Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Mechanistic insight into *anti*-carbometalation of the alkyne via η^2-vinyl-nickel type *E/Z* isomerization

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1. Complete reference for Gaussian 09

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

2. Another possible mechanism

An alternative route in which the ring-expansion product is generated was calculated, too. As shown in Figure S1, after the alkenylnickel intermediate **5a** is generated, the carbonyl is inserted into Ni-C bond via transition state **19-ts** to generate nickel alkoxide intermediate **20** with an activation free energy of 12.6 kcal/mol. However, this process is endergonic with a free energy of 10.7 kcal/mol, which could be attributed to the higher ring strain of the resulting quaternary. Then 1,3-nickel migrate proceeds via transition state **21-ts** to generate ring-expansion intermediate **22** with an energy barrier of 23.0 kcal/mol. Correspondingly, transmetallation via transition state **23-ts** leads to the generation of the ring-expansion borate, which could further undergo protonolysis with water to yield the ring-expansion product. The calculation results showed that the overall activation energy is 33.7 kcal/mol, which is 11.8 kcal/mol higher than the generation pathway of 5,5-bicycle product in Fig. 3. Another possible oxidative addition mechanism has also been calculated via transition state **25-ts**. However, the calculated reaction energy for this process is as high as 39.2 kcal/mol revealing an unfavorable process.

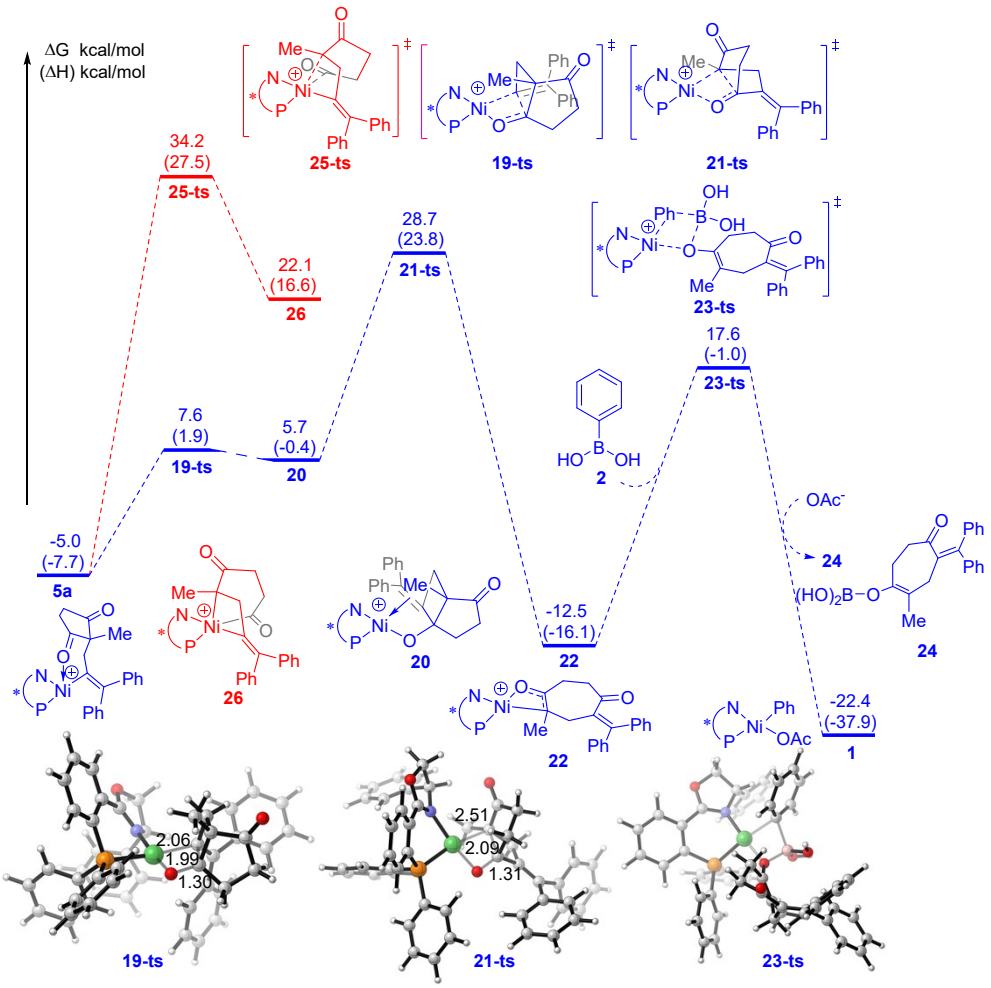

Figure S1. Free energy profile of the synthesis of ring-expansion products of nickel-catalyzed transformation. The bond lengths are given in angstroms.

3. Cartesian coordinates and energies of optimized structures

1
B3LYP SCF energy: -2142.901967 a.u.
B3LYP enthalpy: -2142.300803 a.u.
B3LYP free energy: -2142.411623 a.u.
M06 SCF energy in solution: -2142.274117 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.55142000	-1.11715600	-0.03058300
C	2.92342200	-1.84788400	-1.12382500
C	4.17547800	-2.71912000	-1.16998600
H	4.78010700	-2.58389500	-0.26705600
H	3.87174900	-3.77212400	-1.20186900
H	4.76819400	-2.49221500	-2.05899100
O	2.30792900	-1.86550200	0.02161900
O	2.56071300	-1.19893900	-2.11491200
C	-3.07826700	0.48050100	2.22688200
C	-1.78063900	0.47748700	1.70128900
C	-0.72693300	0.96925900	2.51355400
C	-1.00454900	1.44112100	3.80591000
C	-2.30386000	1.43166200	4.30814100
C	-3.34328100	0.95193600	3.51547900
H	-3.89625500	0.10061700	1.62484500
H	-0.18820000	1.81458600	4.41250100
H	-2.49787400	1.79602900	5.31266000
H	-4.36185500	0.93820000	3.89341900
C	0.66982900	1.04427700	2.04760400
O	1.51524200	1.74443200	2.84337300
C	2.84696800	1.51620900	2.30287200
C	2.57780900	1.06321900	0.85789100
H	3.40732600	2.44661900	2.39061200
H	3.31822000	0.73314800	2.90626100
H	3.20900200	0.22155900	0.57824300
N	1.17825800	0.54811500	0.97122000
P	-1.45214100	-0.18371200	-0.00353100

C	-2.99705300	-1.09666000	-0.41008900
C	-3.94478500	-0.61247800	-1.32289300
C	-3.21698200	-2.34042600	0.20675200
C	-5.09529300	-1.35338200	-1.60577200
H	-3.78731800	0.33829500	-1.82035200
C	-4.36920900	-3.07222000	-0.07244200
H	-2.47360400	-2.75085100	0.88206300
C	-5.31160100	-2.58051300	-0.97955100
H	-5.81868100	-0.96859400	-2.31965500
H	-4.52161000	-4.03538000	0.40632500
H	-6.20503900	-3.15726500	-1.20346600
C	-1.46164100	1.30669900	-1.08167400
C	-0.55081700	1.35029100	-2.14939600
C	-2.34087900	2.38283300	-0.87973600
C	-0.53794500	2.44838000	-3.01185900
H	0.16198600	0.54162700	-2.29377300
C	-2.32237000	3.47755200	-1.74401400
H	-3.03775300	2.36795500	-0.04620200
C	-1.42312100	3.50870600	-2.81322800
H	0.17724300	2.47757400	-3.82829300
H	-3.00616200	4.30637500	-1.58057400
H	-1.40724500	4.36375600	-3.48390600
C	2.68424700	2.17234300	-0.18207200
C	2.28011300	3.48385700	0.11299800
C	3.20127900	1.89307200	-1.45340700
C	2.40646200	4.49814600	-0.83567200
H	1.86212800	3.72048800	1.08854300
C	3.32918400	2.91087200	-2.40187500
H	3.46656200	0.87333700	-1.71566700
C	2.93886800	4.21512600	-2.09584800
H	2.09196100	5.50894900	-0.58916200
H	3.73655800	2.67825400	-3.38233600
H	3.04567600	5.00673400	-2.83315500
C	0.00355700	-3.90270100	0.07748300
C	-0.04965200	-2.76749300	-0.74625000
C	-0.48889400	-2.92944600	-2.06726300
C	-0.87865300	-4.18479100	-2.54795900
C	-0.84247700	-5.30217500	-1.71173300
C	-0.39781900	-5.15715400	-0.39533900
H	0.37807600	-3.81680000	1.09574900
H	-0.52289300	-2.07628700	-2.74101500
H	-1.21120900	-4.28715500	-3.57913300
H	-1.14884900	-6.27706700	-2.08379500
H	-0.34983200	-6.02361500	0.26201400

2

B3LYP SCF energy: -730.400114 a.u.
B3LYP enthalpy: -730.133298 a.u.
B3LYP free energy: -730.196226 a.u.
M06 SCF energy in solution: -730.118661 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.96957200	-0.88434700	0.33901000
C	-1.44881200	-0.78029100	0.54400500
C	-1.14405800	0.72340000	0.56736100
C	-2.25730100	1.48375000	-0.16584400
C	-3.42008300	0.47983600	-0.20141800
H	-3.28771500	-1.68175800	-0.33957900
H	-3.49605800	-1.05232200	1.28785100
H	-0.90074200	-1.22421100	-0.29856200
H	-1.07336000	-1.25428600	1.45452700
O	-4.53198200	0.73141300	-0.61152400
O	-0.18568100	1.23086900	1.10625200
C	-2.63231600	2.80152500	0.52021300
H	-1.77870000	3.48382800	0.50563200
H	-3.47883300	3.26288900	0.00223200
H	-2.91871500	2.63443300	1.56390200
C	-1.84092500	1.72798500	-1.66421800
H	-1.67535200	0.76235200	-2.16455900
H	-2.71092000	2.17978400	-2.15859500
C	-0.65694000	2.56592400	-1.80661600
C	0.34982100	3.23787800	-1.87523400
C	1.55316000	4.00767200	-1.90652400
C	1.88158300	4.80457400	-3.01934500
C	2.43191600	3.97007400	-0.80563000
C	3.06231200	5.54406100	-3.02862500
H	1.20531600	4.83518600	-3.86828500
C	3.60931000	4.71372700	-0.82396800
H	2.17278000	3.35458000	0.05058300
C	3.92883600	5.50152800	-1.93337700
H	3.30676500	6.15568300	-3.89298600
H	4.28027600	4.67839000	0.03013800
H	4.84872500	6.07987900	-1.94413600

3

B3LYP SCF energy: -2644.636413 a.u.
B3LYP enthalpy: -2643.822523 a.u.
B3LYP free energy: -2643.962388 a.u.
M06 SCF energy in solution: -2643.817067 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.04889300	3.56929900	3.92797800
C	0.17217400	6.01832200	7.71276800
C	-0.32294500	5.60005700	6.47175800
C	-0.71689200	6.58724900	5.53547100
C	-0.60630300	7.94657600	5.86697700
C	-0.09980300	8.34153900	7.10366100
C	0.28829400	7.37549300	8.02802200
H	0.47320100	5.27900200	8.44572500
H	-0.91864400	8.69080100	5.14424900
H	-0.01424200	9.39762700	7.33986800
H	0.67953100	7.66833600	8.99787000
C	-1.27335600	6.26029900	4.20945800
O	-1.95389200	7.25649400	3.62211400
C	-2.30181000	6.81456200	2.28432300
C	-1.96053100	5.30217300	2.28281700
H	-3.35988000	7.02623700	2.12872200
H	-1.69565500	7.38944500	1.57895800
H	-1.29895900	5.06811700	1.44921400
N	-1.18129700	5.14942100	3.55015100
P	-0.48231700	3.79604700	6.09428800
C	0.46192700	2.97044200	7.43310600
C	-0.18072700	2.23631800	8.44066700
C	1.86253100	3.08757700	7.45525100
C	0.56700100	1.62993300	9.45305000
H	-1.26016500	2.13333900	8.44168300
C	2.60188700	2.48827300	8.47203000
H	2.37825200	3.63510000	6.67339100
C	1.95567500	1.75567100	9.47200900
H	0.05889000	1.06070100	10.22600200
H	3.68364600	2.58441500	8.47811000
H	2.53480700	1.28288200	10.25992400

C	-2.24435800	3.39889500	6.43208900
C	-2.81458400	2.27247600	5.81889700
C	-3.01282500	4.15157900	7.33505600
C	-4.12246000	1.89144000	6.12007400
H	-2.24094600	1.69179400	5.10301300
C	-4.32590100	3.77511800	7.62264400
H	-2.58924900	5.02532500	7.82053900
C	-4.87962300	2.64184200	7.02196800
H	-4.54991100	1.01427200	5.64357400
H	-4.91247800	4.36363800	8.32223800
H	-5.89820600	2.34581000	7.25609200
C	-3.17744000	4.39915600	2.19457100
C	-4.14300100	4.36503800	3.20929000
C	-3.38960400	3.65410600	1.02650900
C	-5.29862700	3.59825600	3.05818000
H	-3.99669100	4.93633300	4.12227200
C	-4.54733200	2.88679200	0.87574100
H	-2.65300800	3.68916800	0.22712000
C	-5.50414400	2.85747100	1.89142100
H	-6.03895400	3.58134600	3.85250100
H	-4.70511200	2.32022900	-0.03783600
H	-6.40726300	2.26552700	1.77335000
C	0.75543400	0.85285700	4.71930900
C	1.22491800	2.11703600	4.33437400
C	2.60770700	2.28528800	4.16499600
C	3.49401100	1.22442600	4.37997400
C	3.01148000	-0.03196500	4.75307600
C	1.63844200	-0.21611800	4.91635500
H	-0.30654900	0.67588000	4.87300600
H	3.01378700	3.24196900	3.84492000
H	4.56163700	1.37989100	4.24297300
H	3.69843000	-0.85825500	4.91289900
H	1.24786200	-1.18886800	5.20435800
C	-0.50506600	-0.34690500	-1.83125600
C	-0.45969200	1.09414000	-2.37986100
C	-0.21627500	2.00201400	-1.17135900
C	0.31859500	1.16943900	-0.00388100
C	-0.20070300	-0.24392200	-0.33211400
H	-1.47989400	-0.82903400	-1.95658500
H	0.23029900	-1.00971200	-2.30157300
H	-1.37713300	1.40782600	-2.88646900
H	0.35751100	1.24348200	-3.09670600
O	-0.35433500	-1.12432900	0.48230700
O	-0.44389900	3.19569300	-1.14111400
C	1.86981200	1.12156400	-0.08957500
H	2.28723200	2.12446000	0.03575100
H	2.25776700	0.47379500	0.70296000
H	2.21040500	0.72669800	-1.05261600
C	-0.17433700	1.62104800	1.38960200
H	-1.27089600	1.66168800	1.39446300
H	0.11439100	0.85008100	2.11231300
C	0.36496200	2.92193500	1.80506000
C	0.95761700	3.99375900	1.92846500
C	1.59164900	5.26366300	1.70004600
C	2.30661700	5.94770100	2.70011900
C	1.49328400	5.82553000	0.40934500
C	2.91112500	7.17020200	2.41451800
H	2.38683500	5.51766700	3.69364300
C	2.10582900	7.04635400	0.13505400
H	0.94409000	5.28974600	-0.35915600
C	2.81310600	7.72138500	1.13407400
H	3.46479400	7.69057700	3.19056900
H	2.03247100	7.47083300	-0.86205500
H	3.28964600	8.67228500	0.91437300

4-ts

B3LYP SCF energy: -2644.61413 a.u.
B3LYP enthalpy: -2643.801435 a.u.
B3LYP free energy: -2643.936009 a.u.
M06 SCF energy in solution: -2643.79502 a.u.
Imaginary frequency: -281.10 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.02419100	0.20741800	0.43157500
C	4.35371700	-0.03752100	1.83869600
C	3.14464200	-0.49543800	1.30164600
C	2.60473700	-1.70360800	1.80853400
C	3.27493800	-2.40418400	2.82294400
C	4.46761500	-1.91868800	3.35513700
C	5.00886500	-0.73586000	2.85783100
H	4.79323500	0.87931700	1.46303300
H	2.85234600	-3.33294700	3.18863400
H	4.97022500	-2.46639900	4.14622000
H	5.94318300	-0.35040000	3.25552400
C	1.37572300	-2.30689100	1.26659500
O	1.26118900	-3.63554100	1.43147200
C	-0.06904900	-4.00077000	0.96497600
C	-0.49830800	-2.79720000	0.10467500
H	0.01722300	-4.93798300	0.41662100
H	-0.70287000	-4.13227000	1.84691300
H	-1.52470300	-2.51706400	0.33066400
N	0.41060000	-1.72429400	0.63040800
P	2.28761400	0.44105600	-0.05423300
C	3.09145500	2.09346400	-0.01656100
C	3.78385600	2.60689500	-1.12381200
C	2.98624300	2.87825000	1.14512700
C	4.36310800	3.87647200	-1.06623200
H	3.87912200	2.01917400	-2.03032400
C	3.57533700	4.14008500	1.20164800
H	2.45133800	2.50190300	2.01205000
C	4.26363800	4.64342400	0.09477700
H	4.89833600	4.26032300	-1.93006400
H	3.49357800	4.73168800	2.10902800
H	4.72118400	5.62760400	0.13921200
C	2.89673500	-0.32882100	-1.60739600
C	2.06799300	-0.29524500	-2.73876900
C	4.18599100	-0.87483100	-1.71685600
C	2.52776100	-0.77753300	-3.96499100
H	1.05860200	0.09797000	-2.66061400
C	4.63746500	-1.36851800	-2.94094700
H	4.84046100	-0.91040700	-0.85118400
C	3.81239200	-1.31371600	-4.06734100
H	1.87721900	-0.74594100	-4.83364400
H	5.63589100	-1.78991300	-3.01604000
H	4.16983100	-1.69190600	-5.02091200
C	-0.36864600	-2.99743700	-1.39555100
C	0.73948100	-3.65121600	-1.95425200
C	-1.40228800	-2.56613000	-2.23713400
C	0.80637400	-3.88033400	-3.32776100
H	1.55297600	-3.99142700	-1.31775700
C	-1.33092200	-2.79060200	-3.61454700
H	-2.27344000	-2.07196700	-1.81459100
C	-0.23037600	-3.45179600	-4.16146400
H	1.66548400	-4.39636600	-3.74652000

H	-2.14553500	-2.46446100	-4.25536800
H	-0.18309900	-3.64156800	-5.23024600
C	-0.19971500	2.74252000	-1.05393400
C	-0.43218200	2.11138700	0.18650700
C	-0.47608200	2.90975100	1.34535400
C	-0.26546700	4.28927600	1.27329400
C	-0.03804200	4.89732600	0.03809000
C	-0.00509200	4.11885500	-1.12578900
H	-0.17611600	2.15420200	-1.96791400
H	-0.71848500	2.45369500	2.30122600
H	-0.30681500	4.88996900	2.17799700
H	0.09972100	5.97280700	-0.02403200
H	0.17217200	4.58953100	-2.08896200
C	-6.55907000	1.78672200	-1.75716900
C	-6.34914900	0.26774300	-1.61117500
C	-4.95266200	0.08852300	-1.01077000
C	-4.50099000	1.39093500	-0.34875700
C	-5.34942700	2.45170800	-1.09291900
H	-6.60144400	2.11585000	-2.80101000
H	-7.47739100	2.14901900	-1.28210100
H	-6.41278700	-0.28808700	-2.55087300
H	-7.07812500	-0.18776900	-0.92858800
O	-5.08512500	3.63052400	-1.13366600
O	-4.29917200	-0.93370900	-1.08672200
C	-4.98428800	1.42905200	1.12872100
H	-4.49927000	0.64980500	1.72019400
H	-4.74477000	2.40739600	1.55780800
H	-6.06799200	1.28600700	1.20290000
C	-3.00611400	1.73537800	-0.50065700
H	-2.72213900	1.63119600	-1.55519300
H	-2.90770900	2.80138900	-0.27215300
C	-2.02392900	0.95539900	0.32382400
C	-1.79849100	0.02900600	1.17243000
C	-2.24725700	-0.90843400	2.19139200
C	-1.59370600	-0.93630800	3.43939400
C	-3.32551500	-1.78995500	1.97268600
C	-2.01697200	-1.80385800	4.44451000
H	-0.75921200	-0.26381700	3.61606000
C	-3.73566900	-2.66449200	2.97983900
H	-3.82599300	-1.78582600	1.01060000
C	-3.08742700	-2.67333600	4.21741200
H	-1.51045200	-1.80223500	5.40551100
H	-4.56871700	-3.33752500	2.79676900
H	-3.41486700	-3.35129100	5.00027200

5Z

B3LYP SCF energy: -2644.675489 a.u.
B3LYP enthalpy: -2643.860649 a.u.
B3LYP free energy: -2643.998025 a.u.
M06 SCF energy in solution: -2643.855353 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.22458100	3.58968800	1.52280100
C	3.41587800	-0.15118500	2.59233700
C	2.73122500	0.73656200	1.75391100
C	1.77947500	0.20504000	0.84767800
C	1.56295200	-1.17947800	0.78839400
C	2.25294900	-2.04409400	1.63613700
C	3.17604900	-1.52797300	2.54220300
H	4.15050800	0.23153400	3.29168100
H	0.84080400	-1.57077400	0.08096200
H	2.06699400	-3.11239000	1.58631500
H	3.71995400	-2.19069600	3.20878300
C	0.97436600	1.05522400	-0.04340900
O	0.42926000	0.45732700	-1.11432800
C	-0.24295300	1.48700300	-1.89085500
C	-0.20169300	2.74291500	-0.98232200
H	0.31341300	1.61539700	-2.82248600
H	-1.25191700	1.13593200	-2.11105400
H	-1.18711600	2.91780400	-0.53414500
N	0.70618100	2.30856500	0.11534000
P	3.14919800	2.54356400	1.78274500
C	4.09353400	2.76700500	3.33528500
C	5.48012400	2.97590000	3.33654500
C	3.39879800	2.72487200	4.55684600
C	6.16224500	3.14065300	4.54476200
H	6.02891500	3.01456900	2.40167400
C	4.08619000	2.88219700	5.75888900
H	2.32344200	2.57186900	4.56743600
C	5.46888900	3.09424600	5.75455400
H	7.23576900	3.30530100	4.53643300
H	3.54404000	2.84418400	6.69940300
H	6.00137700	3.22253700	6.69249500
C	4.35210700	2.74372200	0.40849500
C	4.54159700	4.02135000	-0.14315800
C	5.10452100	1.66228100	-0.08026000
C	5.47786700	4.21202600	-1.16037500
H	3.96458300	4.86538900	0.21912900
C	6.03274400	1.85973000	-1.10356500
H	4.97186900	0.66787100	0.33371800
C	6.22210800	3.13380000	-1.64362500
H	5.62240700	5.20592000	-1.57398700
H	6.60872800	1.01741800	-1.47579500
H	6.94757800	3.28463900	-2.43791500
C	0.24810800	4.02500800	-1.65562900
C	1.47593000	4.09643700	-2.33074100
C	-0.57116100	5.15947100	-1.60980900
C	1.86952300	5.27999100	-2.95353300
H	2.13177900	3.23005700	-2.36797600
C	-0.17640800	6.34639300	-2.23194600
H	-1.52531400	5.11886200	-1.08963900
C	1.04328700	6.40704000	-2.90715700
H	2.82014200	5.32126900	-3.47735700
H	-0.82447300	7.21658700	-2.18980000
H	1.34839600	7.32594800	-3.39959200
C	-0.95372300	3.64935200	2.53067000
C	-0.34215000	4.07446500	3.73300400
C	-0.63168300	3.37369300	4.91743800
C	-1.46859600	2.26095500	4.89118400
C	-2.04460200	1.82521100	3.68811100
C	-1.79319900	2.52352400	2.51161900
H	-0.91828200	4.33088000	1.67477400
H	-0.18391800	3.69186200	5.85496700
H	-1.67756700	1.72424900	5.81250300
H	-2.70498500	0.96318100	3.68346800
H	-2.27556100	2.22037900	1.58604000
C	-0.32194700	9.85909000	4.18313800
C	-0.18615300	9.30121700	2.75730000
C	-0.65591900	7.84639200	2.82872300
C	-0.67995100	7.36149800	4.28284800
C	-0.42920400	8.63895400	5.10504900
H	0.50221200	10.50245900	4.50411000
H	-1.24265400	10.44572700	4.30246400
H	0.86186600	9.28817200	2.42693000

H	-0.75232100	9.84431500	1.99529100
O	-0.32838800	8.66118600	6.31129500
O	-0.97089600	7.17073300	1.86832600
C	-2.05446000	6.76604100	4.64445500
H	-2.28554300	5.90710800	4.01145100
H	-2.06108000	6.45876600	5.69468100
H	-2.85040000	7.50652300	4.50621500
C	0.51201900	6.37861000	4.57868400
H	1.44772000	6.94442800	4.54875500
H	0.37976000	6.05515000	5.61919400
C	0.63126400	5.18967900	3.65037000
C	1.54402400	5.07488000	2.65665000
C	2.59006800	6.06251700	2.32341800
C	3.72387200	6.25975900	3.13633200
C	2.46767100	6.83495500	1.14853200
C	4.70001300	7.19366300	2.78605800
H	3.83400500	5.67698400	4.04556400
C	3.44435700	7.77157800	0.80564900
H	1.58950400	6.71178700	0.52096000
C	4.56642400	7.95111700	1.61993700
H	5.56460200	7.33324600	3.42922300
H	3.32613900	8.36418500	-0.09772300
H	5.32581000	8.68024000	1.35198900

3a

B3LYP SCF energy: -2644.630459 a.u.
B3LYP enthalpy: -2643.816867 a.u.
B3LYP free energy: -2643.957223 a.u.
M06 SCF energy in solution: -2643.814722 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.07257700	3.61045800	4.05732600
C	-0.24049000	6.12502200	7.83941100
C	-0.60273700	5.63728500	6.57796900
C	-1.06466300	6.55903400	5.60499900
C	-1.13597000	7.92564700	5.92252800
C	-0.75555900	8.39096700	7.17935800
C	-0.31229000	7.48785700	8.14141700
H	0.10805100	5.43467200	8.59839100
H	-1.49303600	8.62183100	5.17363100
H	-0.81092800	9.45211900	7.40115900
H	-0.02016600	7.83419800	9.12837500
C	-1.52516200	6.16230300	4.26022600
O	-2.24992400	7.09822000	3.62412400
C	-2.47530500	6.62419700	2.27400900
C	-2.10542900	5.12214600	2.34729200
H	-3.51975700	6.80980600	2.02423400
H	-1.82254900	7.19785800	1.60827000
H	-1.44001200	4.85227800	1.52691800
N	-1.33324500	5.04693900	3.62370500
P	-0.48330000	3.82910500	6.21687300
C	0.50876100	3.14466200	7.60168400
C	-0.04524400	2.23573900	8.51565300
C	1.85178100	3.53311400	7.75073800
C	0.73217500	1.72361300	9.55702700
H	-1.07899900	1.92267100	8.42253000
C	2.61955500	3.02472100	8.79583400
H	2.30339700	4.22592200	7.04926700
C	2.06239800	2.11625900	9.70002000
H	0.29183100	1.01883900	10.25637000
H	3.65599100	3.33233400	8.89895700
H	2.66474100	1.71644100	10.51061700
C	-2.17663200	3.16777300	6.48580500
C	-2.50778100	1.92788700	5.91600700
C	-3.11881200	3.82889600	7.28901900
C	-3.75456200	1.35154600	6.15971000
H	-1.79230900	1.41003000	5.28347100
C	-4.37086300	3.25438900	7.51873300
H	-2.87827100	4.78505100	7.74346300
C	-4.68794800	2.01388400	6.96051100
H	-3.99726100	0.38809900	5.72102700
H	-5.09326200	3.77277300	8.14271900
H	-5.65837000	1.56436400	7.15087300
C	-3.31754900	4.20767500	2.29658700
C	-4.17859700	4.04961800	3.39005200
C	-3.64063900	3.58637800	1.08226700
C	-5.34023700	3.28505100	3.26752600
H	-3.94512300	4.51377800	4.34350500
C	-4.80400300	2.82545800	0.95803900
H	-2.97937700	3.70050400	0.22617200
C	-5.65748000	2.67361400	2.05249900
H	-5.99693400	3.16949300	4.12454100
H	-5.04051400	2.35182400	0.00960600
H	-6.56455500	2.08338500	1.95893500
C	1.50922300	1.16879900	4.80498000
C	1.56792200	2.54169500	4.54198400
C	2.81751100	3.17776100	4.56093000
C	3.98664200	2.45230500	4.81922600
C	3.91861800	1.08154900	5.07284200
C	2.67740600	0.44322200	5.06606300
H	0.55788100	0.64231900	4.80134200
H	2.89947100	4.24918200	4.38012700
H	4.94763600	2.96163200	4.82337600
H	4.82414700	0.51661700	5.27555600
H	2.61286100	-0.62393300	5.26405500
C	3.89157500	6.00582700	-1.04468300
C	4.29101300	4.53182000	-0.85165500
C	3.10057900	3.83455500	-0.18132700
C	1.98039800	4.84947900	0.10575300
C	2.62713700	6.21031500	-0.20950200
H	4.65505000	6.72788300	-0.74216500
H	3.64678300	6.22965800	-2.09141300
H	5.15836500	4.41996100	-0.18922100
H	4.54566800	4.01157400	-1.78048600
O	2.18413800	7.27391700	0.16460200
O	3.04756900	2.65279100	0.07911600
C	0.82279200	4.61650300	-0.89414200
H	0.39556900	3.62053100	-0.74747700
H	0.04634400	5.37596200	-0.74911900
H	1.16782500	4.68545300	-1.93158800
C	1.49791600	4.84692700	1.58087400
H	2.36663500	4.95658200	2.24206500
H	0.89195800	5.75018300	1.72503700
C	0.75185400	3.64490300	1.97575400
C	0.16557400	2.56265600	1.99564300
C	-0.27100800	1.20501800	1.86516400
C	-1.57209200	0.79155000	2.20883300
C	0.65070300	0.26929100	1.34996100
C	-1.93938900	-0.54216600	2.04485100
H	-2.28548200	1.51538600	2.58726900
C	0.26614300	-1.05836600	1.18400900
H	1.64537300	0.60536800	1.07642200
C	-1.02412000	-1.46730900	1.53431500
H	-2.94494900	-0.85889100	2.30628700

H	0.97520200	-1.77605600	0.78209100
H	-1.31768900	-2.50515300	1.40501600

4a-ts

B3LYP SCF energy: -2644.611774 a.u.
B3LYP enthalpy: -2643.799353 a.u.
B3LYP free energy: -2643.936437 a.u.
M06 SCF energy in solution: -2643.789107 a.u.
Imaginary frequency: -277.99 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.26402500	-0.03632100	-0.04450600
C	-3.83270700	2.00425600	0.56904900
C	-2.77758700	1.39800900	-0.12526300
C	-2.35909800	1.98439000	-1.34343900
C	-2.99419700	3.14121200	-1.82467600
C	-4.02714300	3.73696300	-1.10585000
C	-4.44903500	3.16361600	0.09199300
H	-4.18010100	1.56655300	1.49780900
H	-2.66982500	3.56820200	-2.76669200
H	-4.50221300	4.63635700	-1.48530100
H	-5.26130800	3.61033200	0.65790200
C	-1.29611800	1.40789600	-2.18478400
O	-1.39787100	1.68285600	-3.49569600
C	-0.24587800	1.10083800	-4.15786200
C	0.44926700	0.26307900	-3.04963100
H	-0.61017400	0.50143700	-4.99285100
H	0.37277900	1.92149400	-4.53135200
H	1.49064400	0.57481400	-2.94206200
N	-0.29107200	0.67689900	-1.82316300
P	-2.00429400	-0.15611500	0.53302300
C	-2.43370900	-0.08627700	2.31887000
C	-3.27979300	-1.01850500	2.93473000
C	-1.88131300	0.95581000	3.08596200
C	-3.56919800	-0.91174600	4.29758400
H	-3.72122600	-1.82414000	2.35788900
C	-2.18707300	1.06459900	4.44163600
H	-1.22412900	1.68659900	2.62313400
C	-3.02731800	0.12898800	5.05181100
H	-4.22677700	-1.63973200	4.76414600
H	-1.76516400	1.87932400	5.02379300
H	-3.26037900	0.21386100	6.10946100
C	-3.03916700	-1.50314100	-0.18034800
C	-2.66379200	-2.83400800	0.07728500
C	-4.15979200	-1.25627900	-0.98851800
C	-3.40437700	-3.89163000	-0.45063600
H	-1.79963900	-3.04321100	0.70016000
C	-4.88884600	-2.31914400	-1.52755700
H	-4.47344100	-0.23847600	-1.19537400
C	-4.51608300	-3.63690900	-1.25824500
H	-3.11078600	-4.91474600	-0.23303400
H	-5.75428700	-2.11360300	-2.15111200
H	-5.09026400	-4.46106200	-1.67174200
C	0.42949600	-1.23468000	-3.29953000
C	-0.74375100	-1.98855200	-3.16713500
C	1.59685300	-1.86692800	-3.74678600
C	-0.74373300	-3.35162600	-3.46711800
H	-1.66094200	-1.51919800	-2.82431000
C	1.59605600	-3.22859400	-4.05444500
H	2.51009000	-1.28755800	-3.86738200
C	0.42487900	-3.97470800	-3.91146400
H	-1.65963600	-3.92372800	-3.35276100
H	2.50771700	-3.70429200	-4.40445500
H	0.42184300	-5.03468200	-4.14864000
C	0.73767900	-2.52476200	1.40688700
C	0.88770600	-1.12489200	1.47927000
C	1.02622600	-0.52422300	2.74147500
C	0.95992000	-1.29513800	3.90762800
C	0.78631700	-2.67724600	3.82443400
C	0.68079000	-3.29141600	2.56921600
H	0.68171800	-3.01563000	0.43807100
H	1.17815100	0.54865100	2.80871800
H	1.04938900	-0.81454100	4.87830700
H	0.74777300	-3.27817000	4.72861000
H	0.56446700	-4.37013000	2.50066500
C	2.69212500	5.52243400	0.34209500
C	1.56004900	4.97328400	1.23194400
C	1.53290900	3.45657000	1.01623400
C	2.77886000	3.01201600	0.24882900
C	3.25301700	4.31698100	-0.41909700
H	2.36371900	6.27920500	-0.37645100
H	3.50296800	5.97728400	0.92368000
H	0.57368500	5.37879100	0.98317700
H	1.71548300	5.17555200	2.29841500
O	3.95194600	4.36643500	-1.40493400
O	0.63910400	2.72485700	1.39778300
C	3.86760800	2.59824400	1.27710800
H	3.55399200	1.69910500	1.81379600
H	4.80551700	2.39191800	0.75119500
H	4.05731400	3.38864000	2.01153800
C	2.53590700	1.91700600	-0.81839700
H	1.80247000	2.29952100	-1.53485000
H	3.48084500	1.79582500	-1.36429200
C	2.08916900	0.60951100	-0.26378400
C	2.48278500	-0.45914000	0.29709800
C	3.54671700	-1.43705400	0.47231900
C	4.20090200	-1.90709500	-0.68282100
C	3.99734200	-1.85730000	1.73600700
C	5.29172200	-2.76718700	-0.57232100
H	3.84144400	-1.59816200	-1.65890900
C	5.09169300	-2.71163100	1.83775100
H	3.48796300	-1.51264400	2.62871400
C	5.74072400	-3.16949400	0.68711900
H	5.78935600	-3.12403400	-1.46943700
H	5.43879900	-3.02412700	2.81831500
H	6.59059100	-3.84045600	0.77279500

5a

B3LYP SCF energy: -2644.669280 a.u.
B3LYP enthalpy: -2643.854347 a.u.
B3LYP free energy: -2643.989467 a.u.
M06 SCF energy in solution: -2643.842662 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.36802900	0.87839100	0.23508300
C	-2.65781600	4.25958300	0.21101500
C	-1.81572500	3.28756900	-0.33893400
C	-0.91413000	3.67678800	-1.36040300
C	-0.89386700	5.00855100	-1.80532900
C	-1.73515500	5.96271600	-1.23620200
C	-2.61795400	5.58709700	-0.22607400
H	-3.35503600	3.97911100	0.99313100

H	-0.21177900	5.28972500	-2.59953600
H	-1.70141600	6.98996900	-1.58570700
H	-3.28205700	6.32022200	0.22248500
C	0.00728300	2.73413000	-2.02305500
O	0.38419700	3.08374300	-3.26499800
C	1.40175000	2.13734400	-3.69101100
C	1.28655300	0.97936200	-2.67303000
H	1.17862700	1.84921500	-4.71779200
H	2.36712000	2.65061300	-3.64823000
H	2.26688500	0.71401100	-2.27640200
N	0.50278000	1.62390000	-1.57107300
P	-1.88419900	1.53252900	0.23875300
C	-2.77852400	1.60772000	1.84382400
C	-4.08103400	1.11012700	2.00245900
C	-2.10178300	2.13520000	2.95972200
C	-4.69744400	1.14273700	3.25605900
H	-4.61562100	0.69743800	1.15329400
C	-2.72711800	2.17141600	4.20562700
H	-1.09531300	2.52715900	2.84690500
C	-4.02404500	1.67241700	4.35746800
H	-5.70582900	0.75461200	3.36791500
H	-2.19981100	2.58584100	5.06039700
H	-4.50626900	1.69629400	5.33046200
C	-3.03924900	0.70988800	-0.92713100
C	-2.93001500	-0.67968400	-1.09612400
C	-4.04332000	1.40954500	-1.61680600
C	-3.82304100	-1.35904000	-1.92590500
H	-2.14894800	-1.23029600	-0.58061100
C	-4.92614300	0.72689100	-2.45473400
H	-4.14130300	2.48463100	-1.50024500
C	-4.82072300	-0.65794400	-2.60605300
H	-3.73153800	-2.43440600	-2.04728500
H	-5.69894300	1.27660500	-2.98449200
H	-5.51338900	-1.18754700	-3.25405200
C	0.62743100	-0.27524800	-3.21692000
C	-0.58011100	-0.21121600	-3.92719000
C	1.25953100	-1.51449900	-3.06215200
C	-1.13885500	-1.36439000	-4.47625100
H	-1.08793700	0.74135800	-4.05980300
C	0.69984300	-2.67074900	-3.61022000
H	2.19894100	-1.57546400	-2.51847100
C	-0.49888300	-2.59715400	-4.32044300
H	-2.07193200	-1.29948400	-5.02806000
H	1.20657400	-3.62420300	-3.49111900
H	-0.93009500	-3.49363500	-4.75687500
C	1.14635600	-2.91036700	0.73131600
C	1.31798700	-1.54926100	1.03653100
C	0.26346000	-0.87070300	1.69934100
C	-0.93206100	-1.53612900	2.02615500
C	-1.08235800	-2.88134300	1.70708500
C	-0.03769700	-3.56309600	1.06340100
H	1.94602500	-3.44948900	0.23326100
H	0.47299200	0.10216500	2.16809900
H	-1.71470900	-1.00565300	2.55969700
H	-1.99228800	-3.40943700	1.97625200
H	-0.15201900	-4.61710200	0.82487800
C	3.78743200	5.06195600	1.72953500
C	2.32356800	4.78117000	2.11743200
C	2.04490100	3.32671900	1.73437100
C	3.33310400	2.61699700	1.34549800
C	4.29155200	3.78504000	1.04613000
H	3.91053100	5.90956000	1.04915800
H	4.42153800	5.26647300	2.60039700
H	1.60368200	5.41964400	1.59334600
H	2.12585500	4.91070500	3.18814800
O	5.28634400	3.69920700	0.36459100
O	0.92725500	2.83070100	1.74899100
C	3.87445700	1.89816100	2.61693600
H	3.20785600	1.07612700	2.89034000
H	4.86809100	1.49290400	2.40355800
H	3.95737500	2.57769500	3.47248500
C	3.23747600	1.64185100	0.13937700
H	2.98199400	2.23751700	-0.74587300
H	4.25478100	1.26936000	-0.02424900
C	2.24673800	0.52752400	0.33981700
C	2.51931100	-0.75894300	0.66811100
C	3.86194500	-1.40560700	0.73885600
C	4.77775400	-1.30934300	-0.32309300
C	4.23357100	-2.15134700	1.87193500
C	6.02993600	-1.92014600	-0.24840500
H	4.50009400	-0.76340400	-1.22112600
C	5.48548500	-2.76099500	1.94832200
H	3.53693400	-2.24779700	2.70074600
C	6.38916400	-2.64544300	0.88928900
H	6.72148300	-1.83550300	-1.08202100
H	5.75574900	-3.32659700	2.83571400
H	7.36344900	-3.12193200	0.94793700

OAc$^-$

B3LYP SCF energy: -228.4931536 a.u.
B3LYP enthalpy: -228.4394566 a.u.
B3LYP free energy: -228.4736896 a.u.
M06 SCF energy in solution: -228.563056 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.61975400	0.04255100	-0.00003900
O	-0.78018500	-0.89240600	-0.00038100
C	-3.13366800	-0.39429900	0.00037100
H	-3.64637600	0.02115200	-0.87990000
H	-3.25217900	-1.48562600	0.00022000
H	-3.64579100	0.02084900	0.88112400
O	-1.44084700	1.28752200	0.00019800

6-ts

B3LYP SCF energy: -2644.615102 a.u.
B3LYP enthalpy: -2643.801896 a.u.
B3LYP free energy: -2643.929917 a.u.
M06 SCF energy in solution: -2643.799703 a.u.
Imaginary frequency: -294.07 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.21292700	-0.18623500	-0.33545800
C	-3.27414900	-2.01616600	2.03789000
C	-2.28492600	-1.92702500	1.05097800
C	-1.56735000	-3.09834400	0.70837100
C	-1.86519800	-4.31312600	1.34664600
C	-2.84193600	-4.37572700	2.33787300
C	-3.54608000	-3.22484300	2.68450300
H	-3.84444300	-1.13454800	2.30732400
H	-1.31994400	-5.20571300	1.06302200
H	-3.05317900	-5.32068000	2.82867400

H	-4.31615100	-3.26217000	3.44948700
C	-0.49814200	-3.12068200	-0.30751400
O	-0.24044100	-4.32833700	-0.83570800
C	0.73131700	-4.12289500	-1.89620600
C	1.31504500	-2.72515300	-1.58437600
H	0.18979100	-4.16308600	-2.84667800
H	1.46110900	-4.93017300	-1.84403200
N	0.25093000	-2.14381800	-0.71321900
P	-1.99220000	-0.36288100	0.10544000
C	-2.90678300	0.92927000	1.03397400
C	-3.88250000	1.72582000	0.41778600
C	-2.58191000	1.17200200	2.38131900
C	-4.53164100	2.73021600	1.13876000
H	-4.13629200	1.57223500	-0.62456800
C	-3.23843100	2.17041400	3.09893600
H	-1.82624300	0.57531900	2.88320800
C	-4.21712400	2.95136300	2.47907600
H	-5.28491600	3.33850800	0.64688400
H	-2.98513500	2.33737400	4.14197900
H	-4.72832900	3.72929500	3.03869600
C	-2.94278400	-0.68255300	-1.43986200
C	-2.29222800	-0.63926100	-2.68194700
C	-4.30510500	-1.02560100	-1.39333800
C	-2.99291800	-0.91564000	-3.85801500
H	-1.23438900	-0.39763100	-2.72783500
C	-5.00274700	-1.29840200	-2.56908600
H	-4.82222300	-1.08064100	-0.43991000
C	-4.34848900	-1.24179400	-3.80298400
H	-2.47950700	-0.87531800	-4.81454800
H	-6.05598600	-1.55931800	-2.52193800
H	-4.89423900	-1.45594700	-4.71729400
C	0.99823200	0.09313300	2.55077200
C	1.82791100	1.18492700	2.18914900
C	2.92529400	1.46959900	3.04844300
C	3.17688000	0.70216000	4.17701600
C	2.35254700	-0.38472000	4.48980900
C	1.26204300	-0.68688700	3.66929800
H	0.13175100	-0.12370400	1.93992600
H	3.58909500	2.29619000	2.83321500
H	4.01983500	0.94701000	4.81581800
H	2.55229900	-0.98234200	5.37463000
H	0.60821600	-1.51905400	3.91397200
C	3.15884700	2.52387300	-2.97322900
C	1.78121900	1.97781200	-2.56281500
C	2.00615800	1.37945600	-1.14588600
C	3.21259600	2.19621200	-0.51869500
C	3.74185200	3.06702500	-1.67067700
H	3.12438600	3.30263700	-3.73888900
H	3.81481800	1.71889800	-3.33265300
H	1.06669700	2.80199000	-2.55264900
H	1.39859100	1.19795800	-3.22628000
O	4.47173700	4.02136800	-1.54067300
O	1.96669000	0.06252200	-1.03160700
C	4.36382600	1.30103800	-0.03520000
H	4.02582500	0.55884200	0.68998100
H	5.14933800	1.92372400	0.40640700
H	4.80185400	0.74652200	-0.87110200
C	2.52521400	3.05441900	0.58710800
H	2.02901300	3.91345600	0.13131800
H	3.22084600	3.43196500	1.33465800
C	1.51529000	2.01829800	1.04397500
C	0.53879400	1.71494200	0.03069500
C	-0.37627900	2.80219900	-0.41384800
C	-0.61063300	3.93021600	0.40253700
C	-1.10537300	2.72448800	-1.61802100
C	-1.47574700	4.94892500	0.00748700
H	-0.12080700	4.00037600	1.36974100
C	-1.97271200	3.74133900	-2.01427600
H	-0.99283100	1.85229100	-2.25234300
C	-2.15495600	4.86779300	-1.20957100
H	-1.62646100	5.80414300	0.66054400
H	-2.50900000	3.65026500	-2.95517200
H	-2.82845900	5.66192400	-1.51810400
H	1.40121000	-2.11819700	-2.48681100
C	2.67476400	-2.80014000	-0.90635900
C	3.82645400	-2.60811400	-1.67894500
C	2.81377300	-3.15011800	0.44132600
C	5.09422100	-2.76195000	-1.11796500
H	3.73089600	-2.33213700	-2.72665500
C	4.08199900	-3.29789000	1.00678000
H	1.93434100	-3.30155400	1.06120200
C	5.22547500	-3.10541000	0.22955100
H	5.97815800	-2.61179000	-1.73155000
H	4.17539600	-3.56810900	2.05506400
H	6.21153600	-3.22453800	0.66929600

7(S)-ts

B3LYP SCF energy: -2644.648289 a.u.
B3LYP enthalpy: -2643.835600 a.u.
B3LYP free energy: -2643.974713 a.u.
M06 SCF energy in solution: -2643.81171 a.u.
Imaginary frequency: -38.06 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.16890800	0.14488900	-0.48036900
C	2.96652500	-3.29173300	-1.33539300
C	2.59195800	-1.94572500	-1.24860200
C	2.81438400	-1.10932300	-2.37469500
C	3.42708200	-1.63973100	-3.52171800
C	3.78951800	-2.98355200	-3.58568800
C	3.55323100	-3.81254500	-2.49213700
H	2.80355600	-3.94533000	-0.48528000
H	3.60811500	-0.98952000	-4.36948900
H	4.25281300	-3.37530700	-4.48589600
H	3.83011000	-4.86217600	-2.52810900
C	2.42769300	0.31710700	-2.43415600
O	3.08957200	1.05101000	-3.34533000
C	2.61439800	2.41865400	-3.23839000
C	1.43114300	2.33898000	-2.23812700
H	3.44272500	3.02926200	-2.87099000
H	2.32574400	2.75216400	-4.23650500
H	0.47696300	2.43661300	-2.76615900
N	1.51313100	0.93334700	-1.75609500
P	1.83575000	-1.28079800	0.30547900
C	1.44459400	-2.75079300	1.33284000
C	2.35970700	-3.32479800	2.23049300
C	0.15659300	-3.30220700	1.22448300
C	1.99331800	-4.43547300	2.99243800
H	3.35395000	-2.90295600	2.33981100
C	-0.20432700	-4.41639400	1.98215900
H	-0.56666000	-2.85357100	0.54829200
C	0.71460500	-4.98359000	2.86802700
H	2.70729000	-4.87075800	3.68576000
H	-1.20264700	-4.83424000	1.88874500

H	0.43270000	-5.84631000	3.46466500
C	3.24387000	-0.45368000	1.15467600
C	2.95751200	0.54360400	2.10164800
C	4.58322100	-0.79866900	0.90954700
C	3.99014000	1.16736100	2.80330100
H	1.92952900	0.83961700	2.28975500
C	5.61370500	-0.16358800	1.60577300
H	4.82615500	-1.56209100	0.17665400
C	5.31913400	0.81653900	2.55579400
H	3.75490600	1.93208700	3.53819700
H	6.64577000	-0.43809800	1.40694600
H	6.12235900	1.30634300	3.09880200
C	1.47681700	3.37023300	-1.12882200
C	2.52424600	3.38302500	-0.19693400
C	0.48448600	4.35400600	-1.05062300
C	2.57450300	4.36311000	0.79359200
H	3.29986800	2.62278200	-0.23854300
C	0.53631100	5.33888600	-0.06173700
H	-0.33007200	4.35610500	-1.77157100
C	1.58177900	5.34460500	0.86241600
H	3.39125300	4.36175300	1.50976800
H	-0.23718700	6.10016000	-0.01692900
H	1.62559300	6.11107400	1.63084800
C	-2.06519500	1.01230200	-2.54833100
C	-2.00483600	-0.17508400	-1.79225800
C	-1.75648800	-1.39131300	-2.45938800
C	-1.55115000	-1.41439800	-3.83865900
C	-1.60893200	-0.22898400	-4.57760400
C	-1.87219000	0.98122100	-3.93062100
H	-2.31914400	1.93865000	-2.04354200
H	-1.72484900	-2.32028300	-1.89634600
H	-1.35670700	-2.35914900	-4.33818600
H	-1.46808700	-0.25236100	-5.65440900
H	-1.95071500	1.89984300	-4.50591500
C	-6.86461900	-0.56625400	1.38700600
C	-6.33944100	0.87014500	1.22575900
C	-5.19185900	0.79492400	0.21583200
C	-4.81931600	-0.66553400	-0.07309800
C	-5.75174200	-1.47205300	0.85275700
H	-7.12183200	-0.85010200	2.41073600
H	-7.76080800	-0.73652300	0.77525000
H	-5.91903300	1.25448100	2.16538400
H	-7.08659300	1.59803200	0.89626800
O	-5.60632700	-2.64521200	1.11257500
O	-4.65142300	1.75514600	-0.29521900
C	-5.19691300	-0.99990100	-1.53784200
H	-4.65671900	-0.35617800	-2.23472700
H	-4.96279000	-2.04757100	-1.75100900
H	-6.26953300	-0.85359200	-1.70986900
C	-3.34266000	-1.01012600	0.28997800
H	-3.23681500	-0.98301600	1.37853800
H	-3.18593400	-2.05407700	-0.00832000
C	-2.26231400	-0.11771000	-0.31366100
C	-1.50552800	0.68828700	0.46456300
C	-1.59159300	1.24399300	1.78747300
C	-0.85909800	0.69704500	2.87055200
C	-2.39697600	2.38668900	2.02563300
C	-0.94636800	1.25819600	4.14011200
H	-0.25731200	-0.19174600	2.70703500
C	-2.46201700	2.94855100	3.29615400
H	-2.96679800	2.81017600	1.20562600
C	-1.74005700	2.39018300	4.35755400
H	-0.39904600	0.81105700	4.96519400
H	-3.08271700	3.82428800	3.46380200
H	-1.79968900	2.83085700	5.34842700

7-ts

B3LYP SCF energy: -2644.645391 a.u.
B3LYP enthalpy: -2643.831659 a.u.
B3LYP free energy: -2643.966276 a.u.
M06 SCF energy in solution: -2643.815157 a.u.
Imaginary frequency: -23.73 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.08733900	0.24646300	-0.24734700
C	2.68652500	-3.56327500	-1.06668600
C	2.30794500	-2.21514900	-1.05173800
C	2.62171000	-1.41340100	-2.18174900
C	3.30022800	-1.99127700	-3.26933100
C	3.65772300	-3.33724000	-3.26429100
C	3.35111300	-4.12591200	-2.15890400
H	2.45692900	-4.18763800	-0.21065200
H	3.54212100	-1.37355600	-4.12525200
H	4.17377700	-3.76108600	-4.12017800
H	3.62602100	-5.17638800	-2.13798700
C	2.29369600	0.02363100	-2.30310500
O	2.92426300	0.65746200	-3.30854100
C	2.46446200	2.03154300	-3.33388000
C	1.49457200	2.13309100	-2.12341400
H	3.34035800	2.67625500	-3.24233100
H	1.97695500	2.20189400	-4.29659200
H	0.48092300	2.36723700	-2.46243600
N	1.48035600	0.74313600	-1.59686500
P	1.40456900	-1.54030400	0.41366400
C	0.86850900	-3.02165400	1.36223000
C	1.60630200	-3.52598100	2.44636100
C	-0.32533000	-3.66375200	0.99316500
C	1.15352000	-4.64822300	3.14280000
H	2.53079200	-3.04586500	2.75002100
C	-0.77405700	-4.78542900	1.68990700
H	-0.91569600	-3.29553200	0.16128900
C	-0.03505800	-5.27827400	2.76794900
H	1.73194100	-5.02848000	3.98003700
H	-1.70621900	-5.25620700	1.39268700
H	-0.38525100	-6.14827000	3.31614400
C	2.71340300	-0.77179300	1.45654800
C	2.30143600	-0.06897400	2.60303800
C	4.08111300	-0.83767000	1.15297200
C	3.23976300	0.54711000	3.43081300
H	1.24549800	-0.01197800	2.85560900
C	5.01729500	-0.20936600	1.97899000
H	4.42325100	-1.38589100	0.28075700
C	4.60015900	0.48202900	3.11778700
H	2.90839000	1.07751500	4.31910900
H	6.07427900	-0.27156500	1.73566900
H	5.33134300	0.96170700	3.76214600
C	1.91542200	3.16172200	-1.08978300
C	2.99652000	2.92967900	-0.22784300
C	1.25847900	4.39703000	-1.03988900
C	3.40913400	3.91755900	0.66745400
H	3.51419400	1.97448100	-0.24639900
C	1.67610800	5.38884300	-0.15036000
H	0.41696400	4.58591600	-1.70267500
C	2.75274000	5.15080500	0.70564000

H	4.24614000	3.72307600	1.33205600
H	1.15933100	6.34396000	-0.12571800
H	3.08073600	5.92217400	1.39672000
C	-2.49269500	2.07231700	-2.25185200
C	-2.19745400	0.73809700	-1.91507600
C	-2.06120800	-0.20159900	-2.95352300
C	-2.21732800	0.18124700	-4.28554800
C	-2.52058000	1.50691200	-4.60621200
C	-2.66014100	2.45004500	-3.58403700
H	-2.61386000	2.80720500	-1.46124300
H	-1.82267600	-1.23559900	-2.72121400
H	-2.10717100	-0.55844700	-5.07364000
H	-2.65400200	1.80120800	-5.64315700
H	-2.90988600	3.48000000	-3.82340900
C	-5.61527900	-2.66153100	1.46623400
C	-5.77573600	-1.21587300	1.96510100
C	-4.99708200	-0.33424400	0.98445900
C	-4.17974900	-1.19221700	0.01040800
C	-4.41918100	-2.63172000	0.51554300
H	-5.45341600	-3.40436700	2.25168100
H	-6.49421600	-2.98951200	0.89500400
H	-5.32819700	-1.07888300	2.95882100
H	-6.81047500	-0.86923000	2.03970000
O	-3.74119900	-3.58801200	0.20455800
O	-5.05529900	0.87702700	0.95628900
C	-4.84930300	-1.06727200	-1.38234700
H	-4.81372300	-0.03260900	-1.72912500
H	-4.34403500	-1.71088800	-2.10738500
H	-5.90182200	-1.37062300	-1.33659000
C	-2.63894600	-0.95091100	0.03082700
H	-2.28233400	-1.11345000	1.05254000
H	-2.22891400	-1.77900700	-0.55906300
C	-2.01222100	0.34873700	-0.48106100
C	-1.29419700	1.19292300	0.36092600
C	-1.41958100	2.22145700	1.34638000
C	-0.27414300	2.73138100	2.01033700
C	-2.68750100	2.77936000	1.65112300
C	-0.39774800	3.74307900	2.95147800
H	0.70464900	2.33382700	1.76336400
C	-2.79710400	3.79619900	2.59399700
H	-3.56837800	2.39373500	1.15233100
C	-1.65879900	4.27756900	3.24757500
H	0.48715800	4.12812400	3.44911900
H	-3.77386800	4.21282000	2.82177200
H	-1.75091700	5.07179600	3.98312200

8E

B3LYP SCF energy: -2644.663538 a.u.
B3LYP enthalpy: -2643.848318 a.u.
B3LYP free energy: -2643.985471 a.u.
M06 SCF energy in solution: -2643.836419 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.98105600	6.92925000	1.30654400
C	-1.71868600	10.13779700	-0.33558600
C	-0.51845900	9.45808300	-0.09538100
C	0.65544200	10.22474600	0.11154500
C	0.59900900	11.62610700	0.05076800
C	-0.60824700	12.28037600	-0.18329400
C	-1.76892000	11.53411200	-0.37261700
H	-2.62850000	9.57303300	-0.50239200
H	1.50800800	12.19717700	0.20044600
H	-0.63755500	13.36497900	-0.21716900
H	-2.71679400	12.03079700	-0.55752800
C	1.95991400	9.61916400	0.41613900
O	3.04009200	10.39276300	0.22085600
C	4.21031800	9.56177400	0.45836400
C	3.64090200	8.30578300	1.15930400
H	4.65961400	9.33573900	-0.51283500
H	4.91074800	10.13271300	1.06832900
H	3.77824300	8.38752500	2.24512700
N	2.18089700	8.43666400	0.89135300
P	-0.49416900	7.60648800	-0.16490800
C	-2.25379300	7.12618000	-0.02907800
C	-2.97079900	6.63079500	-1.12750400
C	-2.89479600	7.27559700	1.21372800
C	-4.31739100	6.28797700	-0.98482400
H	-2.48575900	6.50729400	-2.08986100
C	-4.24140300	6.93904300	1.34388500
H	-2.34178400	7.64967800	2.06925100
C	-4.95351700	6.44151200	0.24756700
H	-4.86597800	5.90167600	-1.83892400
H	-4.73531700	7.06070200	2.30382300
H	-6.00122200	6.17555000	0.35539400
C	0.02745300	7.23207400	-1.88838300
C	0.43295800	5.92211700	-2.19752100
C	0.01554200	8.20538200	-2.90117900
C	0.81199400	5.59505600	-3.49978400
H	0.44620900	5.15588400	-1.42947900
C	0.40570000	7.87216800	-4.19968400
H	-0.30023400	9.22087900	-2.68643700
C	0.80318500	6.56843600	-4.50168200
H	1.11375700	4.57693300	-3.72866400
H	0.39361200	8.63294000	-4.97489200
H	1.10267800	6.31187400	-5.51379800
C	4.22616300	6.98627500	0.70029800
C	3.97594900	6.49492100	-0.58973300
C	5.05375900	6.25540800	1.56173300
C	4.54487500	5.29133400	-1.00631000
H	3.33069200	7.04717400	-1.26787800
C	5.62803700	5.05380000	1.14175700
H	5.25621600	6.62949000	2.56300800
C	5.37310100	4.56928200	-0.14239500
H	4.34296900	4.91980500	-2.00682200
H	6.27370200	4.49951400	1.81663300
H	5.81977900	3.63508600	-0.47017000
C	-0.15905600	3.01979300	4.04232700
C	0.96661900	3.84173300	3.86202500
C	2.20181500	3.39459300	4.36361100
C	2.30728000	2.16841200	5.02129900
C	1.17846700	1.36658600	5.19794600
C	-0.05515700	1.79798900	4.70540400
H	-1.12328800	3.34621000	3.66672600
H	3.09605900	3.99551100	4.22166200
H	3.27377400	1.83980400	5.39331300
H	1.25934800	0.41407700	5.71372800
H	-0.94071700	1.18294800	4.83944500
C	1.01415000	8.99358900	6.58887100
C	-0.27290600	9.18706900	5.75719000
C	-0.19241000	8.15112900	4.63268100
C	0.76302700	7.02944200	5.03978900
C	1.73661600	7.79497100	5.96348500
H	1.68166700	9.86043600	6.56393200
H	0.81478200	8.78491200	7.64611700

H	-0.37533700	10.18494300	5.32158300
H	-1.18048800	9.00408500	6.34538700
O	2.89902800	7.50643200	6.13496700
O	-0.74856400	8.25234000	3.55651900
C	-0.01866100	6.04020400	5.95517300
H	-0.81105600	5.54533800	5.38873300
H	0.66087300	5.27763800	6.34378800
H	-0.47594800	6.55755800	6.80518600
C	1.51282700	6.35420900	3.86890000
H	1.76652100	7.17280200	3.16798500
H	2.48165400	6.03802800	4.27063400
C	0.86048200	5.16033800	3.15577300
C	0.33887900	5.28189400	1.91031600
C	-0.17799300	4.17820000	1.07680000
C	-1.55267100	3.93170400	0.91180700
C	0.73555800	3.33883000	0.40597500
C	-1.99789400	2.88159200	0.10796600
H	-2.27273100	4.56051500	1.42504400
C	0.28678800	2.28709900	-0.39257000
H	1.80154700	3.50994400	0.53005100
C	-1.08253500	2.05606600	-0.54829800
H	-3.06463600	2.70532400	0.00029000
H	1.00796500	1.64143600	-0.88679000
H	-1.43194300	1.23571600	-1.16874600

9

B3LYP SCF energy: -2644.692818 a.u.
B3LYP enthalpy: -2643.877357 a.u.
B3LYP free energy: -2644.010995 a.u.
M06 SCF energy in solution: -2643.872704 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.01403300	-0.19696700	0.66524000
C	-3.12418200	-2.93046000	-0.98448700
C	-2.57890400	-1.99940600	-0.09288400
C	-2.76878300	-2.20804600	1.29617800
C	-3.49740500	-3.31957400	1.74552600
C	-4.02028100	-4.24100500	0.83993600
C	-3.83215800	-4.04565900	-0.52614500
H	-3.00040500	-2.78564200	-2.05146000
H	-3.64584900	-3.45750400	2.81036200
H	-4.57321300	-5.10162500	1.20323400
H	-4.23933900	-4.75284900	-1.24270300
C	-2.23921900	-1.28547200	2.31564100
O	-2.83818700	-1.33346200	3.51582800
C	-2.19660400	-0.34539400	4.36629300
C	-1.07020000	0.25915000	3.48367300
H	-2.95506300	0.38523600	4.65368200
H	-1.82713900	-0.86061300	5.25514500
H	-0.08701600	-0.02402200	3.86809000
N	-1.25759900	-0.45469400	2.18828400
P	-1.68370600	-0.50692800	-0.72915900
C	-1.43273300	-0.84870800	-2.51392300
C	-2.16400100	-0.17407200	-3.50268700
C	-0.49111400	-1.81851300	-2.89995700
C	-1.95330700	-0.46275100	-4.85315800
H	-2.89427600	0.57840700	-3.22665500
C	-0.29143700	-2.10965900	-4.24809600
H	0.08643700	-2.34829000	-2.14978300
C	-1.01915700	-1.42822500	-5.22827000
H	-2.52273000	0.06952000	-5.60948800
H	0.43637800	-2.86331300	-4.53450600
H	-0.85722400	-1.65112000	-6.27889000
C	-2.93277200	0.84064100	-0.65986600
C	-2.50377700	2.16069100	-0.87659400
C	-4.29459200	0.58726700	-0.43061700
C	-3.42759000	3.20624900	-0.87230600
H	-1.45515900	2.37512200	-1.05191800
C	-5.21128200	1.64064700	-0.41463900
H	-4.64818600	-0.42650300	-0.27343500
C	-4.78051400	2.95018200	-0.63780600
H	-3.08466000	4.22140900	-1.04957600
H	-6.26289500	1.43401400	-0.23741000
H	-5.49747200	3.76631800	-0.63341500
C	-1.11389200	1.77016600	3.35469500
C	-2.25107200	2.42399500	2.85966600
C	-0.01866600	2.53501600	3.77326500
C	-2.28998300	3.81620700	2.78948100
H	-3.10971700	1.84933700	2.52075100
C	-0.05745100	3.92945000	3.70655500
H	0.86761500	2.03674100	4.15788200
C	-1.19451500	4.57241200	3.21496100
H	-3.17676900	4.30935700	2.40261700
H	0.79598300	4.51074700	4.04395300
H	-1.22972000	5.65705100	3.16726900
C	3.95511100	-1.41308600	-2.69915000
C	3.49578800	-0.45995500	-1.77270900
C	4.23695300	0.72649200	-1.62575000
C	5.38813700	0.95306100	-2.38053700
C	5.82463700	-0.00072500	-3.30174300
C	5.10121200	-1.18454000	-3.45941900
H	3.40481300	-2.34013000	-2.83769900
H	3.90350000	1.47989100	-0.91868100
H	5.94497800	1.87661400	-2.24686000
H	6.72139200	0.17475100	-3.88900000
H	5.43150600	-1.93425900	-4.17305300
C	5.01287400	-0.94589800	2.04148700
C	3.81023900	-0.33971600	2.79355900
C	2.59801900	-0.75106600	1.97785600
C	2.88557600	-2.00837800	1.18897500
C	4.43355400	-2.05118200	1.15358300
H	5.47964700	-0.20748400	1.37742900
H	5.79999700	-1.34016700	2.68953800
H	3.83808600	0.74659100	2.91296000
H	3.71275900	-0.77397200	3.79882000
O	5.06849100	-2.86889000	0.53441400
O	1.54996800	-0.10225000	1.96796500
C	2.43176500	-3.23285700	2.03942200
H	1.34434100	-3.22318100	2.16708500
H	2.72487500	-4.14382700	1.50901200
H	2.90042400	-3.25390400	3.02940700
C	2.22842000	-2.06093600	-0.21398500
H	2.75126300	-2.85110300	-0.76328800
H	1.18738200	-2.38241000	-0.08638300
C	2.27507100	-0.72441600	-0.94739500
C	1.29228700	0.17148100	-0.71667800
C	1.17817000	1.52557800	-1.29682100
C	1.07229600	1.72898900	-2.68711100
C	1.12401600	2.65511300	-0.45347500
C	0.92847400	3.01352200	-3.21094500
H	1.11164900	0.87207900	-3.35193000
C	0.98706400	3.93944100	-0.98158100
H	1.19836100	2.52111000	0.62294300
C	0.88551900	4.12382200	-2.36313800

H	0.85461900	3.14844800	-4.28670700
H	0.95976300	4.79547800	-0.31263700
H	0.77873400	5.12308300	-2.77577900

10-RR-ts

B3LYP SCF energy: -2644.664429 a.u.
B3LYP enthalpy: -2643.850165 a.u.
B3LYP free energy: -2643.979565 a.u.
M06 SCF energy in solution: -2643.840711a.u.
Imaginary frequency: -260.15 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.30123200	-0.60693700	-0.62240500
C	-1.43262700	3.61824400	-1.89212700
C	-1.62580100	2.27304300	-1.55581800
C	-2.50456200	1.50052700	-2.35472200
C	-3.15180400	2.08850900	-3.45279400
C	-2.93223700	3.42525100	-3.77845800
C	-2.07277700	4.19113700	-2.99524000
H	-0.77570200	4.23317100	-1.28804600
H	-3.82566600	1.48697400	-4.05117100
H	-3.43452900	3.86189000	-4.63597100
H	-1.89843200	5.23652900	-3.23234500
C	-2.79696100	0.08280400	-2.07954600
O	-3.89224400	-0.40568500	-2.67801600
C	-3.98333200	-1.81950100	-2.35393700
C	-2.79506800	-2.07831400	-1.39030700
H	-4.95882300	-1.99072100	-1.89636900
H	-3.91214100	-2.37727700	-3.29042300
H	-2.08315200	-2.77732200	-1.83024900
N	-2.12157100	-0.74588300	-1.35017100
P	-0.81314100	1.54037100	-0.06248700
C	0.46948600	2.76597600	0.41088300
C	0.45660000	3.38721300	1.66886900
C	1.50154500	3.07536100	-0.49244900
C	1.45526100	4.30142600	2.01314600
H	-0.33065500	3.16374000	2.38028200
C	2.48791900	3.99877200	-0.14937100
H	1.52338300	2.61482200	-1.47624600
C	2.46943200	4.61087200	1.10687500
H	1.43238900	4.77641700	2.98967700
H	3.27065200	4.24128600	-0.86214800
H	3.24047200	5.32733900	1.37452000
C	-2.10275200	1.67041600	1.24110500
C	-2.09392300	0.75755800	2.30646800
C	-3.06357900	2.69600000	1.21898200
C	-3.02624400	0.87756600	3.33905200
H	-1.36502500	-0.04461200	2.33624300
C	-3.99790200	2.80424200	2.24869100
H	-3.08445700	3.41155700	0.40299400
C	-3.97867900	1.89724400	3.31171400
H	-3.00646100	0.16745600	4.16039400
H	-4.73792700	3.59891000	2.22204000
H	-4.70464300	1.98688900	4.11487800
C	-3.19844900	-2.59322000	-0.02156400
C	-4.10808500	-1.89049700	0.78065100
C	-2.69528600	-3.81789400	0.43368900
C	-4.50802700	-2.40539000	2.01345000
H	-4.50874900	-0.93662500	0.44523900
C	-3.09764100	-4.33683400	1.66666700
H	-1.98898900	-4.36752700	-0.18310200
C	-4.00518700	-3.63118400	2.45850600
H	-5.21645400	-1.85232700	2.62337300
H	-2.70998300	-5.29483700	2.00190300
H	-4.32597500	-4.03690100	3.41382800
C	4.79307700	1.11899300	-0.43387900
C	3.98366500	0.12947400	0.16010800
C	4.49530400	-0.55698900	1.28167200
C	5.75743200	-0.25945000	1.78701400
C	6.53478900	0.74299100	1.19968600
C	6.04532400	1.43343100	0.08975900
H	4.43436300	1.65796500	-1.30471700
H	3.90717500	-1.33933800	1.74734400
H	6.13782700	-0.81455700	2.63959400
H	7.51804100	0.97544700	1.59798100
H	6.64539500	2.20761400	-0.37951100
C	3.53823300	-3.47348000	-1.04477200
C	2.09008100	-3.51438400	-0.54194600
C	1.36992900	-2.29353800	-1.14299500
C	2.23251600	-1.70732300	-2.30586000
C	3.53965800	-2.53599300	-2.24779800
H	4.22222600	-3.04918900	-0.29852100
H	3.94109100	-4.45156100	-1.32339500
H	2.00474400	-3.56213500	0.54401600
H	1.55506400	-4.38735600	-0.94001600
O	4.43505100	-2.42254600	-3.05277700
O	0.07663300	-2.34045500	-1.23751100
C	1.57373700	-1.87215300	-3.68235200
H	0.64664500	-1.29326200	-3.73728400
H	2.26500300	-1.52181100	-4.45471700
H	1.33436900	-2.91921900	-3.89575700
C	2.57536100	-0.24307700	-1.96897900
H	3.50115200	0.04624100	-2.47139000
H	1.77724100	0.42143700	-2.32315700
C	2.67726000	-0.21741100	-0.44018800
C	1.56490400	-0.73221000	0.17273800
C	1.28251100	-0.90845300	1.61891400
C	0.50793700	-1.99587200	2.07865900
C	1.68071400	0.05856300	2.56858800
C	0.19746700	-2.13976500	3.43247200
H	0.12735600	-2.72476900	1.37179300
C	1.36245300	-0.08606800	3.91705200
H	2.24862200	0.92321300	2.24496500
C	0.62865600	-1.19084000	4.36033700
H	-0.39351100	-2.99251300	3.75442300
H	1.69034200	0.66906600	4.62624800
H	0.38966400	-1.30352400	5.41386600

11-RR

B3LYP SCF energy: -2644.688431 a.u.
B3LYP enthalpy: -2643.87253 a.u.
B3LYP free energy: -2644.006898 a.u.
M06 SCF energy in solution: -2643.858996 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.21087300	6.93822700	1.25585500
C	-1.65760600	7.05125300	-2.30591800
C	-0.59357500	7.41762400	-1.47114400
C	-0.23673300	8.78531500	-1.39132500
C	-0.93376200	9.73462100	-2.15692100
C	-1.98741000	9.34834200	-2.98156700

C	-2.35054400	8.00505000	-3.05528700
H	-1.95041200	6.00935900	-2.37295900
H	-0.64939300	10.77806500	-2.09150200
H	-2.52174700	10.09588300	-3.55931100
H	-3.17150600	7.69249600	-3.69353500
C	0.84460700	9.28268900	-0.52822300
O	1.29370500	10.50980200	-0.81135400
C	2.40401500	10.80092500	0.08001600
C	2.43417400	9.60142600	1.06283800
H	3.30634300	10.87205800	-0.53131100
H	2.20354300	11.75901700	0.56148400
H	2.07595300	9.91279200	2.05000900
N	1.40205700	8.68961000	0.48262100
P	0.31032900	6.10350300	-0.55341100
C	-0.89822400	4.75458800	-0.36794500
C	-0.87080800	3.63365600	-1.21192700
C	-1.91820300	4.88652100	0.58741000
C	-1.86787200	2.66174000	-1.10592300
H	-0.08091900	3.51837800	-1.94717400
C	-2.91544900	3.91807000	0.67949400
H	-1.93185200	5.73985400	1.25942300
C	-2.89021800	2.80532800	-0.16695100
H	-1.84292200	1.79393200	-1.75829800
H	-3.69838900	4.02128600	1.42390600
H	-3.66477400	2.04798200	-0.08914100
C	1.65846400	5.51650600	-1.63811700
C	2.66473500	4.72297600	-1.05676300
C	1.70847000	5.82115000	-3.00762100
C	3.69981500	4.23041000	-1.85121200
H	2.63103200	4.50494200	0.00719200
C	2.75430700	5.32871200	-3.79059800
H	0.93805900	6.43299300	-3.46630600
C	3.74691900	4.53265400	-3.21515100
H	4.47185100	3.61190600	-1.40266600
H	2.78955100	5.56511900	-4.85004100
H	4.55655900	4.14850100	-3.82893100
C	3.79640800	8.95257500	1.21840900
C	4.35172000	8.17545900	0.19101300
C	4.53692400	9.17117800	2.38729700
C	5.62354800	7.62107900	0.33817900
H	3.79255400	7.99633400	-0.72371500
C	5.81277000	8.62210400	2.53026100
H	4.11845600	9.77653100	3.18845000
C	6.35644200	7.84381000	1.50674100
H	6.04110300	7.01603200	-0.46117000
H	6.37816400	8.80206500	3.43979000
H	7.34769100	7.41430000	1.61780900
C	-2.63337100	4.28218300	5.96087700
C	-1.97453100	3.84617200	4.79562200
C	-2.57515000	2.81223100	4.04973700
C	-3.77532200	2.23579200	4.45956500
C	-4.40917400	2.67385400	5.62562700
C	-3.83129900	3.69927800	6.37454100
H	-2.20004600	5.07352700	6.56424500
H	-2.09585400	2.46449900	3.14208600
H	-4.21730600	1.43853700	3.86756000
H	-5.34318600	2.22059200	5.94545000
H	-4.31169000	4.04850500	7.28429400
C	2.81192000	4.59472500	3.77957900
C	2.82104900	4.79801100	5.29841700
C	1.88170300	5.97642600	5.51938800
C	0.98923400	6.19349500	4.26548900
C	1.38510100	5.01410600	3.32095100
H	3.04832900	3.57428900	3.46982600
H	3.53333400	5.26611500	3.29855200
H	2.40282000	3.92805600	5.82331800
H	3.80484400	4.99420100	5.73473300
O	1.44302600	5.29394000	1.92450500
O	1.82600100	6.68355100	6.50114600
C	1.27698100	7.59200200	3.71707800
H	1.18930900	8.34631000	4.50798100
H	0.52252500	7.88328700	2.95839300
H	2.29751200	7.67230800	3.31597500
C	-0.48891700	5.96867700	4.63487500
H	-1.16689000	6.58678300	4.02528500
H	-0.67236600	6.25559200	5.67609600
C	-0.71559000	4.49187300	4.35965700
C	0.32013800	3.95719400	3.66345300
C	0.54919800	2.52976800	3.33132800
C	0.46327800	1.54738800	4.33598200
C	0.92480800	2.12613600	2.03773500
C	0.72722700	0.20816600	4.05369400
H	0.18690600	1.84188500	5.34409900
C	1.18569500	0.78406300	1.75642200
H	1.00146400	2.87282800	1.25583800
C	1.08787100	-0.18017400	2.76111100
H	0.65644200	-0.53211100	4.84591600
H	1.46745600	0.49091400	0.74816000
H	1.29471800	-1.22384600	2.54124800

12-SS-ts

B3LYP SCF energy: -2644.665814 a.u.
B3LYP enthalpy: -2643.851547 a.u.
B3LYP free energy: -2643.980369 a.u.
M06 SCF energy in solution: -2643.837418 a.u.
Imaginary frequency: -224.71 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.36841300	0.43642900	-0.77708300
C	1.65852400	-4.00774500	-0.69175100
C	1.78183900	-2.61301500	-0.72732900
C	2.77438400	-2.04965700	-1.56656400
C	3.58656500	-2.88723500	-2.34883900
C	3.43141400	-4.27072100	-2.31292400
C	2.47023700	-4.83165700	-1.47631000
H	0.91900800	-4.46449900	-0.04543500
H	4.34273400	-2.44222200	-2.98399200
H	4.06376400	-4.90170000	-2.92963200
H	2.34593600	-5.90937400	-1.42650500
C	3.04500400	-0.60299200	-1.63362400
O	4.21994500	-0.27608400	-2.19159600
C	4.26149500	1.17076600	-2.30292100
C	3.06443200	1.64971600	-1.44339600
H	5.23064300	1.50390600	-1.93147200
H	4.15939700	1.42206200	-3.36261100
H	2.42319600	2.31873900	-2.01580200
N	2.31012000	0.38080700	-1.21882800
P	0.69079100	-1.54936900	0.32325300
C	-0.63991700	-2.70298800	0.86255300
C	-0.82535700	-3.02274500	2.21635100
C	-1.47471900	-3.29961500	-0.10009200
C	-1.82416100	-3.92146100	2.59864300
H	-0.19210200	-2.58086000	2.97709900

C	-2.46404000	-4.20300400	0.28648200
H	-1.35352000	-3.06750100	-1.15246600
C	-2.64202200	-4.51571600	1.63740100
H	-1.95450300	-4.15952600	3.65024800
H	-3.09625500	-4.66011500	-0.46916100
H	-3.41147100	-5.22181000	1.93643400
C	1.67705700	-1.24500900	1.84732200
C	1.24939800	-0.24465200	2.73514500
C	2.81178600	-2.00496700	2.16975900
C	1.93740400	-0.01405000	3.92634300
H	0.36922900	0.34761700	2.50507800
C	3.50649300	-1.76202400	3.35687600
H	3.15401400	-2.79014800	1.50354500
C	3.06985400	-0.77028100	4.23752900
H	1.59137500	0.75822800	4.60702700
H	4.38395700	-2.35611000	3.59572800
H	3.60715400	-0.59027100	5.16421100
C	3.48101000	2.34874200	-0.16128200
C	4.01498900	1.64785000	0.92761700
C	3.41622100	3.74731800	-0.10189600
C	4.47113000	2.33454800	2.05401600
H	4.07091300	0.56318800	0.90667200
C	3.87684100	4.43535900	1.02232200
H	3.00952000	4.30187800	-0.94451400
C	4.40480700	3.72869600	2.10434500
H	4.87918900	1.77717400	2.89205800
H	3.82336000	5.51995100	1.05134000
H	4.76435500	4.26110100	2.98021200
C	-4.16062100	1.58749200	2.01088900
C	-3.34904800	0.65154200	1.33142600
C	-3.68587800	-0.71432600	1.43454000
C	-4.78093100	-1.12703600	2.18617900
C	-5.58069100	-0.18710900	2.84290000
C	-5.26935000	1.17004100	2.74495000
H	-3.95778200	2.64981800	1.93199300
H	-3.07505000	-1.45178400	0.92994600
H	-5.00873800	-2.18626900	2.26103000
H	-6.43832200	-0.51046800	3.42594500
H	-5.88948900	1.91023900	3.24204800
C	-1.88118500	2.80117800	-2.55374400
C	-3.11588900	3.46479000	-1.92997800
C	-2.73553500	3.80551000	-0.48817600
C	-1.32738000	3.27004400	-0.14234100
C	-0.94989900	2.46287700	-1.39861600
H	-2.10163500	1.91987300	-3.16153200
H	-1.32420100	3.49598700	-3.19819500
H	-3.97654900	2.78563100	-1.89590200
H	-3.44953200	4.36616800	-2.45365200
O	0.25947100	2.09913300	-1.63494100
O	-3.43520200	4.40823800	0.29582100
C	-0.37577500	4.46265500	0.07726100
H	-0.73451200	5.05750100	0.92313600
H	0.63725600	4.10903100	0.28790200
H	-0.33561200	5.11854500	-0.79997900
C	-1.40099200	2.32411200	1.05984300
H	-0.38826800	2.06269000	1.39409900
H	-1.89468000	2.81104500	1.90287800
C	-2.15538500	1.08038900	0.56802000
C	-1.65993900	0.54535000	-0.59675800
C	-2.35971300	-0.25112200	-1.62794000
C	-1.62167200	-0.91665100	-2.63058000
C	-3.76759000	-0.25721700	-1.76162000
C	-2.24678000	-1.59272800	-3.68002700
H	-0.53426800	-0.88951500	-2.59630200
C	-4.39251500	-0.93547700	-2.80471400
H	-4.37791700	0.26884300	-1.03683500
C	-3.63870700	-1.61458900	-3.76719800
H	-1.64331700	-2.09274700	-4.43280800
H	-5.47700400	-0.92629100	-2.87159200
H	-4.13099500	-2.13712900	-4.58214200

13-SS

B3LYP SCF energy: -2644.691976 a.u.
B3LYP enthalpy: -2643.875796 a.u.
B3LYP free energy: -2644.009898 a.u.
M06 SCF energy in solution: -2643.856606 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.86069600	0.65981600	-0.41838100
C	5.38801600	-0.33428700	-0.43372700
C	4.19375600	0.39952800	-0.39913200
C	4.23968800	1.78280900	-0.69966800
C	5.47335400	2.38825600	-0.99533500
C	6.64906300	1.64287900	-1.01060700
C	6.60676300	0.27746600	-0.73412300
H	5.36683600	-1.39886100	-0.22500100
H	5.49940200	3.44645800	-1.22539400
H	7.59118500	2.12784400	-1.24587400
H	7.51617500	-0.31552900	-0.75153900
C	3.04386800	2.63638600	-0.76323600
O	3.26325600	3.94670800	-0.92867800
C	1.97828700	4.62763400	-0.86860800
C	0.93694900	3.48414300	-0.90385100
H	1.95095500	5.20115800	0.06108600
H	1.91985800	5.30280200	-1.72266600
H	0.48957500	3.40465000	-1.90133500
N	1.79996700	2.27628900	-0.71358100
P	2.65456000	-0.47989400	0.08924400
C	2.84107100	-2.14638700	-0.63951000
C	2.86152200	-3.29957700	0.15863400
C	2.95128700	-2.26441900	-2.03683300
C	2.99198200	-4.55604900	-0.43764500
H	2.77416000	-3.22160900	1.23716100
C	3.08329900	-3.52119900	-2.62353000
H	2.94105200	-1.37803300	-2.66569500
C	3.10118500	-4.66879100	-1.82434800
H	3.00914200	-5.44525300	0.18550600
H	3.16968100	-3.60582400	-3.70270900
H	3.20092000	-5.64765700	-2.28392100
C	2.68414600	-0.65701700	1.91059700
C	1.47761700	-0.98961000	2.55300800
C	3.85570900	-0.49602800	2.66810300
C	1.45607000	-1.18203200	3.93432900
H	0.56240600	-1.08830400	1.97628700
C	3.81941500	-0.67804800	4.05114000
H	4.79264400	-0.22995600	2.19042100
C	2.62388300	-1.02491100	4.68447700
H	0.52176000	-1.44758300	4.42023300
H	4.72778000	-0.54992300	4.63250000
H	2.60243800	-1.16772500	5.76096500
C	-0.17336100	3.57273500	0.12367600
C	0.11804200	3.64090400	1.49527200
C	-1.50963100	3.58462500	-0.29296200
C	-0.91314100	3.72373400	2.42950400

H	1.15068700	3.62934800	1.83753000
C	-2.54303100	3.66849700	0.64259600
H	-1.74584400	3.53049600	-1.35326200
C	-2.24495600	3.73840700	2.00401200
H	-0.67833400	3.78047900	3.48843700
H	-3.57563700	3.66874300	0.30729500
H	-3.04670600	3.80575600	2.73350300
C	-5.85688700	0.27097300	-1.96907500
C	-4.93794500	0.28138300	-0.90287900
C	-5.33048100	0.89438500	0.30349900
C	-6.59416500	1.46587300	0.43721700
C	-7.49892500	1.43549700	-0.62737900
C	-7.12492600	0.83433900	-1.83023700
H	-5.58772600	-0.19712600	-2.91101400
H	-4.63439500	0.92806600	1.13439900
H	-6.87480800	1.93549600	1.37625400
H	-8.48539800	1.87770800	-0.52016400
H	-7.82062000	0.80332800	-2.66414900
C	-0.96023400	-2.69020400	-0.47735200
C	-1.71620700	-3.49860800	-1.53920400
C	-1.98363800	-2.51132900	-2.67525300
C	-1.62493500	-1.06914800	-2.23526100
C	-1.41277700	-1.22849300	-0.69506100
H	-1.15555700	-3.02295400	0.54583700
H	0.11931500	-2.75109300	-0.65001600
H	-2.68834000	-3.84996600	-1.16897300
H	-1.18194900	-4.37905900	-1.90948200
O	-0.55923000	-0.30153900	-0.05559900
O	-2.40907800	-2.79543800	-3.77294600
C	-0.41589600	-0.61139800	-3.05613500
H	-0.67782300	-0.59756000	-4.11950800
H	-0.10723100	0.40473200	-2.77192400
H	0.44397000	-1.27895600	-2.93209000
C	-2.85238000	-0.15682300	-2.39361700
H	-2.56796600	0.89209700	-2.56664100
H	-3.44839300	-0.46306100	-3.26046800
C	-3.58594600	-0.29256700	-1.07271500
C	-2.82104800	-0.92175700	-0.14595500
C	-3.20190800	-1.31190900	1.23402900
C	-4.26438800	-2.20927000	1.44126600
C	-2.50870500	-0.82640000	2.35781900
C	-4.62457600	-2.60806700	2.72862900
H	-4.81321300	-2.58858000	0.58387200
C	-2.87421800	-1.22373300	3.64545800
H	-1.70152600	-0.11670700	2.21173000
C	-3.93007400	-2.11791100	3.83639000
H	-5.44986500	-3.30138700	2.86552000
H	-2.34098500	-0.82266100	4.50432800
H	-4.21328600	-2.42545500	4.83915200

$PhB(OH)_2$

B3LYP SCF energy: -408.251372 a.u.
B3LYP enthalpy: -408.117603 a.u.
B3LYP free energy: -408.159333 a.u.
M06 SCF energy in solution: -408.131202 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.48943700	-0.67756900	0.92903100
C	2.58538600	-0.88855800	0.07290500
C	2.92573600	0.13626200	-0.82841300
C	2.20071500	1.32705400	-0.87473700
C	1.11552800	1.51554900	-0.01503300
C	0.75993200	0.51065900	0.88832700
H	1.21073900	-1.45739900	1.63265000
H	3.76953500	-0.00785600	-1.49777000
H	2.47921200	2.10760300	-1.57846400
H	0.54851300	2.44276200	-0.04907200
H	-0.08414700	0.65519000	1.55816800
B	3.40014700	-2.21969000	0.12173300
O	4.46145500	-2.36475800	-0.74207400
H	4.93065000	-3.20756200	-0.66749700
O	3.01838100	-3.18379000	1.02625700
H	3.55800600	-3.98670300	1.01294200

14-ts

B3LYP SCF energy: -3052.911355 a.u.
B3LYP enthalpy: -3051.960936 a.u.
B3LYP free energy: -3052.107627 a.u.
M06 SCF energy in solution: -3051.98227 a.u.

Imaginary frequency: -171.46 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.00979500	-0.57525600	0.23480900
C	0.73885400	3.79539200	1.76202100
C	1.29022900	2.55637000	1.41735400
C	2.20630700	1.94750100	2.31091500
C	2.51501500	2.58311900	3.52578700
C	1.93647900	3.80532200	3.86077300
C	1.05558000	4.41792700	2.97300800
H	0.04699300	4.28077900	1.08308000
H	3.21628800	2.11359400	4.20428300
H	2.18192000	4.27580900	4.80762400
H	0.60998000	5.37810600	3.21569500
C	2.93692300	0.70230500	2.00253500
O	4.00141400	0.49158500	2.78913800
C	4.50459500	-0.83434600	2.47980000
C	3.93735100	-1.09822600	1.07357200
H	5.59202500	-0.79732600	2.52422100
H	4.11217700	-1.52122700	3.23718200
H	3.60291600	-2.12843000	0.98523900
N	2.73904800	-0.19152300	1.06999900
P	0.84387500	1.69959900	-0.14588300
C	-0.70511900	2.48194500	-0.74100300
C	-0.81927400	2.88155200	-2.08259700
C	-1.79787200	2.67229100	0.12210400
C	-1.99604300	3.47531400	-2.54229700
H	0.00887100	2.74304000	-2.76813800
C	-2.96378700	3.28138700	-0.33776700
H	-1.73596000	2.36846300	1.16179600
C	-3.06551600	3.68406900	-1.67182600
H	-2.06788000	3.78404300	-3.58113000
H	-3.79633500	3.43097800	0.34186000
H	-3.97697400	4.15480800	-2.02812800
C	2.11756300	2.23085700	-1.35927500
C	2.37719700	1.41985400	-2.47562700
C	2.77653000	3.46411900	-1.22880200
C	3.27529200	1.84906100	-3.45454500
H	1.86507700	0.46830900	-2.57705100
C	3.68102700	3.88017500	-2.20668500
H	2.58427600	4.10418200	-0.37350000
C	3.92778700	3.07626900	-3.32231100

H	3.46846900	1.22038300	-4.31906800
H	4.18516400	4.83648500	-2.09996100
H	4.62578600	3.40700300	-4.08617600
C	4.94642400	-0.78730500	-0.02288800
C	5.25420600	0.52245400	-0.41052000
C	5.68882400	-1.84519400	-0.56652700
C	6.27897300	0.76703800	-1.32637000
H	4.69365300	1.36126500	-0.01113600
C	6.71546300	-1.60112600	-1.47925300
H	5.46641300	-2.86535500	-0.26735100
C	7.01307000	-0.29208900	-1.86249500
H	6.50097500	1.78878700	-1.61942400
H	7.28189800	-2.43275700	-1.88879200
H	7.81209200	-0.09917000	-2.57258000
C	-6.08105400	0.83976500	1.73646500
C	-5.23416300	0.56692000	0.64420300
C	-5.63122700	1.03487800	-0.62500600
C	-6.82838700	1.72701100	-0.79166900
C	-7.66307700	1.97424200	0.30146200
C	-7.28204900	1.52849000	1.56726700
H	-5.81345300	0.49824300	2.73121400
H	-4.99059900	0.86838700	-1.48213200
H	-7.11066900	2.07616300	-1.78129100
H	-8.59793700	2.51096700	0.16744000
H	-7.91949100	1.71404800	2.42718000
C	-2.96823900	-3.32740300	2.05817100
C	-2.23609000	-3.11067200	0.72710700
C	-2.02856100	-1.56227600	0.61247200
C	-2.02838200	-1.02716900	2.10223300
C	-2.34273900	-2.28065200	2.95288500
H	-4.04164500	-3.11037500	1.96202900
H	-2.86481800	-4.33276300	2.47297100
H	-2.78561100	-3.50651700	-0.12616200
H	-1.28179500	-3.63221700	0.74800200
O	-2.08309800	-2.38470200	4.13205700
O	-0.84528100	-1.17685700	-0.19205700
C	-0.78302900	-0.34569800	2.66006900
H	-0.60769500	0.62540900	2.19359000
H	-0.92659200	-0.19246300	3.73449500
H	0.11732200	-0.95946500	2.54480100
C	-3.27234500	-0.09136800	2.20023300
H	-3.93061700	-0.40816400	3.01861600
H	-2.98391200	0.93940100	2.44757700
C	-3.96152700	-0.15962300	0.85608300
C	-3.26863800	-0.92525100	-0.01926100
C	-3.69040300	-1.32159600	-1.39142600
C	-4.81485100	-2.14831300	-1.56618800
C	-2.97615700	-0.91327400	-2.53200900
C	-5.21372000	-2.55700800	-2.83908500
H	-5.38189200	-2.46553200	-0.69550800
C	-3.37884900	-1.32403700	-3.80647400
H	-2.11023700	-0.27056100	-2.42058900
C	-4.49582100	-2.14729900	-3.96475800
H	-6.08507800	-3.19620900	-2.95037500
H	-2.82049100	-0.99178800	-4.67787600
H	-4.80622900	-2.46424700	-4.95631000
C	1.19880000	-3.36721000	1.04925100
C	1.32735900	-2.63317200	-0.15458400
C	2.32285500	-3.07264600	-1.05795300
C	3.07413500	-4.22347800	-0.82409900
C	2.90563000	-4.93442500	0.36862800
C	1.97942000	-4.49199900	1.31837400
H	0.47128100	-3.06563300	1.79669400
H	2.47503600	-2.52509200	-1.98331800
H	3.78960900	-4.56746500	-1.56618100
H	3.49134100	-5.83041300	0.55626300
H	1.85332500	-5.03426600	2.25169900
B	-0.14853700	-2.06267300	-1.17602100
O	-0.73329500	-3.25880300	-1.62183200
H	-1.49861000	-3.05298600	-2.18467800
O	0.33529700	-1.16929200	-2.20007300
H	0.58846400	-1.70309300	-2.96768000

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B3LYP SCF energy: -1138.748278 a.u.
B3LYP enthalpy: -1138.342925 a.u.
B3LYP free energy: -1138.420619 a.u.
M06 SCF energy in solution: -1138.34858 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-9.77741500	-4.51010000	0.59104300
C	-8.92583800	-4.77647300	-0.49722200
C	-9.27872200	-4.25548300	-1.75583400
C	-10.44381500	-3.50890500	-1.92041200
C	-11.28613800	-3.26616500	-0.83302200
C	-10.94786300	-3.77109400	0.42363600
H	-9.53188700	-4.89899800	1.57464600
H	-8.62597100	-4.42455100	-2.60509700
H	-10.69107300	-3.11050200	-2.90090900
H	-12.19448400	-2.68400300	-0.96300600
H	-11.59405500	-3.58773500	1.27800000
C	-6.47778800	-8.96994900	0.64115600
C	-5.66158400	-8.52004800	-0.57718900
C	-5.77936200	-6.97385000	-0.59668400
C	-5.84818600	-6.54303300	0.90292800
C	-6.47641600	-7.77244000	1.59131300
H	-7.52243300	-9.18398000	0.37943900
H	-6.08822300	-9.86374600	1.13873300
H	-6.00996000	-8.98656900	-1.50329100
H	-4.60723600	-8.78994900	-0.44979600
O	-6.91081400	-7.77739200	2.72313800
O	-4.68302700	-6.32410700	-1.24250400
C	-4.49290800	-6.24303400	1.55804800
H	-4.00755100	-5.40248300	1.05558500
H	-4.64404900	-5.99868800	2.61475400
H	-3.81215800	-7.10079700	1.50480500
C	-6.83954900	-5.36839400	0.95025400
H	-7.41615400	-5.38814800	1.88133200
H	-6.32500900	-4.39807700	0.91380100
C	-7.68399000	-5.55674600	-0.29733800
C	-7.11650000	-6.44814100	-1.14323700
C	-7.65740900	-6.93361700	-2.43969600
C	-8.80192400	-7.74925600	-2.46855700
C	-7.02868700	-6.62617700	-3.66065500
C	-9.29849200	-8.24592400	-3.67413700
H	-9.30561200	-7.98457200	-1.53517400
C	-7.52564300	-7.12593500	-4.86735300
H	-6.16964500	-5.96259100	-3.66598000
C	-8.65937700	-7.94054900	-4.87777400
H	-10.18617800	-8.87296100	-3.67241900
H	-7.02931700	-6.86917900	-5.79949700
H	-9.04551500	-8.32843200	-5.81635500
B	-3.81707100	-6.78653000	-2.20041400

O	-4.07790600	-7.76445200	-3.13538700
H	-5.01026400	-8.01867300	-3.17660300
O	-2.58721000	-6.18247900	-2.22950600
H	-2.07871700	-6.50806200	-2.98609800

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B3LYP SCF energy: -2873.373528 a.u.
B3LYP enthalpy: -2872.501128 a.u.
B3LYP free energy: -2872.644794 a.u.
M06 SCF energy in solution: -2872.465647 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.55630100	6.42375100	1.38798000
C	-1.62072000	8.38948300	-1.23894800
C	-0.32450700	8.14826300	-0.77058300
C	0.47271700	9.25705600	-0.38723600
C	-0.03917200	10.55863100	-0.51482500
C	-1.33009100	10.77565900	-0.99099500
C	-2.12417900	9.68853300	-1.34763500
H	-2.24847700	7.55120500	-1.51946400
H	0.58137200	11.39804300	-0.22538100
H	-1.71177100	11.78894900	-1.07307400
H	-3.13636900	9.84331200	-1.71070100
C	1.83476600	9.11894600	0.16260300
O	2.55034000	10.26399300	0.19054600
C	3.74088300	9.99483100	0.97477800
C	3.81889300	8.45282000	1.01545300
H	4.58494600	10.46887100	0.47376600
H	3.59226800	10.44005900	1.96435600
H	3.98822000	8.08255700	2.02526600
N	2.42590000	8.06633000	0.63610500
P	0.33262200	6.43765600	-0.56711600
C	-1.05148700	5.30045700	-0.96865200
C	-1.53119700	5.15829500	-2.28387700
C	-1.61064600	4.52637300	0.05896200
C	-2.57832000	4.27972600	-2.55592000
H	-1.07985900	5.71932100	-3.09682400
C	-2.65558400	3.64142300	-0.22415300
H	-1.19089600	4.60403700	1.05705500
C	-3.14448300	3.52326200	-1.52493700
H	-2.94438600	4.17692900	-3.57407000
H	-3.07592800	3.03925400	0.57640200
H	-3.95663400	2.83411400	-1.74144000
C	1.49364900	6.21191500	-1.97687500
C	2.48943700	5.23090100	-1.83974500
C	1.38027900	6.92411800	-3.18129100
C	3.33511200	4.94810300	-2.91391200
H	2.62551400	4.71578500	-0.89134400
C	2.23716600	6.64107100	-4.24684400
H	0.62441500	7.69727300	-3.29179400
C	3.20834200	5.64533600	-4.11706400
H	4.10431000	4.18962900	-2.80013200
H	2.14127500	7.19419800	-5.17768700
H	3.86982000	5.42038600	-4.94973400
C	4.87816100	7.87796300	0.09103900
C	4.82878400	8.07657400	-1.29524000
C	5.97605400	7.20592200	0.63967700
C	5.85918500	7.61416300	-2.11296000
H	3.97958900	8.58457000	-1.74463900
C	7.00898800	6.74267500	-0.17711800
H	6.02117200	7.04211100	1.71311500
C	6.95341800	6.94759000	-1.55601800
H	5.80293300	7.76947300	-3.18666700
H	7.85255600	6.21943500	0.26470800
H	7.75552800	6.58713200	-2.19448100
C	-4.16688600	2.87978900	4.49434900
C	-2.92926100	2.77611400	3.83247400
C	-2.64749800	1.57601800	3.14971600
C	-3.56076500	0.52309700	3.14114800
C	-4.77948400	0.63889100	3.81516300
C	-5.07700000	1.82244400	4.49249100
H	-4.41382000	3.79249200	5.02868800
H	-1.70530300	1.47690500	2.62076300
H	-3.31976900	-0.39066700	2.60372800
H	-5.49015200	-0.18342700	3.80911400
H	-6.02152400	1.92612100	5.02069800
C	1.01201300	5.69459300	4.66350100
C	0.18033500	6.00047400	5.91367400
C	-1.14188200	6.53241400	5.37227100
C	-1.26521400	6.21565200	3.86599300
C	-0.02264600	5.28581000	3.58165700
H	1.76675400	4.92065400	4.82018200
H	1.54027500	6.59046600	4.33021800
H	-0.04000300	5.08897200	6.48748200
H	0.63357200	6.71398700	6.61003300
O	0.42158500	5.24749400	2.24987300
O	-1.98317300	7.12694400	6.01667900
C	-1.29723800	7.53402800	3.08816900
H	-2.12542500	8.15715900	3.44410900
H	-1.43239500	7.34728300	2.01886400
H	-0.36797000	8.10349700	3.21710100
C	-2.50726300	5.33460500	3.64042800
H	-2.93201900	5.47047100	2.63456300
H	-3.30224100	5.59616700	4.34941900
C	-1.98590400	3.91774300	3.81138400
C	-0.63093900	3.88650700	3.84573500
C	0.24252800	2.71520600	4.08773800
C	0.00276600	1.86429000	5.18310900
C	1.35931400	2.45488400	3.27074600
C	0.84065400	0.78156900	5.44722300
H	-0.84761300	2.05998400	5.83002300
C	2.19515700	1.36922000	3.53926400
H	1.56534200	3.10901200	2.43127100
C	1.94081600	0.52750000	4.62453100
H	0.63628200	0.13896600	6.30019100
H	3.04881600	1.18635500	2.89139800
H	2.59460800	-0.31646500	4.83022000
C	3.66335100	5.09975200	2.28497100
C	4.71284100	4.68144400	3.30867600
H	5.07370900	5.53191500	3.89366600
H	4.25269100	3.96485800	3.99993600
H	5.54498800	4.17926800	2.80840400
O	3.00960300	6.18605900	2.60001100
O	3.46390600	4.41993900	1.27254800

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B3LYP SCF energy: -3281.641487 a.u.
B3LYP enthalpy: -3280.633246 a.u.
B3LYP free energy: -3280.796391 a.u.
M06 SCF energy in solution: -3280.622992 a.u.

Cartesian coordinates

ATOM	X	Y	Z

Ni	1.59676500	6.85501000	-0.35012300
C	-1.49447100	7.91584700	-3.69444800
C	-0.32428900	7.95580500	-2.92635400
C	0.31430700	9.20336400	-2.72767600
C	-0.23627900	10.36198300	-3.30163200
C	-1.40224100	10.30019400	-4.05998000
C	-2.03217600	9.07388800	-4.25968800
H	-2.00001500	6.96794700	-3.84271800
H	0.25690100	11.31285700	-3.14286800
H	-1.81513800	11.20858400	-4.48809500
H	-2.94274400	9.01253100	-4.84878200
C	1.56673400	9.36341200	-1.96358300
O	2.16179900	10.56146500	-2.12163600
C	3.25996200	10.61903300	-1.17559600
C	3.47444700	9.14510300	-0.77304900
H	4.11297300	11.07115700	-1.68153700
H	2.94078500	11.24730900	-0.33762700
H	3.56870700	9.03065400	0.30508400
N	2.18040600	8.52697100	-1.18471600
P	0.34876500	6.42402000	-2.16177700
C	-1.07584000	5.27587600	-2.09660600
C	-1.07528100	4.06168300	-2.79675000
C	-2.18185100	5.61216100	-1.29714900
C	-2.16837300	3.19701400	-2.70192500
H	-0.22487600	3.78409600	-3.41010300
C	-3.27291900	4.74710600	-1.21281900
H	-2.18844500	6.53458500	-0.72458100
C	-3.26746500	3.53736100	-1.91361700
H	-2.15468400	2.25512500	-3.24297200
H	-4.12028100	5.01449000	-0.58797500
H	-4.11444500	2.86130300	-1.83810300
C	1.51046500	5.71835500	-3.39911300
C	2.58778200	4.94831900	-2.92611700
C	1.34797600	5.90813900	-4.78118800
C	3.47693200	4.36663900	-3.83247000
H	2.74804900	4.80991000	-1.85900900
C	2.24634900	5.33013400	-5.67876500
H	0.52420700	6.50670600	-5.15901900
C	3.30883700	4.55557600	-5.20529600
H	4.30556200	3.77314200	-3.45742700
H	2.11438800	5.48281600	-6.74653600
H	4.00510600	4.10334100	-5.90654300
C	4.67735000	8.50208700	-1.44338100
C	4.65983900	8.10380400	-2.78557600
C	5.86746500	8.37684900	-0.71514700
C	5.81058700	7.58997700	-3.38591100
H	3.74465100	8.17438200	-3.36618100
C	7.02030300	7.87010100	-1.31597000
H	5.88853100	8.67287200	0.33076600
C	6.99392300	7.47406700	-2.65463500
H	5.77746000	7.27484000	-4.42510700
H	7.93481000	7.77740400	-0.73653700
H	7.88848500	7.07269200	-3.12281800
C	-3.16478500	2.54187800	5.98879800
C	-2.42390800	2.68669500	4.80273100
C	-2.92163000	2.09601400	3.62630500
C	-4.10944700	1.36699900	3.64516600
C	-4.82666600	1.21371800	4.83512700
C	-4.34987900	1.80539100	6.00659900
H	-2.80123200	2.99718400	6.90631000
H	-2.37008900	2.24146100	2.70312300
H	-4.48050200	0.91914800	2.72606700
H	-5.75190100	0.64285800	4.84812400
H	-4.90194100	1.69538300	6.93689600
C	2.35781300	4.09577600	4.56124700
C	2.25989800	3.84204900	6.06868100
C	1.05595500	4.67016900	6.52201600
C	0.32284000	5.26658300	5.29895800
C	0.91452900	4.42800700	4.11124000
H	2.77739900	3.25698400	4.00001300
H	2.97719800	4.97634500	4.35594000
H	2.04276500	2.78903300	6.29283400
H	3.15331200	4.11156800	6.64229600
O	1.00088500	5.08283800	2.86093600
O	0.72474800	4.84928600	7.67672400
C	0.60362700	6.77437200	5.27494600
H	0.27118400	7.22342500	6.21800000
H	0.07911800	7.25605700	4.44829700
H	1.67392500	6.98424400	5.15931400
C	-1.16323000	4.88887800	5.36501600
H	-1.79031000	5.57719800	4.78031200
H	-1.53027700	4.91673600	6.39863500
C	-1.18658700	3.49598400	4.76354500
C	-0.02414500	3.20088200	4.13353800
C	0.38338900	1.89354200	3.57398800
C	0.10571300	0.70331300	4.27420300
C	1.12587600	1.79637500	2.38196600
C	0.52855100	-0.53414800	3.79133800
H	-0.44444600	0.75624700	5.20860300
C	1.55219100	0.55806800	1.90243100
H	1.35346600	2.69941900	1.83051400
C	1.25377800	-0.61413300	2.60037200
H	0.29870600	-1.43654100	4.35292100
H	2.12213400	0.51149700	0.97738900
H	1.58859800	-1.57813400	2.22507200
C	3.74201300	5.93447200	1.12212400
C	4.87667300	6.10205300	2.12151200
H	5.82038500	6.19914600	1.57178000
H	4.73572800	6.98510400	2.74883800
H	4.94527400	5.20609400	2.74335100
O	3.01368100	6.99619900	0.93595300
O	3.58285000	4.85171800	0.53486000
C	-2.14632300	6.85765200	1.97559800
C	-0.74417300	6.77226200	1.89310000
C	-0.04290500	7.99612600	1.90317600
C	-0.70244000	9.22912100	1.94963400
C	-2.09825200	9.27853900	2.00549700
C	-2.81976300	8.08332000	2.02921300
H	-2.71820500	5.93249700	2.01220400
H	1.04487400	7.97892800	1.91467600
H	-0.12678200	10.15346100	1.96587900
H	-2.61446800	10.23480800	2.05068700
H	-3.90571600	8.10579900	2.09904400
B	0.00053700	5.31256600	1.82993900
O	0.90437100	5.33278300	0.47511800
H	1.72355700	4.81778600	0.65732100
O	-0.90243200	4.20698300	1.65613600
H	-1.40520400	4.33275700	0.83991600

18-ts

B3LYP SCF energy: -3281.625816 a.u.
B3LYP enthalpy: -3280.619653 a.u.
B3LYP free energy: -3280.779567 a.u.
M06 SCF energy in solution: -3280.607769 a.u.
Imaginary frequency: -36.78 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	-1.23785800	-0.14378600	0.37655000
C	-5.73175200	0.53873500	1.17734600
C	-4.37371500	0.84412900	1.02445700
C	-3.80801800	1.82438100	1.87130600
C	-4.61002700	2.46290200	2.83171300
C	-5.95821900	2.14399600	2.96575700
C	-6.52145500	1.17960600	2.13414400
H	-6.17987700	-0.22558500	0.55225600
H	-4.16110800	3.20821400	3.47660100
H	-6.55974700	2.64421500	3.71889900
H	-7.57101600	0.91548300	2.22906800
C	-2.39711600	2.23898400	1.79424700
O	-2.08900600	3.34340000	2.50793800
C	-0.64734100	3.49192300	2.45337200
C	-0.21584600	2.54573300	1.30813800
H	-0.42696000	4.54318600	2.26522700
H	-0.24533200	3.19122500	3.42592500
H	0.59514600	1.88800200	1.61808500
N	-1.42940100	1.70436100	1.12771600
P	-3.38037600	-0.02436700	-0.27773400
C	-4.31587200	-1.58771600	-0.49181700
C	-5.03309600	-1.90532300	-1.65287200
C	-4.30758500	-2.48678700	0.58969400
C	-5.75615900	-3.09887100	-1.72444100
H	-5.03227900	-1.22837500	-2.50076500
C	-5.04099700	-3.67024500	0.51255400
H	-3.72090800	-2.25186200	1.47498400
C	-5.76800000	-3.97761100	-0.64068400
H	-6.31025300	-3.33741100	-2.62838200
H	-5.03760300	-4.35828800	1.35375600
H	-6.33696400	-4.90201000	-0.69610800
C	-3.64820000	0.99776000	-1.78409300
C	-2.52964800	1.36867900	-2.54641200
C	-4.92325300	1.44000900	-2.17784500
C	-2.68889900	2.14726800	-3.69558800
H	-1.53480700	1.06022600	-2.23921300
C	-5.07710700	2.21633300	-3.32560100
H	-5.79743100	1.18434200	-1.58648500
C	-3.95966200	2.56724400	-4.08883600
H	-1.81425600	2.42747300	-4.27540000
H	-6.06778000	2.55043200	-3.62183900
H	-4.08159400	3.17252900	-4.98314000
C	0.19884400	3.26944800	0.03837400
C	-0.72440600	3.96227300	-0.75562200
C	1.55428700	3.30577100	-0.31181400
C	-0.29728300	4.67310500	-1.87809600
H	-1.78175000	3.94225200	-0.50555000
C	1.98474800	4.01717000	-1.43432000
H	2.28446000	2.78160600	0.29873100
C	1.05721100	4.70214300	-2.22085000
H	-1.02522500	5.20318700	-2.48658300
H	3.04120300	4.02886200	-1.68678700
H	1.38634200	5.25566600	-3.09615700
C	5.96456800	1.95452700	-1.51226500
C	5.14145600	1.35976500	-0.53626000
C	4.90190800	2.09319500	0.64506800
C	5.46891600	3.35024200	0.84316800
C	6.29303200	3.91778100	-0.13320100
C	6.53697700	3.21169500	-1.31173200
H	6.17103300	1.42306300	-2.43545600
H	4.26517700	1.66635600	1.41258800
H	5.26434100	3.89073800	1.76408000
H	6.73634500	4.89763200	0.02341400
H	7.17613900	3.63776400	-2.08102400
C	3.79339000	-3.43826500	-0.17807500
C	5.10988200	-3.63339900	-0.93325700
C	4.98414100	-2.73494000	-2.16245500
C	3.72494800	-1.84049600	-2.05619600
C	3.30448800	-2.01848700	-0.55768600
H	3.88199800	-3.56278300	0.90387800
H	3.03329200	-4.14479100	-0.52977100
H	5.97381600	-3.28237800	-0.35199600
H	5.32534900	-4.66602500	-1.22727200
O	1.92538500	-1.97606300	-0.24264300
O	5.75506800	-2.71775100	-3.10043200
C	2.71576700	-2.31866900	-3.10886500
H	3.18369500	-2.29351700	-4.09970500
H	1.83864400	-1.66990400	-3.10890800
H	2.38600500	-3.34624600	-2.91619200
C	4.14945000	-0.37061200	-2.20399900
H	3.33540200	0.24554600	-2.60261300
H	4.99443800	-0.29078200	-2.89819800
C	4.50761200	0.04475200	-0.78512700
C	4.11619400	-0.89149900	0.12041100
C	4.44672900	-0.96089600	1.56357900
C	5.76374800	-0.71964200	2.00366900
C	3.49107200	-1.34777000	2.52122000
C	6.10243900	-0.82725100	3.35115700
H	6.52458200	-0.44969900	1.27719400
C	3.83128700	-1.44925100	3.87103600
H	2.48014700	-1.57799900	2.21345800
C	5.13501700	-1.18603100	4.29426500
H	7.12650400	-0.63807400	3.66402300
H	3.06323600	-1.73710400	4.58378600
H	5.39972600	-1.26864100	5.34552100
C	-1.09306100	-1.50937700	3.19555900
C	-1.59784400	-2.14479900	4.49239800
H	-2.43540200	-1.57070200	4.90032900
H	-1.96718200	-3.15543700	4.27651200
H	-0.79542800	-2.22065100	5.22986200
O	-1.97062500	-1.07016300	2.38965900
O	0.15779400	-1.49468700	3.00432600
C	-1.00134800	-1.86735700	-2.12617000
C	-0.52529000	-1.84787900	-0.79205900
C	-0.79033200	-2.99178600	0.00322000
C	-1.45973600	-4.09831800	-0.51182000
C	-1.89964500	-4.08884800	-1.83975300
C	-1.67211700	-2.97159700	-2.64919900
H	-0.77637600	-1.02052400	-2.76674000
H	-0.41353300	-3.01576100	1.02093800
H	-1.63478200	-4.97182400	0.11122500
H	-2.41910000	-4.95414800	-2.24445400
H	-2.00561500	-2.97238800	-3.68418700
B	0.92884000	-0.95196900	-0.45871300
O	0.60309500	-0.19493400	0.80660800
H	0.55705500	-0.76059700	1.66190100
O	1.10872300	0.00975400	-1.52100500
H	1.48152700	0.82492400	-1.15582400

19-ts

B3LYP SCF energy: -2644.652641 a.u.
B3LYP enthalpy: -2643.839244 a.u.
B3LYP free energy: -2643.969718 a.u.

M06 SCF energy in solution: -2643.825797 a.u.
Imaginary frequency: -242.71 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.05052800	-0.53527200	-0.10504200
C	-3.72624900	-2.01475300	1.90606400
C	-2.71333700	-1.10070800	1.59914800
C	-1.96847900	-0.53160200	2.66393700
C	-2.26236000	-0.88620700	3.98948600
C	-3.26912600	-1.80805500	4.27255800
C	-4.00257200	-2.37051000	3.23052400
H	-4.30418700	-2.46046100	1.10355600
H	-1.69530700	-0.43514200	4.79560000
H	-3.47766500	-2.07997200	5.30252900
H	-4.79212100	-3.08610500	3.44021700
C	-0.91899500	0.48057200	2.44550500
O	-0.65497500	1.27033800	3.49968300
C	0.49244500	2.08734600	3.13442200
C	0.51544900	2.00786400	1.59536900
H	0.32496000	3.08956000	3.52629000
H	1.37553900	1.64083700	3.60316400
H	1.52963100	1.87661500	1.21992200
N	-0.24045300	0.73106100	1.36625200
P	-2.32883700	-0.66073800	-0.15340000
C	-3.11931800	-1.95986200	-1.17264400
C	-4.22455100	-1.68245900	-1.99296400
C	-2.59340400	-3.26384100	-1.14564900
C	-4.79551400	-2.69454800	-2.76687400
H	-4.64364600	-0.68289500	-2.02865500
C	-3.17465800	-4.27129700	-1.91345600
H	-1.72917100	-3.48759100	-0.53181700
C	-4.27448900	-3.98842000	-2.72754100
H	-5.65046400	-2.46893000	-3.39760100
H	-2.76423800	-5.27654900	-1.88141800
H	-4.72213100	-4.77402800	-3.32939100
C	-3.26007300	0.87531300	-0.50489600
C	-2.80678900	1.69841100	-1.54790000
C	-4.44178600	1.20873600	0.17501500
C	-3.53669600	2.82769200	-1.91799300
H	-1.88468100	1.45751400	-2.07000400
C	-5.16335900	2.34546500	-0.19296600
H	-4.80569800	0.58084900	0.98292600
C	-4.71546700	3.15107600	-1.24233800
H	-3.18031500	3.45829000	-2.72687000
H	-6.07869700	2.59627500	0.33547100
H	-5.28337900	4.03075000	-1.53151900
C	-0.12731300	3.20759700	0.91529100
C	-1.37674100	3.69424800	1.33190000
C	0.56064900	3.88682200	-0.09591200
C	-1.91942600	4.83859700	0.75076400
H	-1.92889000	3.18981400	2.12079500
C	0.01513700	5.03231300	-0.68084500
H	1.53237000	3.52972800	-0.42218800
C	-1.22389300	5.51198600	-0.25763000
H	-2.88373700	5.20712500	1.08800900
H	0.56642000	5.55060500	-1.46018200
H	-1.64446900	6.40868500	-0.70402800
C	1.67865800	1.03223400	-2.34240400
C	2.74079100	1.15351700	-1.41758400
C	3.62473200	2.24039600	-1.59131500
C	3.46811400	3.14545800	-2.64174100
C	2.42451000	2.99280100	-3.55447200
C	1.52941900	1.93077200	-3.39526700
H	0.96001600	0.22544400	-2.24820900
H	4.44039900	2.38674600	-0.89360400
H	4.16832200	3.96955400	-2.74458300
H	2.30684500	3.69113900	-4.37796700
H	0.71123500	1.79862900	-4.09800000
C	2.33291200	-2.32301400	-2.35899800
C	3.62043200	-2.97299800	-1.83366400
C	3.23363500	-3.63953500	-0.51248200
C	1.92545400	-3.03022500	0.03127100
C	1.41145000	-2.15551600	-1.15470500
H	2.48466000	-1.38971800	-2.90625600
H	1.79480000	-3.00027100	-3.03799200
H	4.39261700	-2.22463600	-1.61442700
H	4.06582500	-3.70377800	-2.51396500
O	0.15567300	-1.89481300	-1.35839600
O	3.84979200	-4.51988600	0.04164600
C	0.97467000	-4.11230500	0.54059400
H	1.49055400	-4.70427500	1.30308700
H	0.07721200	-3.67114000	0.98620500
H	0.66664800	-4.79287300	-0.26064900
C	2.24559300	-1.89541700	1.04303800
H	1.53987200	-1.92487000	1.88269100
H	3.25419900	-1.95083800	1.46441400
C	1.99323600	-0.72594700	0.09842800
C	2.93042400	0.20126700	-0.28813200
C	4.23743400	0.26606200	0.44748100
C	4.27649200	0.44352400	1.84035900
C	5.45732200	0.10990100	-0.23701300
C	5.49004000	0.46850800	2.52827500
H	3.34607000	0.56360000	2.38920600
C	6.66985100	0.11739900	0.45196900
H	5.45498100	-0.01745200	-1.31598900
C	6.69077400	0.30090000	1.83639200
H	5.49721100	0.61553500	3.60456600
H	7.59884800	-0.01748900	-0.09436400
H	7.63568600	0.31292400	2.37139700

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B3LYP SCF energy: -2644.659747 a.u.
B3LYP enthalpy: -2643.844213 a.u.
B3LYP free energy: -2643.974055 a.u.
M06 SCF energy in solution: -2643.831637 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	0.00566600	-0.46192300	-0.10807400
C	-3.49235900	-2.07935400	1.98101500
C	-2.53818400	-1.10934500	1.65902500
C	-1.81791300	-0.48709900	2.71133800
C	-2.08322300	-0.83966100	4.04270400
C	-3.03323300	-1.81526800	4.34247400
C	-3.73704400	-2.43444400	3.31194700
H	-4.05054900	-2.56529200	1.18809400
H	-1.53678300	-0.34759600	4.83920600
H	-3.22005300	-2.08646800	5.37674400
H	-4.48070700	-3.19344500	3.53580100
C	-0.81622700	0.56341500	2.46427500
O	-0.57104300	1.39104200	3.49018500
C	0.53160700	2.25146200	3.08337900
C	0.55249800	2.11675000	1.54667100

H	0.31531500	3.25777800	3.43874500
H	1.43962700	1.87110700	3.56050500
H	1.57228000	2.00605600	1.17725900
N	-0.16059300	0.80448100	1.36817300
P	-2.21087800	-0.65643100	-0.09800400
C	-3.01489400	-1.92705800	-1.13258700
C	-4.19847100	-1.64128600	-1.83524000
C	-2.45361300	-3.21303200	-1.21818200
C	-4.81237200	-2.63167000	-2.60258200
H	-4.64347600	-0.65405200	-1.78520400
C	-3.07810100	-4.19766900	-1.98186600
H	-1.52630500	-3.43199800	-0.70727500
C	-4.25567400	-3.90963200	-2.67596100
H	-5.72670400	-2.40168400	-3.14163600
H	-2.63825100	-5.18897900	-2.04206500
H	-4.73582500	-4.67815200	-3.27483800
C	-3.13590000	0.88831600	-0.41565400
C	-2.76091900	1.67174600	-1.51854500
C	-4.26380700	1.24553000	0.33904500
C	-3.51853400	2.78725400	-1.87260100
H	-1.88255300	1.40800100	-2.10125200
C	-5.01310300	2.36868400	-0.01583900
H	-4.56868000	0.64405800	1.19025300
C	-4.64589500	3.13465400	-1.12408300
H	-3.22499200	3.38772000	-2.72818200
H	-5.88852900	2.63755200	0.56833300
H	-5.23661900	4.00233200	-1.40346500
C	-0.12076300	3.27209400	0.82220300
C	-1.33964200	3.80113100	1.27560500
C	0.51475400	3.87344700	-0.26975600
C	-1.90209800	4.91390900	0.65353500
H	-1.85077900	3.35650500	2.12599100
C	-0.05188100	4.98594200	-0.89649400
H	1.46449100	3.48489500	-0.62427300
C	-1.25808300	5.51106200	-0.43399900
H	-2.84030000	5.31864800	1.02140600
H	0.45974000	5.44608200	-1.73696600
H	-1.69227200	6.38511900	-0.91116400
C	1.78594700	0.92602700	-2.50364600
C	2.79702600	1.07542500	-1.52569100
C	3.63201000	2.20896900	-1.62974200
C	3.50018300	3.11573800	-2.68240900
C	2.51869500	2.92892100	-3.65506800
C	1.65710500	1.83264300	-3.55172100
H	1.08300100	0.10311000	-2.44470300
H	4.39419400	2.39149500	-0.88289000
H	4.16917900	3.96979700	-2.73648400
H	2.41800900	3.63119900	-4.47752000
H	0.87695900	1.68153300	-4.29269100
C	2.23067100	-2.38287400	-2.56746700
C	3.44606400	-3.25334300	-2.21334300
C	3.01813900	-4.02558200	-0.96634900
C	1.93069000	-3.23650600	-0.22680600
C	1.52652400	-2.06765700	-1.22486100
H	2.48901600	-1.49271800	-3.14433400
H	1.50747300	-2.95969500	-3.15801100
H	4.31593400	-2.63323700	-1.95162800
H	3.76407500	-3.93648100	-3.00511000
O	0.19129600	-1.73963800	-1.37121700
O	3.44444700	-5.10366000	-0.61543900
C	0.87119800	-4.14574500	0.37144600
H	1.34870000	-4.86169000	1.04870700
H	0.12688100	-3.57383000	0.93680400
H	0.35295700	-4.72215100	-0.40253800
C	2.56763600	-2.19467700	0.74597800
H	2.01415700	-2.12824100	1.69043100
H	3.62437000	-2.34107200	0.99616200
C	2.28560800	-1.07446800	-0.25072200
C	2.97219200	0.10534300	-0.40976700
C	4.05006600	0.36416100	0.60502800
C	3.76481600	0.43730400	1.97740500
C	5.39722800	0.42400900	0.20277400
C	4.78352900	0.60273500	2.91676600
H	2.73739800	0.33995900	2.31329400
C	6.41660500	0.57734600	1.14271900
H	5.64919000	0.33404900	-0.84984800
C	6.11373100	0.67822600	2.50213100
H	4.53846900	0.66116200	3.97375400
H	7.44997500	0.61305000	0.81018100
H	6.90840400	0.80185900	3.23174000

21-ts

B3LYP SCF energy: -2644.632856 a.u.
B3LYP enthalpy: -2643.818815 a.u.
B3LYP free energy: -2643.95055 a.u.
M06 SCF energy in solution: -2643.791552 a.u.
Imaginary frequency: -178.92 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-2.93519300	3.23072600	-1.43801500
C	-2.64887000	1.89389800	-1.13834800
C	-3.09794400	0.88291000	-2.02232700
C	-3.80882900	1.24388800	-3.17906400
C	-4.07300900	2.58127600	-3.46762900
C	-3.64244400	3.57596200	-2.59289700
H	-2.59522400	4.01347000	-0.76911900
H	-4.15442900	0.46715900	-3.85006200
H	-4.61641800	2.83963000	-4.37107100
H	-3.84979300	4.62084700	-2.80371100
C	-2.91945600	-0.56122500	-1.76561600
O	-3.75149100	-1.33962600	-2.46837600
C	-3.34075300	-2.71464900	-2.24173600
C	-2.51631300	-2.62749100	-0.94535200
H	-4.24080600	-3.32246300	-2.16041800
H	-2.74183000	-3.02796000	-3.10278100
H	-1.62651700	-3.24740000	-1.04035400
N	-2.10833600	-1.17646900	-0.94822600
P	-1.67121400	1.46272900	0.35528800
C	-0.79592200	2.99648400	0.81843800
C	-1.06652100	3.65362900	2.02915200
C	0.14264900	3.54500400	-0.07366900
C	-0.41682000	4.85054300	2.33609200
H	-1.78565200	3.24138600	2.72843700
C	0.76892200	4.75201400	0.23120700
H	0.38100900	3.03326600	-0.99976400
C	0.49375700	5.40505500	1.43611700
H	-0.63224700	5.35196700	3.27498000
H	1.47302300	5.18230500	-0.47428400
H	0.98860300	6.34283200	1.67145900
C	-2.86232600	1.12139000	1.69953600
C	-2.42344200	0.37125400	2.80255800
C	-4.16991800	1.63152600	1.68440900
C	-3.27678500	0.14698500	3.88236000
H	-1.41546800	-0.03484000	2.81807300

C	-5.02291200	1.39551900	2.76407300
H	-4.52224400	2.21563600	0.83966100
C	-4.57683000	0.65811200	3.86349100
H	-2.92918100	-0.43112200	4.73327800
H	-6.03304800	1.79445100	2.74797300
H	-5.24135100	0.48197700	4.70439700
C	-3.30011200	-3.04024700	0.29022200
C	-4.31830600	-2.24800700	0.83582800
C	-3.06199700	-4.31026000	0.83555600
C	-5.08198300	-2.71742700	1.90530600
H	-4.52095400	-1.25945900	0.43467800
C	-3.82699400	-4.78060800	1.90387700
H	-2.27750600	-4.93568400	0.41550200
C	-4.83957800	-3.98413300	2.44131600
H	-5.86707800	-2.09125400	2.31866600
H	-3.63159300	-5.76737500	2.31372200
H	-5.43711500	-4.34858300	3.27198000
C	3.89049500	2.20273900	-0.21763100
C	4.65427200	1.07803900	-0.57200300
C	5.77802900	1.26133200	-1.40066800
C	6.11057200	2.52393800	-1.88488200
C	5.34399500	3.63600000	-1.52616900
C	4.24129900	3.46998900	-0.68798400
H	3.04190700	2.08666400	0.44775200
H	6.39201900	0.40453700	-1.66237300
H	6.97581400	2.64250200	-2.53104600
H	5.61455800	4.62474500	-1.88608800
H	3.66050800	4.33341800	-0.37738100
C	1.75900600	-0.54884600	-2.20737800
C	1.84136400	-2.05949400	-2.49975800
C	1.01744300	-2.78858400	-1.43749500
C	1.17833900	-2.21328600	-0.07094700
C	1.83834600	-0.32637100	-0.69123100
H	2.57594600	0.00641200	-2.68681400
H	0.81128400	-0.13840500	-2.57883300
H	2.88329500	-2.40067800	-2.43779500
H	1.47114200	-2.31937700	-3.49423000
O	0.25698800	-3.71070600	-1.71031700
C	0.27606500	-2.70737500	1.04652500
H	0.60588300	-3.71703900	1.33846100
H	0.38792900	-2.07359800	1.93419000
H	-0.78195400	-2.77612200	0.81006100
C	2.65629100	-2.17684200	0.42842200
H	2.66453100	-2.21351500	1.52500400
H	3.22896400	-3.04790700	0.08801900
C	3.11552900	-0.84144300	-0.07045700
C	4.34448300	-0.28753400	-0.06223100
C	5.50234900	-1.06921900	0.48144600
C	6.23599700	-0.56519700	1.56781400
C	5.89338500	-2.29235300	-0.08467300
C	7.31261600	-1.28047100	2.09082700
H	5.95674600	0.39067000	2.00245400
C	6.97869900	-3.00286000	0.43122700
H	5.35940500	-2.67827900	-0.94919200
C	7.68674600	-2.50189100	1.52479900
H	7.86406400	-0.88093400	2.93734300
H	7.27396300	-3.94323700	-0.02593400
H	8.53030700	-3.05473400	1.92813600
Ni	-0.45494800	-0.31242100	-0.24224500
O	1.13261100	0.62245300	-0.12676700

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B3LYP SCF energy: -2644.690932 a.u.

B3LYP enthalpy: -2643.874621 a.u.
B3LYP free energy: -2644.00839 a.u.
M06 SCF energy in solution: -2643.857466 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-3.59817700	2.94259200	-1.56210200
C	-3.21397800	1.70736900	-1.02489000
C	-3.95244700	0.55512300	-1.39272000
C	-5.04012200	0.67769100	-2.27381400
C	-5.40137500	1.91608800	-2.79785500
C	-4.67808600	3.05152700	-2.44135600
H	-3.04071600	3.83583400	-1.30332600
H	-5.59736200	-0.21000800	-2.54734100
H	-6.24172400	1.98873600	-3.48102800
H	-4.94708000	4.02376800	-2.84346200
C	-3.64888700	-0.79780900	-0.89410000
O	-4.59445000	-1.72291000	-1.11713800
C	-4.05537400	-3.00991500	-0.70463100
C	-2.77691700	-2.65113000	0.08837300
H	-4.81835100	-3.51367600	-0.11141400
H	-3.84876600	-3.58358700	-1.61211800
H	-1.91362600	-3.20030600	-0.28808500
N	-2.58877100	-1.21136800	-0.27664000
P	-1.82823900	1.63850700	0.20138800
C	-0.78900800	3.09056900	-0.20983700
C	-0.34278100	3.97681700	0.78145300
C	-0.33224100	3.25239100	-1.53085600
C	0.53538000	5.01352600	0.45495800
H	-0.67123600	3.86278600	1.80906000
C	0.53378900	4.29618800	-1.85336500
H	-0.66228200	2.57300700	-2.31271400
C	0.97059900	5.17774100	-0.85999300
H	0.88338300	5.68374100	1.23474400
H	0.86885500	4.41987300	-2.87920400
H	1.64969600	5.98684000	-1.11209500
C	-2.62803800	1.99291200	1.81438300
C	-2.52309000	1.05813700	2.85491200
C	-3.36821700	3.17124400	2.01881600
C	-3.14008800	1.30145600	4.08437400
H	-1.97133200	0.13593600	2.70708300
C	-3.97895500	3.41080100	3.24783300
H	-3.46776100	3.90214700	1.22214300
C	-3.86423700	2.47682900	4.28252300
H	-3.05501400	0.56785900	4.88033600
H	-4.54680100	4.32429500	3.39814900
H	-4.34295000	2.66659900	5.23887300
C	-2.87488900	-2.84861500	1.59121400
C	-3.97059700	-2.35712200	2.31621500
C	-1.86867500	-3.54792800	2.26925200
C	-4.05933500	-2.56620400	3.69250400
H	-4.76475900	-1.81463500	1.80766100
C	-1.95615600	-3.75673200	3.64806100
H	-1.01582500	-3.93073000	1.71532800
C	-3.05139200	-3.26700800	4.36154500
H	-4.91878800	-2.19039200	4.24045800
H	-1.17349500	-4.30888000	4.16039300
H	-3.12524000	-3.43771000	5.43177500
Ni	-0.88709400	-0.37251700	0.10194100
C	2.98262800	2.51415900	3.34851400
C	3.80315200	2.81175200	2.24812400
C	4.21646800	4.14285700	2.06309000

C	3.79209300	5.14914600	2.92942200
C	2.96654700	4.84116500	4.01495800
C	2.57010600	3.51942100	4.22593000
H	2.69361900	1.48447700	3.53408500
H	4.87733600	4.38322200	1.23535000
H	4.12093500	6.17225100	2.76816800
H	2.65217600	5.62244200	4.70143100
H	1.95229600	3.26572000	5.08331100
C	1.97511100	-1.29972900	-1.44654500
C	3.18422900	-0.35702600	-1.61004300
C	3.92927400	-0.15490100	-0.28396300
C	1.09311200	-1.11741000	-0.22847900
H	1.34852100	-1.29721200	-2.34698500
H	2.34186800	-2.33019500	-1.34559200
H	2.87144600	0.60264600	-2.03498600
H	3.88766100	-0.82072400	-2.30686200
O	0.14013200	-1.97560100	-0.06140400
O	4.80424900	-0.93322500	0.05125500
C	0.93356100	-0.41743100	2.20157600
H	0.46214100	0.39072200	2.76862400
H	0.35867600	-1.33470300	2.34327800
H	1.93216200	-0.57904000	2.63320300
C	1.93718800	1.20469300	0.47419500
H	1.70809200	1.60106300	-0.52203900
H	1.63459400	1.98165300	1.17623900
C	3.44358800	0.97606600	0.57632700
C	4.28799500	1.75025100	1.31147600
C	5.77359300	1.68335700	1.17410200
C	6.58242800	1.58267600	2.31797300
C	6.39400600	1.79205000	-0.08070100
C	7.97080300	1.54584700	2.20457200
H	6.11834400	1.51901000	3.29802300
C	7.78322100	1.77219800	-0.19260700
H	5.78248200	1.90642000	-0.97193200
C	8.57596000	1.64129800	0.94923600
H	8.58130700	1.44840200	3.09786900
H	8.24651800	1.86317600	-1.17112500
H	9.65861600	1.62281000	0.86248500
C	1.10461900	-0.04871400	0.72993900

23-ts

B3LYP SCF energy: -3052.908856 a.u.
B3LYP enthalpy: -3051.958627 a.u.
B3LYP free energy: -3052.110154 a.u.
M06 SCF energy in solution: -3051.964731 a.u.
Imaginary frequency: -214.47 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	3.12564700	-3.33219300	-2.43073800
C	3.07509800	-2.06153800	-1.84286400
C	3.81993800	-1.01268400	-2.42992900
C	4.55987800	-1.25735300	-3.59989600
C	4.57831900	-2.52219200	-4.18200200
C	3.87156000	-3.56561000	-3.58849900
H	2.56596600	-4.14908200	-1.99002800
H	5.12627000	-0.44940400	-4.04575700
H	5.15016100	-2.68926000	-5.08933400
H	3.89114500	-4.56046300	-4.02332700
C	3.94787400	0.32663200	-1.82511300
O	4.99428800	1.02034600	-2.29065600
C	4.92732400	2.34857700	-1.71463200
C	3.98101300	2.16327000	-0.51283600
H	5.93937300	2.64644500	-1.44340700
H	4.52386900	3.02027400	-2.47925000
H	3.27218400	2.98496200	-0.46699500
N	3.24656900	0.91123800	-0.89287600
P	2.03690600	-1.75519500	-0.35984200
C	0.74976600	-3.05854000	-0.44754100
C	0.49551300	-3.89489800	0.64946100
C	0.01513900	-3.23802100	-1.63283300
C	-0.46785600	-4.90196300	0.55599200
H	1.05092200	-3.77154800	1.57259200
C	-0.93548900	-4.25329300	-1.72487800
H	0.19915200	-2.60312700	-2.49511700
C	-1.18016500	-5.08692600	-0.62914600
H	-0.65077400	-5.54784300	1.40972400
H	-1.48163500	-4.39679500	-2.65286100
H	-1.91930100	-5.87923000	-0.70316700
C	3.04777800	-2.15009100	1.11531200
C	2.70242600	-1.55069200	2.33954800
C	4.11648600	-3.05965200	1.05890200
C	3.41311200	-1.88058900	3.49534400
H	1.89242500	-0.82722400	2.39963300
C	4.82650200	-3.37330000	2.21827400
H	4.39672200	-3.52408900	0.11833800
C	4.47190500	-2.78906400	3.43736500
H	3.14071300	-1.41851700	4.43957400
H	5.65215500	-4.07735500	2.16926500
H	5.02230600	-3.04097700	4.33939100
C	4.71977100	2.05423900	0.81249400
C	5.29755600	0.85966900	1.25706200
C	4.91890000	3.22344200	1.56109100
C	6.05381000	0.83378500	2.43085100
H	5.15304400	-0.06070100	0.70086300
C	5.67923300	3.19926900	2.73009500
H	4.47939500	4.15867900	1.22430200
C	6.24768400	2.00164400	3.16945900
H	6.48893700	-0.10321700	2.76550600
H	5.82498400	4.11380700	3.29789700
H	6.83790300	1.98017700	4.08100800
Ni	1.46985200	0.45010100	-0.21975800
C	-4.82636900	0.67715100	2.17532200
C	-5.79790600	0.15529100	1.30501600
C	-7.03574700	-0.24524900	1.83775300
C	-7.28064800	-0.16319400	3.20728600
C	-6.30672000	0.35442700	4.06553900
C	-5.08469800	0.78196000	3.54437300
H	-3.87471400	1.02254600	1.78143800
H	-7.80521000	-0.62315800	1.17068100
H	-8.23744000	-0.49189400	3.60349400
H	-6.50471100	0.43319100	5.13092100
H	-4.32918500	1.20593300	4.20060100
C	-1.63841100	-0.00511200	-1.60113300
C	-2.64157300	-0.83021800	-2.42484400
C	-4.11219200	-0.51468400	-2.13115200
C	-1.46811000	-0.39673800	-0.15677800
H	-0.65253300	-0.09562100	-2.08172300
H	-1.90015400	1.06213200	-1.67948000
H	-2.44829200	-1.89777700	-2.26670700
H	-2.49953500	-0.62094700	-3.48848600
O	-0.28258700	0.11498200	0.42598300
O	-4.83258900	-0.17489700	-3.05690200
C	-1.96677000	-1.50440900	2.03401400
H	-2.09497500	-2.58861300	2.15101700

H	-0.95235500	-1.23184200	2.32545900
H	-2.66338500	-1.02705300	2.73394900
C	-3.68342400	-1.56631200	0.15191800
H	-3.57397900	-2.52214400	-0.38285500
H	-4.25617200	-1.80797500	1.04995400
C	-4.52549600	-0.62111700	-0.70082400
C	-5.56739400	0.09176700	-0.17382100
C	-6.56790600	0.88071400	-0.95276300
C	-6.80853900	2.22252700	-0.60667900
C	-7.36401300	0.29151000	-1.94814400
C	-7.78400700	2.96627000	-1.26809500
H	-6.22306300	2.68353500	0.18403100
C	-8.36135500	1.02693700	-2.58653000
H	-7.20173600	-0.74565700	-2.21610300
C	-8.56760200	2.36812100	-2.25747500
H	-7.94264200	4.00727100	-1.00018200
H	-8.97368200	0.55182900	-3.34788000
H	-9.33956700	2.94167000	-2.76318200
C	-2.30012100	-1.10659400	0.61902400
C	0.42457300	2.93774200	-1.06575100
C	0.83239300	2.44533000	0.19869800
C	1.44828400	3.37376500	1.07111100
C	1.59158600	4.71827600	0.73125800
C	1.17868000	5.16920700	-0.52796700
C	0.60596900	4.27292400	-1.43484100
H	-0.05619900	2.27215400	-1.77861100
H	1.77272800	3.03120000	2.04863500
H	2.02098300	5.41845900	1.44348100
H	1.29317600	6.21602100	-0.79646100
H	0.28385700	4.61877900	-2.41362000
B	-0.29546400	1.35984000	1.26756300
O	-1.51471700	2.03957600	1.40798200
H	-1.86380400	2.39961200	0.58266900
O	0.36372200	1.06929500	2.48390000
H	0.02320900	1.64567100	3.18294800

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B3LYP SCF energy: -1138.720231 a.u.
B3LYP enthalpy: -1138.314972 a.u.
B3LYP free energy: -1138.395010 a.u.
M06 SCF energy in solution: -1138.314891 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	10.13362600	-3.42853100	5.04188600
C	11.07999300	-2.73337700	4.27192900
C	12.35256700	-2.51066400	4.82788800
C	12.65423400	-2.93612900	6.12009000
C	11.70008100	-3.62207200	6.87603700
C	10.44133200	-3.87328400	6.32921100
H	9.15166400	-3.63424500	4.62775100
H	13.10578000	-1.99767300	4.23703700
H	13.63952900	-2.73947900	6.53418800
H	11.93921100	-3.96486900	7.87896200
H	9.69624200	-4.42079100	6.90026100
C	7.01909000	-2.18797200	1.38410500
C	7.87514700	-1.02733300	0.85353700
C	9.36974100	-1.12383600	1.15458700
C	6.75283200	-2.20373300	2.87309700
H	6.03266900	-2.12938700	0.90867300
H	7.44231900	-3.15022600	1.05560300
H	7.48835500	-0.08208100	1.25991000
H	7.78970600	-0.96448700	-0.23488500
O	5.56249400	-2.85775700	3.17015000
O	10.17942900	-0.89264000	0.27077400
C	6.96389000	-1.54768400	5.27384500
H	6.97391000	-0.50681600	5.62589500
H	5.94571700	-1.92838300	5.37104000
H	7.61824800	-2.11036900	5.95312800
C	8.79981500	-0.90973700	3.62026400
H	8.61569900	0.15116700	3.38789300
H	9.32963100	-0.90346600	4.57663100
C	9.73318100	-1.48856900	2.56352000
C	10.80072400	-2.27798100	2.87071200
C	11.79604900	-2.80654500	1.88222800
C	11.96785800	-4.19725700	1.76871600
C	12.63576900	-1.96465700	1.13717100
C	12.92347100	-4.73235700	0.90683900
H	11.34379800	-4.86195300	2.36039100
C	13.60998500	-2.50115700	0.29411100
H	12.51841000	-0.89117200	1.21548200
C	13.75198300	-3.88376400	0.16883600
H	13.02767300	-5.81065800	0.81979900
H	14.25331500	-1.83329800	-0.27247900
H	14.50554800	-4.29818200	-0.49565900
C	7.46128800	-1.60967500	3.84995600
B	5.54933900	-4.19198500	3.51693200
O	6.68421000	-4.96418500	3.61015500
H	7.48201900	-4.45158500	3.41112500
O	4.32740300	-4.74322900	3.77255600
H	4.42117900	-5.67846800	4.00213100

25-ts

B3LYP SCF energy: -2644.592016 a.u.
B3LYP enthalpy: -2643.778927 a.u.
B3LYP free energy: -2643.9079 a.u.
M06 SCF energy in solution: -2643.784624 a.u.
Imaginary frequency: -160.37 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.12898200	-1.14930300	0.53161300
C	1.69835300	2.88983200	1.32790900
C	0.71628300	1.89230300	1.38079400
C	-0.61444300	2.24714700	1.04614000
C	-0.90914300	3.56162900	0.64856500
C	0.08883100	4.53090100	0.58063100
C	1.39287700	4.19542300	0.93200400
H	2.72076900	2.65217800	1.59391100
H	-1.93183200	3.81822000	0.40052200
H	-0.15759300	5.53990500	0.26529600
H	2.18062400	4.94238600	0.90112200
C	-1.74744700	1.31190300	1.16283600
O	-2.95583700	1.90274300	1.17728700
C	-3.94114000	0.83687400	1.12860300
C	-3.14350400	-0.40698600	1.56872000
H	-4.30928300	0.77443700	0.09968000
H	-4.75469900	1.10361900	1.80179800
N	-1.72766100	0.02066800	1.27480400
P	1.15824200	0.16518600	1.90045800
C	0.71243900	0.07331400	3.67719400
C	0.16874800	-1.10805100	4.20073300
C	0.97008000	1.15520300	4.53660700
C	-0.09024100	-1.21638800	5.56774000

H	-0.06787900	-1.93804000	3.54389500
C	0.70442100	1.04378300	5.90099700
H	1.38207800	2.08104400	4.14588200
C	0.18153400	-0.14429500	6.41858700
H	-0.51867900	-2.13254600	5.96216900
H	0.90873500	1.88337200	6.55915100
H	-0.02026200	-0.22985600	7.48245800
C	2.99231200	0.16157400	1.85591800
C	3.75167300	-0.11656100	3.00132700
C	3.65452600	0.45144400	0.64979400
C	5.14685400	-0.09459900	2.94166900
H	3.26268900	-0.35171700	3.93942700
C	5.04625900	0.47958300	0.59703500
H	3.08241000	0.67301800	-0.24551200
C	5.79600000	0.20618000	1.74474900
H	5.72286000	-0.31146100	3.83634500
H	5.54513900	0.71286300	-0.33911300
H	6.88115300	0.22812500	1.70321000
C	3.66068700	-1.77226800	-2.52515100
C	3.24540500	-2.78229100	-1.64284100
C	3.55039100	-4.11717600	-1.97035500
C	4.23150000	-4.42786600	-3.14689000
C	4.63418100	-3.41063800	-4.01629700
C	4.34991200	-2.08175500	-3.69965400
H	3.45343100	-0.73394400	-2.28213500
H	3.25715900	-4.91453600	-1.29275600
H	4.45085900	-5.46530700	-3.38329700
H	5.16920000	-3.65270500	-4.92992700
H	4.66727400	-1.28319100	-4.36458000
C	-0.46342100	-4.21848200	-1.81471900
C	-0.44299700	-4.29252200	-0.27501300
C	-1.00598000	-3.00033600	0.30232000
C	-0.89190600	-1.69205000	-1.48463500
C	-1.26397800	-2.99094600	-2.20644400
H	-0.92925000	-5.09862600	-2.26228300
H	0.55404600	-4.13349300	-2.21145700
H	-1.08710400	-5.09311100	0.10194100
H	0.56427300	-4.44921200	0.11499300
O	-2.13870700	-3.00577100	-3.04707000
O	-1.87111900	-2.97105100	1.13202000
C	-1.90282000	-0.60273000	-1.78099900
H	-1.58013800	0.37333200	-1.41575000
H	-2.88995500	-0.83871400	-1.37498800
H	-2.02335200	-0.54034200	-2.87053500
C	0.60373200	-1.35721200	-1.78035900
H	0.68004400	-0.27981800	-1.97944700
H	0.97478400	-1.86560000	-2.68172400
C	1.32381200	-1.75254700	-0.51728600
C	2.46254500	-2.47097300	-0.39728400
C	2.98837400	-3.03727100	0.87756200
C	4.36475600	-3.30821700	1.01358300
C	2.16076400	-3.33518900	1.97666700
C	4.88389100	-3.84399900	2.19023300
H	5.03516300	-3.08507000	0.19109200
C	2.67809400	-3.87204300	3.15569900
H	1.09414900	-3.15459700	1.90761700
C	4.04414400	-4.13242700	3.26834800
H	5.95027900	-4.03849200	2.26372900
H	2.00929600	-4.09885500	3.98157600
H	4.44806300	-4.56177500	4.18068000
C	-3.37644200	-0.76782100	3.02890800
C	-3.23524900	0.19487900	4.04033600
C	-3.83947000	-2.04384200	3.37173200
C	-3.55044300	-0.11339000	5.36264900
H	-2.89018900	1.19713600	3.79892800
C	-4.15336500	-2.35446600	4.69700000
H	-3.96073200	-2.79723800	2.60005000
C	-4.01106900	-1.39020900	5.69517600
H	-3.44164600	0.64531400	6.13233900
H	-4.51817200	-3.34736700	4.94459300
H	-4.26502500	-1.62777500	6.72441000
H	-3.38191000	-1.26536600	0.94613500

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B3LYP SCF energy: -2644.616735 a.u.
B3LYP enthalpy: -2643.802627 a.u.
B3LYP free energy: -2643.933371 a.u.
M06 SCF energy in solution: -2643.803166 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.08744400	2.18775700	3.55714100
C	1.35157100	1.29834700	2.50845100
C	2.28997900	0.25806100	2.73108600
C	2.91565700	0.14672300	3.98577500
C	2.62901100	1.03772900	5.01666800
C	1.71357300	2.06325400	4.80034200
H	0.37234300	2.98867000	3.40972500
H	3.63112500	-0.64991800	4.14680100
H	3.12055500	0.92724400	5.97811100
H	1.47977000	2.76949500	5.59165400
C	2.69246800	-0.73198700	1.71072300
O	3.80533800	-1.41730300	2.01678000
C	3.92775600	-2.49006900	1.04396500
C	3.03631400	-2.01261900	-0.11892400
H	3.55148700	-3.40472800	1.51009400
H	4.98189700	-2.58715800	0.78792000
N	2.13303000	-1.03394500	0.57668900
P	0.51931700	1.53435200	0.86350300
C	1.71903600	2.59484100	-0.04433900
C	2.16421000	2.21678800	-1.31836700
C	2.20549400	3.78382500	0.52914400
C	3.06224500	3.02682000	-2.01843700
H	1.82757000	1.28695300	-1.76283700
C	3.09975400	4.58899200	-0.17365700
H	1.88619700	4.08532800	1.52217200
C	3.52564200	4.21370600	-1.45152600
H	3.40292500	2.71937100	-3.00249200
H	3.46531000	5.50741900	0.27650800
H	4.22179400	4.84365500	-1.99796600
C	-0.92383700	2.60082100	1.25532400
C	-1.12678500	3.84070800	0.63385200
C	-1.88299100	2.13108000	2.17045100
C	-2.25880900	4.60194400	0.93545600
H	-0.41260300	4.21329000	-0.09130900
C	-3.00464300	2.89916700	2.47712100
H	-1.74719900	1.17045600	2.66039600
C	-3.19498700	4.13845900	1.85877500
H	-2.40354900	5.55988800	0.44486200
H	-3.72838800	2.53276300	3.19982500
H	-4.07029500	4.73615700	2.09591400
C	3.82033600	-1.41558300	-1.27506500
C	4.63534000	-0.28847200	-1.10138400
C	3.81466400	-2.06092700	-2.51734100
C	5.42416800	0.18198800	-2.15118200

H	4.66327000	0.22470600	-0.14391600
C	4.60197600	-1.59136300	-3.56992000
H	3.19799200	-2.94507100	-2.66242600
C	5.40908200	-0.46753200	-3.38836600
H	6.05401800	1.05401600	-2.00057500
H	4.58728700	-2.10539700	-4.52662000
H	6.02781900	-0.10311300	-4.20336400
H	2.43635700	-2.84637000	-0.48307000
Ni	0.18452100	-0.72935200	0.04784100
C	-4.76981300	-0.24712300	0.52213100
C	-4.08217000	-0.38936300	-0.69219900
C	-4.74036700	-0.99697700	-1.77393900
C	-6.04868700	-1.46366400	-1.63881700
C	-6.72273700	-1.31975400	-0.42385300
C	-6.08226400	-0.70511500	0.65398900
H	-4.27811200	0.24418800	1.35737200
H	-4.22787500	-1.09069400	-2.72830100
H	-6.54363500	-1.93268100	-2.48463100
H	-7.74282600	-1.67808800	-0.32017000
H	-6.60548700	-0.57895000	1.59792200
C	-0.29008400	-4.04618900	-0.97315100
C	-0.56379000	-2.94480800	-2.01747400
C	0.09765500	-1.62572200	-1.66843900
C	-0.60316000	-2.35675100	0.99258800
C	0.07161400	-3.55982100	0.43017500
H	0.53341300	-4.68934400	-1.29361700
H	-1.17304600	-4.69353800	-0.89024000
H	-0.20948000	-3.23743400	-3.01166200
H	-1.63193700	-2.72313000	-2.10346500
O	0.93051800	-4.15940900	1.06866100
O	0.73312400	-0.93088400	-2.40707200
C	-0.33551100	-2.11552100	2.45998700
H	-0.56442500	-1.08658700	2.75694600
H	0.68740100	-2.36282400	2.74063300
H	-1.00126300	-2.77085000	3.04316700
C	-2.00020100	-1.95997100	0.51350800
H	-2.65508500	-1.78708900	1.37562200
H	-2.49780000	-2.73176100	-0.08969800
C	-1.71556700	-0.68729200	-0.25081800
C	-2.65867400	0.08302200	-0.85362000
C	-2.47023100	1.30149800	-1.67644600
C	-3.55405200	2.18583700	-1.86153800
C	-1.24944700	1.62963200	-2.29494800
C	-3.41494600	3.34948400	-2.61389500
H	-4.51078700	1.96378300	-1.40286000
C	-1.11250900	2.79179700	-3.05305800
H	-0.40808600	0.95852200	-2.21062200
C	-2.19362700	3.65954000	-3.21649500
H	-4.26679900	4.01290900	-2.73464900
H	-0.15857700	3.01255000	-3.52382700
H	-2.08894700	4.56061600	-3.81421600