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Mechanism of formation of active catalytic species in nickel-catalysed asymmetric hydrogenation

Evgeny V. Pospelov, Ivan S. Golovanov, Alexey Yu. Sukhorukov, Jianzhong Chen, Wanbin Zhang and Ilya D. Gridnev

Computational details

DFT calculations were performed with Gaussian 16 Rev.A03. TPSSh DFT functional with def2-SVP basis set was used for geometry optimization, calculations of thermodynamics and kinetics. Calculations were performed in 2,2,2-trifluoroethanol (SMD model). Cartesian coordinates are given in angstroms; absolute energies for all substances are given in hartrees. Starting coordinates of **1** were taken from CCDC 2092186 [P.Yang, Y. Sun, K. Fu, L. Zhang, G. Yang, J. Yue, Y. Ma, J. S. Zhou, and B. Tang, *Angew. Chem. Int. Ed*., 2022, **61**, e202111778]. Analysis of vibrational frequencies was performed for all optimized structures. All compounds, except transition state structures, were characterized by only real vibrational frequencies. TS were characterized by one imaginary frequency. Then total electronic energy was recalculated as single point job with larger def2-TZVPP basis set. Wavefunction stability, using *stable* keyword, was also checked for each molecule.

For calculations of optimized geometries, frequencies and thermodynamics, following keywords were used:

 # opt=(calcfc) freq tpssh def2svp scrf=(smd,solvent=2,2,2-trifluoroethanol) nosymm scf=xqc test

The same parameters were calculated for transition state structures with keywords:

 # opt=(calcall,ts,noeigentest,maxstep=10) tpssh def2svp scrf=(smd,solvent=2,2,2-trifluoroethanol) nosymm scf=xqc test

IRC calculation was performed for TS and proved that TS connects products and reactants:

 # irc=(forward,calcfc,maxcycle=150,MaxPoints=5,ReCorrect=Never,HPC,stepsize=1) tpssh def2svp scrf=(smd,solvent=2,2,2-trifluoroethanol) nosymm scf=xqc test

 # irc=(reverse,calcfc,maxcycle=150,MaxPoints=5,ReCorrect=Never,HPC,stepsize=1) tpssh def2svp scrf=(smd,solvent=2,2,2-trifluoroethanol) nosymm scf=xqc test

Cartesian coordinates and energies

1a

Charge 0; multiplicity 1

Ni	0.00247900	0.00193300	0.01267500
P	-0.00576700	0.03133400	2.17310700
C	1.71991200	-0.00045200	2.79522200
O	-1.89109600	-0.34991700	-0.05703800
C	0.24083800	2.79970000	2.30199000
H	-0.19585600	3.78082900	2.55510900
H	0.38496900	2.76364900	1.21047600
H	1.22451100	2.73210300	2.79252700
C	-0.71593600	1.69019600	2.77060600
C	2.07963600	-0.11845500	4.14791700
H	1.32265900	-0.33030600	4.90574000
C	-0.86420000	1.72220100	4.29894600
H	0.10001300	1.59960400	4.81488200
H	-1.56245800	0.95374800	4.66529300
H	-1.27107900	2.70623700	4.58973500
C	-2.09118000	1.88841700	2.10792400
H	-2.79145200	1.07314000	2.34838400
H	-2.00172200	1.96054000	1.01483700
H	-2.52833400	2.82961700	2.48311900
C	-0.91583000	-1.29642200	3.03971800
H	-0.55405000	-2.26681500	2.66955100
H	-1.98787700	-1.20530900	2.81172300
H	-0.76650100	-1.24109900	4.12816900
C	3.41458400	0.04636000	4.53117000
H	3.69077500	-0.04402000	5.58459600
O	-1.26282300	-2.47543800	-0.39633600
C	-2.13555600	-1.58960000	-0.33307300
C	-3.58904500	-1.91149400	-0.61851600
H	-3.78947200	-2.97565800	-0.43179800
H	-3.79103300	-1.70209400	-1.68271200
H	-4.26247800	-1.28324100	-0.01804200
P	2.16136700	0.08516500	0.07830100
C	2.71736400	0.22609000	1.82114400
C	2.41175900	-2.65933700	0.45553700
H	2.73279400	-3.64463600	0.07667100
H	1.31425100	-2.67247600	0.54942900
H	2.85214100	-2.52347100	1.45574400
C	2.86908600	-1.57061400	-0.53026400
C	4.04879300	0.42887400	2.22009700
H	4.82244500	0.64216000	1.47959000
C	4.40241400	-1.53219900	-0.61115500
H	4.86834200	-1.34288500	0.36747300
H	4.76271200	-0.77732200	-1.32715000
H	4.75814000	-2.51710700	-0.96024000

C	2.28074400	-1.86321800	-1.92239300
H	2.50975300	-1.06689300	-2.64785100
H	1.19015900	-1.99127300	-1.87751300
H	2.72425100	-2.80045700	-2.30007700
C	2.99743700	1.41406300	-0.85810800
H	2.56984500	2.37953300	-0.55060400
H	2.81409600	1.26937200	-1.93281200
H	4.08090000	1.41610100	-0.66777900
C	4.39110500	0.34741100	3.57374200
H	5.42826500	0.50348900	3.88049400
O	-0.01940300	0.24828100	-1.89823700
O	-0.45806200	2.39134100	-1.40507200
C	-0.33103500	1.46094000	-2.22252500
C	-0.57536000	1.68900300	-3.70120000
H	-0.42741400	2.74782200	-3.95501100
H	-1.62095300	1.42028900	-3.92855600
H	0.07676600	1.05230700	-4.31620000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3273.681181 E_0
Sum of electronic and zero-point Energies= -3273.176282 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3273.141031 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3273.140087 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3273.242507 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.504899
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3275.315200 E_0

H_2

Charge 0; multiplicity 1

H	-5.330968000	0.045872000	0.000000000
H	-6.087381000	0.045872000	0.000000000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -1.174983 E_0
Sum of electronic and zero-point Energies= -1.164894 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -1.162533 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -1.161589 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -1.176416 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.010089
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -1.1788821 E_0

2a

Charge 0; multiplicity 1

Ni	-0.33120500	-0.60376000	-0.50720400
P	-0.33356500	-0.37919000	1.64577500
C	1.24226900	0.37997500	2.19244500
O	-3.34965100	-1.10503600	-1.53335500
C	-1.35852900	2.19293200	1.48343400
H	-2.17331800	2.90752900	1.69040000
H	-1.26726500	2.08767100	0.39051100
H	-0.42426000	2.62444000	1.87649300
C	-1.69353600	0.84492900	2.14475100
C	1.62307300	0.55144800	3.53402000
H	1.03079500	0.11016200	4.33830800
C	-1.79195200	1.00441100	3.66878800
H	-0.87200600	1.42154700	4.10513100
H	-2.02430400	0.05361700	4.17328900
H	-2.61199100	1.70827000	3.89360000
C	-3.02411100	0.31326200	1.58341100
H	-3.28554700	-0.67213400	2.00139900
H	-2.99656500	0.23225000	0.48693500
H	-3.82893000	1.01639300	1.85835400
C	-0.55928100	-1.90105800	2.63086300
H	0.22164500	-2.61852600	2.33748100
H	-1.54286500	-2.33643400	2.40463000
H	-0.48206200	-1.69833700	3.70932400
C	2.76206700	1.30082300	3.84414000
H	3.05396100	1.43592500	4.88850400
O	-1.62988600	-1.99887100	-0.38071100
C	-2.76390800	-2.06330500	-1.00880300
C	-3.35442300	-3.46231400	-1.06477900
H	-3.30087900	-3.94653600	-0.07784400
H	-2.76288900	-4.07460300	-1.76577000
H	-4.39599200	-3.42700800	-1.41185400
P	1.58395200	0.41371100	-0.54540500
C	2.04612600	0.91114600	1.16075900
C	2.59649000	-2.15310700	-0.27381000
H	3.34452900	-2.92105800	-0.53546100
H	1.59672800	-2.55350600	-0.50767000
H	2.65792300	-1.98159400	0.81333100
C	2.88609100	-0.86936700	-1.07051400
C	3.16774900	1.69359200	1.48371800
H	3.77810800	2.13917700	0.69558300
C	4.31593200	-0.38476300	-0.78744900
H	4.51474000	-0.28146800	0.28962300
H	4.53774300	0.57376200	-1.28276900
H	5.02213800	-1.13412100	-1.18504400
C	2.72421400	-1.13673600	-2.57793700
H	2.97781200	-0.25007700	-3.18027500

H	1.70159000	-1.45023900	-2.83088600
H	3.41783000	-1.94491200	-2.86646500
C	1.83599100	1.89418600	-1.58840200
H	1.17413100	2.69436300	-1.22682100
H	1.57670300	1.65937200	-2.63009000
H	2.88252700	2.23183000	-1.54013800
C	3.51508700	1.89430100	2.82320200
H	4.38870000	2.50227900	3.07083700
O	-0.45895700	-0.61988500	-2.42193900
O	-1.41273200	1.40469900	-2.25895900
C	-1.08547400	0.39965400	-2.91547900
C	-1.44982500	0.27506400	-4.38077800
H	-1.60670200	1.26753100	-4.82504100
H	-2.39417700	-0.29145500	-4.44641900
H	-0.68273500	-0.27905100	-4.94061500
H	-4.71419900	2.02328300	-2.72826500
H	-4.00131000	1.80276200	-2.60319100

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3274.855923 E_0
Sum of electronic and zero-point Energies= -3274.338369 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3274.300447 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3274.299503 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3274.407464 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.517554
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3276.491598 E_0

TS1a

Charge 0; multiplicity 1

Ni	0.06257300	-0.65276100	-0.13432000
P	0.01016500	-0.66052500	2.04466800
C	1.67599300	-0.22193700	2.67965700
O	-2.70864700	-3.47979400	0.51710700
C	-0.58522600	2.04875600	2.25518000
H	-1.30395800	2.84508000	2.51277900
H	-0.39798000	2.09953300	1.17053000
H	0.35602800	2.25863100	2.78718500
C	-1.18058100	0.68797200	2.65439000
C	2.01821100	-0.17842700	4.04172100
H	1.31214300	-0.51665000	4.80220500
C	-1.37889700	0.61360200	4.17683800
H	-0.43954800	0.75549200	4.73088000
H	-1.83704000	-0.33721500	4.48957000
H	-2.06271000	1.42645300	4.47557300
C	-2.53897100	0.48838500	1.95267000
H	-2.91032100	-0.54603300	2.03254500
H	-2.48445100	0.75975500	0.88747900
H	-3.28029700	1.15131100	2.42943800
C	-0.45026800	-2.22435400	2.86833700
H	0.25298400	-3.00344400	2.53981400
H	-1.46818300	-2.51546500	2.57217000
H	-0.39156100	-2.12061600	3.96209200
C	3.27183100	0.30369700	4.43058500
H	3.53111000	0.34131400	5.49136700
O	-0.73973100	-3.25062000	-0.53706200
C	-1.66896800	-3.94928700	-0.00739000
C	-1.45463300	-5.46148400	0.00751300
H	-0.79074500	-5.71607900	0.85174800
H	-0.95982300	-5.79820000	-0.91589700
H	-2.40634400	-5.99492900	0.14437900
P	2.17393900	-0.20909200	-0.02638500
C	2.62769900	0.15700000	1.70843800
C	2.89173000	-2.84684200	0.47483600
H	3.43751900	-3.75595800	0.17057700
H	1.81705800	-3.08771400	0.49433200
H	3.21804700	-2.58348300	1.49327500
C	3.18837500	-1.72693800	-0.53662900
C	3.87345100	0.66831600	2.10899200
H	4.60312100	0.99528200	1.36526200
C	4.68990800	-1.40216800	-0.55755000
H	5.06692400	-1.11105300	0.43438000
H	4.93357200	-0.60614300	-1.27809500
H	5.23723500	-2.30943500	-0.86599200
C	2.72459500	-2.16590900	-1.93786100
H	2.84189100	-1.36767800	-2.68711100

H	1.67442400	-2.49129600	-1.93121000
H	3.34596700	-3.01993100	-2.25675300
C	2.71852000	1.20552200	-1.04298000
H	2.07302900	2.06588400	-0.81301300
H	2.61286600	0.95004500	-2.10678400
H	3.76607900	1.46325600	-0.82758900
C	4.18565200	0.75216500	3.46914500
H	5.15417000	1.15206100	3.77887500
O	0.08221200	-0.39691100	-2.02955000
O	-0.95882300	1.53196500	-1.56703900
C	-0.50154000	0.70720200	-2.37761800
C	-0.56653500	0.95820800	-3.86945100
H	-1.44122400	1.57841900	-4.10984500
H	-0.59712800	0.01596100	-4.43399000
H	0.33914600	1.51066500	-4.17209700
H	-1.60009700	-0.78829700	-0.17391000
H	-1.36934100	-1.57584400	-0.25786300

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3274.821872 E_0
Sum of electronic and zero-point Energies= -3274.301372 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3274.265357 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3274.264412 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3274.369489 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.520501
Number of imaginary vibrational frequencies = 1; 121*i*
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3276.464123 E_0

3a

Charge 0; multiplicity 1

Ni	-0.57452900	0.15734000	-0.59410200
P	-0.67112700	0.21552200	1.51695000
C	1.00469900	0.61291800	2.18955000
O	-1.36582500	-3.34713800	-0.41605000
C	-1.57047200	2.79837100	1.13279600
H	-2.20444900	3.65218400	1.42896900
H	-1.81013200	2.53619400	0.08953100
H	-0.51944600	3.12905300	1.17744600
C	-1.83287000	1.61166900	2.07638400
C	1.31412100	0.65653600	3.56057800
H	0.56893600	0.36706700	4.30397600
C	-1.60232600	2.03413100	3.53479500
H	-0.61594400	2.49848700	3.68165200
H	-1.70406000	1.18966300	4.23503700
H	-2.36542800	2.78366900	3.80717100
C	-3.28429600	1.12491800	1.91593100
H	-3.53163600	0.32598900	2.63257800
H	-3.48335000	0.75894200	0.89668000
H	-3.96396200	1.97173300	2.11197300
C	-1.18325400	-1.29098000	2.42529300
H	-0.44283200	-2.08178400	2.23458700
H	-2.16204800	-1.62883800	2.05755800
H	-1.24059700	-1.09938900	3.50798400
C	2.57767900	1.08046200	3.98313900
H	2.80893600	1.11533100	5.05074000
O	-2.66245100	-2.11161900	-1.77189600
C	-2.18290500	-3.27238000	-1.32411700
C	-2.74990300	-4.45608900	-2.05614800
H	-2.47652600	-4.39208800	-3.12138600
H	-3.84917700	-4.43928200	-1.99632400
H	-2.36041200	-5.38618900	-1.62529900
P	1.58276000	0.58619500	-0.51801900
C	2.00190100	0.93205900	1.23971600
C	2.17348100	-2.09859700	-0.18863600
H	2.74380100	-2.99763900	-0.47969100
H	1.10422500	-2.30478000	-0.35345600
H	2.33487000	-1.93406900	0.88924900
C	2.64968300	-0.89952000	-1.02611100
C	3.25570400	1.39482800	1.67674100
H	4.01932500	1.68423400	0.95167700
C	4.15227700	-0.67159500	-0.81294200
H	4.40825800	-0.57059900	0.25242900
H	4.52183300	0.21584500	-1.35075800
H	4.70181300	-1.54653000	-1.20245200
C	2.36627200	-1.16229800	-2.51744200
H	2.73873700	-0.34525200	-3.15594900

H	1.29035700	-1.28855700	-2.70944900
H	2.88476000	-2.08730900	-2.82297700
C	2.19645800	2.02611400	-1.47357300
H	1.66388300	2.92222300	-1.12005800
H	1.95433500	1.87578400	-2.53632700
H	3.28058500	2.17747000	-1.36095300
C	3.53675200	1.47850100	3.04366800
H	4.51376400	1.83789800	3.37643500
O	-0.71629100	0.12181500	-2.49833200
O	-2.32635700	1.69116700	-2.57131500
C	-1.62613700	0.81549500	-3.10530600
C	-1.80530600	0.45841900	-4.56957300
H	-2.44254600	1.19526800	-5.07669200
H	-2.27973300	-0.53536900	-4.63304900
H	-0.82942600	0.39044800	-5.07399800
H	-2.04437100	-0.10633400	-0.39903900
H	-2.24978400	-1.35376600	-1.24851700

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3274.841177 E_0
Sum of electronic and zero-point Energies= -3274.318764 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3274.282222 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3274.281278 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3274.388902 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.522413
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3276.482504 E_0

AcOH

Charge 0; multiplicity 1

O	-1.70547800	-3.43447900	-1.06335000
O	-1.63848400	-2.66979900	-3.17383100
C	-1.75430900	-3.65115200	-2.26085000
C	-1.94431400	-4.99637400	-2.89763400
H	-1.09600700	-5.21262700	-3.56564900
H	-2.85622500	-4.98663900	-3.51510000
H	-2.02201100	-5.76837700	-2.12312900
H	-1.51643000	-1.82277800	-2.69843300

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -228.927089 E_0
Sum of electronic and zero-point Energies= -228.866001 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -228.861381 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -228.860437 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -228.893435 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.061088
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -229.195279 E_0

4a

Charge 0; multiplicity 1

Ni	-0.83615200	-0.05938500	-0.21868200
P	-0.72544500	0.32923600	1.84252100
C	1.02029100	0.71069900	2.31277900
C	-1.06471600	3.06019200	1.45795100
H	-1.65047700	3.98171500	1.61845400
H	-1.05923600	2.84394400	0.37741200
H	-0.03076900	3.25833300	1.78283500
C	-1.70688300	1.90705300	2.24926300
C	1.46769200	0.88734500	3.63403600
H	0.79940900	0.69179700	4.47548800
C	-1.70388600	2.22449300	3.75144700
H	-0.69030400	2.41892900	4.13331900
H	-2.15713200	1.41767700	4.34853800
H	-2.30033900	3.13769200	3.92187900
C	-3.15198600	1.70041200	1.76056200
H	-3.64176200	0.84882900	2.26016700
H	-3.17650900	1.52625500	0.67483400
H	-3.73982700	2.60678300	1.98661800
C	-1.27211100	-0.95848900	3.02504200
H	-0.74817200	-1.89416300	2.77647700
H	-2.35348400	-1.12169300	2.90824500
H	-1.05115000	-0.68596700	4.06737600
C	2.77208900	1.32630300	3.88233300
H	3.11152100	1.46384400	4.91210000
P	1.29527800	0.47415800	-0.44060400
C	1.91479300	0.92071500	1.23810400
C	1.75222800	-2.22955200	-0.16173100
H	2.27620500	-3.15652600	-0.45291000
H	0.67284100	-2.37244800	-0.33517100
H	1.90995100	-2.07857600	0.91909700
C	2.29180200	-1.04709800	-0.98513700
C	3.21057000	1.40024100	1.49868900
H	3.89739100	1.60739100	0.67553700
C	3.80506600	-0.90462200	-0.77975400
H	4.07457300	-0.84934500	0.28571400
H	4.21347000	-0.01947700	-1.29309700
H	4.30681600	-1.79279800	-1.20274700
C	1.98750900	-1.26744500	-2.47933400
H	2.43618200	-0.48122400	-3.10721500
H	0.90423500	-1.29377800	-2.67351900
H	2.41864900	-2.23287500	-2.79583600
C	1.83176700	1.85858100	-1.52130200
H	1.39566000	2.78869000	-1.12634100
H	1.44288000	1.69770400	-2.53765100
H	2.92759600	1.95795300	-1.56167400
C	3.63337000	1.60858900	2.81518100

H	4.64350800	1.97817400	3.00903900
O	-1.25967000	-0.39529900	-2.07395800
O	-1.79306500	1.77973200	-2.12414900
C	-1.68435200	0.66460300	-2.67330800
C	-2.01830000	0.49272700	-4.14313900
H	-2.70987000	1.27949900	-4.47488600
H	-2.44856000	-0.50016900	-4.33902300
H	-1.08831500	0.57854200	-4.73075100
H	-2.19719000	-0.52798500	0.20281400

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3045.901390 E_0
Sum of electronic and zero-point Energies= -3045.441062 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3045.410745 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3045.409801 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3045.501327 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.460328
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3047.281439 E_0

5a

Charge 0; multiplicity 1

Ni	-0.88531900	-0.00173700	-0.82785000
P	-0.98779300	-0.13484900	1.27091500
C	0.72146300	-0.03663400	1.97628600
C	-1.52918100	2.55943300	1.03454800
H	-2.03996500	3.47678300	1.37535300
H	-1.81401500	2.37243300	-0.01414800
H	-0.44269300	2.74333000	1.07357600
C	-1.93904800	1.37573700	1.92747700
C	1.01882900	-0.15964100	3.34526200
H	0.23053500	-0.39697700	4.06218500
C	-1.62935600	1.68722100	3.39856000
H	-0.58304600	1.99312800	3.54670100
H	-1.84468400	0.83254800	4.05949500
H	-2.26983800	2.52572500	3.72291200
C	-3.44599900	1.10417300	1.77212400
H	-3.79723900	0.32048500	2.46148300
H	-3.70053200	0.80862700	0.74231300
H	-3.99905900	2.02935100	2.00815300
C	-1.71953700	-1.60282300	2.08892600
H	-1.11710500	-2.48529800	1.82579100
H	-2.74652400	-1.75464600	1.72899400
H	-1.72851300	-1.48396900	3.18343400
C	2.32633600	0.03242800	3.80178300
H	2.54753800	-0.06040200	4.86809400
P	1.31587500	0.11806100	-0.72369400
C	1.76541900	0.21640200	1.05746500
C	1.40765300	-2.64105800	-0.69112700
H	1.78813900	-3.59592500	-1.09301300
H	0.32055500	-2.59926600	-0.86993700
H	1.57883700	-2.64162000	0.39772600
C	2.12523000	-1.46713200	-1.37919000
C	3.06969500	0.44361000	1.53132800
H	3.87582500	0.67772700	0.83271900
C	3.63536700	-1.54472400	-1.12234100
H	3.86868700	-1.60561700	-0.04854200
H	4.17621100	-0.68701400	-1.55270000
H	4.03220900	-2.45833700	-1.59906600
C	1.84423200	-1.50061600	-2.89315800
H	2.38814700	-0.70688400	-3.42946200
H	0.76977800	-1.38488100	-3.10188400
H	2.17489900	-2.47019000	-3.30330700
C	2.18394900	1.51808300	-1.53130800
H	1.85747400	2.44977700	-1.04426100
H	1.88280400	1.55735600	-2.58892500
H	3.27937800	1.43627500	-1.46339800
C	3.34540000	0.36138800	2.89939900

H	4.36178700	0.53736900	3.26065400
O	-1.03421000	0.49708900	-2.65680600
O	-1.99620400	0.79124400	-4.63546100
C	-1.84683900	0.12548800	-3.59848900
C	-2.61779400	-1.16709100	-3.39932100
H	-3.07689500	-1.48523300	-4.34588700
H	-3.41472400	-1.00157700	-2.65559500
H	-1.96683100	-1.96337400	-3.00920100
H	-2.35839700	-0.19325800	-0.63638100
H	-2.92369600	-3.96592500	-0.63228300
H	-2.67189200	-3.25298500	-0.63404000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3047.069889 E_0
Sum of electronic and zero-point Energies=-3046.598180 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies=-3046.564497 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies=-3046.563553 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3046.662662 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.471708
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3048.456720 E_0

TS2a

Charge 0; multiplicity 1

Ni	-0.69824600	0.36141800	-0.45243900
P	-0.76630900	0.53324600	1.65912700
C	0.95823000	0.63950100	2.30451100
C	-0.76342700	3.30711100	1.50838600
H	-1.25609700	4.27248200	1.71551800
H	-0.67959600	3.19736300	0.41478400
H	0.25046300	3.34846000	1.93726000
C	-1.60261500	2.17220300	2.12145000
C	1.28685800	0.61946200	3.67133900
H	0.51650200	0.43373800	4.42280400
C	-1.71551400	2.35165400	3.64210300
H	-0.72912400	2.39447100	4.12832300
H	-2.30740600	1.55137200	4.11310200
H	-2.22675700	3.30800100	3.84790800
C	-3.00277300	2.16954600	1.48207800
H	-3.62928100	1.34477600	1.85818700
H	-2.93127000	2.08002300	0.38771900
H	-3.51105200	3.11803900	1.72580600
C	-1.57444300	-0.78889700	2.63184400
H	-1.13589400	-1.75246900	2.33056400
H	-2.64955700	-0.80311300	2.40077400
H	-1.43064000	-0.64686400	3.71298700
C	2.60391100	0.84948700	4.08055800
H	2.85154400	0.83489100	5.14487600
P	1.47723100	0.69538400	-0.42800300
C	1.97447800	0.84052700	1.34205500
C	1.62630800	-2.05611700	-0.53812400
H	2.08575300	-2.98265700	-0.92367100
H	0.55987400	-2.05771900	-0.81970400
H	1.69314200	-2.07869700	0.56215800
C	2.35181200	-0.83412200	-1.12753100
C	3.28726100	1.10878700	1.76821700
H	4.07423000	1.30722200	1.03806500
C	3.84844400	-0.89507800	-0.79661900
H	4.02696400	-1.03415400	0.28022500
H	4.38721700	0.00589200	-1.13052500
H	4.29273400	-1.75960700	-1.32026000
C	2.15586100	-0.79389200	-2.65484700
H	2.72958000	0.02250700	-3.12092500
H	1.09465100	-0.67260500	-2.92343000
H	2.51138300	-1.74396400	-3.08878900
C	2.23022600	2.15252300	-1.24998300
H	1.89189800	3.05733100	-0.72303700
H	1.87416000	2.20421400	-2.28882300
H	3.33016800	2.11195700	-1.23625400
C	3.59758100	1.11762200	3.13152600

H	4.62166600	1.32278900	3.45324700
O	-1.02336100	2.44825300	-2.37729900
O	-2.28768700	4.08669500	-3.21509500
C	-2.06842500	2.87974400	-3.00130700
C	-3.05099000	1.82793600	-3.50330000
H	-3.94646600	2.30200800	-3.92826400
H	-3.33978000	1.15097900	-2.68365800
H	-2.56712800	1.21051700	-4.27859700
H	-2.12005600	-0.05231200	-0.26590800
H	-0.90813400	0.06577100	-2.01075800
H	-0.93573200	0.94858500	-2.08118300

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3047.045637 E_0
Sum of electronic and zero-point Energies= -3046.571048 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3046.539853 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3046.538909 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3046.633127 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.474589
Number of imaginary vibrational frequencies = 1; 298*i*
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3048.435089 E_0

6a

Charge 0; multiplicity 1

Ni	-0.89830200	-0.61079200	-0.77831300
P	-0.97492700	-0.47707000	1.36648600
C	0.75336800	-0.30520300	1.99973800
C	-1.28927700	2.25064900	1.07103200
H	-1.81182000	3.19309600	1.31027300
H	-1.40320900	2.05768400	-0.00870000
H	-0.21746600	2.39690600	1.28353900
C	-1.88327300	1.10279900	1.90580700
C	1.09951300	-0.30988100	3.36292700
H	0.34205200	-0.51289700	4.12292800
C	-1.74432200	1.40946500	3.40285200
H	-0.70619600	1.64471200	3.68149800
H	-2.09923400	0.57925900	4.03412600
H	-2.35947100	2.29417600	3.64393900
C	-3.36926200	0.91765200	1.54862500
H	-3.84741400	0.13798200	2.16270800
H	-3.49083400	0.64975300	0.48811700
H	-3.90571300	1.86439100	1.73208700
C	-1.69282100	-1.84679300	2.35577400
H	-1.12372200	-2.76338300	2.13659300
H	-2.73697900	-2.00616900	2.04915500
H	-1.65366200	-1.64589800	3.43720900
C	2.41392100	-0.04369100	3.75830100
H	2.67312000	-0.04602300	4.82011800
P	1.24617900	-0.30407100	-0.74114100
C	1.75629300	-0.09190600	1.02545000
C	1.40018100	-3.05922700	-0.73823400
H	1.86032500	-4.00250900	-1.08069300
H	0.33827000	-3.06492700	-1.03633700
H	1.45068700	-3.04066800	0.36306200
C	2.13971400	-1.86281800	-1.36128100
C	3.06571200	0.21529500	1.43735600
H	3.84142800	0.42493900	0.69798900
C	3.62816300	-1.91077300	-0.99254000
H	3.78239100	-1.99627200	0.09359800
H	4.17721800	-1.02818400	-1.35780100
H	4.08304300	-2.80057200	-1.46234500
C	1.98688500	-1.89517400	-2.89325500
H	2.56953100	-1.09776400	-3.38098900
H	0.93291400	-1.79326300	-3.19579500
H	2.36048300	-2.86185000	-3.27247600
C	2.04211900	1.10723400	-1.60763200
H	1.64736300	2.04172900	-1.18065400
H	1.77892000	1.07688000	-2.67452400
H	3.13761200	1.09254500	-1.49944800
C	3.38996400	0.24612600	2.79711600

H	4.41132000	0.48226700	3.10653800
O	-0.99725800	1.73017100	-2.90084000
O	-2.16576100	3.24039700	-4.00950300
C	-2.10402700	2.11140400	-3.55058200
C	-3.20127800	1.08938600	-3.68823700
H	-4.12339000	1.58086400	-4.02249100
H	-3.35985700	0.55835900	-2.73833900
H	-2.89786400	0.33906400	-4.43739100
H	-2.35923000	-0.96876500	-0.81493900
H	-0.97547100	-0.70149900	-2.28945500
H	-1.04567700	0.77786700	-2.55860300

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3047.059175 E_0
Sum of electronic and zero-point Energies= -3046.581511 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3046.550192 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3046.549248 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3046.644086 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.477664
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3048.447997 E_0

7a

Charge 0; multiplicity 1

Ni	0.14619300	-1.88522100	0.26371300
P	1.45670600	-0.36987400	-0.51564500
C	0.56141200	1.25135200	-0.44839800
C	2.43471300	-0.31397100	2.05771700
H	3.26795500	-0.23689400	2.77817500
H	1.94050200	-1.28984600	2.20086800
H	1.70837600	0.48095100	2.29549500
C	2.97006900	-0.18446800	0.62134900
C	1.07712000	2.46333500	-0.94214800
H	2.03334800	2.48077300	-1.46924300
C	3.72221200	1.14098800	0.44924900
H	3.11483100	2.00463200	0.75928300
H	4.05382800	1.29929800	-0.58959900
H	4.62480700	1.12542800	1.08542300
C	3.91747000	-1.35919100	0.31638600
H	4.38803100	-1.26219100	-0.67481000
H	3.38630500	-2.32288500	0.36071500
H	4.72436000	-1.37696300	1.06918500
C	2.12549200	-0.42830500	-2.22699400
H	1.27984500	-0.37201500	-2.92976600
H	2.64082400	-1.38752900	-2.38250600
H	2.82251400	0.39925900	-2.43123800
C	0.37645000	3.65893200	-0.75486500
H	0.78805500	4.59593400	-1.13878000
P	-1.39274500	-0.42671800	0.59876100
C	-0.70458000	1.24041700	0.18291900
C	-2.23072600	-0.84775800	-1.99752000
H	-3.02579300	-1.05838200	-2.73391200
H	-1.51086900	-1.68303400	-2.01761800
H	-1.70726500	0.06740000	-2.31965200
C	-2.84740900	-0.68812600	-0.59714900
C	-1.38203600	2.45401200	0.39916600
H	-2.34126000	2.46407800	0.92134900
C	-3.86739800	0.45763400	-0.59517900
H	-3.43429600	1.39709100	-0.97045000
H	-4.28911100	0.63942300	0.40624000
H	-4.70606700	0.19141300	-1.26258800
C	-3.53596700	-2.00234800	-0.18545000
H	-4.02986400	-1.91969500	0.79598900
H	-2.81017400	-2.82878700	-0.14151700
H	-4.31003800	-2.25653500	-0.92994400
C	-2.14031100	-0.20128000	2.26206000
H	-1.33535600	0.05974300	2.96650300
H	-2.58952400	-1.15098700	2.58809500
H	-2.90506400	0.59022800	2.27879300
C	-0.83959400	3.65800600	-0.06071900

H	-1.37486500	4.59577300	0.10937300
H	1.14060900	-2.99280200	0.00641900
H	-0.64971000	-2.99134300	0.91342800

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -2818.121016 E_0
Sum of electronic and zero-point Energies= -2817.705557 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -2817.680395 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -2817.679450 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -2817.757908 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.415459
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -2819.247808 E_0

4a*AcOH

Charge 0; multiplicity 1

Ni	-1.67397500	0.23856800	-0.45008400
P	-1.30501400	0.24887100	1.61620900
C	0.50800900	0.42091400	1.92465600
C	-1.66118900	2.99167100	1.51653500
H	-2.12059700	3.91596200	1.90714900
H	-1.97524300	2.86928200	0.46663000
H	-0.56746700	3.12627900	1.53620800
C	-2.10434100	1.79580800	2.37780500
C	1.10236100	0.33479800	3.19603500
H	0.50497200	0.06286500	4.06866500
C	-1.68488000	2.01351800	3.83903800
H	-0.61009400	2.22766100	3.93407000
H	-1.93204700	1.15048900	4.47736500
H	-2.23180400	2.88626900	4.23595600
C	-3.63276400	1.63610600	2.29940900
H	-3.99414900	0.80124300	2.92070100
H	-3.96137200	1.46708300	1.26327700
H	-4.10766100	2.56038200	2.67031700
C	-1.81633300	-1.18149200	2.63942500
H	-1.32199600	-2.08148400	2.24257600
H	-2.90458600	-1.31690000	2.56390700
H	-1.53390000	-1.04871700	3.69460500
C	2.46445700	0.60763300	3.35500900
H	2.91900900	0.54099900	4.34666900
P	0.48553500	0.59860100	-0.84779800
C	1.30555200	0.72477000	0.79838300
C	0.75083300	-2.15086400	-0.95159100
H	1.14117500	-3.06327500	-1.43465900
H	-0.35065500	-2.19859400	-0.96449500
H	1.08350600	-2.15731100	0.09940800
C	1.26089300	-0.90921700	-1.70258300
C	2.66518800	1.03668100	0.97692300
H	3.28385200	1.31435900	0.12111500
C	2.79456900	-0.89632500	-1.71832900
H	3.21893400	-0.99382800	-0.70776500
H	3.20018200	0.01516300	-2.18517700
H	3.15065100	-1.75741100	-2.31088500
C	0.72284900	-0.91129600	-3.14587900
H	1.14444700	-0.08591000	-3.74083000
H	-0.37422900	-0.82666300	-3.16600200
H	1.00520400	-1.85750100	-3.63830200
C	1.08167200	2.06652900	-1.77627900
H	0.74546300	2.96999000	-1.24572300
H	0.63535700	2.07029600	-2.78091000
H	2.17879900	2.08137700	-1.86336800
C	3.23852700	0.98500600	2.25105400

H	4.29688500	1.22521100	2.38015000
O	-3.74456200	0.25593600	-3.95411000
O	-2.38844800	0.53118300	-2.21466200
C	-3.20092700	-0.19400800	-2.93790500
C	-3.45765400	-1.61009900	-2.47172500
H	-4.10023800	-1.57824800	-1.57607800
H	-2.52290700	-2.11488500	-2.18648000
H	-3.96992700	-2.18017500	-3.25860000
H	-3.00471600	-0.14538700	0.10312200
H	-2.24728600	2.07509300	-2.56351600
C	-3.04278300	3.88627500	-2.70715400
O	-2.00116300	3.05591300	-2.68626200
O	-2.85685300	5.08397000	-2.87068900
C	-4.40665500	3.27308900	-2.51878700
H	-5.17693100	4.04955400	-2.60343400
H	-4.56777700	2.48612300	-3.27191500
H	-4.46727400	2.79500300	-1.52781900

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3274.837623 E_0
Sum of electronic and zero-point Energies= -3274.315082 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3274.278850 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3274.277905 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3274.383946 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.522541
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3276.482233 E_0

8a*AcO$^-$

Charge 0; multiplicity 1

Ni	-1.08181000	-0.09303200	-0.60110300
P	-0.95316800	0.06349500	1.47813100
C	0.82144600	0.25231700	1.96073100
C	-1.29909900	2.79226500	1.18931600
H	-1.78887600	3.73500000	1.48599900
H	-1.53160500	2.61762000	0.12786700
H	-0.21024300	2.92358100	1.30092300
C	-1.82724800	1.64352200	2.06606100
C	1.27589100	0.25785200	3.29140700
H	0.58647000	0.05293300	4.11279600
C	-1.55644100	1.94104700	3.54856700
H	-0.50049500	2.18487900	3.73762600
H	-1.85109100	1.10668200	4.20473100
H	-2.15581700	2.82039600	3.84090000
C	-3.33906900	1.46536800	1.84251500
H	-3.76315100	0.68514700	2.49463400
H	-3.55474400	1.21556500	0.79451800
H	-3.84726800	2.41634400	2.07477100
C	-1.56711700	-1.32104600	2.50589000
H	-1.04223800	-2.23772700	2.19638200
H	-2.64433500	-1.45606000	2.33414600
H	-1.38244300	-1.14173000	3.57556900
C	2.61620800	0.53769800	3.57504300
H	2.96081500	0.54374300	4.61209900
P	1.10733800	0.20575700	-0.79912300
C	1.73974300	0.46812800	0.90875100
C	1.36774700	-2.53695600	-0.55989700
H	1.79029400	-3.49625600	-0.90521100
H	0.26991800	-2.59628700	-0.64403700
H	1.62742500	-2.41835500	0.50465700
C	1.93027900	-1.38974500	-1.41700900
C	3.07620000	0.78622200	1.20774300
H	3.78632700	0.99449800	0.40486000
C	3.46147700	-1.36345600	-1.32961800
H	3.81533600	-1.31519600	-0.28886200
H	3.89710200	-0.52131100	-1.89025700
H	3.85853200	-2.29459300	-1.77057700
C	1.49196400	-1.57684800	-2.88163800
H	1.89801400	-0.79124800	-3.53854400
H	0.39519100	-1.58001100	-2.97548900
H	1.86812600	-2.54666800	-3.24973300
C	1.81579200	1.57931500	-1.78956800
H	1.41606600	2.52525800	-1.39312800
H	1.49534300	1.47890400	-2.83753800
H	2.91530000	1.60165700	-1.74787100
C	3.50870500	0.82904800	2.53655000

H	4.54969900	1.07463300	2.76090800
O	-2.87950300	0.19189900	-4.33645300
O	-1.58682200	-0.07496200	-2.53789400
C	-2.74933400	-0.30724100	-3.24376700
C	-3.71198100	-1.21049400	-2.54943200
H	-4.26873000	-0.61347000	-1.81060900
H	-3.18967900	-2.01810700	-2.01988800
H	-4.41354200	-1.61282400	-3.29057900
H	-2.44211200	-0.42791000	-0.10907200
H	-1.03583300	0.53274500	-3.07533800
C	-4.10955000	3.21757100	-1.75824400
O	-3.51261000	2.09748200	-1.73101000
O	-4.09828800	4.07335000	-0.83380600
C	-4.94102600	3.52318200	-3.01021100
H	-5.97136900	3.15945700	-2.85019500
H	-4.99489700	4.60666200	-3.19726700
H	-4.53630800	3.00509400	-3.89325300

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3274.801998 E_0
Sum of electronic and zero-point Energies= -3274.278928 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3274.242383 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3274.241439 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3274.347755 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.523071
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3276.450280 E_0

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Charge 1; multiplicity 1

Ni	-0.86116100	-0.11815200	-0.83304900
P	-0.92827700	0.10302800	1.24320500
C	0.79461200	0.32432800	1.87821900
C	-1.54782100	2.69902000	0.55009100
H	-2.07194100	3.65084300	0.74339300
H	-1.86602500	2.32320900	-0.43688100
H	-0.46634100	2.91011000	0.51418500
C	-1.89462400	1.68541100	1.65408800
C	1.11755600	0.42169000	3.24316900
H	0.34411300	0.30319900	4.00427800
C	-1.53603700	2.25617200	3.03381800
H	-0.49090900	2.59564400	3.08405000
H	-1.71190800	1.52910200	3.84233200
H	-2.18038200	3.13066400	3.22835100
C	-3.39817200	1.36105600	1.61346000
H	-3.69984200	0.70392100	2.44378900
H	-3.68784400	0.88548500	0.66315900
H	-3.96453200	2.30298200	1.70842200
C	-1.61677800	-1.23895400	2.27975700
H	-0.99407500	-2.13625700	2.14494500
H	-2.64316600	-1.46740400	1.96088800
H	-1.61370300	-0.95245300	3.34267600
C	2.43393800	0.68039300	3.63666100
H	2.67605700	0.75922500	4.69942000
P	1.34500900	0.03457400	-0.82252000
C	1.81852200	0.42622500	0.90986900
C	1.54807100	-2.65910200	-0.22883000
H	1.90353100	-3.67165500	-0.48556600
H	0.44591600	-2.66204200	-0.26856100
H	1.85702500	-2.44518400	0.80690900
C	2.13424600	-1.64178300	-1.22255600
C	3.13262200	0.71873200	1.31538800
H	3.92603200	0.83315400	0.57352000
C	3.66542500	-1.63162600	-1.13760700
H	4.02011800	-1.42699900	-0.11613800
H	4.11540600	-0.89500700	-1.82145700
H	4.04544100	-2.62726600	-1.42614000
C	1.68195000	-1.99717300	-2.65162800
H	2.07880500	-1.29118000	-3.39867000
H	0.58368100	-2.00560900	-2.72994800
H	2.05325400	-3.00309900	-2.91130600
C	2.20590100	1.27984000	-1.85967200
H	1.77799200	2.26924400	-1.63660300
H	2.03277700	1.05389100	-2.92288700
H	3.28932600	1.30250500	-1.66884200
C	3.43498800	0.85481100	2.67344000
H	4.45879100	1.08092100	2.98155600
O	-2.22033500	-0.03305600	-4.78253200

O	-1.20026000	-0.03038400	-2.79981800
C	-2.21976700	-0.42510900	-3.64028800
C	-3.21853500	-1.32571500	-2.99551800
H	-3.79017500	-0.75540900	-2.24682400
H	-2.71438200	-2.15112900	-2.47282600
H	-3.89620200	-1.71086100	-3.76643800
H	-2.29949400	-0.27287500	-0.47641000
H	-0.58601000	0.53611900	-3.31382900

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3046.341739 E_0
Sum of electronic and zero-point Energies=-3045.868677 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3045.838195 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3045.837251 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3045.928731 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.473062
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3047.722055 E_0

TS3a

Charge 1; multiplicity 1

Ni	-0.93019600	-0.67476500	-0.43461700
P	-0.97953100	0.00635100	1.51570900
C	0.75851600	0.34950500	2.04143300
C	-1.25902800	2.62692900	0.64231400
H	-1.79080600	3.59255500	0.68564700
H	-1.30938300	2.25987900	-0.39527700
H	-0.20461800	2.81163100	0.90281600
C	-1.92922700	1.64135600	1.61476200
C	1.12054500	0.62874300	3.37095000
H	0.37791100	0.58724200	4.17031800
C	-1.91203400	2.20628700	3.04386300
H	-0.89422400	2.45952700	3.37627200
H	-2.36137000	1.51308100	3.77172700
H	-2.50621200	3.13591700	3.05861300
C	-3.37827500	1.37932100	1.16776600
H	-3.89026800	0.65479200	1.82064000
H	-3.41258700	1.00573600	0.13358700
H	-3.93928600	2.32811300	1.21339000
C	-1.65042600	-1.11433700	2.79300200
H	-1.12555600	-2.07828400	2.71417900
H	-2.72209400	-1.27609500	2.60976100
H	-1.50610500	-0.70318000	3.80276400
C	2.44080700	0.96919800	3.68195900
H	2.71367300	1.18463000	4.71792400
P	1.21636900	-0.16243700	-0.64770600
C	1.74478300	0.37422300	1.02816400
C	1.82998900	-2.76042600	0.04859800
H	2.21616000	-3.75624900	-0.22781400
H	0.74443300	-2.84919500	0.22586800
H	2.30989500	-2.45957400	0.99344900
C	2.12316500	-1.76056000	-1.08241800
C	3.06084400	0.74823000	1.34896600
H	3.82278300	0.80335400	0.56854700
C	3.63378800	-1.59360400	-1.28175900
H	4.13860600	-1.27622500	-0.35678600
H	3.86912600	-0.87044700	-2.07812600
H	4.06590200	-2.56556100	-1.57760900
C	1.45753100	-2.24039300	-2.38825000
H	1.63486600	-1.54413300	-3.22332300
H	0.36720100	-2.35185300	-2.26070800
H	1.87021500	-3.22291900	-2.67361000
C	1.84456900	1.12944000	-1.78785400
H	1.27739600	2.05637700	-1.61485700
H	1.69602500	0.80695700	-2.82884300
H	2.91425200	1.32554500	-1.61886200
C	3.40503500	1.04753100	2.67056800

H	4.43187600	1.33197200	2.91294000
O	-2.82928400	1.29435200	-2.75053500
O	-1.03393500	0.30885800	-3.66944300
C	-2.30270700	0.30140000	-3.22313800
C	-2.94036400	-1.05258800	-3.32213500
H	-2.67538100	-1.60949300	-2.40562200
H	-2.56620500	-1.61090800	-4.19047600
H	-4.03184200	-0.94774300	-3.35916400
H	-2.30140600	-1.03844400	0.02351100
H	-0.67037000	1.21110800	-3.55258600

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3046.321809 E_0
Sum of electronic and zero-point Energies= -3045.848517 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3045.818868 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3045.817924 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3045.906372 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.473293
Number of imaginary vibrational frequencies = 1; 25*i*
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3047.703508 E_0

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Charge 1; multiplicity 1

Ni	-0.90655500	-0.71351700	-0.49944000
P	-0.95282700	-0.03058500	1.45025700
C	0.78614100	0.31201100	1.97268200
C	-1.22879700	2.59128500	0.57879600
H	-1.76129100	3.55657200	0.62086400
H	-1.27564100	2.22457100	-0.45903500
H	-0.17531700	2.77651800	0.84263200
C	-1.90139900	1.60504700	1.54891100
C	1.15062700	0.59067300	3.30163100
H	0.40938100	0.54919200	4.10229600
C	-1.88648400	2.16844800	2.97861700
H	-0.86890700	2.41903700	3.31378700
H	-2.33915100	1.47551300	3.70465300
H	-2.47861600	3.09939900	2.99288900
C	-3.34965900	1.34390100	1.09877000
H	-3.86299300	0.61863100	1.74978300
H	-3.38198600	0.97144600	0.06412000
H	-3.91064900	2.29271200	1.14443100
C	-1.62272800	-1.14920100	2.72982800
H	-1.09950200	-2.11401400	2.65067100
H	-2.69499400	-1.30943600	2.54870700
H	-1.47594900	-0.73753600	3.73901300
C	2.47159300	0.93044400	3.61037900
H	2.74644600	1.14535800	4.64592700
P	1.23858200	-0.19791900	-0.71804100
C	1.77043200	0.33698500	0.95746900
C	1.85231600	-2.79721500	-0.02632000
H	2.23799300	-3.79271700	-0.30457900
H	0.76706500	-2.88621400	0.15269300
H	2.33373500	-2.49757500	0.91815200
C	2.14392200	-1.79591500	-1.15649600
C	3.08721700	0.71025700	1.27610000
H	3.84776700	0.76548700	0.49434200
C	3.65431600	-1.62946200	-1.35799300
H	4.16069700	-1.31374600	-0.43330200
H	3.88882400	-0.90521800	-2.15361500
H	4.08548000	-2.60119600	-1.65596100
C	1.47608100	-2.27359600	-2.46207100
H	1.65381300	-1.57702500	-3.29678700
H	0.38558400	-2.38340000	-2.33398900
H	1.88690000	-3.25656500	-2.74859700
C	1.86545300	1.09477600	-1.85826900
H	1.29551800	2.02042800	-1.68755400
H	1.71998700	0.77057300	-2.89908500
H	2.93430600	1.29368600	-1.68734900
C	3.43398900	1.00867600	2.59724500

H	4.46143100	1.29243000	2.83786300
O	-2.76811100	1.23942100	-2.80483000
O	-0.99978100	0.26799100	-3.78866600
C	-2.25460800	0.25314400	-3.30553400
C	-2.89530900	-1.09969900	-3.40069500
H	-2.64539300	-1.64734000	-2.47432700
H	-2.51420600	-1.66828800	-4.25898600
H	-3.98611000	-0.99086000	-3.45048200
H	-2.27519800	-1.08153500	-0.03702400
H	-0.63313100	1.16859900	-3.66851000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3046.321810 E_0
Sum of electronic and zero-point Energies=-3045.848430 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3045.817913 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3045.816969 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3045.908502 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.473380
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3047.703457 E_0

9a

Charge 1; multiplicity 1

Ni	-0.85777300	-0.40676800	-0.66152500
P	-0.93137500	0.04282100	1.35554200
C	0.79985300	0.29355200	1.95114600
C	-1.23451700	2.67975800	0.60967900
H	-1.75743900	3.64757400	0.69287900
H	-1.33502900	2.31934700	-0.42742400
H	-0.16613200	2.85356000	0.81648500
C	-1.85087000	1.67783700	1.60053600
C	1.13459900	0.44004800	3.30855800
H	0.36924200	0.35005300	4.08188100
C	-1.71901600	2.19682700	3.04095000
H	-0.68000900	2.45371400	3.29514100
H	-2.09791400	1.47357500	3.78004900
H	-2.32114100	3.11659100	3.13650000
C	-3.33356600	1.44882000	1.26034500
H	-3.81590600	0.75034200	1.96212000
H	-3.44997200	1.05547600	0.23935400
H	-3.86564500	2.41275300	1.32590500
C	-1.64601700	-1.19092900	2.49681200
H	-1.09555200	-2.13565300	2.37288800
H	-2.70233700	-1.35719600	2.24393000
H	-1.56367700	-0.85651500	3.54186200
C	2.45528900	0.71182300	3.67955700
H	2.70731900	0.82624600	4.73668700
P	1.31074300	0.00061000	-0.75704300
C	1.81249800	0.37790000	0.96825600
C	1.67894500	-2.68178000	-0.23430400
H	2.01838700	-3.68059700	-0.55754900
H	0.57885500	-2.70267200	-0.14718300
H	2.10107300	-2.48579500	0.76422100
C	2.12632900	-1.62749200	-1.26119900
C	3.13036200	0.68041500	1.35117300
H	3.91406300	0.77858000	0.59671800
C	3.65489900	-1.56249200	-1.34557800
H	4.11164100	-1.34846200	-0.36720800
H	3.99823800	-0.80518800	-2.06767600
H	4.03841200	-2.54125700	-1.68312900
C	1.52095200	-1.96219500	-2.63866400
H	1.80789900	-1.22685700	-3.40726900
H	0.41856000	-1.99838700	-2.58784300
H	1.87825600	-2.95238000	-2.96889200
C	2.05752400	1.32183700	-1.78427600
H	1.58021900	2.27756800	-1.51946300
H	1.86050400	1.11288800	-2.84653800
H	3.14301600	1.39927900	-1.62171000
C	3.44755200	0.85098500	2.70208500

H	4.47514700	1.08186300	2.99334800
H	-2.25841600	-0.77446900	-0.30236500

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -2817.386206 E_0
Sum of electronic and zero-point Energies= -2816.976204 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -2816.951608 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -2816.950664 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -2817.028295 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.410002
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -2818.507287 E_0

AcO^-

Charge -1; multiplicity 1

O	-1.96550000	-2.78389800	0.41784000
O	-3.71080600	-3.89816600	-0.46304900
C	-2.86769900	-3.66832200	0.44863800
C	-2.95481800	-4.51502900	1.73055000
H	-3.36723500	-3.89542700	2.54628900
H	-1.94977600	-4.83699700	2.04893000
H	-3.60310100	-5.39460200	1.59858700

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -228.444404 E_0
Sum of electronic and zero-point Energies= -228.396115 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -228.391688 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -228.390744 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -228.423794 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.048289
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -228.724067 E_0

1b

Charge 0; multiplicity 1

Ni	0.02900700	-0.00012900	-0.00620600
C	1.81715400	-0.40907600	2.74473700
O	-1.86154700	-0.26403600	-0.04942700
O	-1.59482400	-2.17508800	-1.20416300
C	-2.29793200	-1.24541900	-0.77921200
C	-3.77196300	-1.15324400	-1.12703500
H	-4.15930700	-2.13327700	-1.43603800
H	-3.88392000	-0.44940900	-1.96932100
H	-4.35530500	-0.75698000	-0.28425300
C	2.71465900	0.44594400	1.85144700
O	0.03586800	0.26951300	-1.89686500
O	-1.05163000	2.22157600	-1.65519400
C	-0.65700700	1.27100700	-2.34730000
C	-1.01037500	1.17728900	-3.82014400
H	-1.16403800	2.17889700	-4.24415200
H	-1.95744800	0.61738300	-3.90668700
H	-0.24462000	0.63106600	-4.38748600
H	1.87445200	-0.08169800	3.79437300
H	2.12329400	-1.46713000	2.70695400
H	2.62314500	1.51104800	2.11955600
H	3.77364500	0.16335300	1.95546700
P	2.17012400	0.35496500	0.07996900
C	3.12077000	-1.01018000	-0.78665300
C	3.16499500	1.75649400	-0.68427900
H	2.49320500	-1.20037600	-1.67178800
C	4.46799200	-0.37924900	-1.23778900
C	3.16445300	-2.28523800	0.03104400
C	4.56643400	1.09941400	-0.79984100
C	2.63150400	2.40524400	-1.94451000
H	3.18465200	2.53279400	0.09495400
H	4.53713200	-0.46550800	-2.33207200
H	5.31997000	-0.94157600	-0.83073200
C	2.09760600	-3.19996900	-0.06386900
C	4.21516600	-2.57658800	0.91980400
H	5.04476000	1.15315400	0.19051200
H	5.19880500	1.67936900	-1.49055800
C	2.81248700	1.85478800	-3.22712500
C	1.98681300	3.65185700	-1.84319400
C	2.08827400	-4.37416000	0.69649300
H	1.26577900	-2.98874700	-0.74225500
C	4.20366800	-3.74970900	1.68428900
H	5.05814600	-1.88840500	1.01878800
C	2.37274100	2.53559100	-4.36763000
H	3.30709900	0.88928400	-3.34699700
C	1.54183400	4.33167200	-2.98151000
H	1.84170300	4.09854700	-0.85577200

C	3.14185200	-4.65452700	1.57555300
H	1.25695600	-5.07688000	0.59542100
H	5.03331400	-3.95713000	2.36554300
C	1.73745400	3.77768500	-4.25130000
H	2.52951600	2.09066000	-5.35394800
H	1.04727400	5.30080500	-2.87439400
H	3.13725200	-5.57358800	2.16732400
H	1.39794200	4.30904200	-5.14426700
P	0.06397400	-0.38046200	2.13485200
C	-0.88324400	0.89129900	3.11681600
C	-0.69175500	-1.81080800	3.09206000
H	-1.87631400	0.82039100	2.64092900
C	-0.96879500	0.31023500	4.54679000
C	-0.38794000	2.30930700	2.92849600
C	-0.73445000	-1.22825500	4.53363600
C	-2.00678200	-2.36292300	2.57927500
H	0.05233000	-2.61920200	3.03494200
H	-1.95406900	0.55957900	4.97031300
H	-0.21903100	0.78062100	5.19732300
C	-0.83653600	3.03478500	1.80751800
C	0.53376400	2.92341200	3.79471800
H	0.22839700	-1.45168600	5.01600400
H	-1.50630100	-1.75366000	5.11620500
C	-3.25189800	-1.81265600	2.93827700
C	-1.99887800	-3.51607000	1.77355800
C	-0.38176900	4.33304700	1.56028300
H	-1.54959000	2.57109500	1.12100600
C	0.98762300	4.22597300	3.54922800
H	0.90349100	2.39188600	4.67459800
C	-4.44680700	-2.39767900	2.50439700
H	-3.29889900	-0.92595100	3.57474000
C	-3.19167300	-4.10298600	1.33972500
H	-1.04244600	-3.96263400	1.48965900
C	0.53352300	4.93633200	2.43255700
H	-0.74559600	4.87292300	0.68214900
H	1.69985400	4.68658400	4.23923700
C	-4.42262100	-3.54602900	1.70431200
H	-5.40181900	-1.95426300	2.79883900
H	-3.15773300	-5.00134100	0.71763800
H	0.88697600	5.95366600	2.24503600
H	-5.35686600	-4.00532700	1.37083700

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3964.001497 E_0
Sum of electronic and zero-point Energies= -3963.289911 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3963.245371 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3963.244427 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies=-3963.373372 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.711586
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3966.340147 E_0

2b

Charge 0; multiplicity 1

Ni	0.07114800	-0.35404100	-0.27921200
C	1.77142300	0.19754900	2.46651800
O	-2.89717900	-0.91353200	0.26036500
O	-1.05066300	-1.85912200	-0.61041100
C	-2.32773300	-1.78163200	-0.42350200
C	-3.13904300	-2.82875400	-1.16210500
H	-2.55438800	-3.73785100	-1.35564700
H	-3.43313900	-2.39379900	-2.13260600
H	-4.05388100	-3.06964900	-0.60281800
C	1.95273600	1.51212500	1.70864100
O	0.27390600	-0.19614500	-2.17206200
O	-1.89126400	0.27659400	-2.55458500
C	-0.76807700	-0.07383200	-2.94018000
C	-0.51460800	-0.43887800	-4.39128000
H	-1.26389000	0.03194600	-5.04212600
H	-0.60507300	-1.53440200	-4.48901600
H	0.49981400	-0.15731200	-4.70687800
H	-5.30746800	0.70278700	-1.60046000
H	-4.70067800	0.37361900	-1.29117800
H	1.27364600	2.28721100	2.09929300
H	2.98305200	1.88979000	1.80092900
H	1.72826800	0.36528900	3.55375200
H	2.61218600	-0.48585600	2.26398100
P	1.49146700	1.27745800	-0.06939300
C	1.26017000	3.03423400	-0.68180200
C	3.05931900	1.03445700	-1.04927600
H	0.69859700	3.54809100	0.11249000
C	2.72504500	3.54903100	-0.71746300
C	0.47369200	3.17415700	-1.96947500
C	3.74162900	2.42371900	-1.06582400
C	3.86687700	-0.17182600	-0.61800600
H	2.65001300	0.82354400	-2.05076800
H	2.96133800	3.95267500	0.27810800
H	2.80243800	4.38954500	-1.42392100
C	-0.91189900	3.41158700	-1.90534500
C	1.08240500	3.12542800	-3.23711600
H	4.18404400	2.58274900	-2.06140300
H	4.57055400	2.45511800	-0.34578000
C	4.91059300	-0.09878000	0.32157100
C	3.53352200	-1.43525500	-1.14572800
C	-1.66673400	3.59652500	-3.06746300
H	-1.40179100	3.45588900	-0.92881300
C	0.32723400	3.30695200	-4.40173900
H	2.15725200	2.95096000	-3.32550900
C	5.60055300	-1.25161300	0.71829400
H	5.20006500	0.86329100	0.75027000
C	4.22138200	-2.58632600	-0.74972900
H	2.72605600	-1.51070100	-1.87934300

C	-1.04944900	3.54582500	-4.32250200
H	-2.74128500	3.78223100	-2.99095400
H	0.82157300	3.26629300	-5.37609700
C	5.25947800	-2.49983300	0.18673000
H	6.41187500	-1.16916300	1.44662400
H	3.94833200	-3.55407000	-1.17919000
H	-1.63645100	3.69300200	-5.23285300
H	5.80157200	-3.39772700	0.49470200
P	0.25213600	-0.69755500	1.87616600
C	0.49835300	-2.39307400	2.64905100
C	-1.14511000	-0.22027100	3.03258600
H	1.56740400	-2.61298500	2.50841100
C	0.21366600	-2.09440800	4.14389500
C	-0.28549100	-3.53725800	2.04053300
C	-0.92409400	-1.05694600	4.32286000
C	-1.30879100	1.28092600	3.17298300
H	-2.02525400	-0.60428200	2.49504300
H	1.13910900	-1.69849000	4.58814300
H	-0.01575800	-3.03114900	4.67547700
C	0.34041900	-4.36790100	1.09177700
C	-1.60645400	-3.83919000	2.41853800
H	-1.87264400	-1.55771900	4.56877900
H	-0.68927700	-0.40691000	5.17646800
C	-0.68688200	2.02402900	4.19296000
C	-2.08786900	1.97476800	2.22587300
C	-0.32697600	-5.46592100	0.54120100
H	1.36865400	-4.15159800	0.78768800
C	-2.27693500	-4.93769000	1.86707400
H	-2.12325900	-3.22172000	3.15587500
C	-0.84209700	3.41413600	4.26561600
H	-0.07535000	1.52268200	4.94675400
C	-2.24535800	3.36240000	2.29972500
H	-2.57586700	1.41348400	1.42493900
C	-1.64061400	-5.75737100	0.92856900
H	0.18360400	-6.09992500	-0.18873800
H	-3.30228400	-5.15436700	2.17861800
C	-1.62176400	4.09024000	3.32096800
H	-0.35153900	3.96893900	5.07001300
H	-2.86435100	3.87598800	1.55915900
H	-2.16352600	-6.61785900	0.50306900
H	-1.74717400	5.17441800	3.38259000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3965.180767 E_0
Sum of electronic and zero-point Energies=-3964.456245 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3964.409046 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3964.408101 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3964.540893 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.724522
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3967.520067 E_0

TS1b

Charge 0; multiplicity 1

Ni	0.24042100	-0.62111400	0.09610600
C	1.71528400	0.10861900	2.90338500
O	-1.29777900	-3.61308500	0.25371800
O	-0.01477500	-3.05611600	-1.49859400
C	-0.84203200	-3.80886100	-0.91701600
C	-1.38210800	-5.01914700	-1.67698200
H	-1.55207600	-5.86530500	-0.99442400
H	-0.70302600	-5.31644700	-2.48904400
H	-2.35613100	-4.74936100	-2.12092500
C	2.72405300	0.63477600	1.87335600
O	-0.00520100	-0.05703200	-1.69274500
O	-2.25736700	-0.14585300	-1.72680800
C	-1.16083500	-0.10764700	-2.29697300
C	-1.05204600	-0.13987000	-3.80785900
H	-0.31550000	0.59476200	-4.16532200
H	-2.03103400	0.04408600	-4.26963500
H	-0.69468400	-1.14146100	-4.09971300
H	-1.34335600	-1.05934100	0.19227700
H	-1.04843000	-1.82682900	0.25372400
P	1.81109500	0.88077500	0.28485200
C	1.20071900	2.65758100	0.30694900
C	2.92677600	1.12066500	-1.21242500
H	1.97414800	3.16304900	0.91029900
C	1.39655200	3.10055900	-1.15834400
C	-0.14399400	2.94748500	0.93048300
C	2.79012900	2.62221400	-1.57204600
C	4.33917800	0.59690100	-1.09128300
H	2.39796700	0.53123500	-1.97715000
H	1.30159200	4.19510800	-1.23648000
H	0.62203600	2.64742300	-1.79805100
C	-1.33451500	2.40060600	0.41875500
C	-0.22665500	3.82551600	2.02605600
H	2.97248800	2.76025700	-2.64913000
H	3.55071300	3.20486300	-1.02810200
C	5.28950400	1.21188300	-0.25378800
C	4.73819700	-0.51953700	-1.84800700
C	-2.57160200	2.72979500	0.98172000
H	-1.29756700	1.70384800	-0.41965600
C	-1.46469800	4.15604800	2.59033900
H	0.68964400	4.26038200	2.43599900
C	6.59711600	0.72190900	-0.17501900
H	5.00802900	2.08426400	0.34199300
C	6.04680800	-1.01024000	-1.77062200
H	4.01397500	-1.00266500	-2.50952200
C	-2.64313500	3.61191700	2.06734200
H	-3.48280300	2.29099600	0.56633200
H	-1.50642800	4.84320600	3.43969800
C	6.98108500	-0.39168200	-0.93256100
H	7.32019900	1.21376400	0.48114100

H	6.33620700	-1.87695300	-2.37088700
H	-3.61109900	3.87126800	2.50418200
H	8.00385000	-0.77257000	-0.87128300
P	0.79267200	-1.28607900	2.10635700
C	1.97372400	-2.74016000	2.37731300
C	-0.57299000	-1.88945600	3.26187800
H	2.95285700	-2.25786100	2.52530800
C	1.46504500	-3.31269900	3.71723200
C	2.13612400	-3.71249700	1.22235100
C	-0.06986600	-3.27408000	3.74326200
C	-0.93853600	-0.87508200	4.32713300
H	-1.44725800	-2.02162800	2.61050300
H	1.86859500	-2.69168200	4.53219900
H	1.84958200	-4.33229100	3.87610200
C	2.87720400	-3.30552000	0.09685800
C	1.64790400	-5.02918300	1.25253400
H	-0.47068500	-4.03171400	3.05334500
H	-0.46214200	-3.50154800	4.74639100
C	-0.30095600	-0.82578100	5.58031100
C	-1.96057300	0.05578100	4.06199200
C	3.12235700	-4.18043500	-0.96410100
H	3.26888700	-2.28532500	0.05427900
C	1.89155800	-5.90858700	0.18930100
H	1.07507800	-5.38796700	2.10953600
C	-0.67732400	0.12313100	6.53807400
H	0.49182400	-1.53628600	5.82396400
C	-2.33662200	1.00481900	5.01808600
H	-2.47176800	0.02780900	3.09558300
C	2.62950900	-5.49026300	-0.92212700
H	3.70258100	-3.83888300	-1.82528200
H	1.50185500	-6.92903100	0.23649900
C	-1.69526700	1.04276000	6.26187700
H	-0.17184300	0.13961900	7.50739200
H	-3.13968400	1.71114400	4.79272700
H	2.82015400	-6.17915900	-1.74919400
H	-1.99050700	1.78044300	7.01254100
H	2.21378500	-0.23137800	3.82463500
H	0.98238900	0.88561900	3.17286500
H	3.18955300	1.57624800	2.20263400
H	3.52659300	-0.09936000	1.69519500

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3965.149387 E_0
Sum of electronic and zero-point Energies= -3964.421693 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3964.376988 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3964.376044 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3964.504229 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.727693
Number of imaginary vibrational frequencies = 1; 74*i*
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3967.494907 E_0

3b

Charge 0; multiplicity 1

Ni	-0.64872200	-0.13802100	-0.53057300
C	0.90446000	-0.31367700	2.32895700
O	-0.07630300	-3.05554100	-1.80971200
O	-2.22304800	-2.49236000	-2.15649800
C	-1.13309900	-3.21930600	-2.40377200
C	-1.34437700	-4.23313100	-3.49236500
H	-1.40390000	-3.70695500	-4.45936700
H	-2.29513900	-4.76547700	-3.34331800
H	-0.50526600	-4.93903700	-3.51447500
C	1.82160900	0.60916000	1.52437200
O	-0.72943100	0.02882600	-2.43922300
O	-2.49710700	1.41338500	-2.37936800
C	-1.70324900	0.67986800	-2.99211400
C	-1.83001500	0.47005200	-4.48941300
H	-2.50106700	1.21896500	-4.93107800
H	-2.24724500	-0.53533900	-4.66780400
H	-0.84367900	0.51016700	-4.97537600
H	-2.08522500	-0.56864200	-0.41995900
H	-2.00453300	-1.78547300	-1.47860800
H	0.85638400	-0.02678500	3.39124300
H	1.26703300	-1.35382800	2.27717500
H	1.59442700	1.66767000	1.73485500
H	2.88408800	0.43953800	1.76089700
P	-0.79640600	-0.36577400	1.56658800
C	-1.60144100	-1.82715400	2.45622100
C	-1.88110200	0.98525500	2.35005200
H	-0.75349800	-2.35888500	2.91198600
C	-2.45247100	-1.16466200	3.56896200
C	-2.31493200	-2.82350700	1.56618000
C	-2.98567800	0.19587200	3.09657500
C	-1.11907700	2.01723100	3.15493100
H	-2.32227300	1.50342200	1.48729100
H	-1.81139600	-1.02648700	4.45356200
H	-3.27580100	-1.83072200	3.87227100
C	-1.63772600	-3.99274500	1.17324200
C	-3.64826300	-2.65793400	1.14583700
H	-3.82439100	0.04467900	2.40018400
H	-3.37602100	0.78558900	3.94108000
C	-0.81649900	1.85344100	4.52012500
C	-0.70560000	3.20631800	2.52358900
C	-2.27027200	-4.97035100	0.39753200
H	-0.60175200	-4.14270600	1.49083300
C	-4.28298600	-3.63438400	0.37039200
H	-4.20620900	-1.76317400	1.42925100
C	-0.12272300	2.84385300	5.22584500
H	-1.12884800	0.95008400	5.04864000
C	-0.01061100	4.19587600	3.22656500
H	-0.94084200	3.35822800	1.46643100
C	-3.59906700	-4.79632900	-0.00538600

H	-1.72300500	-5.87303500	0.11262900
H	-5.32035600	-3.48434400	0.05931000
C	0.28577300	4.01794500	4.58312300
H	0.09679700	2.69504900	6.28659500
H	0.29372900	5.11136300	2.71212600
H	-4.09822100	-5.56002800	-0.60761100
H	0.82556700	4.79075200	5.13662700
P	1.49376400	0.38170900	-0.28134300
C	2.36851400	1.75825900	-1.17974100
C	2.64239700	-0.90668300	-1.04102100
H	3.34232900	1.84320800	-0.66907800
C	2.59534600	1.15061100	-2.59108800
C	1.70348500	3.11529700	-1.15542200
C	2.68790200	-0.40220100	-2.50709300
C	3.96941500	-1.04647300	-0.32936400
H	2.11795600	-1.87069900	-0.99367400
H	3.50510300	1.59025200	-3.02894400
H	1.75462900	1.43387800	-3.24145100
C	2.45029900	4.26368400	-0.83869000
C	0.34303600	3.27012900	-1.47912500
H	1.82606400	-0.84046900	-3.03068200
H	3.59484000	-0.78099900	-3.00290000
C	5.10764600	-0.29501600	-0.67822500
C	4.08700600	-1.97281000	0.72656300
C	1.85658400	5.53221800	-0.85219100
H	3.50875700	4.16228800	-0.58090400
C	-0.25170300	4.53524100	-1.49375600
H	-0.25790500	2.38534700	-1.69876600
C	6.31502700	-0.45549000	0.01336500
H	5.06543800	0.41530900	-1.50716700
C	5.29147500	-2.13423800	1.41753700
H	3.22112000	-2.58270100	1.00050900
C	0.50378900	5.67354500	-1.18292300
H	2.45520300	6.41287500	-0.60364600
H	-1.31186500	4.62516500	-1.74601800
C	6.41248500	-1.37195500	1.06559900
H	7.18574500	0.13759600	-0.27916400
H	5.35674900	-2.86365700	2.22948200
H	0.04017000	6.66356600	-1.19442300
H	7.35646000	-1.49806900	1.60215300

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3965.170097 E_0
Sum of electronic and zero-point Energies= -3964.440371 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3964.394737 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3964.393793 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3964.524924 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.729726
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3967.514149 E_0

4b

Charge 0; multiplicity 1

Ni	-1.18633400	0.10323100	-0.29065900
C	0.79813700	0.38533000	2.25495500
C	1.54904200	1.15318500	1.16563300
O	-1.74729700	-0.11493900	-2.11076800
O	-3.10322900	1.65887500	-1.86744600
C	-2.67056200	0.69010300	-2.51916100
C	-3.25806200	0.37607600	-3.88386400
H	-4.28676300	0.00320800	-3.74384900
H	-2.67520200	-0.38488600	-4.41960800
H	-3.32144400	1.29614600	-4.48401600
H	-2.54396800	-0.26618700	0.20037300
H	1.33830200	2.23225300	1.24376900
H	2.63716700	1.01909100	1.26218400
H	0.90619000	0.86488800	3.24201800
H	1.18132900	-0.64555600	2.34073500
P	0.94893400	0.66500700	-0.53558400
C	2.15457900	-0.64988600	-1.20198300
C	1.67339200	2.05906800	-1.57016500
H	1.52216300	-1.26137700	-1.86344400
C	3.20041500	0.12626300	-2.05352000
C	2.69580400	-1.56472300	-0.12462500
C	3.15363800	1.62450100	-1.72611700
C	0.97619600	2.36404700	-2.88141000
H	1.61501100	2.96293100	-0.94571600
H	2.96385100	-0.02633700	-3.11717000
H	4.21165500	-0.27911100	-1.89673300
C	2.00629900	-2.75102000	0.19134700
C	3.87611300	-1.27429000	0.58555100
H	3.67404400	1.81851600	-0.77364800
H	3.65854900	2.22464600	-2.50056000
C	0.61589800	1.37587300	-3.81697200
C	0.73033200	3.70986900	-3.21509700
C	2.48101400	-3.62034000	1.17930000
H	1.08973100	-2.99748000	-0.35266400
C	4.34973600	-2.14076100	1.57783200
H	4.44240800	-0.36725100	0.35897300
C	0.04525800	1.72526500	-5.04665600
H	0.75958500	0.31802900	-3.58783600
C	0.15554100	4.06107400	-4.44115400
H	0.99830600	4.49373300	-2.50064700
C	3.65538600	-3.31786500	1.87943600
H	1.93473500	-4.54192300	1.39692000
H	5.27057900	-1.89484700	2.11372700
C	-0.18512600	3.06814100	-5.36644200
H	-0.22498700	0.93923900	-5.75673900
H	-0.02531600	5.11424600	-4.67282200

H	4.02997000	-3.99764400	2.64920200
H	-0.63246800	3.33753300	-6.32683000
P	-0.99521700	0.21051200	1.78934200
C	-1.93051400	1.64691700	2.57055600
C	-1.65335700	-1.06023800	3.02915100
H	-2.87508500	1.64573800	2.00218900
C	-2.22957800	1.16012700	3.99666800
C	-1.26610200	2.98759800	2.37269800
C	-2.70461900	-0.28914100	3.86051300
C	-2.09224900	-2.38240700	2.44323100
H	-0.78027900	-1.25031000	3.67372000
H	-2.99004500	1.79816200	4.47585300
H	-1.32203200	1.19843600	4.62222300
C	-1.41205500	3.64635800	1.13499800
C	-0.48446100	3.60046500	3.36760000
H	-2.83929900	-0.77581500	4.83955500
H	-3.67950500	-0.30425100	3.34744300
C	-3.32719400	-2.54008900	1.78534200
C	-1.25125800	-3.50514400	2.55249300
C	-0.79269200	4.87703700	0.89953200
H	-2.01825500	3.18393300	0.34994000
C	0.13622200	4.83435800	3.13126400
H	-0.36006200	3.11974500	4.34061100
C	-3.70292100	-3.77798400	1.25262900
H	-4.00711400	-1.69073600	1.68691400
C	-1.62422000	-4.74395700	2.01853700
H	-0.29332600	-3.40542500	3.07069200
C	-0.01262900	5.47665100	1.89757500
H	-0.92319700	5.37187100	-0.06671800
H	0.73627100	5.29580600	3.92034600
C	-2.85293700	-4.88508200	1.36396200
H	-4.66740400	-3.87712400	0.74720800
H	-0.95411600	-5.60205900	2.12020500
H	0.46999000	6.44058100	1.71587000
H	-3.14895600	-5.85161300	0.94768300

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3736.232674 E_0
Sum of electronic and zero-point Energies= -3735.565333 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3735.525830 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3735.524886 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3735.641851 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.667341
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3738.320035 E_0

5b

Charge 0; multiplicity 1

Ni	-0.96949500	-0.05064700	-0.43237700
C	0.83473900	-0.35442000	2.23749400
C	1.76012400	0.43572600	1.31056200
O	-1.39616200	-0.02726300	-2.31011600
O	-2.43673400	1.91756200	-1.91209200
C	-2.13765800	0.97012300	-2.66278400
C	-2.69076200	0.90998900	-4.07473200
H	-3.70500800	0.47705300	-4.03053900
H	-2.07603100	0.27711700	-4.72899900
H	-2.77599600	1.92285600	-4.49349700
H	-2.39139100	-0.33860800	-0.08738100
H	-2.24587400	-2.37914700	-3.08875200
H	-2.48082300	-3.06760700	-3.29683000
H	1.68983700	1.51355200	1.52976000
H	2.81065200	0.13628600	1.44569400
H	0.92922700	-0.02782100	3.28639200
H	1.07088600	-1.43122800	2.19999000
P	1.22631000	0.27016400	-0.47242300
C	2.28624000	-1.10050700	-1.26385600
C	2.19837700	1.68135200	-1.25336400
H	1.61121900	-1.54461600	-2.01096000
C	3.45341000	-0.36732200	-1.98404900
C	2.67056600	-2.19384700	-0.29083500
C	3.60628500	1.05792100	-1.43789500
C	1.62132000	2.30196400	-2.51081500
H	2.24210900	2.47167900	-0.48947000
H	3.22728700	-0.32726200	-3.06002600
H	4.39273400	-0.93220800	-1.88162800
C	1.84003700	-3.32145800	-0.14563800
C	3.84222500	-2.12772600	0.48727100
H	4.10414500	1.03173800	-0.45431100
H	4.22759300	1.68227300	-2.10047600
C	1.18304900	1.55371000	-3.61972700
C	1.58038200	3.70654800	-2.60514900
C	2.16932200	-4.35024700	0.74353200
H	0.92820800	-3.39508000	-0.74551200
C	4.17063000	-3.15436900	1.38042500
H	4.51512800	-1.27165500	0.39015400
C	0.73528200	2.19038200	-4.78349300
H	1.16805900	0.46271300	-3.58069600
C	1.12814500	4.34477000	-3.76484100
H	1.91310000	4.30734800	-1.75367800
C	3.33631600	-4.27028700	1.51321000
H	1.51463600	-5.22160100	0.82874900
H	5.08763900	-3.08232400	1.97158100
C	0.70793600	3.58725200	-4.86371700

H	0.40267800	1.58730000	-5.63243000
H	1.10628300	5.43709200	-3.80878100
H	3.59690900	-5.07479300	2.20588500
H	0.35640400	4.08080100	-5.77357300
P	-0.92562600	-0.21416800	1.65139700
C	-1.72626700	1.23239200	2.55735700
C	-1.83890200	-1.52437100	2.66838700
H	-2.59991100	1.44874800	1.92099500
C	-2.23315900	0.61520000	3.87053200
C	-0.86795200	2.47298200	2.61313200
C	-2.87038500	-0.72530500	3.49597300
C	-2.36444500	-2.70837300	1.89031500
H	-1.05958800	-1.88976000	3.35643800
H	-2.95251200	1.28873400	4.36431900
H	-1.39946600	0.44746000	4.57259000
C	-0.82519000	3.32787900	1.49314700
C	-0.08610600	2.80285900	3.73450200
H	-3.17074500	-1.30476100	4.38345400
H	-3.77759300	-0.54148600	2.89839800
C	-3.55993200	-2.64835500	1.14885700
C	-1.64856300	-3.91988900	1.89690500
C	-0.02346300	4.47301400	1.49384700
H	-1.42810200	3.08820500	0.61185900
C	0.71731000	3.95068200	3.73500300
H	-0.10427900	2.16633800	4.62204100
C	-4.01770800	-3.76099400	0.43477900
H	-4.14456600	-1.72587100	1.12716900
C	-2.10349900	-5.03334500	1.18137000
H	-0.72450700	-3.99140900	2.47755800
C	0.75414000	4.78925400	2.61589500
H	-0.00998700	5.12390500	0.61543000
H	1.31389700	4.19064100	4.61939500
C	-3.29109200	-4.95771400	0.44492000
H	-4.94963700	-3.69121700	-0.13279200
H	-1.53064300	-5.96442600	1.20570100
H	1.37895300	5.68628800	2.61904500
H	-3.65104700	-5.82624900	-0.11290700

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3737.409691 E_0
Sum of electronic and zero-point Energies= -3736.730089 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3736.687541 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3736.686597 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3736.810859 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.679602
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3739.499417 E_0

TS2b

Charge 0; multiplicity 1

Ni	-0.96978300	-0.60536800	-1.08233700
C	0.57014600	-0.53217500	1.77057300
C	1.48845200	0.29228400	0.86666800
O	-1.79991100	1.45766100	-2.57593600
O	-3.61679600	2.44974100	-1.74377600
C	-3.08765700	1.61118700	-2.49305400
C	-3.93463300	0.71624400	-3.37813000
H	-5.00349700	0.93656900	-3.25551800
H	-3.74300500	-0.33822100	-3.11934700
H	-3.64224500	0.85156900	-4.43175900
H	-2.37681700	-1.08439300	-0.98541600
H	-1.07183000	-0.74427900	-2.66953700
H	-1.37623300	0.15223000	-2.64737700
H	1.26564100	1.36716200	0.96889700
H	2.54662300	0.14353300	1.13047500
H	0.54561800	-0.13309400	2.79652000
H	0.91710600	-1.57753000	1.82559600
P	1.16211400	-0.09717200	-0.92779900
C	2.39762500	-1.43624500	-1.46906900
C	2.05288000	1.30476400	-1.80242300
H	1.84441900	-1.99869400	-2.23593000
C	3.57932100	-0.67707100	-2.14037500
C	2.73681900	-2.40385800	-0.35649700
C	3.52551600	0.82126000	-1.80593300
C	1.47083900	1.68444600	-3.14934600
H	1.95516300	2.18089800	-1.14438300
H	3.50489600	-0.81750200	-3.22900400
H	4.54415000	-1.10942300	-1.83460500
C	1.96376800	-3.56954200	-0.19301500
C	3.79331700	-2.17529000	0.54450000
H	3.94026400	0.99311900	-0.79891900
H	4.13059900	1.41409800	-2.51077100
C	1.24840800	0.75853100	-4.18681900
C	1.12410900	3.02885900	-3.37961800
C	2.23086600	-4.47403300	0.84013200
H	1.14743700	-3.77087400	-0.89294800
C	4.06175300	-3.07947000	1.57925000
H	4.42085600	-1.28664100	0.43799100
C	0.70500400	1.16677800	-5.41008700
H	1.48008000	-0.29938700	-4.04555500
C	0.57795600	3.43875800	-4.60017000
H	1.27774700	3.76285200	-2.58320000
C	3.28072800	-4.23051200	1.73426000
H	1.62018600	-5.37521400	0.94243200
H	4.88901300	-2.88229600	2.26643600
C	0.36682500	2.50785400	-5.62321500

H	0.53860900	0.42774000	-6.19852700
H	0.31349100	4.48910900	-4.74960300
H	3.49326700	-4.93653500	2.54124400
H	-0.06238300	2.82363700	-6.57773400
P	-1.13663400	-0.63506000	1.02958500
C	-2.19026900	0.79981100	1.68473500
C	-1.96477700	-1.96511100	2.07418700
H	-2.82001900	1.07248000	0.82580000
C	-3.07352900	0.17683500	2.80172300
C	-1.37132800	2.01725900	2.05643300
C	-2.47544200	-1.15466900	3.28370600
C	-2.97375500	-2.80823900	1.31786200
H	-1.14436200	-2.63155400	2.38401000
H	-4.07731000	0.00817200	2.38489300
H	-3.19141400	0.88032100	3.64000500
C	-1.16755900	3.03334400	1.10248000
C	-0.79246600	2.17192900	3.32999600
H	-1.61840100	-0.95337100	3.94666400
H	-3.20295900	-1.73672600	3.87209700
C	-4.36077700	-2.72213200	1.52157600
C	-2.49913500	-3.74434700	0.37717100
C	-0.40286300	4.16385400	1.40970400
H	-1.62426800	2.93936200	0.11295800
C	-0.02695000	3.30311200	3.63727700
H	-0.94391200	1.40673700	4.09583300
C	-5.24504500	-3.53810700	0.80201900
H	-4.77015100	-2.02015300	2.25048100
C	-3.37768900	-4.55973100	-0.33943600
H	-1.42174400	-3.83341900	0.20926100
C	0.17446400	4.30231800	2.67793400
H	-0.26381800	4.94306700	0.65523500
H	0.41152500	3.40374200	4.63387800
C	-4.75987500	-4.45765600	-0.13188300
H	-6.32049000	-3.45116200	0.97900700
H	-2.98258900	-5.27971500	-1.06125300
H	0.77029200	5.18639000	2.91981100
H	-5.45078800	-5.09322500	-0.69194000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3737.373072 E_0
Sum of electronic and zero-point Energies= -3736.692314 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3736.652094 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3736.651150 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3736.769735 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.680758
Number of imaginary vibrational frequencies = 1; 787*i*
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3739.463555 E_0

6b

Charge 0; multiplicity 1

Ni	-0.56903800	-0.35646700	-0.52870300
C	1.12807000	-0.53538000	2.26955100
C	1.97003200	0.37580800	1.37013500
O	-1.51161000	2.16558000	-2.29807500
O	-2.77656500	3.39460100	-3.62124300
C	-2.40366300	2.28149200	-3.28627400
C	-2.88549300	1.00699600	-3.92889900
H	-3.68245000	1.23667400	-4.64680900
H	-3.25095700	0.30673800	-3.16234200
H	-2.04774400	0.51737800	-4.45102800
H	-2.02211800	-0.72094300	-0.62268800
H	-0.66887700	-0.18141100	-2.02647300
H	-1.24517600	1.21090500	-2.10725800
H	1.73007500	1.43420900	1.56778600
H	3.04625300	0.23847700	1.55814800
H	1.13372400	-0.17686100	3.31138400
H	1.53227500	-1.56118500	2.26963500
P	1.53845500	0.12289600	-0.43153400
C	2.73900800	-1.17690800	-1.12338200
C	2.43018400	1.57593900	-1.22360500
H	2.16408700	-1.63988300	-1.93968000
C	3.93633500	-0.38470000	-1.72205800
C	3.04553000	-2.26566500	-0.11870000
C	3.89987100	1.08190600	-1.26565900
C	1.87167700	2.05447100	-2.54848300
H	2.34293500	2.40933700	-0.51040300
H	3.86678600	-0.43267500	-2.81912700
H	4.89435800	-0.85300300	-1.44961500
C	2.19654100	-3.38680200	-0.04104700
C	4.13267600	-2.19297800	0.77130200
H	4.31795400	1.16765200	-0.24925100
H	4.50998700	1.72419200	-1.92114400
C	1.60413600	1.19799800	-3.63380900
C	1.62015400	3.42928400	-2.71631100
C	2.42037000	-4.39899700	0.89769800
H	1.35179500	-3.46491600	-0.73206100
C	4.35801000	-3.20546200	1.71225100
H	4.81677000	-1.34150700	0.73183300
C	1.11151600	1.70306400	-4.84292400
H	1.76416900	0.12157600	-3.54337600
C	1.12369300	3.93611500	-3.92186100
H	1.81217400	4.11103600	-1.88261500
C	3.50274800	-4.31111400	1.78216800
H	1.75032100	-5.26237500	0.93380700
H	5.21028000	-3.12879600	2.39295300
C	0.86853300	3.07333400	-4.99344600

H	0.91087200	1.01713300	-5.67047200
H	0.93176800	5.00785700	-4.02127600
H	3.68202200	-5.10170700	2.51546900
H	0.47779300	3.46398800	-5.93662400
P	-0.60975600	-0.67004200	1.59764700
C	-1.65331500	0.50207900	2.61807300
C	-1.31109000	-2.15135800	2.51564800
H	-2.65602300	0.34365400	2.18373600
C	-1.62240200	-0.08697800	4.03817500
C	-1.28772300	1.95520300	2.40969200
C	-1.49322400	-1.63772100	3.97135900
C	-2.55298200	-2.68834900	1.83129600
H	-0.53670500	-2.93231600	2.47667900
H	-2.52713000	0.21687200	4.58856400
H	-0.76428800	0.32116700	4.59217800
C	-1.51468300	2.52084700	1.13801500
C	-0.71186100	2.76292300	3.40388200
H	-0.61859500	-1.95331500	4.55854900
H	-2.36565700	-2.12865600	4.42820600
C	-3.85194100	-2.27797400	2.18049900
C	-2.41212900	-3.62658300	0.78995300
C	-1.16713400	3.84497700	0.86317300
H	-1.96631100	1.90096000	0.35699900
C	-0.36689700	4.09499000	3.13092500
H	-0.53307900	2.36287500	4.40432200
C	-4.97172400	-2.78645400	1.50923400
H	-4.00239300	-1.55714000	2.98782900
C	-3.52762600	-4.13814300	0.12187200
H	-1.41065900	-3.96207900	0.50506300
C	-0.58845700	4.64029600	1.86260700
H	-1.34710900	4.25243200	-0.13522200
H	0.07696100	4.70771500	3.92045000
C	-4.81579300	-3.71785800	0.47806500
H	-5.97135200	-2.45195100	1.79976000
H	-3.39130300	-4.87037000	-0.67862700
H	-0.31696200	5.67839200	1.65332600
H	-5.69031800	-4.11693800	-0.04242600

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3737.388529 E_0
Sum of electronic and zero-point Energies= -3736.704129 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3736.663399 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3736.662455 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3736.783511 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.684400
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3739.480970 E_0

7b

Charge 0; multiplicity 1

Ni	0.14668800	-2.20887500	0.28280000
C	0.42763300	0.86389500	-0.76624800
C	-0.49220400	0.97995300	0.45221300
H	1.04388900	-3.35163700	-0.10586800
H	-0.58750900	-3.29730100	1.02008800
H	1.10350900	1.73016900	-0.83996200
H	-0.16773700	0.82629400	-1.69372600
H	-1.25864500	1.75582100	0.30033400
H	0.08942100	1.25722200	1.34719500
P	1.36236600	-0.75527200	-0.72591600
C	3.05373400	-0.40249700	0.06867600
C	2.03894000	-0.82189200	-2.47893000
H	3.31947200	-1.36744100	0.52579700
C	4.03000200	-0.10089300	-1.10327200
C	2.95771200	0.61285100	1.18572800
C	3.25456500	0.13948100	-2.40805300
C	2.33450100	-2.20362900	-3.02591000
H	1.26017700	-0.37856400	-3.11730500
H	4.70012100	-0.96517200	-1.22468600
H	4.67342900	0.76115900	-0.87014600
C	2.64763900	0.17582100	2.48858700
C	3.13287600	1.99271200	0.97331300
H	2.87147600	1.17300700	-2.42824600
H	3.90278800	0.01865700	-3.29116400
C	3.13152300	-3.15278100	-2.35623800
C	1.81046100	-2.55532400	-4.28454500
C	2.51225000	1.08499200	3.54261200
H	2.51497300	-0.89402300	2.67571000
C	2.99753000	2.90452300	2.02758800
H	3.38306300	2.36546500	-0.02327000
C	3.40241100	-4.39913800	-2.93266300
H	3.54094900	-2.93416600	-1.36786900
C	2.07659400	-3.80211100	-4.86122900
H	1.18338600	-1.83614600	-4.82009100
C	2.68424200	2.45640500	3.31587400
H	2.27660000	0.71965100	4.54599600
H	3.14052800	3.97202600	1.83869700
C	2.87838200	-4.73002200	-4.18755200
H	4.02300800	-5.11840500	-2.39138800
H	1.65516400	-4.04738000	-5.83995700
H	2.58152800	3.16931500	4.13819500
H	3.08935300	-5.70535900	-4.63395800
P	-1.24954200	-0.68178200	0.85714000
C	-2.95411700	-0.72648800	0.01562100
C	-1.94910100	-0.35176200	2.57044400
H	-3.12073000	-1.80144700	-0.15134400

C	-3.97235100	-0.20438700	1.06890400
C	-2.93670300	-0.05992200	-1.34214400
C	-3.24317300	0.44351300	2.25696100
C	-2.13894300	-1.56873500	3.45281300
H	-1.22524500	0.30821000	3.07200600
H	-4.57045400	-1.05760600	1.42263800
H	-4.68177400	0.50502500	0.61636400
C	-2.56083800	-0.81187900	-2.47262000
C	-3.24930800	1.29974900	-1.52427200
H	-2.95472100	1.47608400	2.00007400
H	-3.89296200	0.50209300	3.14522900
C	-2.83133400	-2.72464100	3.04204300
C	-1.62523500	-1.54043200	4.76332500
C	-2.49505600	-0.22618500	-3.74081300
H	-2.32086300	-1.87263700	-2.35299800
C	-3.18401700	1.88791000	-2.79356300
H	-3.55306200	1.91103100	-0.67062700
C	-3.01269400	-3.80312300	3.91540600
H	-3.22698100	-2.80070700	2.02723400
C	-1.80198300	-2.61872000	5.63742500
H	-1.07815100	-0.65539600	5.10178800
C	-2.80460200	1.12972400	-3.90698400
H	-2.20593500	-0.83316700	-4.60323200
H	-3.43389100	2.94597100	-2.91078400
C	-2.50089400	-3.75569800	5.21720800
H	-3.55285500	-4.68919300	3.57110100
H	-1.39141100	-2.56845100	6.64962500
H	-2.75679700	1.58972500	-4.89748000
H	-2.64136500	-4.60056800	5.89654500

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3508.447681 E_0
Sum of electronic and zero-point Energies= -3507.825620 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3507.791032 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3507.790088 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3507.895911 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.622061
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3510.280929 E_0

4b*AcOH

Charge 0; multiplicity 1

Ni	-1.19995700	0.12115700	-0.35653800
C	0.65613500	0.36000800	2.23352600
C	1.56953900	1.00432200	1.18787500
O	-1.43101500	-0.72942500	-2.05710400
O	-3.32024100	0.26641000	-2.76119900
C	-2.43739800	-0.62659900	-2.83866500
C	-2.52435800	-1.64404500	-3.95488600
H	-3.57105200	-1.79529300	-4.25309800
H	-2.06697100	-2.59741300	-3.65626400
H	-1.97293600	-1.25684100	-4.82845800
H	-2.60931600	-0.15131800	0.05304000
H	1.55101500	2.10132100	1.28963700
H	2.61244500	0.67528500	1.31354200
H	0.80619300	0.79335700	3.23532800
H	0.85144500	-0.72359400	2.30514800
P	0.94291900	0.64796500	-0.53611400
C	2.08200700	-0.64005800	-1.35051600
C	1.62717200	2.10948800	-1.50344400
H	1.38384900	-1.25266100	-1.94075800
C	3.00546800	0.16686900	-2.30402400
C	2.74937400	-1.55413000	-0.34648900
C	3.05762600	1.63790900	-1.87226500
C	0.77533500	2.57352800	-2.66852500
H	1.68772900	2.94442400	-0.79006500
H	2.59613100	0.09777200	-3.32327400
H	4.01445900	-0.27234900	-2.33967000
C	2.07326100	-2.71019300	0.08945400
C	4.02461500	-1.28968500	0.18707400
H	3.69264200	1.74198600	-0.97634100
H	3.49260400	2.27777000	-2.65725700
C	0.21242500	1.69403900	-3.61192100
C	0.55027800	3.95325200	-2.83432300
C	2.65178600	-3.57522500	1.02407200
H	1.08222000	-2.93440900	-0.31627100
C	4.60544400	-2.15585300	1.12158600
H	4.57786900	-0.40292400	-0.13257900
C	-0.54153000	2.17981300	-4.68638400
H	0.34216600	0.61532200	-3.50473300
C	-0.20200100	4.44193400	-3.90772900
H	0.97044700	4.65370100	-2.10676000
C	3.92242200	-3.30149100	1.54517000
H	2.10948900	-4.47032900	1.34084700
H	5.59945700	-1.93243000	1.51857700
C	-0.74976700	3.55532400	-4.84169800
H	-0.97115100	1.47694800	-5.40519500
H	-0.36574100	5.51807600	-4.00914900
H	4.37833500	-3.97837300	2.27243300
H	-1.34062700	3.93222900	-5.68062400
P	-1.12189400	0.48113600	1.70304700

C	-1.89880500	2.07700000	2.36738400
C	-2.04501600	-0.63385400	2.91175300
H	-2.63717200	2.31323600	1.58555600
C	-2.65878200	1.63874100	3.63707000
C	-0.95239200	3.24873700	2.49220500
C	-3.22349500	0.24021000	3.37696300
C	-2.35100100	-2.01816700	2.39152700
H	-1.34079700	-0.73227400	3.75515200
H	-3.45152400	2.36684900	3.87232600
H	-1.97675600	1.60032800	4.50167000
C	-0.87187400	4.19388800	1.45090000
C	-0.12711600	3.43070200	3.61862500
H	-3.69152200	-0.19061200	4.27673100
H	-3.99682400	0.29472600	2.59309800
C	-3.53887400	-2.31798500	1.69872700
C	-1.41905200	-3.05493000	2.58911000
C	0.00875500	5.27821500	1.52872400
H	-1.51156000	4.08487500	0.57104000
C	0.75386900	4.51571700	3.69679000
H	-0.17105100	2.72460300	4.45121200
C	-3.78136800	-3.60914300	1.21572500
H	-4.28900900	-1.54119300	1.53628300
C	-1.65769400	-4.34478200	2.10302600
H	-0.49610000	-2.84789200	3.13859300
C	0.82913600	5.44307400	2.65117400
H	0.04771500	6.00035400	0.70851800
H	1.38281800	4.63652300	4.58304700
C	-2.84140300	-4.62744800	1.41115400
H	-4.71333400	-3.81888800	0.68372200
H	-0.91878200	-5.13288900	2.27212400
H	1.51603500	6.29120500	2.71405600
H	-3.03279800	-5.63523500	1.03327500
H	-3.03446800	1.53826100	-1.97633400
C	-3.29911100	3.50506700	-2.08476700
O	-2.78186700	2.42658100	-1.51327300
O	-3.00179000	4.61947800	-1.66854600
C	-4.27087000	3.28444000	-3.21809400
H	-4.52126100	4.24514100	-3.68461400
H	-3.85201500	2.59236500	-3.96281200
H	-5.18757600	2.82015100	-2.81856000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3965.179936 E_0
Sum of electronic and zero-point Energies= -3964.450715 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3964.405274 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3964.404330 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3964.535372 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.729222
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3967.525179 E_0

8b*OAc$^-$

Charge 0; multiplicity 1

Ni	-0.83723500	0.22148300	-0.78321000
C	0.48218300	-0.44859800	2.04823000
C	1.60570600	0.35438100	1.38824400
O	-1.30191600	0.57091500	-4.92436800
O	-0.84688600	0.12751300	-2.78825100
C	-1.71466800	0.51729600	-3.78944300
C	-3.08825300	0.82914400	-3.30873900
H	-3.04548700	1.64433800	-2.56844700
H	-3.51475600	-0.05348700	-2.80816700
H	-3.70639800	1.11667900	-4.16720900
H	-2.30453000	0.04807300	-0.62510500
H	0.02183500	-0.04292700	-3.20892300
P	-1.14885200	-0.02377200	1.26113600
C	-2.35950300	-1.31758000	1.89248800
C	-1.96540900	1.40824500	2.18341200
H	-1.85963800	-1.72119300	2.78924700
C	-3.56441100	-0.47555700	2.35085800
C	-2.61124000	-2.45803900	0.93489400
C	-3.00084900	0.73062900	3.10632600
C	-1.02045400	2.40681700	2.80809600
H	-2.51706300	1.91551600	1.37798200
H	-4.24010200	-1.08008500	2.97698900
H	-4.13973600	-0.11739100	1.48164200
C	-1.78726800	-3.59884600	0.98144900
C	-3.63971900	-2.42011600	-0.02504100
H	-3.79033200	1.45417000	3.36487200
H	-2.52915800	0.39598200	4.04455900
C	-0.40678300	2.18887700	4.05617300
C	-0.73424700	3.60507200	2.12526600
C	-1.97252300	-4.66090100	0.08976300
H	-0.99400800	-3.65679200	1.73237900
C	-3.82919900	-3.48432400	-0.91465800
H	-4.30615100	-1.55672700	-0.07847100
C	0.47490400	3.13268500	4.59592200
H	-0.62157400	1.27814500	4.62072200
C	0.14792100	4.54809200	2.66324700
H	-1.22654600	3.79944700	1.16842600
C	-2.99446900	-4.60662600	-0.86564600
H	-1.32049400	-5.53683200	0.14738300
H	-4.63794400	-3.43471600	-1.64887300
C	0.76015800	4.31364500	3.90051600
H	0.93898500	2.94386900	5.56783700
H	0.35121900	5.47292300	2.11646700
H	-3.14442000	-5.43653700	-1.56119200
H	1.44807600	5.05011200	4.32417800
P	1.35211100	0.39032700	-0.45415200
C	2.34539200	1.87238200	-1.05135800
C	2.48678600	-0.90881300	-1.26140800
H	2.35178000	2.59095400	-0.21595300

C	3.75082000	1.29138500	-1.28209900
C	1.65156900	2.53603200	-2.23236700
C	3.61979700	-0.09045400	-1.94037800
C	2.91445300	-2.00828200	-0.31294900
H	1.85517700	-1.37190200	-2.03401500
H	4.24384000	1.19025400	-0.30169300
H	4.37632200	1.97011600	-1.88453000
C	0.39377700	3.13535900	-2.01875200
C	2.19650900	2.58724300	-3.52591700
H	3.36365800	0.02869600	-3.00397200
H	4.57192800	-0.64192800	-1.90348000
C	4.07548600	-1.91253200	0.47747000
C	2.13445900	-3.17595400	-0.20892100
C	-0.29834600	3.76091700	-3.05806400
H	-0.04785600	3.11066000	-1.01839900
C	1.50199200	3.21148600	-4.57264500
H	3.17424300	2.14697600	-3.73255300
C	4.44376200	-2.95174000	1.34025200
H	4.70704000	-1.02259400	0.41694600
C	2.50058900	-4.21440400	0.65400100
H	1.23313400	-3.27341300	-0.82119100
C	0.25387900	3.79832200	-4.34571400
H	-1.27484800	4.20826200	-2.85637300
H	1.94624700	3.23672800	-5.57141800
C	3.65833900	-4.10631000	1.43386000
H	5.35244100	-2.85713700	1.94088000
H	1.88232300	-5.11450600	0.71043700
H	-0.28628500	4.28100200	-5.16428200
H	3.94905900	-4.91821400	2.10552200
H	0.61813000	-1.52866000	1.86939700
H	0.44574300	-0.29052500	3.13771000
H	1.56722900	1.40802700	1.70991600
H	2.59607400	-0.04412800	1.65593900
C	-4.34954400	3.15180600	-0.62050300
O	-3.10706900	3.25208200	-0.86915200
O	-4.84999800	2.53207300	0.35695500
C	-5.31276200	3.80479500	-1.61618600
H	-5.49819700	3.09823300	-2.44420900
H	-6.28009900	4.03301400	-1.14434000
H	-4.87914100	4.71889600	-2.04943800

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3965.141069 E_0
Sum of electronic and zero-point Energies= -3964.411673 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3964.365730 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3964.364786 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3964.497850 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.729397
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3967.490865E_0

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Charge 1; multiplicity 1

Ni	-0.83247400	0.23935900	-0.67290100
C	0.77983000	-0.41118900	2.04954900
C	1.78930900	0.43234000	1.27192600
O	-1.88742400	1.08420500	-4.62662000
O	-1.04274200	0.59308900	-2.62230600
C	-2.06728700	0.56855200	-3.54954700
C	-3.29850000	-0.13027800	-3.08385400
H	-3.71791800	0.39414400	-2.21231000
H	-3.05550400	-1.15669500	-2.77202300
H	-4.02565300	-0.14387800	-3.90392800
H	-2.28855400	0.14000900	-0.38936100
H	-0.28195400	1.06241600	-3.03407700
P	-0.93558600	-0.15790200	1.37981700
C	-1.91538700	-1.59176700	2.06973500
C	-1.88583300	1.15118000	2.37383100
H	-1.38135500	-1.82475400	3.00719100
C	-3.25474200	-0.93599900	2.46640200
C	-1.98828400	-2.86098600	1.25091600
C	-2.89120400	0.34239800	3.22811600
C	-1.02758400	2.16780400	3.09111400
H	-2.44705800	1.67845500	1.58948600
H	-3.84985200	-1.62586600	3.08529200
H	-3.84531300	-0.70235400	1.56369700
C	-1.70005800	-4.09399800	1.86381100
C	-2.37549500	-2.86148400	-0.10137500
H	-3.77582000	0.96153100	3.44506700
H	-2.43679500	0.06608400	4.19265600
C	-0.42322500	1.90552300	4.33525200
C	-0.81033100	3.42730500	2.49994300
C	-1.80028500	-5.29370300	1.14955300
H	-1.39514300	-4.11261400	2.91417700
C	-2.47626400	-4.05945800	-0.81684400
H	-2.56954500	-1.90774200	-0.59814700
C	0.37479900	2.86944600	4.96235500
H	-0.57724700	0.94218500	4.82771800
C	-0.01188700	4.39121400	3.12453200
H	-1.28443500	3.65471400	1.54068800
C	-2.19116300	-5.28108500	-0.19419600
H	-1.57213700	-6.24049600	1.64647400
H	-2.77681200	-4.03843400	-1.86799100
C	0.58620800	4.11486200	4.35975800
H	0.83222100	2.64434200	5.92952500
H	0.13732700	5.36345000	2.64718400
H	-2.27032400	-6.21666100	-0.75401400
H	1.20816100	4.86695300	4.85207200
P	1.38643000	0.39598600	-0.54140100

C	2.36460400	1.83829000	-1.25807300
C	2.40272500	-0.96444200	-1.39779500
H	2.52483100	2.53161800	-0.41778400
C	3.69940100	1.20103000	-1.68931600
C	1.55958800	2.58164700	-2.31090200
C	3.44558400	-0.20237200	-2.26091100
C	2.93664800	-2.01639300	-0.44878200
H	1.67451700	-1.45688600	-2.05833000
H	4.34148900	1.12629200	-0.79730500
H	4.23018500	1.84127100	-2.41253800
C	0.51575000	3.42930700	-1.88369600
C	1.79884800	2.47176500	-3.69289200
H	3.04707100	-0.12310200	-3.28350500
H	4.38190700	-0.77737200	-2.33017100
C	4.17105400	-1.88130000	0.21428800
C	2.18187400	-3.18221000	-0.21581000
C	-0.26084400	4.13916100	-2.80260600
H	0.31818900	3.53511800	-0.81286100
C	1.01880100	3.18447600	-4.61572500
H	2.60486500	1.83625600	-4.06432500
C	4.63293800	-2.87984200	1.08004300
H	4.78797300	-0.99437700	0.05081300
C	2.64109600	-4.17953700	0.65090100
H	1.22514000	-3.31165000	-0.73009300
C	-0.01300000	4.01837300	-4.17645600
H	-1.06077600	4.79286000	-2.44488700
H	1.22471700	3.08216400	-5.68434200
C	3.87028600	-4.03174500	1.30436500
H	5.59710100	-2.75510800	1.58025100
H	2.03825600	-5.07763600	0.80997700
H	-0.62067000	4.57092600	-4.89735700
H	4.23406100	-4.81102800	1.97907000
H	0.98132300	-1.48699200	1.91251000
H	0.81138800	-0.19910400	3.12978300
H	1.71058900	1.49329200	1.56083700
H	2.82323300	0.10628700	1.46275000

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3736.675284 E_0
Sum of electronic and zero-point Energies= -3735.995212 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3735.955525 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3735.954581 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3736.072484 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.680072
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3738.759351 E_0

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Charge 1; multiplicity 1

Ni	-0.61347400	0.68660600	-0.60228900
C	0.50877700	-0.56783000	2.15513000
C	1.75321500	0.08914000	1.54393100
O	-2.82121000	-1.97295800	-4.31287800
O	-1.38331500	-1.19558100	-2.77569500
C	-1.74176000	-2.04857300	-3.75673400
C	-0.67376900	-3.05865600	-4.05322800
H	-0.99659300	-3.70812300	-4.87523900
H	-0.47854500	-3.66141000	-3.15241300
H	0.26279100	-2.54573200	-4.32091300
H	-2.05055400	1.11113900	-0.55637300
H	-2.12172200	-0.57264100	-2.61115700
P	-1.04650900	0.11044500	1.37252200
C	-2.38621600	-1.14370900	1.82401800
C	-1.70925800	1.44912200	2.52152600
H	-1.85024700	-1.85236200	2.47551800
C	-3.38217900	-0.34673200	2.69464500
C	-2.95815000	-1.91992200	0.65988100
C	-2.57708000	0.66047500	3.51852800
C	-0.65663900	2.38525400	3.06612100
H	-2.37944200	2.02515100	1.86390800
H	-3.95836000	-1.03664100	3.33106900
H	-4.09963300	0.19371000	2.05696200
C	-2.48845300	-3.21869800	0.39271900
C	-3.95960600	-1.38906500	-0.17519000
H	-3.22884500	1.34588200	4.08389600
H	-1.94538500	0.12508600	4.24650400
C	-0.01948400	2.16979700	4.30157200
C	-0.28188400	3.51289300	2.30966500
C	-3.00711700	-3.97008300	-0.66810800
H	-1.71475700	-3.65060900	1.03433400
C	-4.48247700	-2.14072400	-1.23293000
H	-4.34293700	-0.38148100	0.00247100
C	0.96800200	3.05045700	4.76069700
H	-0.29774700	1.31418900	4.92098300
C	0.70518200	4.39123000	2.76640400
H	-0.77969900	3.70522200	1.35504900
C	-4.01125800	-3.43541900	-1.48276500
H	-2.63133100	-4.98048600	-0.85077000
H	-5.26089700	-1.71044500	-1.86846400
C	1.33738200	4.16162700	3.99510600
H	1.44725900	2.86658500	5.72604400
H	0.97642500	5.26232500	2.16384200
H	-4.41998900	-4.01952600	-2.31099000
H	2.10642200	4.84915200	4.35670400
P	1.49524500	0.14273200	-0.28390600

C	2.38621400	1.53243800	-1.15811800
C	2.34119500	-1.28228400	-1.17679800
H	2.99920300	2.12009900	-0.46123700
C	3.27696600	0.85429500	-2.23465100
C	1.23014500	2.39052400	-1.64741700
C	2.82169700	-0.59822900	-2.48528000
C	3.37558300	-2.00721600	-0.34294100
H	1.54205700	-1.99787400	-1.41912700
H	4.31478900	0.86996500	-1.87147600
H	3.25846100	1.43097600	-3.17244300
C	1.15570600	3.75313100	-1.34062300
C	0.13869900	1.79372800	-2.34680300
H	1.97698400	-0.60101400	-3.19282500
H	3.62603300	-1.19030600	-2.94953100
C	4.66080700	-1.49022700	-0.08976600
C	3.03940200	-3.25333600	0.22018900
C	0.02867300	4.50995600	-1.70176300
H	1.97926200	4.22844400	-0.80187400
C	-1.00201900	2.55355600	-2.67064000
H	0.22226800	0.77629400	-2.75278700
C	5.57821500	-2.20205000	0.69120500
H	4.95737900	-0.52394000	-0.50211800
C	3.95422200	-3.96365200	1.00476100
H	2.04755500	-3.67427400	0.03048800
C	-1.05804800	3.91611600	-2.34696100
H	-0.00061800	5.57488400	-1.45637400
H	-1.82124800	2.08089600	-3.21670300
C	5.23002500	-3.44035700	1.24321000
H	6.57216400	-1.78303200	0.86938600
H	3.66975700	-4.93180200	1.42557400
H	-1.94101700	4.50630200	-2.60166300
H	5.94863000	-3.99364700	1.85332500
H	0.50262100	-1.65073400	1.94441300
H	0.47394900	-0.44026300	3.24898200
H	1.85380000	1.13524200	1.87587200
H	2.67613900	-0.44802200	1.81181800

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3736.665154 E_0
Sum of electronic and zero-point Energies= -3735.986880 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3735.946509 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3735.945565 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3736.064899 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.678274
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3738.749224 E_0

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Charge 1; multiplicity 1

Ni	-0.68233900	-0.23881700	-1.02726200
C	0.55033700	-0.33153600	1.96848500
C	1.69527000	0.22040600	1.10671100
H	-2.11881600	0.14753300	-1.06366000
H	0.48765000	0.19282300	2.93460600
H	0.70743900	-1.40342900	2.17710300
H	2.68211000	-0.03066400	1.52514300
H	1.62823100	1.31678300	1.01746800
P	1.47801700	-0.45439000	-0.60037500
C	2.62133500	-1.91003600	-0.94477400
C	2.11157100	0.66347500	-1.95848700
H	2.00164400	-2.81387000	-0.85688200
C	2.98337800	-1.68608700	-2.43783900
C	3.76260100	-2.03763300	0.04139500
C	3.12325700	-0.18621400	-2.77474100
C	0.81248300	1.05685700	-2.64530300
H	2.59288600	1.56377800	-1.55331100
H	2.17664200	-2.12522600	-3.04621400
H	3.90418300	-2.23514900	-2.69019400
C	3.68217100	-3.02219200	1.04492600
C	4.90113200	-1.20900500	0.01507200
H	4.13528300	0.16626700	-2.52858600
H	2.98324000	-0.02138500	-3.85444400
C	-0.09510600	0.04708000	-3.09313300
C	0.43836600	2.39968300	-2.78244100
C	4.70364000	-3.18054200	1.98742200
H	2.80753500	-3.67854800	1.07888000
C	5.92540200	-1.36932300	0.95493900
H	4.99783100	-0.42778500	-0.74131100
C	-1.36258000	0.41211300	-3.59375600
H	0.22356300	-0.99817800	-3.17835100
C	-0.79998100	2.74760200	-3.34607500
H	1.12068900	3.18258400	-2.44201600
C	5.83181000	-2.35360200	1.94586000
H	4.61880500	-3.95670200	2.75275000
H	6.80200700	-0.71742300	0.91186700
C	-1.70994000	1.76366000	-3.73454500
H	-2.04711200	-0.37061300	-3.92831800
H	-1.05859000	3.80385900	-3.45756400
H	6.63334700	-2.47584700	2.67890300
H	-2.68601300	2.03920500	-4.13956000
P	-1.07022200	-0.21690400	1.04132900
C	-2.03415100	1.20530700	1.77843700
C	-2.17526500	-1.48341800	1.86071500
H	-2.92313500	1.22172400	1.12755400
C	-2.45803000	0.70619900	3.18203100

C	-1.36051300	2.55549500	1.67157700
C	-2.43935900	-0.84916100	3.24744700
C	-3.38112200	-1.78883700	0.99365300
H	-1.57869000	-2.40295000	1.96158200
H	-3.46179100	1.10226200	3.40068800
H	-1.78678400	1.10970000	3.95275100
C	-1.63543100	3.37189600	0.55728800
C	-0.43974400	3.02462600	2.62717700
H	-1.63221700	-1.17309000	3.92074700
H	-3.37590600	-1.24464200	3.66922300
C	-4.64147700	-1.20646100	1.20838000
C	-3.23265900	-2.68162900	-0.08623900
C	-1.01016500	4.61296600	0.39922500
H	-2.35429000	3.02791100	-0.19167400
C	0.18566100	4.26727900	2.47056100
H	-0.20566400	2.42227600	3.50803300
C	-5.72199300	-1.50764500	0.36791800
H	-4.79406000	-0.51285000	2.03862800
C	-4.30944700	-2.98462200	-0.92278800
H	-2.25956900	-3.14942800	-0.26437600
C	-0.09487600	5.06660400	1.35647500
H	-1.24485500	5.22998200	-0.47233300
H	0.89439900	4.61277400	3.22799200
C	-5.56148600	-2.39570300	-0.69962300
H	-6.69434900	-1.04393400	0.55439800
H	-4.17320700	-3.68650400	-1.74996100
H	0.39161400	6.03832800	1.23827100
H	-6.40592900	-2.63211000	-1.35217900

DFT TPSSh; Def2-SVP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3507.726226 E_0
Sum of electronic and zero-point Energies= -3507.110288 $E_0 + E_{ZPE}$
Sum of electronic and thermal Energies= -3507.076239 $E_0 + E_{tot}$
Sum of electronic and thermal Enthalpies= -3507.075294 $E_0 + H_{corr}$
Sum of electronic and thermal Free Energies= -3507.179503 $E_0 + G_{corr}$
Zero-point correction (*unscaled*) = 0.615938
Number of imaginary vibrational frequencies = 0
DFT TPSSh; Def2-TZVPP, 2,2,2-trifluoroethanol, SMD model
Total electronic energy= -3509.548683 E_0