95168200	0.94592500	3.54187700
C	-4.40497300	-1.16283800	3.38354000
H	-5.02607600	-1.81457700	2.75249000
H	-4.83285600	-1.20666000	4.39189000
C	-2.96417200	-1.69242200	3.39046800

H	-2.36651700	-1.12261200	4.11547600
H	-2.94256500	-2.73733200	3.72155600
C	-2.31655000	-1.57511900	2.00131000
H	-2.85957300	-2.22289000	1.30176400
H	-1.28611300	-1.94603600	2.03756300
F	1.07039400	0.00875400	-1.56809100
Ni	1.00141500	-0.07794500	0.22895100
P	-1.28887700	0.11743200	-0.04956300
O	1.11106200	-0.37215700	3.09046500
C	1.07022200	-0.24863200	1.94643300
C	5.00713900	-1.22943700	-0.30278800
C	3.60915500	-1.19954400	-0.23637100
C	5.74978600	-0.18164800	0.25427600
C	2.93249200	-0.14136000	0.37647000
C	3.69360700	0.89018000	0.94766900
C	5.08518600	0.88170700	0.87819000
H	3.20598100	1.72348200	1.44908900
H	5.67740400	1.68429700	1.30744700
H	3.05106300	-2.00966400	-0.69807200
H	5.49752900	-2.06202100	-0.79464900
O	7.11755800	-0.10561600	0.24620600
C	7.84059400	-1.15802000	-0.36609700
H	7.59743400	-1.25398900	-1.43272100
H	8.89647400	-0.90097500	-0.26247900
H	7.65591400	-2.12176800	0.12745200

IM5

B3LYP/BSI SCF energy: -1664.216566 a.u.
M06/BSII SCF energy in solution: -1663.674845 a.u.
M06/BSII free energy in solution: -1663.126772 a.u.

Ni	-0.29065200	0.73849800	-1.64684300
P	0.92721100	0.05697400	-0.01266700
F	1.08673300	1.11344800	-2.73256000
C	-2.00276900	0.53151000	-0.93476800
C	-2.62831700	1.47147700	-0.08466200
H	-2.03915200	2.26187300	0.37649200
C	-3.99439400	1.43670300	0.17842400
H	-4.46767900	2.17222000	0.82260200
C	-4.79688200	0.43987600	-0.39648400
C	-4.21217800	-0.51862100	-1.23083200
H	-4.80780500	-1.30256500	-1.68567100
C	-2.83327800	-0.46695900	-1.47794500
H	-2.40776200	-1.23486800	-2.12312500
C	0.03645800	-0.65280500	1.48192700
H	-0.77923400	0.06965700	1.61757400
C	0.83753700	-0.71838900	2.80191800

H	1.67593700	-1.41787700	2.69816300
H	1.26924800	0.25661600	3.04835200
C	-0.06228100	-1.17695900	3.96473900
H	0.53304500	-1.24392600	4.88326600
H	-0.82962100	-0.41113600	4.14522600
C	-0.74651800	-2.51841300	3.66894900
H	0.01559200	-3.30887000	3.60954300
H	-1.41504400	-2.79219500	4.49368600
C	-1.52262700	-2.46263200	2.34611000
H	-1.96115600	-3.44135700	2.11805300
H	-2.36031800	-1.75848100	2.44058000
C	-0.62306000	-2.01662200	1.18162000
H	-1.20931700	-1.95528400	0.26033800
H	0.15638300	-2.77355000	1.02652400
C	1.93901300	1.49535800	0.65253600
H	2.49768500	1.11062600	1.51712400
C	1.00055600	2.62173300	1.14470100
H	0.38591300	2.95914500	0.29943700
H	0.30760500	2.24702400	1.90712200
C	1.78773100	3.81883700	1.70270200
H	1.08784600	4.60207600	2.01725600
H	2.33517700	3.50800500	2.60434300
C	2.77930300	4.36359900	0.66759400
H	2.22236700	4.76599000	-0.18988000
H	3.35299900	5.19701700	1.09010200
C	3.72338400	3.25516500	0.18469100
H	4.35832700	2.93437000	1.02376100
H	4.40059600	3.63868300	-0.58743900
C	2.95822200	2.04152000	-0.37232900
H	3.68162200	1.26303800	-0.63704000
H	2.43627100	2.30227600	-1.29952300
C	2.17876400	-1.13702000	-0.73287000
H	2.71390700	-0.46613000	-1.41649900
C	3.19053300	-1.74411500	0.25998300
H	3.65484600	-0.96361500	0.87378700
H	2.67189000	-2.42273800	0.94961700
C	4.27992400	-2.53573000	-0.48623700
H	4.87181200	-1.84135600	-1.09848800
H	4.97193400	-2.98388600	0.23691500
C	3.67135400	-3.61756300	-1.38985300
H	3.17766300	-4.37490100	-0.76389800
H	4.46250400	-4.13820100	-1.94220800
C	2.64617100	-3.01858300	-2.36387300
H	3.15882500	-2.34672300	-3.06570700
H	2.18705500	-3.80986000	-2.96819800
C	1.55004100	-2.22849400	-1.62788100

H	0.95102200	-2.92108600	-1.02423200
H	0.87590200	-1.76131200	-2.35305200
O	-6.12644400	0.48906300	-0.07524800
C	-6.98732200	-0.48036400	-0.64628000
H	-6.71685700	-1.49910100	-0.33760100
H	-7.98906700	-0.25054900	-0.27877600
H	-6.98609300	-0.43018600	-1.74316400

IM6

B3LYP/BSI SCF energy: -2711.459034 a.u.
M06/BSII SCF energy in solution: -2710.531638 a.u.
M06/BSII free energy in solution: -2709.520968 a.u.

Ni	-0.00294600	-0.22670400	0.02832600
P	-2.26021500	-0.41205100	0.29812400
P	2.24790100	-0.47520900	-0.25238200
F	-0.00112300	-2.07829600	0.23482000
C	0.00460000	1.67162600	-0.15205700
C	-0.02267100	2.52142100	0.96825400
H	-0.05431900	2.09398700	1.96903600
C	-0.01147600	3.92229100	0.87170800
H	-0.03011900	4.51817700	1.77827400
C	0.02246900	4.52741700	-0.38802300
C	0.04650200	3.71591700	-1.52985800
H	0.07158000	4.19472800	-2.50504200
C	0.04026300	2.32619000	-1.40399300
H	0.06318400	1.73812000	-2.31971600
C	-3.32676200	1.11989600	0.02614300
H	-2.70468300	1.90200400	0.48267700
C	-4.71539300	1.18093400	0.70108700
H	-5.37739500	0.41617200	0.27514200
H	-4.64218000	0.96955100	1.77261700
C	-5.35386000	2.56983500	0.50928100
H	-6.34823800	2.58572200	0.97234500
H	-4.74832600	3.31499900	1.04439000
C	-5.44599500	2.96586100	-0.97117000
H	-6.15320600	2.29536500	-1.48080200
H	-5.85405000	3.97927900	-1.06746800
C	-4.07659000	2.87024200	-1.65793300
H	-4.17127500	3.09331900	-2.72772900
H	-3.39677100	3.62496400	-1.24052400
C	-3.45206100	1.47871900	-1.47107200
H	-2.47108800	1.44572200	-1.95298800
H	-4.08710500	0.73708800	-1.97275000
C	-2.68579800	-0.95103000	2.05588700
H	-3.78118200	-0.93475500	2.13818200
C	-2.11357500	0.06442700	3.07027000

H	-1.02113700	0.08750400	2.96007300
H	-2.46838100	1.07784600	2.85035200
C	-2.46701700	-0.30846700	4.51875700
H	-2.02062200	0.41922500	5.20754300
H	-3.55589600	-0.24101400	4.65700100
C	-1.99926200	-1.72974600	4.85912400
H	-0.90085600	-1.76448100	4.83087800
H	-2.29532700	-1.99580300	5.88115100
C	-2.56241800	-2.74542200	3.85617400
H	-3.65592000	-2.79002200	3.96790900
H	-2.18691000	-3.75122900	4.08027800
C	-2.21354000	-2.38051800	2.40291600
H	-2.68328200	-3.10799800	1.73287300
H	-1.13589400	-2.45971900	2.22743900
C	-2.86211500	-1.83607300	-0.76855700
H	-2.29650300	-2.66193800	-0.32143500
C	-4.36556500	-2.16903700	-0.70589100
H	-4.70324200	-2.25973600	0.33293600
H	-4.94505100	-1.35101800	-1.15345100
C	-4.67377500	-3.47221100	-1.46572600
H	-4.18473300	-4.31069400	-0.95009800
H	-5.75165600	-3.67405400	-1.43761700
C	-4.17762500	-3.41397600	-2.91799100
H	-4.75354600	-2.65405300	-3.46590700
H	-4.36566500	-4.36985700	-3.42174100
C	-2.68457900	-3.05937300	-2.98219900
H	-2.09784600	-3.87411100	-2.53525300
H	-2.35898500	-2.97537700	-4.02654600
C	-2.37794200	-1.75175000	-2.23277800
H	-2.86747400	-0.92051200	-2.75338900
H	-1.30196400	-1.55269900	-2.24870400
C	3.33470800	1.06837300	-0.32100800
H	2.71278000	1.74717400	-0.92024900
C	3.50097700	1.73514700	1.06318400
H	2.52820000	1.83825700	1.55242100
H	4.12521000	1.09939200	1.70435900
C	4.16996100	3.11450300	0.93900200
H	4.29420200	3.55532700	1.93585700
H	3.50304400	3.78498000	0.38056800
C	5.52527900	3.02062700	0.22487700
H	5.96462800	4.01809600	0.10311100
H	6.22429300	2.44556000	0.84951800
C	5.38398700	2.33160200	-1.13871000
H	6.36573400	2.22036200	-1.61536200
H	4.78393000	2.96829000	-1.80403200
C	4.70626300	0.95383300	-1.02217700

H	5.36129300	0.27579200	-0.46060900
H	4.60128900	0.52890800	-2.02482800
C	2.61453400	-1.34733800	-1.88662300
H	3.70775400	-1.37091900	-1.99278000
C	2.03684500	-0.53121600	-3.06487500
H	0.94723400	-0.46749000	-2.94393700
H	2.41067400	0.49887300	-3.04818200
C	2.35679700	-1.17803200	-4.42216600
H	1.90776500	-0.58601700	-5.22901100
H	3.44370000	-1.15660000	-4.58789400
C	1.86280600	-2.62937600	-4.47994800
H	0.76449600	-2.63873800	-4.43308800
H	2.13916400	-3.08949600	-5.43642100
C	2.42592700	-3.44721900	-3.30987200
H	3.51608400	-3.53583300	-3.42721100
H	2.02827800	-4.46909300	-3.33304900
C	2.11062800	-2.80567300	-1.94706500
H	2.57780300	-3.40255500	-1.15708500
H	1.03481700	-2.82845200	-1.74635400
C	2.87889200	-1.67360000	1.04731100
H	2.29034700	-2.56213500	0.78998200
C	2.44874000	-1.29777100	2.48253400
H	2.96145000	-0.38602500	2.81130500
H	1.37460300	-1.08784400	2.49609100
C	2.77556600	-2.43716000	3.46325000
H	2.49298200	-2.14427100	4.48206800
H	2.16423200	-3.31392500	3.20791600
C	4.26169000	-2.82264700	3.41398200
H	4.86623400	-1.97924900	3.77823500
H	4.46101500	-3.66319100	4.08966400
C	4.69907800	-3.17377900	1.98456500
H	4.18027700	-4.08702600	1.66068500
H	5.77267000	-3.39747500	1.95700500
C	4.37618100	-2.03602000	0.99874700
H	4.67717400	-2.32856500	-0.01382100
H	4.97992500	-1.15815400	1.26371000
O	0.03399000	5.88298500	-0.61031800
C	0.01389400	6.73641000	0.51754600
H	0.89130600	6.58498500	1.16138000
H	0.02874200	7.75670800	0.12914300
H	-0.89329200	6.59605100	1.12142300

TS4

B3LYP/BSI SCF energy: -2600.14303 a.u.
M06/BSII SCF energy in solution: -2599.268854 a.u.
M06/BSII free energy in solution: -2598.371287 a.u.

Ni	-0.14458900	-0.45332500	-0.10318300
P	2.15104200	-0.69554600	-0.02958400
F	-0.51560500	-1.82483500	1.35651800
C	3.21331600	0.65761000	-0.79603800
H	2.65322800	0.87325300	-1.71636300
C	4.65641300	0.28904300	-1.20652400
H	5.25510600	0.06407800	-0.31565300
H	4.67067600	-0.61097100	-1.82879700
C	5.31713600	1.44801100	-1.97554900
H	6.34656300	1.17612300	-2.23906800
H	4.78180600	1.59969000	-2.92345600
C	5.29819400	2.75354100	-1.16826900
H	5.93618900	2.63744700	-0.28010100
H	5.73120700	3.57091800	-1.75736900
C	3.87343300	3.11102400	-0.72246900
H	3.88347700	4.01064500	-0.09542900
H	3.26063700	3.35107700	-1.60205400
C	3.21249200	1.95393200	0.04491000
H	2.19160500	2.23070900	0.32492500
H	3.76754100	1.78512700	0.97676800
C	2.58476500	-2.24427600	-1.01211100
H	3.67094300	-2.39466200	-0.92932000
C	2.22423800	-2.05970700	-2.50485100
H	1.15200800	-1.84901700	-2.59109800
H	2.73575300	-1.18815400	-2.92560000
C	2.57706100	-3.31055500	-3.32646600
H	2.28642000	-3.15420600	-4.37216000
H	3.66766700	-3.45505800	-3.32386600
C	1.89878400	-4.56676800	-2.76434100
H	0.81006600	-4.46905100	-2.87519800
H	2.19658100	-5.45265000	-3.33837600
C	2.23872600	-4.75414500	-1.27997200
H	3.31305800	-4.96615400	-1.17733500
H	1.70894800	-5.62299800	-0.87148800
C	1.88649600	-3.50508400	-0.45328500
H	2.16579900	-3.67580000	0.59208800
H	0.79973700	-3.35547800	-0.46849400
C	2.70793800	-1.07963200	1.72587400
H	2.18231000	-2.02567800	1.91646500
C	4.21438100	-1.32926300	1.94115400
H	4.59508500	-2.06345700	1.22196500
H	4.76706100	-0.39800000	1.76327100
C	4.49812000	-1.80801600	3.37614900
H	4.03339600	-2.79299500	3.52540600
H	5.57718400	-1.94892800	3.51344800
C	3.94839800	-0.82413500	4.41886700

H	4.50033800	0.12415600	4.34601800
H	4.12210900	-1.20817000	5.43124700
C	2.45275900	-0.55620200	4.19691800
H	1.88636500	-1.47934100	4.38528400
H	2.08773700	0.18528200	4.91783700
C	2.16188900	-0.07317800	2.76557800
H	2.62975900	0.90769900	2.61885900
H	1.08463600	0.06559600	2.63264700
C	-2.70867400	-0.09682100	3.26963000
C	-3.74768900	-0.99001600	2.47898000
C	-3.71831200	-0.29620600	-2.32716200
C	-3.29456300	-1.81883100	-2.37152200
C	-4.77405600	-0.16771900	1.69161900
H	-4.28943800	0.54349000	1.02122900
H	-5.37681200	-0.84615600	1.08129900
H	-5.45121500	0.36796900	2.36402800
C	-4.47010100	-2.03575700	3.33116100
H	-5.07618000	-1.55694400	4.10802400
H	-5.13953300	-2.62278100	2.69586000
H	-3.77082000	-2.72520300	3.80721400
C	-2.09178000	-0.81238200	4.48117600
H	-1.25944100	-0.21183700	4.85899700
H	-2.81643500	-0.94205100	5.29118700
H	-1.70059700	-1.79532700	4.20493700
C	-3.22093100	1.28136500	3.68384700
H	-2.42130900	1.83141200	4.18934000
H	-3.54085400	1.86551300	2.81936000
H	-4.06199600	1.19508200	4.38017300
C	-2.98738900	-2.35854500	-3.76787400
H	-2.18783500	-1.79354000	-4.24965200
H	-2.66761700	-3.40206200	-3.69244100
H	-3.87716100	-2.32376200	-4.40607200
C	-4.26458200	-2.75874400	-1.64501100
H	-5.22477300	-2.83168900	-2.16559600
H	-3.82029100	-3.75737700	-1.60331700
H	-4.43284300	-2.43111400	-0.61732900
C	-5.21713600	-0.04758100	-2.16467400
H	-5.39973900	1.02710100	-2.07301300
H	-5.76659600	-0.40968200	-3.04044400
H	-5.61980300	-0.53667600	-1.27704900
C	-3.18176600	0.52933100	-3.50482000
H	-3.66830600	0.24961600	-4.44464200
H	-3.38856700	1.58657800	-3.31469400
H	-2.10114200	0.41536700	-3.61429400
O	-2.90255800	-1.70490700	1.53653700
O	-1.64656600	0.08389000	2.29682200

O	-2.05707500	-1.82405900	-1.60172200
O	-3.03388600	0.19207800	-1.13222100
B	-1.69982700	-1.00743600	1.41580000
B	-2.00210100	-0.67387200	-0.83921200
O	0.18997000	0.67105400	-2.52260900
C	-0.12724200	0.91295100	-1.35946300
C	-0.31663100	4.69979400	-1.50160600
C	-0.12603600	3.36414400	-1.84794000
C	-0.77258100	5.01757800	-0.21306700
C	-0.37689800	2.33054000	-0.93404900
C	-0.83482300	2.66368300	0.35244500
C	-1.03054600	3.99075300	0.70927700
H	-1.05127100	1.87609400	1.06755400
H	-1.38921500	4.26279100	1.69692600
H	0.22146000	3.09751400	-2.84116800
H	-0.11306900	5.47666300	-2.22940700
O	-0.99553300	6.28474700	0.23589500
C	-0.77066500	7.36720300	-0.65392600
H	-1.01807200	8.27176400	-0.09612000
H	0.27767500	7.41750000	-0.97500300
H	-1.41388600	7.30297300	-1.54078700

IM7

B3LYP/BSI SCF energy: -2088.955146 a.u.
M06/BSII SCF energy in solution: -2088.232652 a.u.
M06/BSII free energy in solution: -2087.514855 a.u.

Ni	0.39539300	-0.68701800	0.03833800
P	-1.86276100	-0.26732400	0.10848900
C	-2.30786100	1.52745600	-0.25387600
H	-1.60644800	2.05468000	0.40944900
C	-3.72939200	2.01736600	0.09707800
H	-4.46608900	1.52485700	-0.54776300
H	-3.99167300	1.75591600	1.12727500
C	-3.84172600	3.54149100	-0.09011300
H	-4.86258200	3.86849200	0.14192700
H	-3.18187100	4.04221700	0.63242900
C	-3.45382100	3.96850300	-1.51273300
H	-4.18911600	3.56344000	-2.22309100
H	-3.49915800	5.05997000	-1.60766100
C	-2.05465400	3.45857100	-1.88817600
H	-1.81989300	3.71955500	-2.92706700
H	-1.30097100	3.95767800	-1.26400100
C	-1.93309400	1.93743600	-1.69513100
H	-0.91337000	1.61087400	-1.92663700
H	-2.60153200	1.43444700	-2.40670100
C	-2.60085100	-0.61411300	1.80454100

H	-3.69009000	-0.47424800	1.74431200
C	-2.03119500	0.36622200	2.85793100
H	-0.93860400	0.27188700	2.87784700
H	-2.25544800	1.40374600	2.58634500
C	-2.59141000	0.07639100	4.26097800
H	-2.14911100	0.77458600	4.98145300
H	-3.67548100	0.26302400	4.26888500
C	-2.32194000	-1.37260100	4.68664000
H	-1.23871500	-1.52203200	4.78989600
H	-2.76379900	-1.57070500	5.67067800
C	-2.87143500	-2.35920400	3.64809200
H	-3.96907000	-2.29282200	3.62798600
H	-2.62684500	-3.38990700	3.93141100
C	-2.31976600	-2.07046500	2.24135500
H	-2.75702600	-2.78282200	1.53282900
H	-1.23465500	-2.24058500	2.23222500
C	-2.78810800	-1.43286900	-1.04922100
H	-2.72025000	-2.38652400	-0.50611600
C	-4.28222300	-1.15801000	-1.30969400
H	-4.82634100	-1.03794200	-0.36595800
H	-4.38831900	-0.21405600	-1.85850700
C	-4.91710100	-2.28592100	-2.14328800
H	-4.90535700	-3.21722100	-1.55941100
H	-5.97122500	-2.05437400	-2.33819600
C	-4.16397500	-2.50272800	-3.46376700
H	-4.27859200	-1.60991200	-4.09512800
H	-4.60699400	-3.33652200	-4.02111800
C	-2.67009900	-2.76025300	-3.21831600
H	-2.54979900	-3.71667700	-2.68999200
H	-2.13794000	-2.86183800	-4.17152200
C	-2.02850700	-1.64156700	-2.38015500
H	-2.02612200	-0.70994400	-2.95987900
H	-0.97682500	-1.88190200	-2.17861600
C	4.33348300	-2.13300500	-0.58343000
C	3.47691400	-3.41929400	-0.28418100
C	4.06107100	-4.36264200	0.76598800
H	4.20101100	-3.85801900	1.72322500
H	3.37727600	-5.20173800	0.92487200
H	5.02455200	-4.76868300	0.43808700
C	3.09473700	-4.20824000	-1.54478100
H	3.95442700	-4.73122300	-1.97583400
H	2.33893500	-4.95255300	-1.27812300
H	2.66792600	-3.55146000	-2.30797100
C	5.22024100	-2.21367400	-1.82476800
H	5.74340200	-1.26289800	-1.96267700
H	5.97413300	-3.00163200	-1.71861600

H	4.63666300	-2.40917500	-2.72630600
C	5.15542000	-1.65390700	0.62184400
H	5.99145400	-2.32714500	0.83672400
H	5.56014800	-0.66236500	0.40073000
H	4.53244100	-1.57037000	1.51643200
O	2.24529400	-2.85120300	0.24560200
O	3.30715200	-1.12546200	-0.81353600
B	2.14122900	-1.53845600	-0.19210300
O	1.50941900	0.07801800	2.32513900
C	1.44138300	0.31792800	1.12319300
C	2.65287900	3.91417200	1.00266300
C	2.23768600	2.66484700	1.46080600
C	2.77310700	4.13656800	-0.37703600
C	1.93270800	1.62776400	0.56967300
C	2.06144100	1.86511700	-0.80844700
C	2.47668600	3.10224300	-1.27999400
H	1.85329800	1.05664300	-1.50266800
H	2.59219100	3.29475800	-2.34184200
H	2.14617900	2.47055700	2.52500900
H	2.88056800	4.69762600	1.71626400
O	3.17072000	5.31424700	-0.93797800
C	3.51152200	6.38946300	-0.07715000
H	3.80904100	7.21369100	-0.72737600
H	2.65758600	6.70458400	0.53637600
H	4.34894400	6.12965600	0.58287600

TS5

B3LYP/BSI SCF energy: -2088.926214 a.u.
M06/BSII SCF energy in solution: -2088.201025 a.u.
M06/BSII free energy in solution: -2087.479929 a.u.

Ni	-0.44636000	0.06923100	-0.23476300
P	1.73196200	0.04282600	-0.07083600
C	2.72884000	1.51331700	-0.69603600
H	2.24322500	1.69191900	-1.66524800
C	4.23652700	1.31123300	-0.96357900
H	4.76709600	1.11418700	-0.02412100
H	4.40561500	0.44300900	-1.60793900
C	4.84451600	2.55783100	-1.63339600
H	5.91936200	2.40460200	-1.78897700
H	4.39860600	2.67994700	-2.63035000
C	4.59846500	3.82986400	-0.81076000
H	5.14502000	3.75784800	0.14088800
H	5.00108600	4.70470600	-1.33501200
C	3.10328900	4.02210000	-0.52126300
H	2.94695700	4.90283400	0.11322400
H	2.56920800	4.21381300	-1.46191800

C	2.49679200	2.78105100	0.15402800
H	1.42510100	2.93612500	0.32153300
H	2.95920000	2.65384700	1.14198400
C	2.41026400	-1.41295500	-1.05498900
H	3.50578900	-1.36382700	-0.98028100
C	2.01549600	-1.27202200	-2.54369900
H	0.92089400	-1.25075900	-2.61739000
H	2.36564200	-0.31826800	-2.95270400
C	2.56312500	-2.43370300	-3.38848000
H	2.23737700	-2.31407700	-4.42864200
H	3.66226800	-2.39303200	-3.39907700
C	2.11252300	-3.79225000	-2.83603200
H	1.02073100	-3.87598300	-2.92970300
H	2.54261700	-4.60850900	-3.42896900
C	2.50596600	-3.93871400	-1.36064900
H	3.60285300	-3.96724200	-1.28182900
H	2.14109300	-4.89171100	-0.95921300
C	1.96184100	-2.78366200	-0.50149100
H	2.31351000	-2.91659900	0.52750500
H	0.86765400	-2.82835800	-0.46337000
C	2.12977300	-0.35658800	1.72166200
H	1.69230800	-1.35932300	1.81958500
C	3.62407700	-0.45703900	2.09096400
H	4.15392700	-1.11502600	1.39284900
H	4.09210700	0.53240600	2.00909300
C	3.80114900	-0.96975300	3.53135600
H	3.42842500	-2.00173300	3.59482200
H	4.86807700	-1.00715200	3.78250700
C	3.04372800	-0.09254700	4.53843900
H	3.49701800	0.90921000	4.55657800
H	3.14938800	-0.49970600	5.55098600
C	1.55886100	0.02947500	4.16581300
H	1.07774700	-0.95366500	4.26328300
H	1.04386500	0.69894000	4.86511700
C	1.36935400	0.53727100	2.72618200
H	1.72671000	1.57231400	2.65873000
H	0.30309200	0.54613800	2.47177300
C	-2.65200800	-3.51370200	0.87885600
C	-3.55834900	-2.93739700	-0.26751800
C	-5.05016200	-2.85527300	0.05680000
H	-5.23706500	-2.23267300	0.93356700
H	-5.58404900	-2.41154300	-0.78893800
H	-5.47141100	-3.85088200	0.23735900
C	-3.35797400	-3.64476100	-1.61693200
H	-3.78187900	-4.65448400	-1.61819100
H	-3.85501700	-3.06166700	-2.39747300

H	-2.29667800	-3.71084700	-1.87186700
C	-2.28660400	-4.99185200	0.74494300
H	-1.62298600	-5.28146800	1.56554900
H	-3.17900800	-5.62603500	0.79378800
H	-1.76722800	-5.19453600	-0.19348900
C	-3.20262400	-3.23955200	2.28663500
H	-4.08944000	-3.84377400	2.50473200
H	-2.43081600	-3.48522700	3.02195200
H	-3.46016000	-2.18402300	2.40818400
O	-3.04339200	-1.58787400	-0.41854200
O	-1.43978000	-2.72302900	0.73873000
B	-1.74033800	-1.52749400	0.07440800
O	-0.03375700	1.66477600	-2.43881800
C	-0.48556600	1.49813000	-1.32307700
C	-3.79941900	3.35359400	-1.15465000
C	-2.69919100	2.64293600	-1.62654100
C	-3.87683700	3.68761900	0.20643600
C	-1.66545200	2.25516000	-0.76238200
C	-1.75494700	2.59686300	0.59897200
C	-2.84286600	3.31023800	1.07889800
H	-0.95664100	2.31149700	1.27804900
H	-2.91983700	3.58986200	2.12434300
H	-2.62688800	2.38578500	-2.67847600
H	-4.58314900	3.64188200	-1.84508000
O	-4.90126400	4.37940000	0.77371000
C	-5.99128200	4.77306300	-0.04780400
H	-6.69065500	5.29080600	0.61011200
H	-5.67132600	5.45707500	-0.84395400
H	-6.49129100	3.90594300	-0.49687300

IM8

B3LYP/BSI SCF energy: -2600.145284 a.u.
M06/BSII SCF energy in solution: -2599.266367 a.u.
M06/BSII free energy in solution: -2598.367871 a.u.

C	-1.85535800	1.00123200	1.70795000
H	-2.17909100	1.79746600	1.02163700
C	-0.47024400	1.43186100	2.23918100
H	-0.11175000	0.70541200	2.97599700
H	0.27015700	1.44653700	1.43721100
C	-0.56195200	2.81034300	2.91447600
H	-0.83728400	3.56328700	2.16342600
H	0.42418300	3.10096100	3.29659500
C	-1.59295700	2.81197800	4.05325700
H	-1.23797100	2.15536900	4.86065800
H	-1.68454400	3.81513300	4.48648900
C	-2.96432200	2.31712500	3.57069300

H	-3.38609700	3.04673400	2.86492000
H	-3.66602400	2.25581900	4.41136100
C	-2.86808000	0.94747300	2.87265100
H	-3.86146900	0.64031400	2.52906800
H	-2.54174200	0.19540600	3.60229400
C	-3.62523600	-0.61071700	-0.03467100
H	-4.18174900	-0.99110900	0.83162800
C	-4.29050900	0.72342700	-0.44269000
H	-4.25518600	1.44371800	0.38110000
H	-3.74849200	1.16261300	-1.28416100
C	-5.75926800	0.49750600	-0.84577200
H	-6.32888300	0.15019600	0.02892000
H	-6.20460800	1.45329400	-1.14700500
C	-5.88867300	-0.53211000	-1.97617500
H	-6.94472400	-0.69956200	-2.21985400
H	-5.41400100	-0.13366400	-2.88299900
C	-5.21407800	-1.85554200	-1.59249700
H	-5.25957200	-2.56490000	-2.42746300
H	-5.76616400	-2.31720600	-0.76066000
C	-3.74846000	-1.64374800	-1.17686700
H	-3.17128300	-1.28058600	-2.03520300
H	-3.31068300	-2.60335400	-0.87899800
C	-1.55186600	-2.07719800	1.52259600
H	-1.30289100	-2.78865000	0.72532100
C	-2.75657300	-2.65614200	2.29666600
H	-3.61679000	-2.79442900	1.63490500
H	-3.07193000	-1.95747500	3.08158300
C	-2.40546000	-4.01274800	2.93615500
H	-3.26890800	-4.38385100	3.50136000
H	-2.21841100	-4.74517100	2.13793400
C	-1.16841900	-3.92451300	3.83850500
H	-1.39367800	-3.28025700	4.70073600
H	-0.92293000	-4.91316000	4.24410200
C	0.02751800	-3.34612900	3.07159700
H	0.33164400	-4.04979000	2.28536800
H	0.89182700	-3.23337200	3.73701300
C	-0.31139000	-1.98637000	2.43882900
H	-0.51338900	-1.27597000	3.24940800
H	0.54833900	-1.60492200	1.87991500
Ni	-0.25343200	-0.30225900	-1.02194500
P	-1.83256200	-0.47800600	0.54137700
F	1.40455800	-0.00304500	-1.99757000
B	2.15133200	-1.26749300	-1.37701800
O	0.91760700	-2.01544000	-0.92459100
O	2.73856800	-2.04119600	-2.39933800
C	0.86250300	-3.26098800	-1.69311500

C	1.77430600	-2.94833400	-2.94092300
C	-0.57921900	-3.61264000	-2.04958500
C	1.46277900	-4.34565600	-0.78839700
C	1.01750800	-2.27110100	-4.09977000
C	2.52936200	-4.16573400	-3.48637500
H	-0.60065800	-4.48649300	-2.70989000
H	-1.08546800	-2.78890400	-2.55620200
H	-1.14901400	-3.86973300	-1.15137600
H	1.43302200	-5.33118100	-1.26312400
H	0.88791200	-4.39895000	0.14034100
H	2.49949600	-4.10829100	-0.53735200
H	0.35262700	-2.97272600	-4.61506200
H	1.75386500	-1.90582400	-4.82114100
H	0.43470600	-1.41233900	-3.76266400
H	1.84040300	-4.94955500	-3.82086700
H	3.20658600	-4.58402800	-2.73976200
H	3.13167800	-3.85767100	-4.34601700
B	3.19379300	-0.63747200	-0.16346500
O	4.50656100	-1.01874900	0.01476500
O	2.82662200	0.33357700	0.76496000
C	5.13771900	-0.10530200	0.94744200
C	3.90308800	0.47983000	1.73278600
C	6.13795100	-0.89047200	1.79562100
C	5.87694100	0.94378300	0.10412400
C	3.51518800	-0.35482000	2.96110700
C	4.01722400	1.95386700	2.11954300
H	6.60410600	-0.24786600	2.55046400
H	5.66475300	-1.73480100	2.30017900
H	6.92933900	-1.28539300	1.15210800
H	6.44419700	1.64237100	0.72735700
H	6.57455900	0.42979800	-0.56253500
H	5.18010200	1.51346400	-0.51669800
H	4.25231700	-0.26156300	3.76468100
H	2.55014800	-0.00511600	3.33899100
H	3.41501100	-1.41248200	2.70212500
H	4.85753700	2.11553600	2.80347600
H	4.15708300	2.59040800	1.24383900
H	3.10303000	2.27458300	2.62851200
O	-1.87982200	1.01656500	-2.59655400
C	-0.99159000	1.22663100	-1.77800400
C	-0.70660100	5.00021500	-1.89417000
C	-1.15705500	3.69614800	-2.07813300
C	0.48788600	5.22213200	-1.19090200
C	-0.45019300	2.60024300	-1.56004800
C	0.74813200	2.83682800	-0.86133000
C	1.21256200	4.13160300	-0.68195200

H	1.33201000	2.00275600	-0.48654900
H	2.14088200	4.32938100	-0.15605600
H	-2.07002200	3.50613900	-2.63387300
H	-1.27843000	5.82679400	-2.29945400
O	1.02437300	6.44938100	-0.95217400
C	0.35915000	7.59288700	-1.46901200
H	0.96422200	8.45126000	-1.17365200
H	0.28942700	7.55904300	-2.56340600
H	-0.64858600	7.69992600	-1.04794400

IM9

B3LYP/BSI SCF energy: -2088.938025 a.u.
M06/BSII SCF energy in solution: -2088.220526 a.u.
M06/BSII free energy in solution: -2087.497579 a.u.

Ni	-0.31742400	0.84865700	0.32853800
P	1.64036400	0.07842700	-0.13018000
C	3.01361300	1.30630100	0.27551000
H	2.58579700	2.23469500	-0.12630000
C	4.39932800	1.10467400	-0.37558100
H	4.87590200	0.19682400	0.01382800
H	4.31219600	0.97306300	-1.45903000
C	5.31293400	2.31284400	-0.09252300
H	6.30107600	2.13938100	-0.53650600
H	4.89631700	3.19890600	-0.59129400
C	5.44375600	2.59470900	1.41072700
H	5.97540300	1.75971800	1.89026200
H	6.05635100	3.48916500	1.57628000
C	4.06592900	2.76002000	2.06749600
H	4.17497700	2.90572600	3.14925100
H	3.57333900	3.65885600	1.67430100
C	3.16588200	1.54401300	1.79321900
H	2.18210600	1.69573400	2.25032500
H	3.61098300	0.65959000	2.26792800
C	1.85691100	-0.21757400	-1.97610900
H	2.91695500	-0.46315500	-2.12794000
C	1.54082500	1.07003200	-2.77088500
H	0.49249600	1.34276100	-2.59020000
H	2.14426700	1.91063100	-2.41272000
C	1.76622000	0.87266500	-4.27906200
H	1.50454500	1.79359200	-4.81389100
H	2.83552600	0.69707100	-4.46650300
C	0.95508300	-0.31178200	-4.82152500
H	-0.11654500	-0.08069700	-4.74341300
H	1.16690500	-0.46425500	-5.88675400
C	1.25266000	-1.59193100	-4.02878200
H	2.29667200	-1.89123600	-4.20183200

H	0.62864700	-2.41839600	-4.38987900
C	1.02136900	-1.39459700	-2.52025300
H	1.27263500	-2.32210400	-1.99358600
H	-0.04128900	-1.20176000	-2.33524000
C	1.97769500	-1.58643800	0.67557300
H	1.22892200	-2.22042200	0.18247900
C	3.36702900	-2.21032300	0.43623900
H	3.62066200	-2.21294700	-0.63018100
H	4.13308200	-1.60834600	0.94060000
C	3.42234800	-3.64693500	0.98808300
H	2.72654900	-4.27741400	0.41639900
H	4.42387000	-4.06632700	0.83219500
C	3.04506000	-3.69568500	2.47582700
H	3.81278000	-3.16615200	3.05839600
H	3.04512100	-4.73291100	2.83231000
C	1.67853800	-3.04222300	2.72809100
H	0.88972500	-3.63534100	2.24651400
H	1.45329200	-3.03636300	3.80154700
C	1.61887000	-1.60774600	2.17798900
H	2.31800300	-0.97856500	2.74143700
H	0.61484600	-1.19881200	2.31961800
C	-2.65773800	-2.72948000	0.71742400
C	-2.99684600	-2.31846000	-0.76495100
C	-4.48653500	-2.15618900	-1.06993300
H	-4.94651000	-1.40017500	-0.43117000
H	-4.61367900	-1.84008000	-2.10983100
H	-5.02386400	-3.10189900	-0.93687000
C	-2.35314200	-3.23412200	-1.81580300
H	-2.82272000	-4.22298900	-1.83749100
H	-2.47107900	-2.77751300	-2.80287500
H	-1.28383900	-3.36194000	-1.62922100
C	-2.33290900	-4.20890900	0.92684200
H	-2.07562800	-4.38210800	1.97620600
H	-3.19393300	-4.84137300	0.68334000
H	-1.48574600	-4.52759300	0.31651100
C	-3.72148100	-2.28727100	1.73361700
H	-4.64537800	-2.86681700	1.63761200
H	-3.32719400	-2.43507300	2.74327700
H	-3.96129900	-1.22738300	1.61679700
O	-2.36266900	-1.01588000	-0.88239100
O	-1.46268700	-1.94978900	0.99321600
B	-1.40772500	-0.85701300	0.12312800
O	0.76217600	3.62143900	0.16891300
C	0.03517000	2.67828200	0.41580500
C	-3.70620900	3.07814100	-0.26595800
C	-2.33346100	3.23472400	-0.36520300

C	-4.25318900	2.34873400	0.81219300
C	-1.46487000	2.70971800	0.61715200
C	-2.02631900	1.95244100	1.67201000
C	-3.41166700	1.79526400	1.77832600
H	-1.38481200	1.57990100	2.46877800
H	-3.85330100	1.24757000	2.60394100
H	-1.90875600	3.79496400	-1.19369600
H	-4.35017800	3.51984000	-1.01745900
O	-5.58503800	2.13591100	0.99083400
C	-6.49598800	2.67189900	0.04088300
H	-7.48926300	2.37239300	0.37794200
H	-6.44373200	3.76720200	0.00336100
H	-6.31761500	2.26660500	-0.96274100

TS6

B3LYP/BSI SCF energy: -2088.93662 a.u.
M06/BSII SCF energy in solution: -2088.216627 a.u.
M06/BSII free energy in solution: -2087.494376 a.u.

Ni	-0.34286100	-0.79288900	-0.10728000
P	1.70354800	-0.14911400	0.13956100
C	2.93144900	-1.55160700	-0.16114600
H	2.45511800	-2.36684800	0.40031200
C	4.37451800	-1.40482900	0.36788600
H	4.90011300	-0.61490800	-0.18148500
H	4.38115900	-1.10991900	1.42269700
C	5.14781400	-2.72814000	0.20745400
H	6.17808500	-2.59876200	0.56127000
H	4.68868600	-3.48989600	0.85307900
C	5.13918800	-3.22589900	-1.24525600
H	5.71071300	-2.52423500	-1.87029200
H	5.65120400	-4.19306400	-1.31628500
C	3.70810400	-3.33565400	-1.78973400
H	3.72469600	-3.63420400	-2.84500200
H	3.16243000	-4.12012500	-1.24882200
C	2.94663700	-2.00914800	-1.63551200
H	1.92259200	-2.12114400	-2.00683100
H	3.43481500	-1.24518100	-2.25481700
C	2.06258000	0.36487800	1.91466100
H	3.14442300	0.54866100	1.97272400
C	1.71510900	-0.78194400	2.89122100
H	0.64373100	-1.00691000	2.80070200
H	2.24843000	-1.69979900	2.62132400
C	2.03772700	-0.40710800	4.34707900
H	1.75019200	-1.23089200	5.01139900
H	3.12485700	-0.28335500	4.45724100
C	1.33484300	0.89115900	4.76558200

H	0.24791900	0.72828600	4.77014000
H	1.61587600	1.16476300	5.78971700
C	1.66890900	2.03295900	3.79626200
H	2.73817000	2.27686700	3.87859900
H	1.12095400	2.94162900	4.07323200
C	1.34068000	1.66082500	2.33966100
H	1.62406600	2.49231700	1.68470800
H	0.25873100	1.52624100	2.22864500
C	2.14568100	1.35678800	-0.89339900
H	1.49213700	2.11680600	-0.44541700
C	3.59884600	1.86318100	-0.80381600
H	3.92008600	1.96218800	0.23947100
H	4.27261300	1.13586300	-1.27401500
C	3.75234200	3.21426300	-1.52543000
H	3.15452500	3.97251600	-0.99996900
H	4.79603000	3.54752600	-1.47136100
C	3.29194100	3.12664700	-2.98760700
H	3.97155700	2.45976400	-3.53788000
H	3.36526900	4.10987000	-3.46799700
C	1.85823400	2.58562900	-3.09120500
H	1.15818100	3.30724100	-2.64905200
H	1.56897200	2.47619600	-4.14347500
C	1.69546400	1.23848600	-2.36684500
H	2.29301200	0.47771000	-2.88340100
H	0.64882400	0.92402400	-2.40667700
C	-2.48418700	2.81926800	-0.92072100
C	-2.73994200	2.69783200	0.62688200
C	-4.21024500	2.71524800	1.04650300
H	-4.76787600	1.89981000	0.58250300
H	-4.28302500	2.59698300	2.13201500
H	-4.68792700	3.66405800	0.77745900
C	-1.95364700	3.72190500	1.45806400
H	-2.35280300	4.73492500	1.34271800
H	-2.02040200	3.44576200	2.51448100
H	-0.89711000	3.73050900	1.17772100
C	-2.10483800	4.21598300	-1.41400600
H	-1.90768300	4.18229600	-2.48978600
H	-2.91802100	4.93038500	-1.24329500
H	-1.20634100	4.58968500	-0.91910600
C	-3.63517500	2.26454900	-1.77474900
H	-4.52283400	2.90407800	-1.73074500
H	-3.30476300	2.20730200	-2.81595100
H	-3.91280700	1.25623300	-1.45615700
O	-2.19261100	1.38682300	0.92994700
O	-1.35052500	1.93340000	-1.11771900
B	-1.31358400	0.99238800	-0.08211100

O	0.18674700	-3.69025400	-0.05401900
C	-0.25038400	-2.57583200	-0.13586900
C	-1.86447000	-2.27765900	-0.28777200
C	-2.69949100	-2.36406900	0.83661200
C	-2.45869000	-2.24844100	-1.56569000
C	-4.08482800	-2.42577400	0.70723400
H	-2.25903200	-2.38878700	1.82979900
C	-3.83608600	-2.30474300	-1.71134100
H	-1.82854300	-2.18789800	-2.44932400
C	-4.65779400	-2.39549800	-0.57367500
H	-4.70335800	-2.49174200	1.59436700
H	-4.30711200	-2.28477400	-2.68881400
O	-5.99292100	-2.45322800	-0.81957400
C	-6.88405200	-2.55297200	0.28308000
H	-7.88673100	-2.58950600	-0.14487900
H	-6.70514800	-3.46614000	0.86412400
H	-6.80478400	-1.68235900	0.94582900

IM10

B3LYP/BSI SCF energy: -2089.007193 a.u.
M06/BSII SCF energy in solution: -2088.293982 a.u.
M06/BSII free energy in solution: -2087.570611 a.u.

Ni	0.08987700	-0.86891900	1.17710900
P	1.08120300	0.83732600	0.04292600
C	2.92541900	0.45734400	-0.10600000
H	3.22726200	0.45974600	0.95086100
C	3.80552200	1.48978600	-0.83942000
H	3.53137500	1.51960500	-1.90129500
H	3.63432100	2.49786700	-0.44440200
C	5.29906500	1.13501900	-0.71984900
H	5.89999900	1.86190800	-1.28007000
H	5.60554400	1.22262300	0.33236000
C	5.58523900	-0.29081900	-1.21274000
H	5.39166800	-0.34455300	-2.29385900
H	6.64550100	-0.53450600	-1.07427200
C	4.70091000	-1.31798100	-0.49048100
H	4.88384600	-2.32400100	-0.88674500
H	4.97507500	-1.34683700	0.57395900
C	3.20747600	-0.97275800	-0.61733900
H	2.60319500	-1.69418700	-0.05630700
H	2.90805600	-1.06637300	-1.66736900
C	1.07222000	2.46468300	1.01035900
H	1.50209200	3.23791700	0.36056900
C	1.91756000	2.43044600	2.30123700
H	1.57085400	1.61855000	2.95019000
H	2.96692000	2.22186100	2.06949500

C	1.83707500	3.76281200	3.06841400
H	2.42514100	3.68908400	3.99105100
H	2.30117100	4.55674700	2.46532300
C	0.38832300	4.15394700	3.38709500
H	-0.04048700	3.41851100	4.08219600
H	0.35777000	5.12369200	3.89830300
C	-0.45947600	4.19550800	2.10959100
H	-0.10311800	5.01057700	1.46301000
H	-1.50510900	4.42364000	2.35001500
C	-0.38221500	2.86557100	1.34120000
H	-0.98071300	2.93467100	0.42471800
H	-0.83069600	2.06765200	1.94822900
C	0.41369500	1.36956300	-1.65728100
H	-0.66953000	1.26185700	-1.50687500
C	0.66953100	2.81295800	-2.14538500
H	0.37473400	3.54666000	-1.38920600
H	1.74128000	2.96380800	-2.32790500
C	-0.11351100	3.10021100	-3.44095000
H	-1.18955300	3.06616200	-3.21840900
H	0.10072800	4.12003500	-3.78402000
C	0.20353700	2.08637300	-4.54890800
H	1.24901300	2.21253800	-4.86544800
H	-0.41482600	2.28427700	-5.43289900
C	-0.00232700	0.64628000	-4.05866700
H	-1.06837000	0.47321500	-3.85651200
H	0.29093000	-0.06662500	-4.83929500
C	0.79838600	0.37455200	-2.77466300
H	1.86800000	0.47353200	-3.00035400
H	0.64011000	-0.65491800	-2.44499500
C	-4.21761300	0.20789200	-0.95842400
C	-4.41676000	0.06900300	0.60469600
C	-5.80074300	-0.41226700	1.04047700
H	-6.04408900	-1.38484200	0.60967600
H	-5.82529800	-0.51118900	2.12945100
H	-6.57524900	0.30493300	0.74850300
C	-4.03309600	1.33069000	1.38715200
H	-4.75498900	2.13866100	1.23278900
H	-4.00913500	1.08986300	2.45361400
H	-3.04157600	1.68770500	1.10107700
C	-4.34729500	1.62784400	-1.50603700
H	-4.15834300	1.62392600	-2.58359700
H	-5.35723400	2.01793900	-1.34212700
H	-3.63238500	2.30803800	-1.03955600
C	-5.09963200	-0.74971300	-1.77206500
H	-6.15329900	-0.45654000	-1.74210800
H	-4.76819400	-0.73624600	-2.81410700

H	-5.01402000	-1.77624500	-1.40504700
O	-3.45040300	-0.95824600	0.95055200
O	-2.84501100	-0.23678000	-1.14231200
B	-2.51923400	-1.03899900	-0.06217000
O	0.90885700	-0.86951000	3.97178800
C	0.57557600	-0.87777100	2.85788500
C	-1.30799500	-2.00284300	-0.03323700
C	-0.96500500	-2.70992200	1.16366300
C	-0.76555800	-2.50814200	-1.26735200
C	-0.07081900	-3.82701100	1.11440600
H	-1.59296100	-2.60189600	2.04215000
C	0.08725500	-3.57851900	-1.30491600
H	-1.08243400	-2.04298300	-2.19616000
C	0.46372100	-4.23122100	-0.09218200
H	0.15632200	-4.35157400	2.03509500
H	0.48117300	-3.96736200	-2.23848700
O	1.32780400	-5.27522400	-0.25956000
C	1.73835000	-5.98986100	0.89452700
H	2.43688100	-6.75288100	0.54704500
H	2.24428800	-5.33455500	1.61539600
H	0.88906800	-6.47648800	1.39168200

Pr1

B3LYP/BSI SCF energy: -757.479511 a.u.
M06/BSII SCF energy in solution: -757.157989 a.u.
M06/BSII free energy in solution: -756.896603 a.u.

C	-3.04170700	0.98108700	-0.11610000
C	-3.68311700	-0.25603600	0.03184900
C	-2.91983400	-1.42615000	0.17681800
C	-1.53472000	-1.35301400	0.17059700
C	-0.86084000	-0.12296200	0.02299200
C	-1.64702300	1.03098300	-0.11771400
H	-3.61197800	1.89588200	-0.22801000
H	-1.15582800	1.99359300	-0.23195100
H	-0.95361500	-2.26442100	0.28147300
H	-3.44102700	-2.37143900	0.29017800
O	-5.03576600	-0.42886600	0.04780700
C	-5.86329200	0.71384100	-0.10135500
H	-5.69259500	1.21545800	-1.06257600
H	-6.89090500	0.34863600	-0.06501600
H	-5.70849300	1.43580700	0.71076900
C	2.86450400	-0.72122400	-0.10193400
C	2.78752700	0.84540600	0.08534800
C	3.64248400	1.65969300	-0.88394100
H	3.37561300	1.45967100	-1.92309400
H	3.49204400	2.72696400	-0.69728000

H	4.70641000	1.43918400	-0.74678800
C	3.04938800	1.29815100	1.52824800
H	4.10240500	1.18626000	1.80389900
H	2.77915100	2.35353700	1.62249400
H	2.44184400	0.73033100	2.23844500
C	3.81641400	-1.44465500	0.84893500
H	3.77298300	-2.52153400	0.66192100
H	4.84937400	-1.11580000	0.69285100
H	3.54983100	-1.27423100	1.89342900
C	3.13987700	-1.14813500	-1.55008400
H	4.17161700	-0.93691000	-1.84728300
H	2.96970700	-2.22460100	-1.63912700
H	2.46649400	-0.64202200	-2.24743400
O	1.38774800	1.12076000	-0.19285100
O	1.50496100	-1.13528800	0.20376000
B	0.68469100	-0.04582400	0.01228500

CO

B3LYP/BSI SCF energy: -113.306914 a.u.
M06/BSII SCF energy in solution: -113.281208 a.u.
M06/BSII free energy in solution: -113.29531 a.u.

O	0.00000000	0.00000000	0.48760100
C	0.00000000	0.00000000	-0.65013500

PCy_3

B3LYP/BSI SCF energy: -1047.202489 a.u.
M06/BSII SCF energy in solution: -1046.793758 a.u.
M06/BSII free energy in solution: -1046.358237 a.u.

C	0.75824000	-1.50793100	-0.30869700
H	0.03770500	-2.33353300	-0.41166000
C	1.95571700	-1.88256100	-1.21215900
H	2.71491600	-1.09076800	-1.17090600
H	1.62965700	-1.94449300	-2.25653400
C	2.59700800	-3.21103100	-0.77594000
H	1.87761900	-4.02686800	-0.93719400
H	3.46556600	-3.43355400	-1.40805800
C	3.00715000	-3.18553700	0.70379700
H	3.81490800	-2.45231300	0.84196500
H	3.41603900	-4.15819000	1.00330700
C	1.82370800	-2.80373500	1.60474800
H	1.06219300	-3.59546300	1.55861700
H	2.14573300	-2.74278900	2.65182300
C	1.19242800	-1.46806600	1.16951000
H	0.34353400	-1.22594400	1.81966200

H	1.93349900	-0.67083400	1.30946100
C	-1.83446500	-0.12430400	-0.04162100
H	-1.61102200	-0.07141600	1.03389700
C	-2.59580800	-1.44233800	-0.30836100
H	-1.99908800	-2.30485600	0.00788400
H	-2.75130800	-1.55231300	-1.39114300
C	-3.95683700	-1.48605600	0.40690100
H	-3.79370100	-1.49356300	1.49419800
H	-4.47263300	-2.42329800	0.16405500
C	-4.83178300	-0.28172500	0.03624400
H	-5.77777500	-0.31031700	0.59052100
H	-5.09180200	-0.33793200	-1.03045000
C	-4.09213700	1.03467600	0.30656100
H	-4.70433800	1.88916900	-0.00736500
H	-3.93495800	1.14610600	1.38907500
C	-2.73193200	1.07902700	-0.41060000
H	-2.89680800	1.07793700	-1.49768000
H	-2.22862100	2.02325900	-0.17601100
C	0.55136000	1.56657400	-0.46616300
H	-0.07404600	2.29747800	-1.00284500
C	0.52141000	1.96757800	1.02458600
H	-0.49455000	1.89390000	1.42721700
H	1.13827800	1.27814700	1.61189100
C	1.05069500	3.40091200	1.22287900
H	1.04362100	3.65705000	2.28968200
H	0.36924200	4.10838200	0.72873000
C	2.46241800	3.57127500	0.64308800
H	3.16458000	2.94897700	1.21656200
H	2.79959400	4.60840700	0.75973500
C	2.51212400	3.15486800	-0.83396800
H	1.90560900	3.85260800	-1.42874900
H	3.53749400	3.22909500	-1.21676900
C	1.97810900	1.72699900	-1.03451300
H	2.65297700	1.02461300	-0.52751500
H	1.99396400	1.46391700	-2.09886300
P	-0.22803400	-0.06549000	-1.04628600

B1[B_2pin_2]
B3LYP/BSI SCF energy: -822.56502 a.u.
M06/BSII SCF energy in solution: -822.240172 a.u.
M06/BSII free energy in solution: -821.92382 a.u.

B	0.85293000	-0.00006700	0.00000200
O	1.61586700	-1.08081200	-0.37277800
O	1.61580500	1.08073500	0.37282500
C	3.00436300	-0.78751600	-0.04629200
C	3.00431600	0.78749400	0.04636700

C	3.89172800	-1.37803000	-1.14091800
C	3.29213800	-1.47967000	1.29312300
C	3.29210200	1.47954800	-1.29311100
C	3.89166800	1.37820900	1.14088100
H	4.94564000	-1.13986600	-0.96148700
H	3.61411300	-1.00852300	-2.12964500
H	3.78752500	-2.46676100	-1.14767900
H	4.33928700	-1.36731500	1.59013000
H	3.07404900	-2.54649800	1.19380200
H	2.65973200	-1.07973500	2.09053300
H	4.33922000	1.36711000	-1.59016800
H	3.07407900	2.54640000	-1.19383100
H	2.65959800	1.07963700	-2.09044400
H	4.94566100	1.14074200	0.96102500
H	3.61466200	1.00837300	2.12965500
H	3.78675000	2.46687100	1.14784500
B	-0.85292900	0.00004000	-0.00001300
O	-1.61585100	1.08080100	0.37275600
O	-1.61581900	-1.08075600	-0.37281800
C	-3.00435200	0.78751900	0.04628500
C	-3.00432600	-0.78749200	-0.04635800
C	-3.89170100	1.37805400	1.14091300
C	-3.29213100	1.47966300	-1.29313400
C	-3.29211700	-1.47953100	1.29312700
C	-3.89168900	-1.37820700	-1.14086400
H	-4.94561800	1.13990600	0.96149000
H	-3.61408700	1.00855000	2.12964100
H	-3.78748000	2.46678300	1.14766600
H	-4.33928300	1.36731100	-1.59013300
H	-3.07403600	2.54649100	-1.19382500
H	-2.65973300	1.07971800	-2.09054400
H	-4.33923300	-1.36707400	1.59018800
H	-3.07411100	-2.54638700	1.19385600
H	-2.65960400	-1.07962200	2.09045400
H	-4.94567800	-1.14072800	-0.96100600
H	-3.61468200	-1.00838200	-2.12964200
H	-3.78678100	-2.46687100	-1.14782000

FBpin

B3LYP/BSI SCF energy: -511.186169 a.u.
M06/BSII SCF energy in solution: -511.031053 a.u.
M06/BSII free energy in solution: -510.880752 a.u.

B	1.59171800	-0.00004800	-0.00011700
O	0.85676900	-1.07674400	0.41038600
O	0.85678300	1.07674600	-0.41039400
C	-0.52602400	-0.79001000	0.04873400

C	-0.52601200	0.79001400	-0.04873300
C	-1.43717800	-1.37522100	1.12439200
C	-0.77916300	-1.47913100	-1.29770600
C	-0.77915300	1.47912100	1.29771500
C	-1.43716400	1.37524700	-1.12438100
H	-2.48521100	-1.13174300	0.92120600
H	-1.17831800	-1.00536600	2.11800200
H	-1.33915900	-2.46441800	1.13401200
H	-1.81963400	-1.37113100	-1.61743500
H	-0.55779200	-2.54503900	-1.19724000
H	-0.13205800	-1.07170000	-2.07977100
H	-1.81962700	1.37113200	1.61743700
H	-0.55776600	2.54502700	1.19726400
H	-0.13206000	1.07167000	2.07978100
H	-2.48519700	1.13176300	-0.92120000
H	-1.17830200	1.00540900	-2.11799700
H	-1.33914700	2.46444400	-1.13398100
F	2.91838100	0.00000700	0.00004900

TS7

B3LYP/BSI SCF energy: -2535.029564 a.u.
M06/BSII SCF energy in solution: -2534.160558 a.u.
M06/BSII free energy in solution: -2533.322396 a.u.

Ni	0.16884600	-0.28445100	0.43519000
P	-2.01101500	-0.90104700	0.19910200
F	0.85097000	-1.84275100	-0.79167500
C	-3.33431600	0.35542500	0.67477800
H	-2.89513600	0.79889000	1.57851600
C	-4.73319900	-0.17890800	1.05537300
H	-5.21304500	-0.63701900	0.18208800
H	-4.66188400	-0.95932400	1.81876200
C	-5.62688800	0.95962500	1.58153500
H	-6.62092600	0.56470600	1.82456900
H	-5.20390300	1.34031600	2.52181900
C	-5.74031100	2.11217600	0.57438700
H	-6.27581500	1.75938300	-0.31908800
H	-6.34171200	2.92668100	0.99574500
C	-4.35484900	2.62719600	0.16082600
H	-4.44980000	3.40644800	-0.60498200
H	-3.86152300	3.09568200	1.02334200
C	-3.46482600	1.48994500	-0.36646300
H	-2.47966500	1.88394700	-0.63187000
H	-3.91130700	1.09113100	-1.28676300
C	-2.34097700	-2.36249500	1.34597500
H	-3.39454300	-2.64652700	1.21526800
C	-2.12473500	-1.95482000	2.82276800

H	-1.09221200	-1.60989200	2.95478300
H	-2.75532600	-1.10104100	3.08971000
C	-2.40806600	-3.12501900	3.77897500
H	-2.21875200	-2.80732600	4.81111200
H	-3.47363500	-3.39276900	3.72511300
C	-1.56046100	-4.35616600	3.43314800
H	-0.49964400	-4.12327000	3.60228100
H	-1.80759000	-5.19207600	4.09866900
C	-1.76012800	-4.76460800	1.96782700
H	-2.79491400	-5.10839600	1.82528200
H	-1.11311000	-5.61281000	1.71363000
C	-1.47767500	-3.59789300	1.00519900
H	-1.65846300	-3.92997300	-0.02249000
H	-0.41514600	-3.32988700	1.06336600
C	-2.33782900	-1.58766600	-1.52444800
H	-1.67446600	-2.46345600	-1.53839800
C	-3.76998100	-2.07939300	-1.81750100
H	-4.11504400	-2.76609200	-1.03605300
H	-4.45715400	-1.22392000	-1.81051000
C	-3.85251100	-2.77064200	-3.19012100
H	-3.24813500	-3.68868000	-3.16857200
H	-4.88556200	-3.08256500	-3.38652600
C	-3.34512400	-1.85581000	-4.31366800
H	-4.02171100	-0.99438800	-4.41028400
H	-3.37334200	-2.38307600	-5.27478900
C	-1.92451600	-1.35267700	-4.02030100
H	-1.22799500	-2.20298500	-4.03833800
H	-1.59411600	-0.66387400	-4.80715000
C	-1.83183200	-0.65679200	-2.65147000
H	-2.42966900	0.26194900	-2.67797600
H	-0.79704900	-0.35775100	-2.45850300
C	3.09289700	-0.42207200	-3.02694100
C	4.05729100	-1.39564400	-2.22031200
C	5.18002700	-0.67613000	-1.46289600
H	4.79847100	0.13215100	-0.83855000
H	5.67335900	-1.39708500	-0.80503600
H	5.92940600	-0.27052300	-2.15008800
C	4.65687200	-2.53205600	-3.05203800
H	5.30055700	-2.13989400	-3.84663100
H	5.26860500	-3.16788200	-2.40559700
H	3.88427000	-3.15721200	-3.50273200
C	2.45394400	-1.07879600	-4.25873700
H	1.68497000	-0.41020000	-4.65614400
H	3.18797300	-1.26478300	-5.04889400
H	1.97461000	-2.02687000	-3.99990700
C	3.71198100	0.91953000	-3.41556900

H	2.96694500	1.53023500	-3.93451800
H	4.05111200	1.47238300	-2.53825200
H	4.56216400	0.77815600	-4.09119800
O	3.16430200	-1.99197400	-1.24657800
O	2.01425600	-0.17193700	-2.08373000
B	2.05079800	-1.18762200	-1.13744900
O	-0.55882000	1.10909300	2.62396400
C	-0.19987100	1.20767600	1.45665700
C	-0.38599400	4.97846500	0.99962400
C	-0.43423000	3.70319600	1.55936000
C	-0.00858700	5.12731100	-0.34349100
C	-0.11148600	2.56521700	0.80906600
C	0.26781200	2.73082300	-0.53440400
C	0.31794300	3.99428400	-1.10708000
H	0.54129700	1.85837800	-1.12352400
H	0.61380500	4.13677100	-2.14155100
H	-0.72260000	3.56623500	2.59707400
H	-0.63872900	5.83976500	1.60720400
O	0.07373700	6.32135900	-0.99491800
C	-0.22275400	7.50674900	-0.27260100
H	-0.08386300	8.32997100	-0.97510800
H	-1.25890500	7.51271900	0.08927400
H	0.45496500	7.64128300	0.57988800
C	2.09848100	-0.15103800	0.87433300
C	2.92348700	1.00070900	0.85587500
C	2.49788900	-1.16183400	1.77732700
C	4.04613600	1.13390900	1.66155500
H	2.68141800	1.81927000	0.18372400
C	3.62422700	-1.06003900	2.59827600
H	1.91890000	-2.08177900	1.84193100
C	4.40275900	0.10171700	2.54535600
H	4.66523500	2.02606600	1.63386800
H	3.88058600	-1.87665200	3.26394400
O	5.51953800	0.32435600	3.29728100
C	5.91187800	-0.67132300	4.22791700
H	5.13225800	-0.85430600	4.97854100
H	6.15681700	-1.61873500	3.73030600
H	6.80452400	-0.28628500	4.72396400

IM11

B3LYP/BSI SCF energy: -2023.847641 a.u.
M06/BSII SCF energy in solution: -2023.128703 a.u.
M06/BSII free energy in solution: -2022.463493 a.u.

Ni	-0.72511900	-0.61767500	0.02719800
P	1.55466600	-0.73337600	-0.01746000
C	2.47182000	0.87622900	-0.35640600

H	1.92340800	1.24585900	-1.23525200
C	3.96376200	0.79981500	-0.74664500
H	4.55663900	0.46201700	0.11080000
H	4.12719700	0.07099300	-1.54671000
C	4.47667100	2.18056100	-1.19616400
H	5.54110700	2.11449100	-1.45214500
H	3.95240100	2.47531600	-2.11616200
C	4.25149200	3.25005800	-0.11760500
H	4.87981600	3.01941100	0.75487500
H	4.57649500	4.23161200	-0.48285700
C	2.78044700	3.30351000	0.31959400
H	2.65055900	4.02447100	1.13547700
H	2.16052400	3.66111600	-0.51395100
C	2.26673400	1.92218300	0.76115900
H	1.20909700	1.98934300	1.03423300
H	2.81387300	1.60916400	1.66036500
C	2.13601200	-1.90058800	-1.37738700
H	3.22118300	-2.03792800	-1.26789000
C	1.85283400	-1.30542000	-2.77706600
H	0.78151900	-1.09085100	-2.86792800
H	2.36892500	-0.34746900	-2.90169500
C	2.28882400	-2.26383500	-3.89790500
H	2.04946300	-1.81918800	-4.87106600
H	3.38157900	-2.38722400	-3.87060800
C	1.62144000	-3.63808000	-3.75943900
H	0.53753100	-3.52937900	-3.90295100
H	1.97611100	-4.31719100	-4.54406900
C	1.89033100	-4.23923400	-2.37376300
H	2.96380900	-4.45586900	-2.27362000
H	1.36757700	-5.19660100	-2.26180800
C	1.45939300	-3.28486900	-1.24693500
H	1.69115600	-3.74400500	-0.27943400
H	0.36912700	-3.15213800	-1.27962500
C	2.18267200	-1.54202900	1.56787000
H	1.79522100	-2.56610100	1.45990000
C	3.70861600	-1.65021900	1.76574300
H	4.18922700	-2.08180600	0.88039000
H	4.13192100	-0.64626900	1.89747700
C	4.04829000	-2.49368000	3.00785000
H	3.71413000	-3.52802700	2.84471800
H	5.13608500	-2.53538400	3.14093600
C	3.37566000	-1.93370500	4.26942400
H	3.80230200	-0.94625100	4.49668700
H	3.59396800	-2.57322500	5.13276800
C	1.85807000	-1.79644700	4.07800200
H	1.41373800	-2.79635900	3.97245600

H	1.40061400	-1.34528900	4.96645500
C	1.51248300	-0.96034600	2.83401100
H	1.84528900	0.07333400	2.99047800
H	0.42490500	-0.91906900	2.69993300
O	-1.05389400	0.46345900	-2.36984500
C	-1.10241500	0.71247200	-1.17384200
C	-1.52462600	4.48288900	-1.17837000
C	-1.30997800	3.16959000	-1.59139400
C	-1.80362600	4.74443600	0.17196400
C	-1.35929900	2.10465000	-0.68122400
C	-1.64109600	2.38270500	0.66601100
C	-1.86328800	3.68419700	1.09161100
H	-1.70468800	1.55796400	1.36917700
H	-2.09470300	3.91118100	2.12723300
H	-1.10625100	2.94759000	-2.63435400
H	-1.48075800	5.28621000	-1.90456100
O	-2.03269800	5.98408100	0.68639600
C	-2.02020100	7.09635000	-0.19590000
H	-2.24026700	7.97025000	0.41904500
H	-1.03881300	7.22675500	-0.66958500
H	-2.78562900	7.00164000	-0.97633200
C	-2.55627000	-1.00798100	0.22979800
C	-3.36758800	-1.47573800	-0.81914000
C	-3.09447000	-1.11208200	1.53454700
C	-4.62145300	-2.05611500	-0.59769000
H	-3.01594300	-1.38138400	-1.84450200
C	-4.33946800	-1.68791400	1.77809500
H	-2.53138500	-0.74204600	2.39078400
C	-5.10932900	-2.16736300	0.71005600
H	-5.20400300	-2.40875000	-1.44205900
H	-4.73985700	-1.77204500	2.78447600
O	-6.31921000	-2.71641600	1.04764600
C	-7.14151000	-3.20771800	0.00517100
H	-7.42598100	-2.41474800	-0.69943300
H	-6.65310500	-4.01765300	-0.55325500
H	-8.04095300	-3.59762200	0.48577700

TS8

B3LYP/BSI SCF energy: -2023.82359 a.u.
M06/BSII SCF energy in solution: -2023.105781 a.u.
M06/BSII free energy in solution: -2022.439731 a.u.

Ni	0.48806000	0.78476000	0.62660700
C	2.18092000	1.68499500	0.30796600
C	2.49286200	2.36403600	-0.90086800
C	3.08869400	1.92250200	1.36749600
C	3.58956600	3.20737400	-1.04089300

H	1.85333500	2.22683600	-1.77297000
C	4.20050500	2.76574200	1.26046000
H	2.92649700	1.43660000	2.32926700
C	4.45217700	3.41519700	0.04597700
H	3.80501400	3.71839100	-1.97535500
H	4.85300000	2.90867600	2.11535400
C	-0.83093300	-1.44284800	-1.57303200
H	-1.81779300	-1.05498100	-1.28125500
C	-0.30995600	-0.51460300	-2.69208500
H	0.66732100	-0.86443500	-3.04116000
H	-0.15070900	0.49689600	-2.30531200
C	-1.28668200	-0.49357600	-3.87967700
H	-2.24005200	-0.05240700	-3.55598900
H	-0.89386800	0.15601200	-4.67089900
C	-1.53700100	-1.90682200	-4.42736300
H	-0.60578000	-2.29223500	-4.86650100
H	-2.27434100	-1.87683600	-5.23819900
C	-2.00409700	-2.86223000	-3.31984700
H	-2.99969700	-2.55460600	-2.97009100
H	-2.11344000	-3.87976300	-3.71402300
C	-1.03393800	-2.87033400	-2.12394800
H	-1.41424900	-3.54445100	-1.34911800
H	-0.06751400	-3.27594700	-2.44932700
C	-0.82011500	-2.41711100	1.23095400
H	-0.67690100	-3.43669500	0.84833300
C	-2.34334700	-2.16802300	1.28521000
H	-2.79062200	-2.27108300	0.29044600
H	-2.54176000	-1.14577700	1.62037400
C	-3.02764800	-3.14988500	2.25344700
H	-2.92611400	-4.17412000	1.86593400
H	-4.10276400	-2.93641000	2.28955200
C	-2.41877000	-3.07568500	3.66007300
H	-2.90173700	-3.80406200	4.32255900
H	-2.61358600	-2.08193600	4.08562500
C	-0.90365200	-3.31564300	3.61555900
H	-0.47026100	-3.21036400	4.61717600
H	-0.71004100	-4.35109700	3.29848300
C	-0.20524800	-2.34361200	2.64941300
H	-0.30188000	-1.31831300	3.02259100
H	0.86647900	-2.57123800	2.61714400
C	1.81553900	-2.12173200	-0.07522700
H	2.28911000	-1.76309000	0.84979600
C	1.85609300	-3.66655500	-0.04981100
H	1.28800700	-4.06711900	0.79448600
H	1.39367400	-4.06753600	-0.96046800
C	3.30756500	-4.17486500	0.04778400

H	3.31207400	-5.27167000	0.03661300
H	3.72404700	-3.87176200	1.01880800
C	4.19329700	-3.62164600	-1.07613400
H	3.85477300	-4.03135800	-2.03889400
H	5.22850400	-3.95777900	-0.94232300
C	4.12667000	-2.08971000	-1.12734000
H	4.57884900	-1.66934300	-0.21861500
H	4.71375600	-1.70863900	-1.97125900
C	2.67650200	-1.59058000	-1.24202900
H	2.26178100	-1.94788600	-2.19383700
H	2.65796900	-0.49754100	-1.25794900
P	0.11449300	-1.28744400	0.04818300
O	5.50484900	4.25949000	-0.18339500
C	6.39898300	4.51868700	0.88418200
H	5.88845200	4.97857400	1.74059600
H	6.90571400	3.60530800	1.22333800
H	7.14300600	5.21601100	0.49431900
O	-1.14479100	0.88962600	2.64096500
C	-1.16524400	1.01885200	1.41878200
C	-4.60459500	2.53497400	0.88705700
C	-3.49129000	1.94728200	1.48131800
C	-4.56550800	2.86733200	-0.47638600
C	-2.33452900	1.66449000	0.74016900
C	-2.31133800	2.00610300	-0.62255200
C	-3.40735200	2.60386500	-1.22690600
H	-1.41433400	1.81532100	-1.20275000
H	-3.39615200	2.88300400	-2.27540100
H	-3.50072000	1.69503100	2.53708900
H	-5.48729500	2.73316200	1.48374500
O	-5.59034300	3.44463000	-1.15891100
C	-6.78369800	3.75827600	-0.45453500
H	-7.45237400	4.21442600	-1.18577800
H	-7.25811200	2.85853300	-0.04296500
H	-6.59663700	4.47062500	0.35849900

IM12

B3LYP/BSI SCF energy: -2023.832098 a.u.
M06/BSII SCF energy in solution: -2023.118688 a.u.
M06/BSII free energy in solution: -2022.453368 a.u.

Ni	-0.45931300	-0.71836100	-0.01155100
P	1.59036900	-0.03071500	0.11070000
C	2.65666700	-0.86079100	-1.19058200
H	2.54964800	-1.91553200	-0.90326100
C	4.15624000	-0.50052300	-1.19279100
H	4.28553100	0.54382800	-1.50485000
H	4.58439400	-0.58334300	-0.18725200

C	4.93328100	-1.40992900	-2.16231000
H	5.99163800	-1.12188800	-2.17261700
H	4.89315500	-2.44412300	-1.79287200
C	4.34962000	-1.35477300	-3.58140800
H	4.50215800	-0.34698700	-3.99427900
H	4.88927400	-2.04590300	-4.23984300
C	2.84834600	-1.67882800	-3.58111400
H	2.43883500	-1.58255400	-4.59399400
H	2.69772300	-2.72356600	-3.27756600
C	2.07165300	-0.76529700	-2.61797800
H	1.01421500	-1.04891700	-2.60636100
H	2.12114500	0.26666400	-2.98431000
C	2.39039900	-0.50600500	1.74812700
H	3.38360700	-0.03680100	1.75011200
C	2.59264300	-2.02600300	1.92386800
H	1.62284500	-2.53384300	1.86713800
H	3.19992100	-2.43455000	1.11056700
C	3.26153800	-2.34754200	3.27179400
H	3.36726300	-3.43384200	3.37632100
H	4.28011800	-1.93325900	3.28060600
C	2.47112500	-1.77012700	4.45347100
H	1.49410700	-2.27052200	4.51353500
H	2.98759200	-1.97857900	5.39799600
C	2.25454000	-0.26047000	4.28433700
H	3.22401000	0.25467100	4.34395200
H	1.64213100	0.13443800	5.10381200
C	1.58836200	0.06771200	2.93768800
H	1.46672300	1.15200500	2.84112000
H	0.57677800	-0.36058800	2.91905100
C	1.76701400	1.84593100	0.05446700
H	0.96373700	2.15206500	0.73738000
C	3.08579300	2.46427100	0.56801300
H	3.33987500	2.08660600	1.56348100
H	3.91546500	2.18826800	-0.09414500
C	2.97769800	4.00004500	0.62894100
H	2.22767000	4.27376300	1.38420000
H	3.93131600	4.42204900	0.96920000
C	2.57563900	4.60414000	-0.72402200
H	3.38725600	4.43996000	-1.44779100
H	2.45564300	5.69029000	-0.63221600
C	1.28630100	3.96391700	-1.25653700
H	0.44398900	4.22522500	-0.60220400
H	1.04593100	4.36153300	-2.24991300
C	1.40567500	2.43266000	-1.32709800
H	2.18773400	2.17335600	-2.05234000
H	0.46573400	2.00300700	-1.68466400

O	0.67723700	-3.34181300	-0.72954300
C	-0.11531600	-2.50121100	-0.34845400
C	-1.62730400	-2.65044600	-0.35282800
C	-2.37831500	-2.26222300	0.76960900
C	-2.31642500	-3.01102800	-1.53567000
C	-3.77826300	-2.25272300	0.73764400
H	-1.87146800	-2.01651600	1.70005300
C	-3.69559500	-3.00747500	-1.57476400
H	-1.74254600	-3.31167800	-2.40769700
C	-4.43804900	-2.61676800	-0.43795800
H	-4.32789300	-1.95442600	1.62164500
H	-4.24069800	-3.30053700	-2.46644400
O	-5.78622400	-2.63898400	-0.59336900
C	-6.59993900	-2.20890500	0.49090000
H	-7.62966800	-2.27944400	0.13837600
H	-6.47358900	-2.85431600	1.36905600
H	-6.37987600	-1.17123500	0.76904900
C	-2.54647600	2.77777600	1.40143900
C	-1.69634500	1.67519100	1.31995900
C	-3.24628300	3.20733000	0.26667600
C	-1.49909500	0.93652400	0.12974000
C	-2.22364800	1.40692800	-0.98364100
C	-3.08259000	2.51581000	-0.93718200
H	-2.12841200	0.89724800	-1.94313200
H	-3.60965400	2.82265600	-1.83471500
H	-1.17154400	1.38258900	2.22970900
H	-2.68288300	3.32428900	2.33105600
O	-4.05597300	4.30454600	0.43904900
C	-4.77444100	4.77852900	-0.68296500
H	-5.34554500	5.64276100	-0.33729400
H	-4.10538200	5.09325800	-1.49575400
H	-5.46978000	4.02307900	-1.07430000

TS9

B3LYP/BSI SCF energy: -2023.828074 a.u.
M06/BSII SCF energy in solution: -2023.115157 a.u.
M06/BSII free energy in solution: -2022.451013 a.u.

Ni	-0.52656900	-0.65198900	-0.10705700
P	1.62610800	-0.24912400	0.10439600
C	2.59402700	-1.16836100	-1.22138200
H	2.39826400	-2.21391600	-0.94535800
C	4.12228100	-0.95995300	-1.23810300
H	4.34738500	0.07598600	-1.52118700
H	4.55057500	-1.11383300	-0.24097300
C	4.79773800	-1.90864600	-2.24516400

H	5.87837300	-1.72211600	-2.26149700
H	4.66471900	-2.94596500	-1.90724800
C	4.20583300	-1.75338000	-3.65338200
H	4.44575000	-0.75108600	-4.03645600
H	4.67089400	-2.46931600	-4.34133800
C	2.68131700	-1.93829900	-3.64012100
H	2.26884300	-1.77385200	-4.64272300
H	2.44228900	-2.97610200	-3.36954800
C	2.00274400	-0.98866800	-2.63832000
H	0.92366400	-1.17543900	-2.61568300
H	2.13749000	0.04509000	-2.97669400
C	2.31057600	-0.92038600	1.72776800
H	3.36700100	-0.62244000	1.77176900
C	2.25397300	-2.45971700	1.82901100
H	1.21649700	-2.79536000	1.71654700
H	2.81881800	-2.92416300	1.01446300
C	2.81222300	-2.95551700	3.17467800
H	2.72835800	-4.04759800	3.22378700
H	3.88540800	-2.72277200	3.22942900
C	2.09449500	-2.30825800	4.36631500
H	1.04561700	-2.63692000	4.37959800
H	2.54000400	-2.64627700	5.30944300
C	2.14180900	-0.77762500	4.27030700
H	3.18227400	-0.43832800	4.37626100
H	1.58109600	-0.32322500	5.09578000
C	1.57889900	-0.27955400	2.92905900
H	1.63928000	0.81323300	2.88661400
H	0.51170000	-0.53244400	2.86787500
C	2.09547200	1.57505200	0.13301900
H	1.31097100	1.98355600	0.78350800
C	3.46252700	1.95910200	0.74107500
H	3.59260400	1.51770800	1.73428100
H	4.27737500	1.57185600	0.11721600
C	3.59679400	3.48938400	0.85409700
H	2.85402000	3.86025900	1.57409300
H	4.58229800	3.74252500	1.26376700
C	3.38229400	4.18569500	-0.49615200
H	4.19851500	3.90836200	-1.17917400
H	3.43548000	5.27410200	-0.37370900
C	2.03956100	3.78187700	-1.12165200
H	1.21385600	4.16202200	-0.50565200
H	1.92725600	4.23981300	-2.11183400
C	1.90785900	2.25413000	-1.24134200
H	2.67011700	1.88728300	-1.94126500
H	0.92769900	1.99925000	-1.65489400
O	-0.30386400	-3.51728700	-0.64916800

C	-0.57545300	-2.38377200	-0.42010100
C	-2.22771200	-1.83757500	-0.41744400
C	-3.00045200	-2.05158300	0.73228400
C	-2.88808000	-1.73262800	-1.65729000
C	-4.39087700	-2.13258700	0.66894400
H	-2.51322600	-2.15513800	1.69863200
C	-4.26875400	-1.81365500	-1.73870600
H	-2.30990900	-1.58990400	-2.56684400
C	-5.03037900	-2.00937400	-0.57302700
H	-4.95988600	-2.28879200	1.57775000
H	-4.78919900	-1.73103100	-2.68752900
O	-6.37587200	-2.07740100	-0.75683900
C	-7.20754100	-2.26164000	0.38002500
H	-8.23112600	-2.27783000	0.00314500
H	-6.99434300	-3.21144300	0.88656000
H	-7.09889700	-1.43841900	1.09700600
C	-1.96643500	3.06547000	1.50678900
C	-1.34955500	1.82350100	1.35373100
C	-2.55184600	3.69713400	0.40310200
C	-1.28809400	1.13779300	0.11852900
C	-1.89524500	1.80911800	-0.95955400
C	-2.51341900	3.06328100	-0.84209300
H	-1.90517400	1.34586700	-1.94654200
H	-2.96215400	3.52232200	-1.71701200
H	-0.90762800	1.37558700	2.24363600
H	-2.00649700	3.56513700	2.47121600
O	-3.13104100	4.92059500	0.64559200
C	-3.75186200	5.58245600	-0.43859100
H	-4.15100400	6.51700300	-0.03859300
H	-3.03863200	5.81303600	-1.24226100
H	-4.57659100	4.99210400	-0.86125000

IM13

B3LYP/BSI SCF energy: -2023.842567 a.u.
M06/BSII SCF energy in solution: -2023.131076 a.u.
M06/BSII free energy in solution: -2022.467137 a.u.

Ni	-0.70432500	-0.77109700	-0.16714600
P	1.57239200	-0.39786900	0.09243600
C	2.55707500	-1.37199500	-1.18684200
H	2.33547800	-2.40782400	-0.89139700
C	4.09107700	-1.20993200	-1.17245400
H	4.35486400	-0.18810000	-1.47188900
H	4.48969300	-1.35396200	-0.16162500
C	4.76085000	-2.20154100	-2.14149300
H	5.84651100	-2.04699000	-2.13718000
H	4.59038400	-3.22642200	-1.78253100

C	4.20549500	-2.06415900	-3.56663000
H	4.48201000	-1.07873600	-3.96796900
H	4.66556000	-2.80921300	-4.22627100
C	2.67665700	-2.20630900	-3.58532300
H	2.29172700	-2.05498500	-4.60064700
H	2.40301000	-3.23121000	-3.29748200
C	2.00319500	-1.21371000	-2.62239100
H	0.91761900	-1.36397900	-2.62621000
H	2.17764300	-0.19351900	-2.98178500
C	2.19931700	-1.06558600	1.74381000
H	3.26206300	-0.79736400	1.81234500
C	2.09967100	-2.60093900	1.87185700
H	1.05259900	-2.91011800	1.76166400
H	2.66079300	-3.09834300	1.07395400
C	2.62753700	-3.08592400	3.23409700
H	2.51824100	-4.17474600	3.30156000
H	3.70472000	-2.87594200	3.29778600
C	1.90788600	-2.40088000	4.40326500
H	0.85289300	-2.70929800	4.40963400
H	2.33519400	-2.72925700	5.35799000
C	1.98566500	-0.87351100	4.27834000
H	3.03015700	-0.55065400	4.39506100
H	1.41971300	-0.39355200	5.08540600
C	1.45392500	-0.39225700	2.91838300
H	1.52559900	0.69861200	2.85613000
H	0.38582100	-0.63563400	2.84223500
C	2.12004400	1.40621700	0.09489100
H	1.31780400	1.87361400	0.68143000
C	3.46328900	1.75245700	0.77348200
H	3.50782500	1.34900100	1.78971200
H	4.29448000	1.29967800	0.21924000
C	3.66605500	3.27846400	0.83489800
H	2.90072400	3.71285000	1.49292700
H	4.63644100	3.50118600	1.29508200
C	3.56808200	3.92870200	-0.55166400
H	4.41097900	3.58868700	-1.17095400
H	3.66463600	5.01761200	-0.46639000
C	2.24951400	3.56040000	-1.24529200
H	1.40453800	4.00019900	-0.69939200
H	2.22154400	3.98095600	-2.25787800
C	2.05567300	2.03676000	-1.31429800
H	2.84577600	1.60948700	-1.94504900
H	1.09668900	1.80885800	-1.78767900
O	-0.62867200	-3.67782000	-0.60120000
C	-0.59977100	-2.54035200	-0.42841800
C	-2.61529100	-1.07065300	-0.34813300

C	-3.43141600	-1.29777900	0.76500100
C	-3.22753700	-1.10575900	-1.61351600
C	-4.80716200	-1.53514600	0.64091500
H	-3.00677500	-1.27445700	1.76649400
C	-4.59324900	-1.33734100	-1.75771400
H	-2.63583200	-0.94047200	-2.51201000
C	-5.39348200	-1.55381200	-0.62824500
H	-5.40043100	-1.69698900	1.53425800
H	-5.06226600	-1.35686400	-2.73720300
O	-6.72561200	-1.77463600	-0.87236200
C	-7.57602000	-1.98673800	0.23831100
H	-8.57838700	-2.13334500	-0.16893000
H	-7.28772200	-2.87946800	0.81022300
H	-7.58684100	-1.12211000	0.91582700
C	-1.66796100	2.99296500	1.55060200
C	-1.32745300	1.65336400	1.36410000
C	-1.91278300	3.81795400	0.44589200
C	-1.21247100	1.07575200	0.08304900
C	-1.48572500	1.92366500	-1.00026800
C	-1.82213500	3.27612400	-0.83978100
H	-1.45893000	1.53276000	-2.01593600
H	-2.02432500	3.88069500	-1.71748100
H	-1.15555400	1.04882800	2.25220900
H	-1.75565100	3.41962800	2.54599600
O	-2.23528300	5.12283900	0.72834200
C	-2.51946900	5.98270500	-0.35832500
H	-2.75290300	6.95688700	0.07601900
H	-1.65839600	6.08847000	-1.03289100
H	-3.38244900	5.63398000	-0.94170800

TS10

B3LYP/BSI SCF energy: -2023.827765 a.u.
M06/BSII SCF energy in solution: -2023.120162 a.u.
M06/BSII free energy in solution: -2022.457609 a.u.

C	2.29773300	-2.06156900	-0.29742100
H	2.23734700	-2.55498200	0.68369800
C	1.43893100	-2.92010100	-1.25407300
H	1.45191600	-2.48525500	-2.26059200
H	0.39415000	-2.91846600	-0.92452400
C	1.96975300	-4.36173100	-1.32744700
H	1.84998400	-4.83942900	-0.34465100
H	1.36480200	-4.94470100	-2.03208200
C	3.45013100	-4.40148500	-1.73455800
H	3.55120000	-4.03675300	-2.76702100
H	3.81843700	-5.43427400	-1.73261500
C	4.30841600	-3.52918800	-0.80707900

H	4.30911800	-3.96396900	0.20264500
H	5.35203500	-3.52408300	-1.14442300
C	3.77691200	-2.08604600	-0.73304200
H	4.39819800	-1.49801000	-0.04819800
H	3.87423400	-1.62221300	-1.72266900
C	2.56965700	0.26507900	1.50934700
H	3.60614400	0.32228900	1.14866100
C	2.55275500	-0.66629000	2.74163400
H	2.90814100	-1.66865400	2.47990700
H	1.51942000	-0.78204000	3.09356900
C	3.41858700	-0.10684400	3.88425300
H	4.47089700	-0.09406700	3.56560100
H	3.36355900	-0.77871300	4.74914600
C	2.99290800	1.31338000	4.27921900
H	3.65362300	1.70550900	5.06161900
H	1.98204200	1.28153500	4.70985700
C	2.99295300	2.24543900	3.06032700
H	2.63439200	3.24303100	3.34062100
H	4.02474600	2.37390900	2.70198800
C	2.12402900	1.68652100	1.92134900
H	1.07643700	1.65510800	2.24392900
H	2.15546500	2.37071600	1.06727100
C	1.87149700	0.82644700	-1.31022100
H	1.22535800	1.67100900	-1.02981300
C	3.30716500	1.37204800	-1.47195700
H	3.68873900	1.76892700	-0.52636500
H	3.98521000	0.56264800	-1.76754000
C	3.35533100	2.48228500	-2.53854500
H	4.38601200	2.83937500	-2.65386600
H	2.76505200	3.34060100	-2.18787100
C	2.80121600	2.00473300	-3.88792600
H	3.46602900	1.23082400	-4.29793600
H	2.79969000	2.82835300	-4.61190500
C	1.38767900	1.42540000	-3.73385500
H	0.69469300	2.22543500	-3.43946000
H	1.02852500	1.03484000	-4.69378100
C	1.34872000	0.31510600	-2.67046300
H	1.97191600	-0.52118100	-3.01222900
H	0.32973600	-0.07307100	-2.56618100
Ni	-0.73181000	-0.68365500	0.62409700
P	1.51134400	-0.38871300	0.08975900
O	-0.77202100	-2.95653600	2.48849100
C	-0.71559900	-2.11134900	1.70290400
C	-2.62749300	-0.61653800	0.21505200
C	-3.69472500	-0.59864400	1.12737000
C	-2.87948100	-1.18156600	-1.05447400

C	-4.94302000	-1.14079700	0.81451100
H	-3.56008700	-0.14673700	2.10631200
C	-4.11341000	-1.73852400	-1.37434800
H	-2.09839700	-1.18595100	-1.81177300
C	-5.15809100	-1.72345700	-0.44114000
H	-5.73358400	-1.10514900	1.55585700
H	-4.29458500	-2.18004600	-2.34987600
O	-6.33925500	-2.28340900	-0.85297200
C	-7.42219200	-2.29416400	0.05874100
H	-8.24950200	-2.78488300	-0.45742900
H	-7.18261100	-2.85823200	0.97029000
H	-7.72822000	-1.27780800	0.34166400
C	-1.66147600	3.21584200	1.32420100
C	-1.68197100	3.88448500	0.09283800
C	-1.65376500	3.13291900	-1.08858600
C	-1.57869200	1.73827800	-1.02768300
C	-1.52419300	1.04089500	0.19259500
C	-1.60666600	1.82677400	1.36782400
H	-1.71108600	3.80476200	2.23545000
H	-1.63364600	1.34197000	2.34144800
H	-1.58920000	1.18713800	-1.96370500
H	-1.70094600	3.61614600	-2.05839600
O	-1.75166500	5.25191600	0.15169500
C	-1.81152300	5.96733700	-1.06839000
H	-2.70116600	5.70090900	-1.65484300
H	-1.86466300	7.02390300	-0.79934000
H	-0.91798300	5.79894200	-1.68500600

Pr2

B3LYP/BSI SCF energy: -692.35866 a.u.
M06/BSII SCF energy in solution: -692.041209 a.u.
M06/BSII free energy in solution: -691.835714 a.u.

C	-0.73925600	-0.05869000	-0.05715000
C	-1.55736300	1.01307100	0.32595300
C	-1.37889400	-1.25385200	-0.44086600
C	-2.95067100	0.91447400	0.33054600
H	-1.10014100	1.94227100	0.65371700
C	-2.76163200	-1.37033200	-0.43819400
H	-0.77941600	-2.09727900	-0.77079100
C	-3.56160000	-0.28459900	-0.05236300
H	-3.54072000	1.76779900	0.64371600
H	-3.24993700	-2.29017100	-0.74366000
O	-4.91047700	-0.49787400	-0.08501500
C	-5.76609400	0.56871300	0.28956500
H	-6.78427500	0.18951300	0.18788800
H	-5.59947500	0.87725500	1.32997000

H	-5.63965900	1.44063500	-0.36557700
C	2.76177200	1.37040600	-0.43812000
C	3.56159700	0.28461900	-0.05238100
C	2.95051100	-0.91444200	0.33047000
C	1.55731100	-1.01291600	0.32585200
C	0.73926600	0.05894300	-0.05719000
C	1.37898600	1.25400400	-0.44085700
H	3.24996600	2.29032200	-0.74351000
H	0.77968900	2.09758100	-0.77074300
H	1.09991100	-1.94197900	0.65377300
H	3.54057900	-1.76764900	0.64390900
O	4.91054100	0.49761300	-0.08505700
C	5.76602600	-0.56902100	0.28961600
H	5.63932800	-1.44113600	-0.36520500
H	6.78428500	-0.19009600	0.18763900
H	5.59960400	-0.87724600	1.33017000

IM14

B3LYP/BSI SCF energy: -2535.051057 a.u.
M06/BSII SCF energy in solution: -2534.182804 a.u.
M06/BSII free energy in solution: -2533.338638 a.u.

C	2.33623100	2.47288300	0.39048300
H	1.47279200	3.15302900	0.35421500
C	3.05667900	2.61365500	-0.97050800
H	3.94989200	1.98082500	-0.98888700
H	2.42054100	2.25901300	-1.78619500
C	3.48559400	4.07186700	-1.20396300
H	2.59240200	4.70823600	-1.28123000
H	4.00850900	4.15229400	-2.16412500
C	4.38004600	4.58367500	-0.06491300
H	5.32629300	4.02398000	-0.07206900
H	4.64013400	5.63662100	-0.22531200
C	3.70202200	4.40835200	1.30171100
H	2.82442200	5.06792400	1.35904400
H	4.37772600	4.72009000	2.10725400
C	3.25112300	2.95456600	1.53712800
H	2.74420700	2.88033000	2.50543800
H	4.13745400	2.30967200	1.59516000
C	0.55040200	1.01941500	2.26712900
H	1.32494400	1.12521000	3.03825800
C	-0.34498400	2.27413800	2.33582200
H	0.23966400	3.18044500	2.14341100
H	-1.10988700	2.21520800	1.55458500
C	-1.00824400	2.39175000	3.72030600
H	-0.23076100	2.55851900	4.48021000
H	-1.65631800	3.27631800	3.74142100

C	-1.81093500	1.13445100	4.08198700
H	-2.22337800	1.22623600	5.09410700
H	-2.66397100	1.04071200	3.39864700
C	-0.94891100	-0.13076000	3.97063300
H	-1.55906300	-1.02270900	4.15398500
H	-0.17157400	-0.11536400	4.74874100
C	-0.28472500	-0.24151400	2.58748100
H	-1.06173600	-0.35861200	1.82243800
H	0.33411800	-1.14531400	2.54856000
C	2.75654800	-0.52960700	1.02539200
H	2.19179600	-1.44919900	0.82212100
C	3.26027200	-0.61006100	2.48574000
H	2.42771800	-0.66059900	3.19190200
H	3.82987200	0.29480800	2.73287800
C	4.15368000	-1.84825500	2.69397100
H	4.51285300	-1.86710600	3.73002200
H	3.54297600	-2.75213100	2.55968600
C	5.33363300	-1.88564100	1.71510200
H	6.01469700	-1.05132700	1.93640700
H	5.91303000	-2.80606600	1.85444300
C	4.84713000	-1.76851800	0.26560200
H	4.26893600	-2.66229700	-0.00575800
H	5.70014600	-1.72821400	-0.42234500
C	3.97007000	-0.52097600	0.06528500
H	4.57939000	0.36785200	0.27054200
H	3.65210600	-0.45583000	-0.97694200
Ni	0.04607000	0.39073500	-1.01828400
P	1.47351400	0.81749700	0.63899400
F	-1.41928300	-0.15967300	-2.21768700
B	-2.48290700	0.66308200	-1.43827100
O	-1.59860100	1.71123900	-0.81970700
O	-3.32619700	1.34123900	-2.35947000
C	-1.71056200	2.91169300	-1.65410700
C	-3.15979300	2.75345000	-2.25744800
C	-1.52390700	4.14220300	-0.76689400
H	-2.18801100	4.12253300	0.09886000
H	-0.49283200	4.19764900	-0.40381100
H	-1.72265300	5.05713800	-1.33541600
C	-0.62310900	2.88869500	-2.73752900
H	-0.73664800	2.03305300	-3.40556800
H	-0.64507800	3.80480600	-3.33611000
H	0.36233200	2.82714800	-2.26631100
C	-3.33419900	3.36574600	-3.65182400
H	-4.36021800	3.19367900	-3.98991900
H	-3.15903900	4.44753600	-3.64239500
H	-2.66327400	2.90437400	-4.37821200

C	-4.25922500	3.30384400	-1.32942500
H	-4.15273700	2.92122600	-0.31163800
H	-4.26047300	4.39828400	-1.29216800
H	-5.22834800	2.97020400	-1.70990100
C	1.19624800	-0.79415500	-1.86280500
O	1.93880300	-0.29583600	-2.69793300
C	1.11081700	-2.26891000	-1.66132600
C	0.18935300	-2.83884800	-0.76581900
C	1.96711900	-3.11639500	-2.38028500
C	0.12830500	-4.21295200	-0.59074800
H	-0.49760100	-2.19610600	-0.22364800
C	1.92218200	-4.49697100	-2.20969200
C	0.99686200	-5.05176800	-1.30958200
H	-0.58807300	-4.66527900	0.08694000
C	-3.17693800	-0.35456100	-0.40856500
C	-3.28928800	-1.73237100	-0.68485100
C	-3.78958500	0.08997500	0.77139200
C	-3.96246600	-2.60829300	0.16138600
H	-2.83904700	-2.12581300	-1.59159500
C	-4.47399100	-0.76744600	1.64153300
H	-3.73933700	1.14446000	1.03246100
C	-4.56101400	-2.12956400	1.33456200
H	-4.04634800	-3.66655100	-0.06791700
H	-4.93403000	-0.36562000	2.53752100
O	-5.20118600	-3.06439400	2.10563200
C	-5.84764600	-2.62361700	3.28523500
H	-5.13970900	-2.17861600	3.99792000
H	-6.63737900	-1.89171500	3.06892700
H	-6.29668700	-3.51075800	3.73596200
H	2.66884900	-2.67041400	-3.07822600
H	2.59579500	-5.12879800	-2.77647300
O	0.86404600	-6.38218300	-1.06657200
C	1.68984200	-7.29141700	-1.78096400
H	1.40289800	-8.28723700	-1.44057900
H	1.52750500	-7.21828500	-2.86337100
H	2.75287600	-7.12790300	-1.56376300

TS11

B3LYP/BSI SCF energy: -2535.030172 a.u.
M06/BSII SCF energy in solution: -2534.169996 a.u.
M06/BSII free energy in solution: -2533.325292 a.u.

C	-2.16635100	2.48496800	-0.05826300
H	-2.93156800	1.77956100	0.29305100
C	-2.37339500	2.62037200	-1.58497300
H	-1.62142300	3.29365700	-2.00990600
H	-2.23007100	1.65070800	-2.07207400

C	-3.77244000	3.17838300	-1.90072800
H	-4.53356900	2.44929000	-1.58944600
H	-3.88272600	3.29683700	-2.98489200
C	-4.02943700	4.51294400	-1.18688100
H	-3.34554000	5.27572400	-1.58610900
H	-5.04600100	4.86721200	-1.39452600
C	-3.81141000	4.38381900	0.32702500
H	-4.57086500	3.70987700	0.74817900
H	-3.94877400	5.35404900	0.81961600
C	-2.41141400	3.83200000	0.65217200
H	-2.29781900	3.73048900	1.73745400
H	-1.66010700	4.56020600	0.32290100
C	-0.71312800	1.31940600	2.26115600
H	-0.73174500	2.32286000	2.70620300
C	-2.00128400	0.59106700	2.69140500
H	-2.88678300	1.14081300	2.35803600
H	-2.04150500	-0.38894000	2.20300800
C	-2.06604100	0.41766100	4.21916600
H	-2.14746700	1.40712300	4.69188000
H	-2.97813300	-0.12920200	4.48622300
C	-0.82882600	-0.30369800	4.76958700
H	-0.87966300	-0.36764900	5.86294300
H	-0.81576400	-1.33726200	4.39564700
C	0.45932200	0.40668900	4.33368900
H	1.33966700	-0.14726200	4.68122600
H	0.50792200	1.39733500	4.80815200
C	0.52189700	0.56846200	2.80581900
H	0.55799000	-0.42414300	2.33953400
H	1.44968800	1.07897300	2.52578500
C	0.89467000	2.75942100	0.24051300
H	1.74563400	2.06923500	0.29938400
C	1.08420800	3.80472100	1.36556700
H	1.06913200	3.33419900	2.35246200
H	0.26171700	4.52966900	1.34971200
C	2.41999400	4.55385300	1.19845200
H	2.52038400	5.30196500	1.99422200
H	3.24667600	3.84217400	1.33343500
C	2.54260300	5.21586900	-0.17989700
H	1.79334500	6.01600900	-0.26591300
H	3.52316000	5.69540700	-0.28470900
C	2.32065400	4.19369800	-1.30206800
H	3.13648900	3.45817800	-1.29828600
H	2.34867200	4.68745600	-2.28074900
C	0.97959400	3.45801600	-1.13721900
H	0.16853000	4.19206800	-1.21892200
H	0.84455100	2.74160300	-1.95084100

Ni	-0.49301200	-0.38309300	-0.70991000
P	-0.58005900	1.57483800	0.39571400
F	-1.42946200	-1.98089800	-2.58591900
B	-1.63267300	-2.48581700	-1.25542900
O	-2.27901700	-1.40423100	-0.41511500
O	-2.57648900	-3.57115300	-1.23945500
C	-3.71306000	-1.60328200	-0.56045200
C	-3.78035900	-3.18432000	-0.58713300
C	-4.46328700	-0.97275200	0.61087000
H	-4.07581900	-1.30447200	1.57489000
H	-4.39670900	0.11897700	0.56918200
H	-5.52523600	-1.23657000	0.55948200
C	-4.19074300	-0.96613400	-1.87494900
H	-3.69639800	-1.41577500	-2.73594700
H	-5.27537900	-1.06242600	-1.98796400
H	-3.94709300	0.09982400	-1.86563700
C	-4.96924600	-3.74152000	-1.37931100
H	-4.94451100	-4.83492300	-1.34362800
H	-5.92695900	-3.41138100	-0.95991400
H	-4.91940700	-3.44237300	-2.42749400
C	-3.78064300	-3.80242800	0.82457700
H	-2.97964100	-3.38405400	1.43985700
H	-4.73324100	-3.66179000	1.34721100
H	-3.59890400	-4.87623000	0.72583400
C	1.01689100	0.07306000	-1.67226500
O	0.67895700	0.40577000	-2.79882000
C	2.45229700	0.01047600	-1.27534800
C	2.86103700	-0.44952600	-0.01352100
C	3.43072200	0.43235200	-2.18841400
C	4.20368700	-0.47190500	0.33252500
H	2.11498200	-0.80866400	0.68577400
C	4.78230700	0.41552800	-1.85527400
C	5.17462400	-0.03618000	-0.58466200
H	4.53436500	-0.83351200	1.30055800
C	-0.14452600	-2.77737900	-0.63359200
C	0.90372100	-3.20663400	-1.48546200
C	0.07880100	-2.93233800	0.74999800
C	2.07203700	-3.77110100	-0.99627700
H	0.76645900	-3.10376900	-2.55771400
C	1.25120400	-3.48785800	1.27047600
H	-0.70811300	-2.64350200	1.44180800
C	2.25201100	-3.91986500	0.38892900
H	2.86260500	-4.11121000	-1.65801000
H	1.36550100	-3.59900800	2.34301100
O	3.42802700	-4.49248700	0.77551400
C	3.65076600	-4.70796600	2.15911500

H	3.66588300	-3.76441200	2.72064800
H	2.89031000	-5.36892200	2.59437600
H	4.62888200	-5.18545800	2.23705800
H	3.11094000	0.77474100	-3.16749100
H	5.51583200	0.74840200	-2.58015100
O	6.46135300	-0.09064600	-0.15017000
C	7.49594900	0.31263600	-1.03714100
H	8.42937800	0.18073700	-0.48836600
H	7.51674800	-0.30847700	-1.94101700
H	7.39214400	1.36609900	-1.32574000

IM15

B3LYP/BSI SCF energy: -2535.031478 a.u.
M06/BSII SCF energy in solution: -2534.171607 a.u.
M06/BSII free energy in solution: -2533.3284 a.u.

C	-2.46629300	2.01112800	-0.52445000
H	-3.11790900	1.31035300	0.01407100
C	-2.55217300	1.61756200	-2.01938700
H	-1.86501300	2.23242200	-2.60960100
H	-2.24275100	0.57696400	-2.15379200
C	-3.97852800	1.80798300	-2.56310000
H	-4.65011500	1.08465600	-2.08184800
H	-3.99034100	1.57380600	-3.63384500
C	-4.50751200	3.22766600	-2.31789900
H	-3.90874300	3.94669300	-2.89564800
H	-5.53884600	3.32039100	-2.67886800
C	-4.43396400	3.59270500	-0.82894100
H	-5.11254800	2.94013700	-0.26131800
H	-4.78043300	4.62042800	-0.66486900
C	-3.00461500	3.43684100	-0.27784800
H	-2.99215800	3.68039600	0.79129200
H	-2.35526600	4.16822500	-0.77430300
C	-0.99939700	1.87719100	2.07568700
H	-1.18768800	2.94916000	2.21378600
C	-2.19159700	1.11252200	2.67780100
H	-3.12367500	1.38307400	2.17073300
H	-2.04483100	0.03979500	2.51751900
C	-2.33576000	1.39385100	4.18381400
H	-2.58688400	2.45403100	4.33155400
H	-3.17725700	0.81661600	4.58497500
C	-1.04878800	1.06599700	4.95284800
H	-1.16011500	1.32558800	6.01224200
H	-0.87069000	-0.01801400	4.91309600
C	0.15713400	1.79613900	4.34646000
H	1.08056800	1.50459900	4.86107600
H	0.04399900	2.87895000	4.49961900

C	0.28967300	1.50690000	2.84188500
H	0.47895300	0.43516600	2.69740500
H	1.16091900	2.03222000	2.43623200
C	0.46307100	2.96740600	-0.24860200
H	1.42380500	2.47834500	-0.03789500
C	0.42743600	4.26982300	0.58655900
H	0.46993100	4.06046000	1.65858800
H	-0.51406700	4.80372700	0.40695000
C	1.60868400	5.19095300	0.22602800
H	1.54397100	6.11290000	0.81675500
H	2.54607800	4.69789600	0.52060100
C	1.65685200	5.51418700	-1.27247700
H	0.78077400	6.12206900	-1.54043100
H	2.54002900	6.12258400	-1.50155200
C	1.65362700	4.22904400	-2.10884300
H	2.58695700	3.67468400	-1.93753900
H	1.62522400	4.46800000	-3.17858800
C	0.46049900	3.32501400	-1.75509900
H	-0.46588000	3.85978900	-1.99842900
H	0.48621700	2.42387600	-2.36898400
Ni	-0.27763500	-0.53299500	-0.32846400
P	-0.78573000	1.61009800	0.22120600
F	-1.79336100	-1.78622600	-2.24255100
B	-1.57504800	-2.50299500	-1.02257400
O	-2.08273700	-1.71518400	0.14777400
O	-2.31170900	-3.74128300	-1.00902000
C	-3.40666000	-2.23670700	0.44869600
C	-3.23694800	-3.76219400	0.06704200
C	-3.75784800	-2.01335900	1.91884900
H	-2.94184700	-2.31672600	2.57861800
H	-3.98735000	-0.96230600	2.10969300
H	-4.64743200	-2.59462300	2.18534600
C	-4.43515000	-1.52326300	-0.44177700
H	-4.21096600	-1.67706200	-1.49863600
H	-5.45279500	-1.87016600	-0.23581700
H	-4.40281800	-0.44926300	-0.23737000
C	-4.53111500	-4.43079300	-0.41564700
H	-4.32623000	-5.47966700	-0.65066100
H	-5.31352800	-4.40378800	0.35200400
H	-4.90767300	-3.95541600	-1.32289400
C	-2.64404300	-4.60568300	1.21377000
H	-1.74696100	-4.14287600	1.63143600
H	-3.36004000	-4.77181100	2.02593200
H	-2.35610400	-5.57893300	0.80633400
C	1.24131000	-0.00814800	-1.25858700
O	1.05801800	0.23565200	-2.44063400

C	2.61337500	0.08873900	-0.66411800
C	2.87411300	-0.16502900	0.69118200
C	3.68276800	0.45935600	-1.49382600
C	4.15810500	-0.04711100	1.20471900
H	2.05752700	-0.46575400	1.33738600
C	4.97663500	0.57979700	-0.99588900
C	5.21974700	0.32530800	0.36352000
H	4.37137300	-0.23893400	2.25144600
C	0.05976900	-2.65642100	-0.81685400
C	0.88080900	-2.91180800	-1.95150300
C	0.63534700	-2.94548400	0.44109500
C	2.15351400	-3.43538400	-1.83753800
H	0.47687900	-2.68975000	-2.93420000
C	1.93081400	-3.45516000	0.58404300
H	0.03125400	-2.81170300	1.33468400
C	2.69060300	-3.70838500	-0.56267200
H	2.76773500	-3.64320100	-2.70821500
H	2.32511900	-3.65947300	1.57277400
O	3.95214400	-4.21535200	-0.55775100
C	4.56911800	-4.48265500	0.69294400
H	4.66418600	-3.57075300	1.29546000
H	4.01463000	-5.23772500	1.26429900
H	5.56349000	-4.86749700	0.46141800
H	3.47621800	0.65021000	-2.54210000
H	5.78191600	0.86574500	-1.66218800
O	6.44003100	0.41266700	0.95762200
C	7.55835900	0.77895900	0.16038300
H	8.41730700	0.78310000	0.83275500
H	7.73314900	0.05590100	-0.64584000
H	7.43415100	1.77898000	-0.27345000

TS12

B3LYP/BSI SCF energy: -2535.017888 a.u.
M06/BSII SCF energy in solution: -2534.154203 a.u.
M06/BSII free energy in solution: -2533.312832 a.u.

C	3.21897000	0.78381600	-0.14594200
H	2.94458500	1.52583800	0.61644000
C	3.13600500	1.51980800	-1.50419500
H	3.39094900	0.83332800	-2.31820500
H	2.11751300	1.86540300	-1.69146600
C	4.11393100	2.70749500	-1.54297500
H	3.80039700	3.45961500	-0.80615500
H	4.05915900	3.19313700	-2.52450800
C	5.55588500	2.27654800	-1.24021700
H	5.91410700	1.61841600	-2.04478200
H	6.22287600	3.14712400	-1.23002300

C	5.63934700	1.52646700	0.09643600
H	5.39590700	2.21683700	0.91687600
H	6.66291300	1.17627700	0.27810500
C	4.66769300	0.33337900	0.13684500
H	4.74664000	-0.16859600	1.10746900
H	4.97711000	-0.39740500	-0.62052500
C	2.14861100	-1.08927100	1.87909300
H	3.17014800	-1.48913200	1.92206400
C	2.04922200	0.05199000	2.91069900
H	2.74813200	0.86096200	2.67215100
H	1.04020200	0.48018700	2.86492000
C	2.32355100	-0.45273600	4.33855600
H	3.36651500	-0.79397800	4.40464700
H	2.22297300	0.37692600	5.04884800
C	1.38730600	-1.60534400	4.72582200
H	1.63982600	-1.98208000	5.72413400
H	0.35619800	-1.22854300	4.78542800
C	1.44936200	-2.73827000	3.69245800
H	0.72846100	-3.52515600	3.94392300
H	2.44454200	-3.20483500	3.72334000
C	1.17317900	-2.22066500	2.27097400
H	0.14732700	-1.83897500	2.21867100
H	1.22248100	-3.05181400	1.56066900
C	2.29097500	-2.06007500	-0.90812500
H	1.35135200	-2.62654300	-0.85515900
C	3.40915000	-2.98775400	-0.37995100
H	3.25898500	-3.24340400	0.67279700
H	4.37935300	-2.48040300	-0.44414600
C	3.46483700	-4.28923600	-1.20291200
H	4.27400400	-4.92764200	-0.82713600
H	2.53018100	-4.84668300	-1.04753200
C	3.64842900	-4.01731100	-2.70236100
H	4.64397400	-3.58116200	-2.86966200
H	3.62412800	-4.95939900	-3.26347600
C	2.57970600	-3.04887100	-3.22693000
H	1.59131100	-3.52591100	-3.18679200
H	2.76615700	-2.80924300	-4.28055900
C	2.53848000	-1.75172900	-2.40265600
H	3.50352700	-1.24049400	-2.50862000
H	1.76202400	-1.08931600	-2.79056900
Ni	-0.21563800	0.39616300	-0.32498700
P	1.86728000	-0.51322400	0.10342300
F	-0.11810400	2.43228900	-2.19468100
B	-0.61514000	2.76108500	-0.96397600
O	0.23391000	2.55183800	0.16527800
O	-1.31407500	3.95193900	-0.84863100

C	0.12112000	3.69604700	1.06817900
C	-1.00291500	4.61871200	0.38156500
C	-0.24156300	3.20909800	2.47246500
H	-1.18094300	2.65592800	2.48896100
H	0.54854100	2.55624100	2.84938400
H	-0.33139200	4.05531600	3.16070900
C	1.51186300	4.34228500	1.11765700
H	1.86225900	4.61756100	0.12137100
H	1.51638800	5.23630800	1.74868900
H	2.22618500	3.63006000	1.54080300
C	-0.51387300	6.02691100	0.00958200
H	-1.31608600	6.54229500	-0.52528000
H	-0.26130900	6.61856600	0.89558300
H	0.35358600	5.99230600	-0.65200600
C	-2.29973800	4.75643200	1.19391700
H	-2.75222500	3.78890300	1.41082100
H	-2.13452200	5.29434700	2.13286300
H	-3.01836500	5.32633700	0.59837800
C	-0.81947100	-1.10453000	-1.23833800
O	-0.53877300	-1.20673100	-2.42587300
C	-1.60614700	-2.19972800	-0.56941500
C	-2.11956000	-2.08623500	0.73178200
C	-1.83908600	-3.38932100	-1.27381300
C	-2.83639900	-3.12347000	1.31153800
H	-1.96531900	-1.16367400	1.28085900
C	-2.55052700	-4.44368000	-0.70587000
C	-3.05476900	-4.31226700	0.59673500
H	-3.24559800	-3.04071900	2.31335400
C	-2.02326000	1.17221000	-0.70998700
C	-2.68547600	1.11346300	-1.96286900
C	-2.87226700	1.29199900	0.41192400
C	-4.06383300	1.21341800	-2.08876500
H	-2.08840300	0.99806100	-2.86215300
C	-4.26299200	1.37269400	0.32092200
H	-2.43794100	1.32781000	1.40950700
C	-4.86560800	1.34129000	-0.94463700
H	-4.54938000	1.18734700	-3.05967400
H	-4.85917900	1.46089800	1.22257100
O	-6.20877000	1.42720600	-1.16469600
C	-7.06859100	1.55363000	-0.04444300
H	-6.99398800	0.68680800	0.62505400
H	-6.85752500	2.46606800	0.52834400
H	-8.08179300	1.60947000	-0.44608200
H	-1.45420100	-3.46768300	-2.28578800
H	-2.71097700	-5.35019400	-1.27796700
O	-3.76509800	-5.27292300	1.25127000

C	-4.03632700	-6.49121900	0.57466400
H	-4.61549800	-7.09959300	1.27098500
H	-4.62505000	-6.32558900	-0.33634800
H	-3.11281100	-7.02327100	0.31294700