

Supporting Information

Theoretical Studies on Coupling Reactions of Carbon Dioxide with Alkynes Mediated by Nickel(0) Complexes

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Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T., Jr.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, revision B05; Gaussian, Inc.: Pittsburgh, PA, 2003.

Cartesian coordinates for all the species calculated in this study:

1A

E = -1209.9783588 a.u.

Ni	0.04751200	1.79240800	-0.29303400
C	0.34444100	3.37197700	-1.24560100
C	-0.92436400	3.22391900	-1.03147100
H	1.05678200	4.05161400	-1.70573700
C	-2.27132900	3.83581700	-1.22233600
H	-2.91802400	3.19918100	-1.84370500
H	-2.79208500	3.96034300	-0.26267600
H	-2.22403700	4.82371800	-1.70500700
N	1.87167300	0.97495600	0.15766900
N	-1.13749500	0.48880900	0.73100400
N	-3.15574000	-0.70673300	1.17805200
C	-0.76833100	0.34889200	2.15266500
C	-1.28674200	-0.95889000	2.76242700
C	-2.80062200	-1.03640300	2.57101900
C	-4.51077900	-1.09257200	0.74528400
C	-4.55511500	-2.29703200	-0.21559700
C	-4.19156300	-1.93826500	-1.66755500
C	-2.81591900	-1.26767400	-1.84470500
C	-2.65343900	0.08985400	-1.11454800
C	-2.27480200	-0.02510500	0.34770800
H	-1.16077300	1.21185800	2.71098600
H	0.32191700	0.39671900	2.20824500
H	-0.80526900	-1.80842500	2.26094900
H	-1.03972500	-1.02143400	3.82847200
H	-3.30819300	-0.34635400	3.26324400
H	-3.16644600	-2.04749000	2.79265200
H	-5.01980800	-0.23319000	0.28969300
H	-5.06802800	-1.33124300	1.65743600
H	-3.87854700	-3.07405400	0.16726500
H	-5.56907800	-2.72160900	-0.19786000
H	-4.96307000	-1.26015800	-2.06484300
H	-4.23409200	-2.84682800	-2.28391800
H	-2.65387800	-1.09496100	-2.91694600
H	-2.01953000	-1.95211100	-1.51796000
H	-1.85396000	0.67818100	-1.57369900
H	-3.57541300	0.67887000	-1.22627100
N	3.76148000	-0.44795200	-0.16394400
C	2.72055700	1.88199400	0.95577500
C	3.79068700	1.11798200	1.74396100
C	4.63189600	0.28679400	0.77507200
C	4.39310800	-1.54944100	-0.91106600
C	3.95955600	-2.95920700	-0.46069400
C	2.58710800	-3.38795900	-1.01100000
C	1.42493900	-2.43783800	-0.66456500
C	1.57953800	-0.99613900	-1.20882900
C	2.43447000	-0.08323600	-0.35422900
H	2.06367900	2.44566000	1.62265600
H	3.18498000	2.61409900	0.28029400
H	3.30427900	0.45788600	2.47405600
H	4.43547300	1.80630200	2.30204400
H	5.32089500	0.93834100	0.21546100
H	5.24448100	-0.44113300	1.32316500
H	4.21066000	-1.43035400	-1.98743300
H	5.47303500	-1.43745600	-0.76872200
H	4.71701900	-3.68146100	-0.79718300
H	3.95706900	-2.98954800	0.63794500
H	2.65865100	-3.46641700	-2.10727100
H	2.35257500	-4.39693200	-0.64484300
H	1.28302100	-2.39779900	0.42479800
H	0.50037700	-2.86019000	-1.08131900
H	0.60277300	-0.50894600	-1.26298000
H	1.97277600	-1.03046600	-2.23577700

2A

E = -1398.5542654 a.u.

Ni	0.06729600	1.12227000	-0.32500100
C	-0.57440300	2.81260100	-0.84789200
C	0.69937400	2.88403000	-0.81865000
H	-1.51646400	3.30457700	-1.04431800
C	1.94522800	3.68373500	-0.91146400

H	2.53347200	3.55911900	0.00368000
H	2.57114500	3.35768800	-1.75284600
H	1.73178200	4.75237100	-1.04889300
N	-1.66028900	-0.07826900	-0.81763000
O	1.87818700	1.92483700	1.81439600
O	-0.28041200	1.24821600	2.29265600
C	0.73436100	1.56282700	1.70778100
N	1.18549300	-0.56998300	0.04467200
N	3.15315900	-1.89889800	0.15390200
C	0.52162000	-1.58531100	0.89305500
C	1.48093300	-2.12420400	1.95902200
C	2.68506600	-2.75592800	1.26498200
C	4.49520100	-2.21887200	-0.36772200
C	5.61764300	-1.31243100	0.17400700
C	5.68284300	0.05636400	-0.52616900
C	4.37932300	0.87579800	-0.47457000
C	3.15575400	0.20370700	-1.15000000
C	2.43443200	-0.79857400	-0.27414200
H	0.16244900	-2.41130700	0.25907500
H	-0.34846600	-1.11580700	1.34972400
H	1.79970500	-1.29455400	2.60063800
H	0.98591600	-2.86462900	2.59729100
H	2.42748300	-3.75110100	0.87252600
H	3.51418500	-2.88843800	1.97284100
H	4.48413300	-2.18629800	-1.46418200
H	4.69008400	-3.26075500	-0.09141300
H	5.47315700	-1.18076300	1.25538700
H	6.57932200	-1.82854700	0.04274000
H	5.95860100	-0.10385800	-1.58089800
H	6.49540000	0.64738000	-0.08252500
H	4.55769800	1.83136400	-0.98377100
H	4.11453900	1.12542300	0.55993700
H	2.41127800	0.96159700	-1.40016900
H	3.46587000	-0.27168700	-2.09297600
N	-3.98496500	-0.55273200	-1.04403000
C	-1.41677400	-0.84761300	-2.05240100
C	-2.37364500	-2.03853400	-2.18122500
C	-3.81368300	-1.52819500	-2.13906800
C	-5.37745900	-0.25863000	-0.65625900
C	-5.82346100	-0.90868900	0.66871000
C	-5.32404000	-0.16013300	1.91789400
C	-3.79672500	0.02176300	1.99618100
C	-3.17229100	0.83934800	0.83683100
C	-2.89680400	0.03641700	-0.41705500
H	-0.37492600	-1.17949200	-2.03441000
H	-1.52552200	-0.17897700	-2.92037400
H	-2.19957200	-2.73288500	-1.34913100
H	-2.19901900	-2.58917600	-3.11259900
H	-4.08203600	-1.06177600	-3.09944400
H	-4.51143300	-2.36001300	-1.97535600
H	-5.53079300	0.82701600	-0.60860100
H	-6.00630100	-0.62277300	-1.47566300
H	-6.92211700	-0.94178500	0.68865600
H	-5.47476300	-1.95118800	0.68273600
H	-5.79715700	0.83420200	1.94213700
H	-5.67266900	-0.68791200	2.81611300
H	-3.30321500	-0.95913700	2.05041400
H	-3.55394500	0.53745500	2.93364500
H	-2.21310700	1.24188500	1.16231600
H	-3.81996600	1.69710400	0.60186000

3A

E = -936.5668394 a.u.

Ni	1.70537700	-0.07672800	-0.33619900
C	3.49458500	-0.43800600	-0.78258400
C	3.08513500	0.53732600	-1.49399800
O	1.99466400	1.08729400	2.23226900
O	1.25552700	-1.03712200	1.59346300
C	1.69349100	0.10669900	1.61320000
N	-0.10152100	0.78808100	-0.46985200
C	3.24690500	1.59537100	-2.51960700
H	4.23034300	1.53479700	-3.00371200
H	2.47847400	1.51684200	-3.29735600

H	3.15362500	2.59127100	-2.06949100
H	4.29568000	-1.10648400	-0.50467500
N	-2.47647600	0.73331500	-0.50353100
C	-0.15266800	2.25363600	-0.28442900
C	-1.35753100	2.66446100	0.56792300
C	-2.63760000	2.14402600	-0.08474800
C	-3.72700500	-0.01342500	-0.75063900
C	-4.10621100	-1.00242000	0.36988900
C	-3.32658500	-2.32923200	0.31196900
C	-1.79434100	-2.18798900	0.36372400
C	-1.18550100	-1.35791400	-0.79473900
C	-1.23496100	0.14247400	-0.58311500
H	-0.19892400	2.73821400	-1.27137000
H	0.78024700	2.56001400	0.19201800
H	-1.24321600	2.23973500	1.57246000
H	-1.40991400	3.75328700	0.67481000
H	-2.90168400	2.75691200	-0.95915600
H	-3.47715900	2.19775000	0.61929500
H	-3.66418400	-0.54006700	-1.71133200
H	-4.51344700	0.73949000	-0.86316300
H	-3.95179000	-0.51036400	1.34026400
H	-5.18082800	-1.21879900	0.29192600
H	-3.60125600	-2.85495700	-0.61627600
H	-3.65538900	-2.97334000	1.13821500
H	-1.35241400	-3.19156500	0.32443600
H	-1.47386700	-1.75245900	1.31815600
H	-0.13064100	-1.62015700	-0.91302900
H	-1.68187500	-1.61950600	-1.74079200

3A'

E = -936.5667145 a.u.

Ni	-0.74119700	2.06694900	0.02962200
C	0.19558600	3.71869800	-0.05603300
C	-0.28236200	3.53423000	1.11137700
O	1.36736000	0.16976700	-0.13135000
O	-0.22277100	0.86045600	-1.70172900
C	0.46947000	0.72539100	-0.69708200
N	-1.89364800	0.63891600	0.86073200
C	0.97048900	4.49902600	-1.05169300
H	1.90071900	3.97650700	-1.30486300
H	0.40889300	4.62134100	-1.98468400
H	1.23199400	5.49498900	-0.67230200
H	-0.42579900	3.85935700	2.13075800
N	-3.74289800	-0.85021700	0.92805000
C	-1.37677700	0.03155400	2.10492000
C	-1.68995300	-1.46697300	2.16496800
C	-3.19795700	-1.67420400	2.02994500
C	-5.07459400	-1.24349300	0.42580800
C	-5.04781400	-1.98728700	-0.92392600
C	-4.88000600	-1.05389900	-2.13737300
C	-3.62728000	-0.15826600	-2.10485200
C	-3.55731500	0.81060600	-0.89707800
C	-3.01900000	0.18321300	0.37384000
H	-1.81976400	0.55085000	2.96791000
H	-0.29924400	0.20380100	2.13441000
H	-1.16348800	-1.97449600	1.34761100
H	-1.33633900	-1.90398900	3.10504400
H	-3.70943800	-1.41460500	2.96861300
H	-3.42328700	-2.72604000	1.81385700
H	-5.72237200	-0.36063300	0.35527100
H	-5.51295300	-1.88613300	1.19593700
H	-4.23967100	-2.73160400	-0.89906600
H	-5.98865600	-2.54465800	-1.03268700
H	-5.77083300	-0.40984800	-2.20808000
H	-4.86455000	-1.65792600	-3.05427100
H	-3.61088400	0.44638200	-3.02036300
H	-2.71397500	-0.76629500	-2.12564700
H	-2.89205500	1.64325700	-1.13926000
H	-4.55012400	1.24559200	-0.71085600

TS₍₃₋₄₎A'

E = -936.5402856 a.u.

Ni	-1.50003200	0.02169000	-0.18543400
C	-3.58241300	0.03754700	0.19269800
C	-2.82629900	1.10669000	0.41581100
H	-4.66698000	0.01966100	0.25558900

C	-3.09245200	2.49059100	0.89545400
H	-2.55871100	2.68177100	1.83573100
H	-2.74751200	3.23987500	0.17190300
H	-4.16210600	2.65960000	1.07635600
O	-4.20427200	-2.27566700	-0.11162800
O	-2.00022000	-1.92717400	-0.52181100
C	-3.19041700	-1.61109300	-0.20375300
N	0.20205300	0.84072100	-0.08684100
N	2.53531000	0.74932900	0.32568500
C	0.32442000	2.26828100	-0.44936600
C	1.66829300	2.55303800	-1.12568500
C	2.80021900	2.10617500	-0.20274200
C	3.70881800	0.02773800	0.86660100
C	4.24197200	-1.09181000	-0.04783400
C	3.42250000	-2.39283600	0.03221800
C	1.92443400	-2.23626700	-0.28540400
C	1.15749600	-1.27534500	0.66092600
C	1.28236100	0.18792400	0.28638400
H	0.21173300	2.87943300	0.45790300
H	-0.50632100	2.51354400	-1.11281300
H	1.71852700	2.00518300	-2.07447100
H	1.77092500	3.61916500	-1.35379200
H	2.91738400	2.80971000	0.63425300
H	3.75186700	2.07999400	-0.74644500
H	3.47035700	-0.37653300	1.85795400
H	4.48379700	0.78496600	1.01995300
H	4.27057100	-0.71964300	-1.08145500
H	5.28048300	-1.30672400	0.23937400
H	3.52500600	-2.80968000	1.04628500
H	3.85901400	-3.13417600	-0.64976300
H	1.44554500	-3.21992300	-0.21389800
H	1.78553700	-1.90519200	-1.32351400
H	0.09649500	-1.53634300	0.64055300
H	1.49608400	-1.42342800	1.69620100

TS₍₃₋₄₎A'

E = -936.5352436 a.u.

Ni	1.37338100	0.18019900	0.06389600
C	3.50621800	0.48034600	-0.19636200
C	2.59754800	1.42068700	-0.38982800
O	4.25399300	-1.88253400	0.10483100
O	2.01936600	-1.71083800	0.43362500
C	3.18846200	-1.30966700	0.17130000
N	-0.36844700	0.91808800	-0.04154300
H	2.67677400	2.46874700	-0.66358700
C	5.00485700	0.64447000	-0.26021700
H	5.26325400	1.68623300	-0.47772400
H	5.46786500	0.34885800	0.68636300
H	5.42985800	-0.00560600	-1.02977300
N	-2.70705400	0.69880900	-0.37157600
C	-0.54118900	2.36581900	0.20016500
C	-1.87627000	2.65507300	0.89158700
C	-3.01492300	2.08397100	0.04888100
C	-3.86163800	-0.11070900	-0.81905200
C	-4.31827500	-1.17880700	0.19340800
C	-3.44600000	-2.44721700	0.18565900
C	-1.94791000	-2.20515100	0.44653400
C	-1.25082400	-1.28678100	-0.59118600
C	-1.42937600	0.19503600	-0.32626000
H	-0.48070200	2.89665400	-0.76105100
H	0.29815200	2.70113600	0.81055300
H	-1.87650000	2.19274700	1.88624300
H	-2.01753200	3.73235300	1.02866800
H	-3.18788600	2.70721400	-0.84048200
H	-3.94776800	2.06589000	0.62472200
H	-3.63513600	-0.57866700	-1.78500700
H	-4.67403900	0.59887500	-1.00314700
H	-4.33325600	-0.73024200	1.19650500
H	-5.35421100	-1.45809200	-0.04341000
H	-3.55698400	-2.94332100	-0.79112000
H	-3.83157400	-3.15235700	0.93357400
H	-1.42945900	-3.17118000	0.43414900
H	-1.79744500	-1.79048200	1.45254800
H	-0.17923200	-1.50110300	-0.58925200
H	-1.61130600	-1.52693700	-1.60146600

4A

E = -936.5943831 a.u.

Ni	-1.52645000	0.23816000	-0.61873700
O	-3.15358600	-0.30983000	-1.16297100
O	-5.16631900	-0.97017900	-0.38856500
N	0.28486700	0.87590400	-0.45134900
C	-4.02815200	-0.57867100	-0.19112200
C	-3.42790300	-0.33664700	1.15281500
C	-2.15532600	0.08895700	1.14580200
H	-4.01900300	-0.50545400	2.05462600
C	-1.32794700	0.40726100	2.35468000
H	-0.43393300	-0.22803800	2.41310200
H	-0.97574300	1.44797900	2.34502700
H	-1.90907500	0.26014700	3.27648200
N	2.63851100	0.58551900	-0.41286700
C	0.46363900	2.33330600	-0.26156400
C	1.69306900	2.63530900	0.60019100
C	2.92237500	1.99000200	-0.03657300
C	3.82157200	-0.27071000	-0.65586700
C	4.10708300	-1.28929100	0.46430300
C	3.20718600	-2.53617200	0.40532200
C	1.69580300	-2.24613800	0.45522600
C	1.16248700	-1.37652900	-0.71247200
C	1.35670600	0.11522600	-0.52297600
H	-0.44793800	2.71802900	0.20151500
H	0.55746400	2.81600500	-1.24506500
H	1.53718200	2.23189000	1.60795100
H	1.84644900	3.71517300	0.69616800
H	3.23605700	2.55025700	-0.92889400
H	3.76417800	1.98818700	0.66542900
H	3.71162300	-0.78770800	-1.61715300
H	4.67058700	0.41045600	-0.76557400
H	5.15647400	-1.60398600	0.38416500
H	4.00141200	-0.78573700	1.43524400
H	3.42935500	-3.08735400	-0.52150300
H	3.47060300	-3.20779700	1.23258400
H	1.43146000	-1.76863300	1.40858100
H	1.15737500	-3.20134800	0.43058900
H	0.08455500	-1.53750800	-0.81643000
H	1.62354000	-1.69834000	-1.65700100

4A'

E = -936.5952581 a.u.

Ni	-0.99179800	0.99870300	-0.80136000
O	-1.29684200	2.76138400	-1.04862600
O	-0.53473400	4.79916800	-0.45819900
N	-0.88133500	-0.91815900	-0.76605600
C	-0.47002500	3.58092600	-0.40647000
C	0.55797100	2.82886900	0.39583900
C	0.42026500	1.49763700	0.30071700
C	1.58124000	3.59465100	1.18459600
H	2.26210100	2.92518000	1.72199400
H	2.17127100	4.24260200	0.52453300
H	1.09254200	4.25758800	1.90943200
H	1.05920600	0.76833800	0.80543900
N	-1.60538800	-3.06906700	-0.08060700
C	0.22664700	-1.53376000	-1.53031300
C	0.73191100	-2.80725700	-0.84583900
C	-0.43646300	-3.77317200	-0.65696700
C	-2.64323200	-3.92897800	0.53020700
C	-2.64389400	-3.92072700	2.07013000
C	-3.31977100	-2.67836700	2.67798200
C	-2.72555200	-1.33009400	2.22916800
C	-2.81184600	-1.05696600	0.70499800
C	-1.70510000	-1.70288000	-0.10545900
H	1.01980900	-0.78707900	-1.61108100
H	-0.11833300	-1.75765700	-2.55001300
H	1.16530400	-2.54787100	0.12774300
H	1.51781700	-3.28406600	-1.44066500
H	-0.72088100	-4.22992700	-1.61565300
H	-0.16034500	-4.58462600	0.02650000
H	-3.63115600	-3.64131900	0.15020300
H	-2.45221500	-4.94168600	0.16258300
H	-3.17087200	-4.81885000	2.42007500
H	-1.60690900	-4.00526700	2.42394100
H	-4.38885500	-2.69587900	2.41516600

H	-3.27176200	-2.74365900	3.77265200
H	-1.67806400	-1.24822300	2.54920100
H	-3.26658100	-0.52509200	2.74137800
H	-2.73400300	0.02144900	0.53149400
H	-3.79463900	-1.36960000	0.32493500

5A

E = -1398.608839 a.u.

Ni	-0.00722900	1.00967100	0.01621900
O	-1.29641300	2.09623200	-0.75673400
O	-1.85034000	4.25077700	-1.08687600
N	-1.21857200	-0.57759800	-0.52981700
N	1.36207900	-0.20103100	0.73141300
C	-1.08665400	3.40337500	-0.63890800
C	0.16240200	3.70138400	0.11371600
C	0.86193000	2.63467300	0.53656800
H	0.42986500	4.74290600	0.30739900
C	2.10536100	2.77083900	1.37313000
H	1.98792600	2.27462100	2.34826200
H	2.97828600	2.30343800	0.89897300
H	2.35345700	3.82514000	1.56564200
N	-3.47468600	-1.18333000	-0.98169900
N	3.29532500	-1.57290200	0.59804300
C	-0.78590800	-1.32233400	-1.72258200
C	-1.68357900	-2.53243200	-2.00551600
C	-3.13224300	-2.06035900	-2.11865000
C	-4.91493700	-0.92703600	-0.77259200
C	-5.50243100	-1.59149800	0.48653500
C	-5.17397300	-0.83516000	1.78536300
C	-3.67012700	-0.62039200	2.03957000
C	-2.94186300	0.23392900	0.97131100
C	-2.49697000	-0.53542200	-0.25670200
C	1.05977900	-0.75216900	2.06637300
C	2.33942300	-1.11169400	2.82846000
C	3.17769500	-2.07048000	1.98482500
C	4.33753900	-2.20994100	-0.23259400
C	5.55237600	-1.31524500	-0.54087200
C	5.28957100	-0.29677100	-1.66267500
C	4.10616300	0.65256700	-1.40034900
C	2.72522400	-0.03893800	-1.26864800
C	2.42223900	-0.62792600	0.09702700
H	0.24750300	-1.64344100	-1.55830800
H	-0.78242100	-0.64203100	-2.58751900
H	-1.59217200	-3.25666000	-1.18580200
H	-1.38117200	-3.03833700	-2.92947100
H	-3.28757300	-1.52201600	-3.06550600
H	-3.81804000	-2.91672900	-2.11030000
H	-5.09947800	0.15398500	-0.75037700
H	-5.42470500	-1.30987400	-1.66235300
H	-6.59423700	-1.64717000	0.37305000
H	-5.13532000	-2.62608300	0.54287400
H	-5.66635900	0.14877500	1.75404700
H	-5.61212400	-1.37345600	2.63682800
H	-3.16480400	-1.59229100	2.13835300
H	-3.55656600	-0.11311000	3.00671400
H	-2.03712200	0.66972400	1.40002200
H	-3.55955100	1.08891100	0.66983800
H	0.41178800	-1.63259200	1.95009000
H	0.48485200	0.00306000	2.60917000
H	2.90842700	-0.19596400	3.02867900
H	2.10310600	-1.57248400	3.79373300
H	2.72629700	-3.07440800	1.98167700
H	4.18771300	-2.16674800	2.40162000
H	3.89587200	-2.57363100	-1.17003000
H	4.66377700	-3.09719500	0.31920200
H	5.85339700	-0.79935200	0.38136100
H	6.39249500	-1.96059200	-0.83323200
H	5.10457800	-0.84380200	-2.60052800
H	6.19694200	0.29899200	-1.82807800
H	4.03974700	1.36432400	-2.23257300
H	4.29954500	1.25058200	-0.50066300
H	1.93432000	0.69344400	-1.45881700
H	2.63302400	-0.81657200	-2.04155800

5A'

E = -1398.6122595 a.u.

Ni	0.05259500	0.79480800	0.03592900	N	-1.68717300	0.75007300	0.40527500
O	-1.15234800	2.09091100	-0.53415200	C	2.03344500	2.42648400	0.56166400
O	-1.46585900	4.31654700	-0.62602700	O	1.43893100	2.38304000	1.62439200
N	-1.30835100	-0.62905600	-0.55794300	O	3.13018000	2.25703300	0.07375200
N	1.34377200	-0.55356300	0.62487000	N	-3.66765800	-0.55108800	0.61209500
C	-0.77451000	3.34504400	-0.33676600	C	-1.91773100	1.28722000	1.76516700
C	0.58868400	3.45082100	0.28640600	C	-2.55536100	0.23387500	2.67695900
C	1.14726100	2.25359300	0.53047800	C	-3.85977700	-0.25590300	2.04800200
C	1.15127800	4.81824700	0.56231500	C	-4.71394700	-1.37145400	-0.02701800
H	2.14931800	4.75967900	1.01228000	C	-4.29084800	-2.82299600	-0.33125400
H	1.21620500	5.40882000	-0.36080400	C	-3.42696000	-2.96360400	-1.59844200
H	0.49511600	5.38279500	1.23722400	C	-2.13680100	-2.12309500	-1.59992800
H	2.13833600	2.17343500	0.99169400	C	-2.36089700	-0.59412900	-1.49315400
N	-3.59420600	-1.08929900	-1.02620400	C	-2.56487000	-0.08438100	-0.08167000
N	3.38611900	-1.76024600	0.55016400	H	-2.56885800	2.17068900	1.68880600
C	-0.91520100	-1.38128100	-1.76069300	H	-0.95622200	1.63132100	2.15162200
C	-1.88349100	-2.53036000	-2.06384900	H	-1.86082400	-0.60653200	2.80072100
C	-3.30059600	-1.96936100	-2.17453800	H	-2.75318700	0.64578600	3.67256500
C	-5.01763500	-0.75618000	-0.81246800	H	-4.64910700	0.50166400	2.16674900
C	-5.64558100	-1.41478000	0.43003100	H	-4.20746300	-1.17080200	2.54463500
C	-5.27625100	-0.71020900	1.74689800	H	-5.06503200	-0.88447100	-0.94623600
C	-3.76316800	-0.59035800	2.00803700	H	-5.56360000	-1.37424700	0.66321200
C	-2.98364200	0.24709400	0.96257000	H	-3.75596200	-3.22217300	0.54197000
C	-2.58210300	-0.51662900	-0.28387500	H	-5.19822300	-3.43125400	-0.45262000
C	0.99385200	-1.24133500	1.88269500	H	-4.03488200	-2.67532600	-2.47042400
C	2.24139200	-1.51788200	2.72823400	H	-3.16896300	-4.02177300	-1.74052300
C	3.23711000	-2.33379000	1.90484400	H	-1.59731700	-2.32138600	-2.53547900
C	4.56163200	-2.21484500	-0.21939600	H	-1.47237300	-2.44404900	-0.78662300
C	5.69571600	-1.17714000	-0.32947900	H	-1.48592700	-0.06446200	-1.87485700
C	5.43323700	-0.09422400	-1.39071600	H	-3.21215400	-0.30083600	-2.12522400
C	4.13131300	0.70226200	-1.19062100	N	2.70715500	-1.81456600	-0.61596100
C	2.83294800	-0.14229800	-1.24635100	C	1.46645200	-0.11157500	-2.35902500
C	2.47881900	-0.84989200	0.04663600	C	2.99153900	-0.21129000	-2.47814700
H	0.09715000	-1.76305600	-1.59481700	C	3.43293000	-1.54506100	-1.87855900
H	-0.86650600	-0.69164400	-2.61674000	C	3.25934200	-2.90679400	0.20701600
H	-1.83920300	-3.26980600	-1.25397500	C	4.20561700	-2.44398300	1.33154700
H	-1.60936100	-3.04100300	-2.99389200	C	3.46270400	-1.88078400	2.55620300
H	-3.41865700	-1.40948800	-3.11442200	C	2.51507400	-0.70586500	2.25131300
H	-4.03732700	-2.78219800	-2.18126600	C	1.33783400	-1.05496300	1.30140600
H	-5.14012600	0.33289200	-0.76485900	C	1.69236900	-0.98950600	-0.17054000
H	-5.54647900	-1.08803900	-1.71161600	H	1.09739200	0.82174200	-2.78834700
H	-6.73851900	-1.40410800	0.31426800	H	0.98748200	-0.94609800	-2.89804000
H	-5.33953600	-2.47008800	0.46184100	H	3.43123600	0.62569500	-1.92487200
H	-5.70977500	0.30154700	1.73823300	H	3.31702000	-0.14489700	-3.52226400
H	-5.74803100	-1.24161900	2.58461900	H	3.24723300	-2.36989800	-2.58269900
H	-3.31551100	-1.59224100	2.08375100	H	4.50976800	-1.53306100	-1.66263700
H	-3.62254400	-0.11432100	2.98743800	H	2.43858600	-3.49971300	0.62972000
H	-2.05687600	0.61903000	1.40206000	H	3.79472500	-3.56809700	-0.48350600
H	-3.55085500	1.14403200	0.68485700	H	4.82103200	-3.29937500	1.64508800
H	0.46757300	-2.17802800	1.64789300	H	4.89389600	-1.68964800	0.92586400
H	0.29184100	-0.60242100	2.42317700	H	2.88366600	-2.69577300	3.02064100
H	2.69164100	-0.56279600	3.02435200	H	4.19937100	-1.56088400	3.30523900
H	1.98279600	-2.06001600	3.64427200	H	3.07222700	0.13999900	1.83271700
H	2.90560500	-3.38027600	1.82770600	H	2.08714700	-0.34811500	3.19566800
H	4.22258800	-2.33694100	2.38704800	H	0.52810300	-0.34095400	1.45072100
H	4.24885400	-2.53346300	-1.22226300	H	0.94347400	-2.05180400	1.55246200
H	4.92893200	-3.11229500	0.28881300				
H	5.84922700	-0.71715100	0.65657900				
H	6.62573000	-1.70593900	-0.58109100				
H	5.40617000	-0.57344200	-2.38213000				
H	6.28157500	0.60262900	-1.40945700				
H	4.06403600	1.46350800	-1.97782200				
H	4.16119900	1.24958400	-0.23974500				
H	1.98877900	0.51607400	-1.46898600				
H	2.90189900	-0.87177500	-2.06737100				

TS_{(1-5)A'}
E = -1398.5409956 a.u.

TS_{(1-5)A}
E = -1398.5455919 a.u.

Ni	-0.05853000	1.50142300	-0.44486500
C	0.89945000	3.19211800	-0.86948900
C	-0.39819600	3.29731600	-0.70128300
H	1.63127300	3.73172000	-1.46365200
C	-1.51388000	4.27087300	-0.83568800
H	-2.40183000	3.81344500	-1.28876900
H	-1.81389600	4.62813600	0.16020900
H	-1.23264600	5.15391400	-1.42690800
N	1.05565400	-0.14355000	-0.93774100

Ni	0.09173400	1.53138400	-0.19930500	C	-0.61001700	0.12675400	2.16517400
C	1.16506100	3.28392000	-0.44463400	C	-1.13320100	-1.17206800	2.78880100
C	-0.11909600	3.35832000	-0.21988100	C	-2.64823600	-1.23734600	2.60469800
N	1.00765500	-0.17253600	-0.87606600	C	-4.38667000	-1.25825800	0.80456400
N	-1.64341600	0.90270600	0.51698400	C	-4.49230800	-2.47108700	-0.13878100
C	2.23476600	2.05674100	0.74306600	C	-4.13689000	-2.13978500	-1.59856500
O	1.68188800	1.87729100	1.81786200	C	-2.74056600	-1.51965000	-1.79566600
O	3.30256300	1.88041200	0.19185600	C	-2.52237100	-0.15591600	-1.09173600
H	-0.90169400	4.11086500	-0.26681000	C	-2.13215500	-0.25571200	0.36918200
C	2.19164100	4.12369000	-1.14751200	H	-0.99769100	0.99581700	2.71760700
H	1.71909100	4.83830500	-1.83296900	H	0.48129500	0.17057900	2.21848200
H	2.80059200	4.68760800	-0.42936100	H	-0.66079700	-2.03009200	2.29332200
H	2.88765400	3.49161000	-1.70762700	H	-0.88195100	-1.22604200	3.85412700
N	-3.83170200	-0.02673100	0.48730000	H	-3.14755900	-0.53468600	3.28915100
C	-1.84254700	1.29889500	1.92875200	H	-3.02318500	-2.24231600	2.83697500
C	-2.71866000	0.28681600	2.67361100	H	-4.86496700	-0.38309000	0.34793300
C	-4.05128900	0.13401300	1.94029000	H	-4.93477500	-1.46254600	1.73014200
C	-4.97342300	-0.54828600	-0.28739900	H	-3.84115500	-3.27074600	0.24202800
C	-4.80526900	-2.00291400	-0.77027400	H	-5.52170500	-2.85446700	-0.10057400
C	-3.91465600	-2.13909000	-2.01867700	H	-4.88786600	-1.43858300	-1.99328700
C	-2.49534600	-1.55955700	-1.87080100	H	-4.21667200	-3.05208200	-2.20533500
C	-2.44351900	-0.04140300	-1.56538400	H	-2.58328100	-1.36758800	-2.87155900
C	-2.62827800	0.31377300	-0.10456500	H	-1.96627900	-2.22837200	-1.46621800
H	-2.30262800	2.29731700	1.94993300	H	-1.71096700	0.38812100	-1.57940200
H	-0.85598700	1.39580000	2.38655400	H	-3.41288700	0.47675700	-1.20579600
H	-2.20215200	-0.68058300	2.71605500	N	3.88282000	-0.27043600	-0.20526900
H	-2.89614000	0.60908600	3.70547800	C	2.73115900	1.98434400	0.96920300
H	-4.68981000	1.01155000	2.12279200	C	3.83490100	1.25147400	1.73928000
H	-4.59385000	-0.74686500	2.30636500	C	4.71573400	0.48569100	0.75231700
H	-5.17922500	0.10769700	-1.14336800	C	4.56421000	-1.34240200	-0.95563100
H	-5.84592100	-0.47835200	0.36992100	C	4.16878600	-2.77097800	-0.53018200
H	-4.39935200	-2.60188700	0.05691700	C	2.82432700	-3.24023000	-1.11489100
H	-5.79986100	-2.41083800	-0.99911300	C	1.62235700	-2.33774700	-0.77880600
H	-4.41318100	-1.63393600	-2.86085200	C	1.74217800	-0.88191400	-1.29329900
H	-3.84422600	-3.19977600	-2.29522000	C	2.54763100	0.04046600	-0.40175700
H	-1.95315000	-1.73387600	-2.80953800	H	2.04419200	2.48992400	1.65216000
H	-1.94279700	-2.10044800	-1.09061200	H	3.16149800	2.76139600	0.32126600
H	-1.46843600	0.36105500	-1.84654000	H	3.37929900	0.55162000	2.45165200
H	-3.19177500	0.48387400	-2.17712200	H	4.44508500	1.95572400	2.31555900
N	2.35198200	-2.12173800	-0.70787500	H	5.37168300	1.18152200	0.20742700
C	1.52342700	-0.00535300	-2.25348200	H	5.36179800	-0.22425800	1.28387300
C	3.00922000	-0.37144000	-2.33002100	H	4.39698000	-1.21394600	-2.03312500
C	3.17602600	-1.82788300	-1.90295700	H	5.63649700	-1.19568700	-0.79172600
C	2.69145700	-3.37163100	-0.00138400	H	4.95789700	-3.46193900	-0.85868400
C	3.59127600	-3.18024400	1.23531200	H	4.14495600	-2.81500400	0.56767900
C	2.82276800	-2.69643000	2.47839600	H	2.92082000	-3.30015400	-2.21032500
C	2.04940500	-1.37879600	2.28972600	H	2.61881800	-4.26188400	-0.76783700
C	0.94164600	-1.42932400	1.20500900	H	1.45166800	-2.32195500	0.30661500
C	1.44037900	-1.21187600	-0.20970200	H	0.72245600	-2.78069000	-1.22582700
H	1.36045800	1.03489700	-2.54186800	H	0.74930900	-0.43197400	-1.36042600
H	0.93737900	-0.63903800	-2.93961100	H	2.16119100	-0.88305200	-2.31013700
H	3.55677200	0.29540700	-1.65607700				
H	3.40013300	-0.23383200	-3.34443800				
H	2.88636500	-2.51019000	-2.71619500				
H	4.22543500	-2.03728400	-1.65674300				
H	1.77145900	-3.89787300	0.28289700				
H	3.19674600	-4.00842500	-0.73554200				
H	4.07794700	-4.13884500	1.46502000				
H	4.39072100	-2.46990000	0.98326400				
H	2.11467000	-3.48553600	2.78014500				
H	3.52823200	-2.58128800	3.31222200				
H	2.73146200	-0.55189100	2.06316900				
H	1.57111200	-1.11828900	3.24241200				
H	0.21284500	-0.64131100	1.39119500				
H	0.40538700	-2.38874700	1.27071100				

1B

E = -1262.9260077 a.u.

Ni	0.05976800	1.69844800	-0.23288900
C	0.12182900	3.33576100	-1.10673900
C	-1.12329500	3.01389200	-0.88350900
H	0.67614700	4.15065100	-1.56467100
N	1.93491400	1.05989100	0.13672600
N	-0.98503000	0.25201200	0.74347000
C	-2.46750900	3.34254800	-1.01703600
N	-3.62314200	3.52327600	-1.09700900
N	-3.00709300	-0.91967800	1.20924100

TS_{(3-4)B}

E = -989.4690092 a.u.

Ni	1.39400800	-0.24039900	0.16097700
C	3.53624400	-0.24894500	-0.11742200
C	2.79783300	0.84613600	-0.25732200
H	4.61820900	-0.31004300	-0.18427400
O	4.06197500	-2.61203800	0.07685400
O	1.84253100	-2.21957700	0.38853700
C	3.05499700	-1.94539500	0.16137500
N	-0.22323900	0.72516300	0.12174900
C	3.04493200	2.19469800	-0.54379000
N	3.16836000	3.33367400	-0.77206000
N	-2.55062800	0.83945600	-0.30014200
C	-0.21096800	2.15635200	0.49805000
C	-1.53262800	2.56148200	1.15426800
C	-2.69007000	2.22021300	0.21870800
C	-3.78172300	0.23036700	-0.85335800
C	-4.40919200	-0.85405200	0.04320300
C	-3.70611100	-2.21970700	-0.05556600
C	-2.20110400	-2.19884800	0.26944900
C	-1.35394700	-1.29082200	-0.66126600
C	-1.35523000	0.17288300	-0.26493000
H	-0.01697500	2.76016800	-0.39853900
H	0.62655400	2.31704300	1.17823800
H	-1.64801000	2.02494700	2.10399500

H	-1.53693600	3.63308800	1.37797400
H	-2.72916000	2.92431900	-0.62439900
H	-3.64659400	2.28619800	0.74947400
H	-3.57845600	-0.17383800	-1.85255600
H	-4.48834300	1.05392900	-0.99110200
H	-4.40826700	-0.49645200	1.08227500
H	-5.46150400	-0.97423700	-0.24818500
H	-3.83948300	-2.61063800	-1.07613500
H	-4.20758800	-2.93071200	0.61358800
H	-1.80903000	-3.21897800	0.18224500
H	-2.03919200	-1.89665600	1.31308900
H	-0.31973900	-1.64486700	-0.65332500
H	-1.70343800	-1.39342300	-1.69807100

TS_{(3-4)B'}

E = -989.4582239 a.u.

Ni	1.18465800	0.07602000	0.14359900
C	3.34024300	0.38782100	-0.25670500
C	2.37753600	1.26916700	-0.48152900
O	4.21105700	-1.92597600	0.37594300
O	1.94741000	-1.77580000	0.63534100
C	3.11832400	-1.43571300	0.36791600
N	-0.51550400	0.88961900	0.03009900
H	2.37499900	2.28399400	-0.86797300
C	4.72462600	0.61204500	-0.45660100
N	5.86034700	0.81497200	-0.62364100
N	-2.84746200	0.76213200	-0.37119300
C	-0.64501200	2.32870700	0.34437200
C	-1.98954100	2.62446600	1.01419800
C	-3.12129700	2.13555300	0.11227500
C	-4.01805300	0.01057200	-0.88037400
C	-4.52419400	-1.09242500	0.06849000
C	-3.69038000	-2.38546400	0.01124600
C	-2.19156200	-2.20507500	0.31325200
C	-1.44856500	-1.25379000	-0.66118500
C	-1.59162600	0.21694400	-0.32251000
H	-0.54090700	2.90749600	-0.58456600
H	0.18647700	2.60323800	0.99531100
H	-2.03232000	2.11265500	1.98322300
H	-2.10033700	3.69720100	1.20296300
H	-3.24841200	2.80666400	-0.74887800
H	-4.06989500	2.11862400	0.66089500
H	-3.78550200	-0.41380000	-1.86470800
H	-4.80450700	0.75345600	-1.04247800
H	-4.54658200	-0.69518500	1.09275400
H	-5.56264900	-1.32792100	-0.20115800
H	-3.79612000	-2.82755200	-0.99151800
H	-4.11173700	-3.11535800	0.71431000
H	-1.70287100	-3.18497000	0.25690800
H	-2.04886900	-1.85042600	1.34307500
H	-0.38153000	-1.49461000	-0.65343900
H	-1.79206800	-1.43177600	-1.68969800

TS_{(1-5)B}

E = -1451.4814257 a.u.

Ni	-0.08359300	1.39808400	-0.25477600
C	0.48623100	3.36543400	-0.64838400
C	-0.77092500	3.11264900	-0.34305000
H	0.92323000	4.16976200	-1.23388300
N	1.21784300	-0.01937700	-0.87802100
N	-1.57907800	0.41783000	0.53954800
C	1.97747000	2.65548900	0.29592600
O	1.66070600	2.32844200	1.43216100
O	2.95235900	2.78917900	-0.41420700
C	-2.03155700	3.71260800	-0.38198600
N	-3.12070800	4.13966200	-0.37121700
N	-3.54119300	-0.91728300	0.55161800
C	-1.86580000	0.84681500	1.92748900
C	-2.55166500	-0.26715300	2.72263200
C	-3.82000400	-0.70037400	1.98857000
C	-4.56021200	-1.68088600	-0.19728700
C	-4.11393200	-3.09547700	-0.61540900
C	-3.20988200	-3.11319400	-1.86057500
C	-1.92691100	-2.26935800	-1.74073000
C	-2.16598900	-0.75727200	-1.50018200
C	-2.42783100	-0.37968700	-0.05666500

H	-2.49825800	1.74424300	1.89109900
H	-0.91953400	1.14170200	2.38736300
H	-1.86900000	-1.12022000	2.82515700
H	-2.80423600	0.07581500	3.73161700
H	-4.60520500	0.06150500	2.09928200
H	-4.20744300	-1.63760900	2.40607500
H	-4.88249000	-1.11236100	-1.07905100
H	-5.43178300	-1.74949800	0.46042700
H	-3.60409900	-3.56894000	0.23517600
H	-5.01127800	-3.69534600	-0.82115100
H	-3.79107500	-2.74682500	-2.72101900
H	-2.93776000	-4.15147900	-2.09291100
H	-1.35654400	-2.37536600	-2.67270900
H	-1.28665300	-2.66372300	-0.93973700
H	-1.28204700	-0.19303200	-1.80232900
H	-2.99499200	-0.40707800	-2.13175500
N	2.94171300	-1.63399300	-0.64986200
C	1.66276800	0.20511400	-2.27333600
C	3.18532300	0.10243000	-2.39437900
C	3.62854800	-1.27590800	-1.91284500
C	3.56394700	-2.72929600	0.12082100
C	4.42364300	-2.25829200	1.30993400
C	3.59350100	-1.87974100	2.54994700
C	2.53176800	-0.78973700	2.31633500
C	1.45192200	-1.15210000	1.26308000
C	1.87164300	-0.90991200	-0.17340000
H	1.32145400	1.19817300	-2.57354600
H	1.17274700	-0.53019600	-2.93172500
H	3.62935300	0.89211400	-1.77951200
H	3.50720600	0.25704200	-3.43006600
H	3.41550800	-2.04469100	-2.67042200
H	4.71006000	-1.28771500	-1.72744700
H	2.79001400	-3.42494900	0.46837600
H	4.18284100	-3.28619600	-0.59012500
H	5.11917800	-3.06558200	1.57898700
H	5.03625600	-1.40575200	0.98610400
H	3.09344000	-2.78777800	2.92424800
H	4.27210200	-1.55173400	3.34846100
H	2.99348900	0.16377100	2.03582100
H	2.01677300	-0.60291000	3.26757100
H	0.56520500	-0.54131000	1.42638900
H	1.14723900	-2.20192000	1.39182100

TS_{(1-5)B'}

E = -1451.4737935 a.u.

Ni	0.13455100	1.40029100	-0.06731000
C	1.50152000	3.01244900	-0.07488400
C	0.19023400	3.21320500	0.02772500
N	0.91437200	-0.29202100	-0.88011000
N	-1.65950300	0.94846900	0.55637700
C	2.35135400	1.74706900	1.06190100
O	1.59566800	1.42381300	1.97350300
O	3.48142800	1.55686300	0.67186900
H	-0.44178800	4.08731800	-0.11125800
C	2.45780200	3.79333300	-0.76690000
N	3.24878100	4.41616700	-1.35732800
N	-3.91492300	0.22601700	0.41127600
C	-1.86032100	1.28836800	1.98324100
C	-2.85679800	0.33257800	2.64489000
C	-4.17033000	0.34872000	1.86374800
C	-5.06839700	-0.17669100	-0.41885400
C	-4.99506100	-1.62223600	-0.94919000
C	-4.07966600	-1.78316300	-2.17644200
C	-2.62559900	-1.32003100	-1.96752600
C	-2.46966700	0.17657400	-1.59752500
C	-2.67156600	0.48123400	-0.12762800
H	-2.21735100	2.32621200	2.04829500
H	-0.88353300	1.25615800	2.46996500
H	-2.43944100	-0.68228300	2.65357300
H	-3.03837700	0.62093000	3.68574500
H	-4.72333500	1.27853000	2.06272800
H	-4.81186700	-0.48656200	2.16982800
H	-5.19207200	0.52364000	-1.25478700
H	-5.95353100	-0.06024600	0.21383100
H	-4.66163700	-2.27873400	-0.13347800
H	-6.01002900	-1.94416100	-1.22037300
H	-4.51202800	-1.21209300	-3.01280400

H	-4.08102800	-2.83553000	-2.49003800
H	-2.07054400	-1.49626600	-2.89792200
H	-2.13665700	-1.93079900	-1.19664600
H	-1.45926100	0.50951800	-1.83992500
H	-3.15884800	0.78218600	-2.20347700
N	2.19793600	-2.28170200	-0.81057400
C	1.52236400	-0.01958900	-2.20422100
C	3.00706200	-0.39813300	-2.20488600
C	3.12394900	-1.88986900	-1.90194200
C	2.45586500	-3.60944600	-0.21757800
C	3.26841100	-3.57294900	1.09094800
C	2.42066200	-3.20177200	2.32077600
C	1.69145100	-1.84962500	2.22182000
C	0.66889100	-1.74536200	1.05964300
C	1.27777400	-1.40359700	-0.28607700
H	1.39110900	1.04220400	-2.42303200
H	0.98082200	-0.59089200	-2.97567600
H	3.51632000	0.19669100	-1.43907300
H	3.47185200	-0.17563800	-3.17122700
H	2.89536000	-2.49127500	-2.79382700
H	4.14569200	-2.13919600	-1.58807400
H	1.50479600	-4.13179200	-0.05515400
H	2.99666100	-4.18100400	-0.97915200
H	3.71779000	-4.56311500	1.25056900
H	4.09780700	-2.86255200	0.97208300
H	1.67704200	-3.99840200	2.48639700
H	3.06511000	-3.19363100	3.20973600
H	2.40461200	-1.02188000	2.14214000
H	1.14509500	-1.68323700	3.15908100
H	-0.05093300	-0.95663500	1.27822900
H	0.10174600	-2.68593300	0.98171300

5B

E = -1451.5561931 a.u.

Ni	-0.05024900	0.90065100	-0.10363100
O	-1.24021000	2.14572600	-0.81170500
O	-1.58334900	4.35561400	-1.07823200
N	-1.38867600	-0.52716900	-0.60017500
N	1.21890000	-0.40516700	0.59462600
C	-0.89943500	3.41872400	-0.68824500
C	0.41799500	3.58798500	0.00104900
C	1.01077900	2.43369000	0.36810400
H	0.80621600	4.58990400	0.17883000
C	2.24268700	2.38827700	1.06814100
N	3.25126200	2.25399000	1.64631000
N	-3.67465300	-1.09000000	-0.91684500
N	3.19541600	-1.70688500	0.57463800
C	-1.01799000	-1.36822100	-1.75049600
C	-1.96963800	-2.55636200	-1.92538200
C	-3.40367100	-2.03805200	-2.01653800
C	-5.09932200	-0.80942600	-0.63745000
C	-5.61716200	-1.40800400	0.68346100
C	-5.21261200	-0.59192900	1.92342200
C	-3.69622600	-0.37454400	2.08235300
C	-3.02461300	0.41574900	0.92978400
C	-2.65260100	-0.42956700	-0.27259800
C	0.93342000	-0.87945200	1.96412500
C	2.22954200	-1.06646500	2.76022500
C	3.13624300	-2.04363600	2.01526700
C	4.30301500	-2.32581400	-0.18274800
C	5.47635100	-1.37679100	-0.49027900
C	5.20323000	-0.43840800	-1.67875400
C	3.95744400	0.45226100	-1.51913300
C	2.61694500	-0.31907900	-1.39401700
C	2.30678000	-0.82977400	0.00065300
H	0.00500600	-1.71810800	-1.58565900
H	-1.00988400	-0.74942600	-2.66014800
H	-1.87369500	-3.23297000	-1.06664900
H	-1.71950500	-3.12774300	-2.82610800
H	-3.57365700	-1.54482200	-2.98502200
H	-4.11821500	-2.86594500	-1.93769700
H	-5.27407500	0.27323600	-0.65632700
H	-5.66154900	-1.22804000	-1.47782900
H	-6.71363900	-1.46160300	0.63430600
H	-5.25215700	-2.44122300	0.76910900
H	-5.70319800	0.39214100	1.87299900
H	-5.60313800	-1.08566800	2.82335900

H	-3.18914600	-1.34242200	2.20560700
H	-3.52630200	0.18400500	3.01197300
H	-2.09938200	0.87032900	1.28658600
H	-3.65995000	1.25345900	0.61669800
H	0.36612400	-1.82065300	1.90996600
H	0.28981400	-0.13800000	2.44409200
H	2.72619100	-0.09540200	2.85974800
H	2.01913100	-1.44707400	3.76555600
H	2.77832600	-3.07744200	2.13220300
H	4.15574700	-1.99958200	2.41722200
H	3.91694700	-2.75838000	-1.11482400
H	4.65204900	-3.16576600	0.42627600
H	5.70455100	-0.79224500	0.41109500
H	6.36492500	-1.98469500	-0.71081100
H	5.09521500	-1.04657000	-2.59124400
H	6.08004400	0.20270000	-1.83779100
H	3.88158200	1.10228100	-2.40014300
H	4.07266500	1.11271200	-0.65192300
H	1.79319200	0.34703800	-1.66631600
H	2.60249400	-1.15332400	-2.11151600

5B'

E = -1451.5431776 a.u.

Ni	0.04710700	0.68775000	-0.00124300
O	-1.11267200	2.00720400	-0.61010900
O	-1.34657000	4.23853400	-0.77333800
N	-1.36611000	-0.70475000	-0.54530900
N	1.29125900	-0.68640000	0.62795700
C	-0.68943500	3.25267600	-0.45441600
C	0.67891000	3.32949500	0.16167000
C	1.19511000	2.12148600	0.44307000
H	2.18433200	2.02072200	0.90422300
C	1.30571400	4.71630500	0.39720200
N	1.77239800	5.74884800	0.57256600
N	-3.66866000	-1.09746700	-0.99282000
N	3.28877900	-1.96746100	0.58743300
C	-1.00449900	-1.50909000	-1.72399100
C	-2.01442300	-2.63183700	-1.98736400
C	-3.41090800	-2.02416000	-2.11272700
C	-5.07846000	-0.70669200	-0.78652400
C	-5.72511900	-1.30180800	0.47820600
C	-5.32604100	-0.56877100	1.77062900
C	-3.80870400	-0.49498000	2.02405000
C	-3.00344600	0.27970200	0.95007900
C	-2.63402100	-0.53783600	-0.27192300
C	0.92145600	-1.32014800	1.90827200
C	2.16132500	-1.61386500	2.75928700
C	3.12419800	-2.49120200	1.96035800
C	4.44447000	-2.48863000	-0.16984800
C	5.61460100	-1.49643800	-0.31628900
C	5.38726700	-0.43965400	-1.41143900
C	4.11544500	0.40914100	-1.23409900
C	2.78746200	-0.38958800	-1.25924500
C	2.41287000	-1.04184700	0.05686700
H	-0.00588600	-1.92142800	-1.54829500
H	-0.93421200	-0.84967300	-2.60206700
H	-1.99373900	-3.34583800	-1.15404900
H	-1.76211700	-3.18178900	-2.90102600
H	-3.51222000	-1.49107400	-3.06998000
H	-4.17630800	-2.80979700	-2.09129600
H	-5.16168100	0.38704700	-0.77395600
H	-5.62209100	-1.04822200	-1.67314500
H	-6.81738300	-1.25562500	0.36482500
H	-5.45696800	-2.36585100	0.54347100
H	-5.72306600	0.45709700	1.73021900
H	-5.81353600	-1.05553900	2.62629000
H	-3.39696000	-1.50932800	2.13111800
H	-3.64758700	0.00710000	2.98715400
H	-2.06237200	0.63211100	1.37501400
H	-3.53915600	1.18699500	0.64481300
H	0.36111200	-2.24442700	1.70525200
H	0.24473800	-0.63929300	2.42946500
H	2.64656800	-0.66650100	3.02318000
H	1.88677300	-2.11647200	3.69305100
H	2.75513700	-3.52704800	1.91800300
H	4.11066200	-2.51417000	2.44000400
H	4.11686600	-2.82804900	-1.16109000

H	4.78120900	-3.38180300	0.36629600
H	5.78804500	-1.01063500	0.65395700
H	6.52415900	-2.06616200	-0.55289100
H	5.33947600	-0.94937900	-2.38672300
H	6.25995400	0.22530200	-1.45483600
H	4.07264900	1.14647500	-2.04540300
H	4.16834700	0.98548000	-0.30154600
H	1.96662700	0.29114700	-1.50105000
H	2.82727500	-1.14722300	-2.05634500

1C

E = -1285.1817473 a.u.

Ni	-0.04269200	1.61654800	0.04129900
C	0.05981700	3.35562300	-0.69632000
C	-1.16600600	2.97107100	-0.48510400
H	0.67299700	4.16559100	-1.07054000
N	1.86815400	0.95685900	0.32327400
N	-1.02797200	0.04645900	0.86812500
O	-2.46491400	3.35810100	-0.59986200
C	-2.62203000	4.66605000	-1.14049500
H	-3.69612000	4.86844500	-1.18973400
H	-2.13276800	5.41322000	-0.50089700
H	-2.18600700	4.72690000	-2.14728500
N	-2.91217000	-1.38287900	1.18325300
C	-0.54904000	-0.33118300	2.21155000
C	-0.91573300	-1.77500600	2.57179100
C	-2.42876800	-1.94981000	2.45627600
C	-4.26516500	-1.79361000	0.76499500
C	-4.29458600	-2.78348700	-0.41624600
C	-4.07946700	-2.11231400	-1.78442000
C	-2.77804800	-1.29669400	-1.90567100
C	-2.65619400	-0.10543000	-0.92325200
C	-2.15297400	-0.47630900	0.45627800
H	-0.97218800	0.36461500	2.95137900
H	0.53483100	-0.19300500	2.21891100
H	-0.40874600	-2.46082900	1.88073200
H	-0.58551600	-2.02388100	3.58687600
H	-2.93487900	-1.45987200	3.30272800
H	-2.69814100	-3.01363900	2.48700200
H	-4.86878600	-0.90883200	0.52571200
H	-4.73008000	-2.25574500	1.64229000
H	-3.53116900	-3.55575500	-0.24512800
H	-5.26805900	-3.29452600	-0.41942000
H	-4.93034600	-1.44237700	-1.98393400
H	-4.10161800	-2.88059700	-2.56959000
H	-2.71827200	-0.89687700	-2.92655300
H	-1.90881200	-1.95948000	-1.78256400
H	-1.94501000	0.62967200	-1.30627500
H	-3.61824200	0.42038200	-0.84848400
N	3.86882700	-0.20706100	-0.25737100
C	2.65485900	1.82056900	1.22601600
C	3.83130600	1.06713700	1.85686200
C	4.70436300	0.47827600	0.74871600
C	4.57318700	-1.11930800	-1.17646100
C	4.28481300	-2.61604400	-0.94110700
C	2.94028700	-3.08700000	-1.52344500
C	1.70882800	-2.31844900	-1.00928000
C	1.71114100	-0.80277600	-1.32603200
C	2.50807500	0.04864900	-0.35891200
H	1.97491000	2.20607800	1.98939100
H	3.01120800	2.69003100	0.65614800
H	3.44861800	0.26066800	2.49595000
H	4.42999200	1.73186700	2.48983100
H	5.29395400	1.27344700	0.26652000
H	5.41457700	-0.24897900	1.16303500
H	4.34728900	-0.85556400	-2.21857200
H	5.64232100	-0.92881400	-1.03695300
H	5.09385100	-3.20204800	-1.40006700
H	4.32297800	-2.81378100	0.13934800
H	2.97971500	-2.99108400	-2.61985200
H	2.81370500	-4.15791600	-1.31298900
H	1.60292500	-2.45936300	0.07571400
H	0.81241000	-2.75863200	-1.46674200
H	0.69224500	-0.41020300	-1.28582500
H	2.07103900	-0.64065200	-2.35305900

TS_{(3-4)C}

E = -1011.7461259 a.u.

Ni	1.32115500	0.17553800	-0.33425400
C	3.27331700	0.52991100	-0.11040600
C	2.80510700	-0.68953700	0.19654300
H	4.28481700	0.80941700	-0.37584000
O	3.29067200	3.01543600	-0.02564000
O	1.24844700	2.18432700	-0.61683500
C	2.45651200	2.17862600	-0.25964100
N	-0.33513700	-0.76188200	-0.16020200
O	3.32364600	-1.85069500	0.58861300
C	4.71104500	-1.82063300	0.96079300
H	4.88516200	-1.03215800	1.70122000
H	4.93986800	-2.80055300	1.38319600
H	5.33703300	-1.63930800	0.07932900
N	-2.64009700	-0.99126000	0.34825700
C	-0.29051300	-2.19205100	-0.53876400
C	-1.60628600	-2.63406400	-1.18394800
C	-2.75733600	-2.35224700	-0.22078700
C	-3.87002200	-0.44741100	0.96342100
C	-4.58363400	0.62381300	0.11586700
C	-3.93780500	2.01785600	0.21351700
C	-2.44718900	2.06960500	-0.16877000
C	-1.52303000	1.18299700	0.70649300
C	-1.47156600	-0.26839800	0.27732500
H	-0.07747700	-2.78982900	0.35925700
H	0.54903000	-2.32886800	-1.22141200
H	-1.75454600	-2.08066600	-2.11944700
H	-1.57985500	-3.70049000	-1.43197600
H	-2.76830500	-3.09017700	0.59458400
H	-3.72059800	-2.42288900	-0.74052800
H	-3.64275100	-0.04976400	1.96004400
H	-4.53486300	-1.30313900	1.11644300
H	-4.60954300	0.28592900	-0.92968600
H	-5.62770400	0.69087900	0.45195800
H	-4.04837400	2.38299200	1.24657900
H	-4.49756100	2.71763600	-0.42097000
H	-2.09648100	3.10440600	-0.07673600
H	-2.31309700	1.79548800	-1.22396800
H	-0.50802000	1.57746600	0.65326600
H	-1.83616100	1.24721300	1.75842200

TS_{(3-4)C'}

E = -1011.7299943 a.u.

Ni	-1.12387500	-0.01360200	-0.13844100
C	-3.25405100	0.16811200	0.12876000
C	-2.41214600	1.17654600	0.30637600
O	-3.86061800	-2.27399600	-0.16978000
O	-1.62646500	-1.96618700	-0.48556400
C	-2.82316600	-1.67348900	-0.24074200
N	0.55294200	0.86298600	-0.01298000
H	-2.50333000	2.22120200	0.57649300
O	-4.60266300	0.11814800	0.16845200
C	-5.23554600	1.35831500	0.45848300
H	-6.30959500	1.16208300	0.45362800
H	-4.92989400	1.73297600	1.44463100
H	-4.98959500	2.11142900	-0.30247400
N	2.89137000	0.83613100	0.38166200
C	0.61972500	2.31227400	-0.29385300
C	1.94574200	2.68297300	-0.96355300
C	3.10343300	2.22716400	-0.07737000
C	4.09281700	0.13038300	0.87912300
C	4.65618600	-0.92472600	-0.09230800
C	3.88296700	-2.25608000	-0.07327800
C	2.37802500	-2.13663000	-0.37554200
C	1.58806200	-1.25001400	0.62261800
C	1.65808500	0.23358100	0.32039300
H	0.49594000	2.86374000	0.64946400
H	-0.22865400	2.56372800	-0.93144700
H	2.00613000	2.19265000	-1.94289600
H	2.00756300	3.76336600	-1.13150400
H	3.20669100	2.88917400	0.79455800
H	4.04897400	2.26254400	-0.63138700
H	3.87771700	-0.32851700	1.85201300
H	4.84344100	0.90513400	1.06267700
H	4.66436300	-0.50127400	-1.10634900

H	5.70351600	-1.11806200	0.17772500
H	4.00608300	-2.71907300	0.91819700
H	4.34055200	-2.94680500	-0.79350800
H	1.93490200	-3.13928800	-0.35033200
H	2.22150600	-1.75894700	-1.39518700
H	0.53625100	-1.54623200	0.60583000
H	1.94293100	-1.43696700	1.64594200

TS_{(1-5)C'}

E = -1473.7517645 a.u.

Ni	-0.11160300	1.40230400	-0.42563900
C	0.89228900	3.00292100	-0.81826000
C	-0.39663100	3.20606600	-0.59655600
N	1.08493300	-0.16048500	-0.98377100
N	-1.64183400	0.47745900	0.48584500
C	2.08227300	2.45977800	0.84976900
O	1.41823600	2.44157300	1.85432400
O	3.16939100	2.32063100	0.35472400
H	1.63890100	3.46186200	-1.45561100
O	-1.23680800	4.24682600	-0.64297600
C	-2.61960100	3.94093000	-0.47152500
H	-2.81293500	3.56044900	0.53791900
H	-3.16252300	4.87719300	-0.62080500
H	-2.94788500	3.19680800	-1.20672000
N	-3.50552800	-0.98525900	0.70485900
C	-1.81005700	0.86727900	1.90345400
C	-2.28989400	-0.31501600	2.75232400
C	-3.60004600	-0.84965400	2.17435600
C	-4.53936900	-1.82104800	0.06542100
C	-4.04353600	-3.20478000	-0.40068700
C	-3.26707700	-3.16727200	-1.72976200
C	-2.03978600	-2.23670400	-1.74137100
C	-2.35851400	-0.74366900	-1.47889200
C	-2.49227100	-0.37654600	-0.01522800
H	-2.53588500	1.69246600	1.96128800
H	-0.85492700	1.26206500	2.25653500
H	-1.52646100	-1.10289700	2.74115300
H	-2.43735600	-0.01487300	3.79545200
H	-4.43275300	-0.17722800	2.42985500
H	-3.83410000	-1.83494700	2.59762100
H	-4.99003600	-1.28211000	-0.77821000
H	-5.33346900	-1.94639000	0.80857700
H	-3.42149200	-3.64014300	0.39393500
H	-4.91453900	-3.86462600	-0.51858700
H	-3.95549700	-2.84834000	-2.52806900
H	-2.94942600	-4.18659000	-1.98785600
H	-1.56054700	-2.31190000	-2.72636800
H	-1.29496800	-2.57705800	-1.00970700
H	-1.55359600	-0.11718800	-1.86952800
H	-3.27263400	-0.46214900	-2.02259400
N	2.84754500	-1.72817800	-0.73884700
C	1.48881900	-0.05434600	-2.40336100
C	3.01735000	-0.01718100	-2.51629400
C	3.56732300	-1.33426800	-0.91640700
C	3.45842200	-2.83384600	-0.82804800
C	4.37368300	-2.38871500	-1.92359500
C	3.59634000	-1.94014800	-3.55343400
C	2.59142300	-0.79914500	-2.71806400
C	1.43494700	-1.15250300	-1.73624800
C	1.78042600	-0.99362900	-0.25457400
H	1.03874600	0.85267700	0.40254400
H	1.08917200	-0.91640700	-0.70313900
H	3.38452300	0.82804800	1.44576700
H	3.34114900	0.12370900	0.82451900
H	3.46453300	-2.13681200	2.83951900
H	4.63590400	-1.23913400	3.20196900
H	2.67064000	-3.49576400	1.81620200
H	4.03273000	-3.42168000	3.14652800
H	5.03307900	-3.22682300	1.39407600
H	5.02181800	-1.57527200	1.41060600
H	3.05742800	-2.80966700	0.82451900
H	4.31114600	-1.62766600	2.83951900
H	3.11193600	0.09220200	3.20196900
H	2.14531100	-0.51606700	1.81620200
H	0.58959100	-0.48968000	3.14652800
H	1.08785800	-2.17861800	1.39407600

TS_{(1-5)C'}

E = -1473.7389776 a.u.

Ni	-0.11160300	1.40230400	-0.42563900
C	0.89228900	3.00292100	-0.81826000
C	-0.39663100	3.20606600	-0.59655600
N	1.08493300	-0.16048500	-0.98377100
N	-1.64183400	0.47745900	0.48584500
C	2.08227300	2.45977800	0.84976900
O	1.41823600	2.44157300	1.85432400
O	3.16939100	2.32063100	0.35472400
H	1.63890100	3.46186200	-1.45561100
O	-1.23680800	4.24682600	-0.64297600
C	-2.61960100	3.94093000	-0.47152500
H	-2.81293500	3.56044900	0.53791900
H	-3.16252300	4.87719300	-0.62080500
H	-2.94788500	3.19680800	-1.20672000
N	-3.50552800	-0.98525900	0.70485900
C	-1.81005700	0.86727900	1.90345400
C	-2.28989400	-0.31501600	2.75232400
C	-3.60004600	-0.84965400	2.17435600
C	-4.53936900	-1.82104800	0.06542100
C	-4.04353600	-3.20478000	-0.40068700
C	-3.26707700	-3.16727200	-1.72976200
C	-2.03978600	-2.23670400	-1.74137100
C	-2.35851400	-0.74366900	-1.47889200
C	-2.49227100	-0.37654600	-0.01522800
H	-2.53588500	1.69246600	1.96128800
H	-0.85492700	1.26206500	2.25653500
H	-1.52646100	-1.10289700	2.74115300
H	-2.43735600	-0.01487300	3.79545200
H	-4.43275300	-0.17722800	2.42985500
H	-3.83410000	-1.83494700	2.59762100
H	-4.99003600	-1.28211000	-0.77821000
H	-5.33346900	-1.94639000	0.80857700
H	-3.42149200	-3.64014300	0.39393500
H	-4.91453900	-3.86462600	-0.51858700
H	-3.95549700	-2.84834000	-2.52806900
H	-2.94942600	-4.18659000	-1.98785600
H	-1.56054700	-2.31190000	-2.72636800
H	-1.29496800	-2.57705800	-1.00970700
H	-1.55359600	-0.11718800	-1.86952800
H	-3.27263400	-0.46214900	-2.02259400
N	2.84754500	-1.72817800	-0.73884700
C	1.48881900	-0.05434600	-2.40336100
C	3.01735000	-0.01718100	-2.51629400
C	3.56732300	-1.33426800	-0.91640700
C	3.45842200	-2.83384600	-0.82804800
C	4.37368300	-2.38871500	-1.92359500
C	3.59634000	-1.94014800	-3.55343400
C	2.59142300	-0.79914500	-2.71806400
C	1.43494700	-1.15250300	-1.73624800
C	1.78042600	-0.99362900	-0.25457400
H	1.03874600	0.85267700	0.40254400
H	1.08917200	-0.91640700	-0.70313900
H	3.38452300	0.82804800	1.44576700
H	3.34114900	0.12370900	0.82451900
H	3.46453300	-2.13681200	2.83951900
H	4.63590400	-1.23913400	3.20196900
H	2.67064000	-3.49576400	1.81620200
H	4.03273000	-3.42168000	3.14652800
H	5.03307900	-3.22682300	1.39407600
H	5.02181800	-1.57527200	1.41060600
H	3.05742800	-2.80966700	0.82451900
H	4.31114600	-1.62766600	2.83951900
H	3.11193600	0.09220200	3.20196900
H	2.14531100	-0.51606700	1.81620200
H	0.58959100	-0.48968000	3.14652800
H	1.08785800	-2.17861800	1.39407600

5C

E = -1473.8253596 a.u.

Ni	-0.05024400	0.74208500	-0.14516700
O	-1.19979900	1.98732300	-0.88723500
O	-1.45090300	4.18703100	-1.27328700
N	-1.48803800	-0.65991900	-0.51585700
N	1.17764900	-0.57159700	0.60935600

C	-0.77998400	3.25156100	-0.85040800	H	0.34356000	5.31617200	1.82280000
C	0.56291900	3.39582000	-0.23887600	N	-3.63062000	-1.26221900	-0.98291200
C	1.09990900	2.22334800	0.16573900	N	3.30845800	-1.98640500	0.60983000
H	0.99660200	4.38825500	-0.14942700	C	-0.95687100	-1.61636100	-1.71253700
O	2.31831800	2.08684000	0.78364800	C	-1.93510700	-2.77407000	-1.94086700
C	3.04896100	3.28448600	1.03090200	C	-3.34881100	-2.21062700	-2.07878300
H	2.48014600	3.96589000	1.67648600	C	-5.05169100	-0.91625900	-0.77372900
H	3.97476200	2.98868200	1.53174600	C	-5.66596700	-1.50188500	0.51162400
H	3.28573500	3.80516200	0.09390700	C	-5.28357600	-0.72190200	1.78147400
N	-3.80880500	-1.05870500	-0.84333600	C	-3.76796100	-0.58500600	2.01920500
N	3.19970600	-1.79886500	0.69579700	C	-3.00083500	0.18893800	0.91686500
C	-1.17257000	-1.59588100	-1.60758500	C	-2.61076500	-0.65154400	-0.28287600
C	-2.21381000	-2.71335100	-1.73058000	C	0.92617400	-1.34079400	1.90979700
C	-3.59944000	-2.08776200	-1.88079800	C	2.16117400	-1.62802600	2.76992000
C	-5.20667000	-0.63192100	-0.62598700	C	3.13147000	-2.50709900	1.98219000
C	-5.81141600	-1.09593800	0.71212100	C	4.47587400	-2.50401700	-0.13253000
C	-5.35643700	-0.24917400	1.91345600	C	5.64008300	-1.50413400	-0.27244100
C	-3.82956000	-0.16528300	2.09893900	C	5.41632700	-0.45544600	-1.37569600
C	-3.06412900	0.49709000	0.92472300	C	4.13706600	0.38596200	-1.21621900
C	-2.74359500	-0.44379400	-0.21974600	C	2.81482500	-0.42229400	-1.25022400
C	0.93220800	-0.91544500	2.02299300	C	2.43209600	-1.07023500	0.06584700
C	2.24813000	-0.93465600	2.80794700	H	0.05294000	-1.99494600	-1.52612000
C	3.19102200	-1.95192600	2.16737800	H	-0.90512900	-0.98099900	-2.60936300
C	4.30535200	-2.47127700	-0.01404600	H	-1.89202400	-3.46372300	-1.08804400
C	5.44887200	-1.53315400	-0.44535900	H	-1.66920600	-3.34216800	-2.83941500
C	5.12534200	-0.72020300	-1.71160600	H	-3.46707800	-1.70629500	-3.04954200
C	3.85339100	0.14275300	-1.62082700	H	-4.09121700	-3.01691400	-2.03403500
C	2.53959800	-0.64858200	-1.39967200	H	-5.17386300	0.17373800	-0.78719800
C	2.26698000	-1.02026900	0.04463300	H	-5.59024500	-1.29866900	-1.64656900
H	-0.18212200	-2.01477000	-1.40510200	H	-6.76005900	-1.49857900	0.40716200
H	-1.10379100	-1.03548400	-2.55214100	H	-5.35837500	-2.55337200	0.60131900
H	-2.18613100	-3.34156900	-0.83101400	H	-5.71934400	0.28707100	1.71952400
H	-1.99755000	-3.35698000	-2.59067100	H	-5.74508900	-1.20463300	2.65361400
H	-3.71201300	-1.64054800	-2.87986900	H	-3.31769600	-1.57999200	2.14903900
H	-4.38084600	-2.84950700	-1.77063000	H	-3.61773200	-0.05163800	2.96706600
H	-5.27950100	0.45885400	-0.71599500	H	-2.07103900	0.58973000	1.32331500
H	-5.78529000	-1.04970500	-1.45588900	H	-3.57562100	1.06438400	0.59005000
H	-6.90666900	-1.04622500	0.63504400	H	0.36415700	-2.26547100	1.71317100
H	-5.55132800	-2.15251500	0.86808200	H	0.24918800	-0.65314600	2.42180600
H	-5.74915300	0.77207800	1.79320500	H	2.64306100	-0.67863500	3.03257900
H	-5.81157100	-0.64942400	2.82964900	H	1.88113700	-2.12654500	3.70422900
H	-3.41848200	-1.16825100	2.28531900	H	2.76350400	-3.54333600	1.93905400
H	-3.62784700	0.42436600	3.00292000	H	4.11347400	-2.52806800	2.47073600
H	-2.10865600	0.88682400	1.27793800	H	4.16104700	-2.85137200	-1.12515300
H	-3.61156900	1.37057100	0.55016100	H	4.81268900	-3.39161200	0.41258800
H	0.43039000	-1.89311300	2.08047800	H	5.80010800	-1.01160800	0.69669200
H	0.24579900	-0.17026400	2.43075800	H	6.55609800	-2.06859500	-0.49646400
H	2.68693500	0.06826700	2.76744100	H	5.38233000	-0.97090700	-2.34854700
H	2.07988500	-1.19207800	3.85925700	H	6.28451300	0.21562700	-1.41396200
H	2.88786400	-2.97729200	2.42663600	H	4.09707700	1.11821000	-2.03199400
H	4.21608200	-1.81056300	2.53361100	H	4.17655000	0.96916600	-0.28742700
H	3.91250500	-3.00787700	-0.88706400	H	1.99282200	0.25283500	-1.50260000
H	4.68772300	-3.23493700	0.67139000	H	2.86720400	-1.18346400	-2.04316800
H	5.68607400	-0.85991200	0.39015300				
H	6.34687100	-2.13963000	-0.62911500				
H	5.02218700	-1.41705400	-2.55863700				
H	5.98018000	-0.07317100	-1.94977700				
H	3.74860800	0.70186500	-2.55938500				
H	3.94434400	0.88942100	-0.82352600				
H	1.69447900	-0.03182800	-1.71787600				
H	2.53722500	-1.55053100	-2.03016100				

5C'

E = -1473.8144684 a.u.

Ni	0.04974300	0.62935800	-0.03019900
O	-1.12141000	1.93036800	-0.67677500
O	-1.33296000	4.14034200	-1.01759400
N	-1.33956400	-0.78777500	-0.55720000
N	1.30246500	-0.71970800	0.62493900
C	-0.70067400	3.17607900	-0.59523800
C	0.65253100	3.25991400	0.06683200
C	1.18522000	2.07324300	0.39941000
H	2.17640300	2.01838200	0.85567600
O	1.32133300	4.45518900	0.19126900
C	0.59506800	5.53784700	0.77402100
H	1.26590500	6.40144100	0.74753000
H	-0.31761900	5.74777100	0.21316200

1D

E = -1618.6499772 a.u.

Ni	-0.38807600	-0.98819200	0.41519400
C	-1.75699700	-2.22885400	-0.08739900
C	-0.60225800	-2.80413800	0.08165700
C	0.08566500	-4.12886200	0.04770300
H	0.89491400	-4.13889500	-0.69623900
H	0.55409400	-4.35296300	1.01588000
H	-0.59803900	-4.95519200	-0.19447100
N	-1.24095500	0.87095400	0.68066800
N	1.51228500	-0.51039400	0.97579900
S	-3.52524900	-2.38860400	-0.53502500
N	3.89718300	-0.63239900	0.90742300
C	1.60598500	0.11996100	2.30669600
C	2.86530900	0.98157500	2.45562100
C	4.09602900	0.12774500	2.15582700
C	5.11213200	-1.18739100	0.28332400
C	5.55400300	-0.46790200	-1.00703800
C	4.73964900	-0.87442800	-2.24833400
C	3.21916000	-0.66603300	-2.11985300
C	2.54417300	-1.48042400	-0.98787500
C	2.62785400	-0.84488600	0.38476600
H	1.58867400	-0.66528700	3.07735700

H	0.70695400	0.72558000	2.44166100	C	-2.33803000	-1.43726800	1.52344300
H	2.81491400	1.82128300	1.75026900	C	-2.51596500	-1.50468000	0.02085800
H	2.93751400	1.40197600	3.46524800	H	-1.50422100	-2.47566400	-2.46908500
H	4.29341900	-0.56276000	2.99087600	H	-0.83107800	-0.86062700	-2.67708400
H	4.98534600	0.76049700	2.03943200	H	-3.10810900	0.14528100	-2.43482100
H	4.97860800	-2.25900700	0.08487400	H	-3.14493900	-1.05686700	-3.73068400
H	5.90512700	-1.11096200	1.03459300	H	-4.19951100	-2.71798300	-2.32082500
H	5.48496700	0.61681800	-0.84345700	H	-5.07328800	-1.21008800	-2.00909800
H	6.61430000	-0.69541200	-1.18766900	H	-4.57374100	-3.02386200	1.07260500
H	4.92930900	-1.93860900	-2.45923200	H	-5.66954400	-2.60210400	-0.23069500
H	5.11028300	-0.31745900	-3.11977900	H	-5.58708000	-0.16362500	0.64026700
H	2.75074000	-0.95659600	-3.06952800	H	-6.48306600	-1.34122800	1.60124600
H	2.99738400	0.40159200	-1.97909200	H	-4.63600500	-1.58846000	3.19248600
H	1.47478900	-1.59282800	-1.18793400	H	-5.11319500	0.10057700	3.07058900
H	2.96789200	-2.49509300	-0.96445600	H	-2.67578700	-0.09805700	3.17939700
N	-1.98135200	3.04059500	0.01498400	H	-3.12559100	0.58277200	1.62241700
C	-2.16774900	0.93327000	1.82806300	H	-1.27199300	-1.26254100	1.68636700
C	-2.32426400	2.36158800	2.36375000	H	-2.57200700	-2.41453900	1.97141900
C	-2.78764500	3.27545700	1.22910200	N	-0.09405700	3.38272300	0.93578800
C	-2.06758900	4.07465400	-1.03190300	C	0.66581300	1.01635400	2.11872800
C	-0.80185300	4.94253200	-1.17831700	C	1.57421300	2.28633300	2.34660700
C	0.32888200	4.25585900	-1.96498300	C	0.75403300	3.49994200	2.14328300
C	0.78887600	2.90209700	-1.39092600	C	-0.64328400	4.65214900	0.42319200
C	-0.30725100	1.80922400	-1.33965000	C	0.15715400	5.26853800	-0.74063900
C	-1.22662200	1.88538000	-0.13804600	C	-0.12704300	4.59646100	-2.09603400
H	-1.78498200	0.26084300	2.60032500	C	0.12395400	3.07767400	-2.13054100
H	-3.14212100	0.53061500	1.51749800	C	-0.76190900	2.25146200	-1.16081700
H	-1.36049700	2.71368700	2.75462900	C	-0.22902800	2.18650200	0.25651200
H	-3.04521300	2.39605000	3.18834500	H	1.22187300	0.08501800	2.24240300
H	-3.85237900	3.10040000	1.01078100	H	-0.15936400	1.01465900	2.85011300
H	-2.68270200	4.32970100	1.51685700	H	2.39233900	2.17953400	1.62045700
H	-2.31879700	3.61533600	-1.99721800	H	2.00614700	2.21850900	3.35338300
H	-2.91781100	4.71072300	-0.76481100	H	0.11569900	3.69858500	3.01749600
H	-1.07523900	5.87449700	-1.69328600	H	1.41569600	4.36717900	2.01677100
H	-0.45295100	5.22447800	-0.17495400	H	-1.68889800	4.50889300	0.12302300
H	-0.01059800	4.09859600	-3.00074200	H	-0.65851100	5.34278600	1.27347700
H	1.19015600	4.93550900	-2.02349700	H	-0.09194800	6.33709100	-0.80991100
H	1.20536700	3.04156300	-0.38314500	H	1.22817600	5.20638500	-0.50331000
H	1.61102500	2.52738100	-2.01563300	H	-1.17681100	4.79134500	-2.37018900
H	0.15297500	0.81876400	-1.28727400	H	0.48659200	5.07766800	-2.86941300
H	-0.89672000	1.83351000	-2.26816000	H	1.17680000	2.85159400	-1.92747800
C	-4.62178600	-2.41642400	1.01799400	H	-0.06893900	2.71595400	-3.14802100
H	-5.68634300	-2.47885200	0.75326600	H	-0.81000800	1.22192600	-1.51247900
H	-4.37678100	-3.28073600	1.64836600	H	-1.78802900	2.64996200	-1.16410000
H	-4.47438600	-1.51311800	1.62355100	C	5.35337900	-1.34451700	-0.88217900
C	-3.87983300	-3.98011900	-1.51521400	H	6.36425600	-1.51375200	-0.48721200
H	-4.94198400	-4.05652600	-1.78629600	H	5.24493500	-1.93970200	-1.79775100
H	-3.29139900	-4.00810500	-2.44120400	H	5.25592600	-0.28727100	-1.14864200
H	-3.61743400	-4.86852700	-0.92634000	C	4.28299900	-3.65462000	0.82852100
C	-4.06127000	-0.91355700	-1.60461200	H	5.27761700	-3.81142700	1.26823700
H	-3.51274100	-0.91135700	-2.55552000	H	3.53755800	-3.99920100	1.55644600
H	-5.13588000	-0.94222700	-1.83019500	H	4.21061500	-4.29346800	-0.06071000
H	-3.83987100	0.03169400	-1.09298300	C	4.29918200	-0.81550700	1.98148500
				H	5.31384100	-0.96191200	2.37577900
				H	4.15671500	0.24944500	1.77283900
				H	3.58772000	-1.11878400	2.76066900

TS_(1-5D)

E = -1807.212782 a.u.

Ni	0.36646600	-0.78842900	-0.19486000
C	2.31327400	-1.55865800	-0.27322500
C	1.28547900	-2.34965800	-0.48102200
C	0.94610900	-3.78548200	-0.67974500
H	0.04777800	-4.06840400	-0.11773200
H	0.72719400	-3.96701500	-1.74187400
H	1.76573000	-4.45705300	-0.39479800
N	0.10706500	1.02332800	0.74892000
N	-1.47550300	-1.27733100	-0.73427300
C	2.26886700	0.21177100	-1.16117900
O	1.65266500	0.15145600	-2.21739200
O	3.01539800	0.96840500	-0.56381800
S	4.04348400	-1.81837200	0.39651300
N	-3.77954700	-1.79571400	-0.46107500
C	-1.63861900	-1.41786600	-2.19769500
C	-3.01737800	-0.92664700	-2.65049800
C	-4.09960900	-1.70526300	-1.90232700
C	-4.89029600	-2.19732500	0.42288000
C	-5.47359100	-1.05260500	1.27633800
C	-4.62968200	-0.71699900	2.51911400
C	-3.16695300	-0.33376500	2.22612200

TS_(1-5D)

E = -1807.2099177 a.u.

Ni	0.40335600	-0.80555500	-0.06342000
C	0.80651800	-2.81333100	-0.25374100
C	1.83596300	-2.01613700	-0.07120600
N	-1.40260000	-0.23371200	-0.85015700
N	1.13836000	0.90180500	0.63607400
C	-0.73163600	-2.60553100	0.89935600
O	-0.44266600	-2.07319300	1.96886300
O	-1.67523700	-3.19644500	0.39809600
C	0.59776600	-4.11822200	-0.97189200
H	1.40890500	-4.31979300	-1.68056200
H	0.54392300	-4.95193700	-0.26014600
H	-0.35912600	-4.10967800	-1.50178200
S	3.68762800	-1.99630000	-0.13367600
N	1.82828400	3.17678900	0.60511400
C	1.42491000	0.85468800	2.08697900
C	1.10673600	2.19442000	2.75850200
C	1.90807800	3.30319800	2.07656200
C	2.23860000	4.36425600	-0.16832900

C	1.07144500	5.14572200	-0.80525700	H	-5.21139400	-0.05604200	-1.84728300
C	0.53655100	4.50854100	-2.10027600	C	-4.59447700	0.99553600	1.98340600
C	0.05703600	3.05210200	-1.95670500	H	-5.57578100	0.72395600	2.39654100
C	1.14810800	2.05401400	-1.49623400	H	-3.84646200	0.82598800	2.76767400
C	1.38043300	2.01599600	-0.00018900	H	-4.62278600	2.06906300	1.76216500
H	2.48604400	0.60151400	2.22810100	C	-4.64123800	-1.85492900	0.93315200
H	0.84131200	0.03596400	2.51235200	H	-3.97532600	-2.19247900	1.73775800
H	0.03232600	2.39854300	2.67003400	H	-5.67389000	-1.93679000	1.29833800
H	1.34813600	2.16350400	3.82660600	H	-4.51679000	-2.52607800	0.07920800
H	2.96125800	3.26287200	2.39249600	N	3.73157200	0.73743600	0.35448700
H	1.51930900	4.29000000	2.35906800	C	1.60682000	2.19203100	-0.71098500
H	2.96286200	4.07751300	-0.94178400	C	2.98990400	2.37603100	-1.34247900
H	2.77667300	5.01238300	0.53068900	C	4.06241200	2.01410500	-0.31646100
H	0.26565600	5.23892500	-0.06374000	C	4.84663700	0.07496500	1.06509800
H	1.41648700	6.16507300	-1.02849600	C	5.42927700	-1.14890100	0.33197300
H	1.33180100	4.54242800	-2.86136500	C	4.57891000	-2.42303200	0.48830700
H	-0.28675800	5.12303600	-2.48882500	C	3.11477200	-2.28649600	0.03174900
H	-0.31757900	2.71603200	-2.93266300	C	2.29307600	-1.22321400	0.80588700
H	-0.79331500	2.99550300	-1.26416100	C	2.47155600	0.19144400	0.29286900
H	0.86253500	1.03839100	-1.77670600	H	1.46998300	2.89463000	0.12393200
H	2.09280800	2.27226100	-2.01531800	H	0.81542600	2.38836100	-1.43634100
N	-3.74837700	0.11730500	-0.85310800	H	3.07445300	1.72552000	-2.22148700
C	-1.53089300	-0.66887400	-2.25871100	H	3.13008300	3.40810100	-1.68063200
C	-2.79654000	-1.51168700	-2.45023100	H	4.16080500	2.80930400	0.43687600
C	-4.00592000	-0.65091300	-2.09268800	H	5.03813900	1.90042500	-0.80402800
C	-4.94164400	0.71198900	-0.22174000	H	4.52594800	-0.20791100	2.07537700
C	-5.54169200	-0.12750000	0.92296600	H	5.62156600	0.83781100	1.18942100
C	-4.76547400	0.00635800	2.24569200	H	5.55080400	-0.89798600	-0.73104000
C	-3.27100000	-0.35342900	2.15792600	H	6.43575300	-1.34188100	0.72813400
C	-2.44371600	0.54990800	1.20491000	H	4.59002700	-2.72474500	1.54731500
C	-2.50656100	0.12863400	-0.24931500	H	5.05380700	-3.24105900	-0.06890200
H	-0.63540800	-1.24117200	-2.51059500	H	2.61541400	-3.25365400	0.16487500
H	-1.55896300	0.21610100	-2.91575500	H	3.06773000	-2.06441200	-1.04290000
H	-2.73147300	-2.37839500	-1.78339300	H	1.22867200	-1.46256400	0.72543100
H	-2.88548100	-1.87174100	-3.48122400	H	2.54051100	-1.26757100	1.87611900
H	-4.24289100	0.04869200	-2.90822900				
H	-4.89148700	-1.27967900	-1.93072400				
H	-4.70393500	1.72074900	0.13822000				
H	-5.67993300	0.83592000	-1.02183200				
H	-6.58204600	0.19042600	1.08170000				
H	-5.57519000	-1.17967900	0.60830100				
H	-4.86328800	1.04374300	2.60563300				
H	-5.24179400	-0.62848900	3.00478700				
H	-3.13818000	-1.39965700	1.85912100				
H	-2.83257200	-0.26912600	3.15978900				
H	-1.39318000	0.50471000	1.48899300				
H	-2.76796300	1.59673500	1.31169300				
C	4.36857500	-2.12331400	1.63008200				
H	4.04863900	-3.06081200	2.10090200				
H	5.46645100	-2.09707100	1.63170900				
H	4.00698100	-1.29930300	2.25701100				
C	4.35575400	-3.45376800	-1.14939100				
H	3.99661800	-3.41422800	-2.18557100				
H	5.45390400	-3.44048600	-1.17417600				
H	4.03991900	-4.41290200	-0.72123900				
C	4.30523000	-0.38782500	-0.92241900				
H	3.97060800	0.48216800	-0.34496900				
H	5.40199700	-0.36726100	-0.97157100				
H	3.91843800	-0.28200900	-1.94418700				

TS_{(3-4)D}
E = -1807.183840 a.u.

Ni	-0.27645600	-0.00735700	-0.37965000
C	-2.42526100	0.08816900	-0.04985700
C	-1.59045900	1.07736200	0.24298600
C	-1.61431000	2.42167800	0.88315800
H	-0.94343600	2.44948800	1.75125300
H	-1.25966700	3.18537100	0.17880900
H	-2.61563200	2.71417300	1.21468300
O	-3.06909500	-1.52699200	-1.76112300
O	-0.94297900	-1.84446800	-1.04983800
C	-2.06977700	-1.27450500	-1.10330100
N	1.42865100	0.81117100	-0.21344000
Si	-4.26553100	-0.07033900	0.44338200
C	-5.39085200	0.53537400	-0.94551800
H	-6.44697100	0.43891900	-0.65932700
H	-5.19969900	1.59050700	-1.17867800

TS_{(3-4)D'}
E = -1807.178993 a.u.

Ni	-0.73367400	0.80952200	0.64839900
C	-2.83031000	0.99564500	0.03656900
C	-2.11669600	-0.11114700	-0.13140100
O	-2.97856000	3.46988200	0.01052900
O	-1.11478400	2.77048100	1.09028600
C	-2.19131100	2.65151900	0.44303200
N	0.83485400	-0.26472000	0.79086800
C	-4.32257500	1.16290800	-0.14233000
H	-4.79884300	0.21129900	-0.39105200
H	-4.77345500	1.55739300	0.77514600
H	-4.52545900	1.89588300	-0.92679100
Si	-2.33787500	-1.87694800	-0.69160900
C	-3.85895400	-2.08694400	-1.80267900
H	-3.88038500	-3.10181900	-2.22223000
H	-4.79494900	-1.93578300	-1.25257500
H	-3.84194400	-1.37731300	-2.63858100
C	-2.52582900	-0.99952300	0.82355300
H	-2.61831800	-4.05206100	0.52446700
H	-1.66434800	-2.91287200	1.49655300
H	-3.42205200	-2.73121600	1.39641300
C	-0.81514200	-2.40980400	-1.68217700
H	-0.67766300	-1.76780800	-2.56147500
H	0.09473000	-2.34971700	-1.07422700
H	-0.92464400	-3.44376700	-2.03459100
N	3.05400800	-0.84490800	0.18619800
C	0.94369100	-1.12904900	1.98723200
C	2.36895400	-1.11768700	2.54800400
C	3.34254800	-1.55285000	1.45397700
C	4.14523400	-0.83958300	-0.81247400
C	4.89079500	0.50446300	-0.92843000
C	4.14092800	1.55756100	-1.76484400
C	2.72029800	1.88845900	-1.27105700
C	1.74723900	0.68143500	-1.25624800
C	1.86294800	-0.19384100	-0.02526000
H	0.64502900	-2.15248000	1.71767200
H	0.22822700	-0.76588100	2.72787200
H	2.61418100	-0.10489300	2.88987500
H	2.45373700	-1.78712600	3.41044500
H	3.28001900	-2.63821200	1.28928300

H	4.37440100	-1.32295800	1.74502300
H	3.75252400	-1.13966700	-1.79173300
H	4.84121800	-1.62566100	-0.50416900
H	5.08645200	0.88756500	0.08285100
H	5.87006400	0.31678900	-1.38989300
H	4.07736600	1.19913900	-2.80418000
H	4.73472000	2.48040900	-1.79424000
H	2.29246700	2.65403900	-1.92976300
H	2.75716300	2.33421100	-0.26801200
H	0.71530100	1.04218100	-1.28138400
H	1.89138700	0.07610800	-2.16215500

5D

E = -1807.2650892 a.u.

Ni	-0.02418200	0.15963000	-0.00862800
O	-0.80383300	1.60332100	-0.84928100
O	-0.51367000	3.76636600	-1.33761400
N	-1.75822900	-0.88878400	-0.48799500
N	0.79753200	-1.45838600	0.74349600
C	-0.11173000	2.72853600	-0.80908900
C	1.18137500	2.62791200	-0.04188900
C	1.38440700	1.38068400	0.44995700
C	2.53128100	0.97546500	1.33901500
H	2.15685600	0.58624600	2.29727100
H	3.11954700	0.16226700	0.89583400
H	3.21366800	1.79987100	1.56267200
S	2.15148200	4.25943300	0.04918300
N	-4.07747900	-0.62560400	-0.95280100
N	2.07979400	-3.45416700	0.62916900
C	-1.64164300	-1.81917700	-1.62180700
C	-2.93272200	-2.61100300	-1.85777400
C	-4.09167500	-1.63131900	-2.03358200
C	-5.32053400	0.15347000	-0.77431100
C	-6.09793800	-0.17778000	0.51329200
C	-5.50546700	0.47970300	1.77175600
C	-4.02536400	0.14469800	2.03506300
C	-3.04501700	0.60365200	0.92598200
C	-2.92598100	-0.35114100	-0.24568600
C	0.33072600	-1.83625000	2.09112500
C	1.39902300	-2.62528900	2.85516800
C	1.81315900	-3.84281500	2.03040800
C	2.80603500	-4.44577900	-0.19079200
C	4.25794000	-4.06167500	-0.53254500
C	4.36829200	-3.04357900	-1.68036700
C	3.61717500	-1.72196200	-1.43780300
C	2.08247100	-1.86225700	-1.27506900
C	1.61012300	-2.26418200	0.11055300
H	-0.81107300	-2.49948600	-1.40920400
H	-1.37419600	-1.25143300	-2.52574300
H	-3.12619400	-3.26224300	-0.99565100
H	-2.84536900	-3.25071800	-2.74323100
H	-4.02651500	-1.13062700	-3.01109600
H	-5.05210300	-2.15987900	-1.99744800
H	-5.09469700	1.22616900	-0.81452400
H	-5.94402700	-0.06428500	-1.64707800
H	-7.13593700	0.16164100	0.38965500
H	-6.13272300	-1.26996700	0.63238400
H	-5.60445800	1.57198300	1.67778200
H	-6.10384800	0.18937500	2.64601500
H	-3.90949100	-0.93617400	2.20263500
H	-3.72541900	0.63635200	2.96986900
H	-2.03983900	0.70366100	1.33964100
H	-3.31252800	1.60448400	0.56520800
H	-0.59485200	-2.42193600	1.99695500
H	0.07632800	-0.91436600	2.62066100
H	2.26786900	-1.97979200	3.03025400
H	1.02322500	-2.94703100	3.83245900
H	1.02549200	-4.61107500	2.05828900
H	2.72509200	-4.29311800	2.44096400
H	2.24673600	-4.64754800	-1.11426200
H	2.79740300	-5.37741000	0.38383800
H	4.74134900	-3.67041300	0.37324600
H	4.80001900	-4.97576900	-0.81237100
H	3.98218700	-3.50669500	-2.60195900
H	5.42804200	-2.82514500	-1.86665900
H	3.79840100	-1.05650500	-2.29107400
H	4.03162400	-1.21203100	-0.55882000

H	1.60623500	-0.89941600	-1.48527000
H	1.70153800	-2.57476100	-2.02167200
C	1.09041900	5.57276200	0.90828600
H	0.89404900	5.30259900	1.95436700
H	1.58543200	6.55334500	0.89974800
H	0.13132100	5.65805900	0.38762200
C	3.80045100	4.17495800	0.99949800
H	4.28400200	5.16036900	0.93824200
H	3.66428600	3.94324200	2.06312600
H	4.49593300	3.44127200	0.57315200
C	2.57208500	4.81631700	-1.71211800
H	3.26317600	4.11310800	-2.19572800
H	1.65325600	4.86114600	-2.30496800
H	3.04390500	5.80836100	-1.71365600

5D'

E = -1807.2562328 a.u.

Ni	-0.15935500	0.54095100	-0.22325900
O	-1.25502000	1.60692500	-1.26137300
O	-1.28680300	3.52409300	-2.42483400
N	-1.73364600	-0.82799400	-0.39681300
N	0.91401500	-0.88484200	0.63281300
C	-0.73459300	2.75627800	-1.64305200
C	0.58743400	3.04623200	-0.98508300
C	1.05424400	2.08011300	-0.15269000
C	1.15011300	4.41165200	-1.30851200
H	2.18572400	4.54530400	-0.98934600
H	1.08650000	4.58278400	-2.38904200
H	0.54214500	5.20046100	-0.84448800
S	2.52180400	2.44463600	0.98146700
N	-4.09364900	-0.86697500	-0.70520400
N	2.22429800	-2.86018200	0.42765800
C	-1.57369100	-1.78128100	-1.50548400
C	-2.77026100	-2.73160300	-1.62972700
C	-4.05000400	-1.90580300	-1.75420500
C	-5.40590500	-0.22366700	-0.48397300
C	-6.05100400	-0.54261100	0.87788100
C	-5.45752600	0.26733600	2.04352000
C	-3.93532300	0.11535200	2.22142300
C	-3.08951300	0.59574600	1.01554300
C	-2.94037000	-0.41792900	-0.10129900
C	0.38992400	-1.36189100	1.92954500
C	1.38814700	-2.25681400	2.66991600
C	1.83270700	-3.39091000	1.74997900
C	3.00257800	-3.77757100	-0.43116100
C	4.46501900	-3.35739300	-0.66637300
C	4.61865400	-2.25211100	-1.72446400
C	3.83367300	-0.96441600	-1.41808300
C	2.29419900	-1.13163900	-1.34882900
C	1.76283700	-1.63705500	-0.02029900
H	-0.65254400	-2.34758700	-1.33071700
H	-1.43784300	-1.21581800	-2.43924800
H	-2.82672400	-3.37088700	-0.73914100
H	-2.66238100	-3.38687900	-2.50149200
H	-4.10680100	-1.43447100	-2.74647700
H	-4.93393500	-2.54499700	-1.64057100
H	-5.31512400	0.86200900	-0.61501800
H	-6.05718100	-0.57803300	-1.28882600
H	-7.12704600	-0.32976100	0.80918100
H	-5.95193900	-1.62009800	1.07067200
H	-5.68537100	1.33236400	1.88394100
H	-5.96172700	-0.02042000	2.97599400
H	-3.68711500	-0.93169300	2.44850700
H	-3.63271200	0.70240200	3.09856000
H	-2.07528900	0.83400600	1.34472600
H	-3.49371300	1.53210200	0.61034500
H	-0.55355200	-1.89268700	1.74618000
H	0.14835200	-0.47981500	2.52897100
H	2.25654900	-1.66332000	2.97514500
H	0.93409300	-2.66991400	3.57761800
H	1.02403900	-4.12857300	1.62980300
H	2.69497500	-3.91669100	2.17670300
H	2.49392300	-3.90994500	-1.39568400
H	2.97679600	-4.75154600	0.06726000
H	4.89620600	-3.03364000	0.29091800
H	5.03141300	-4.24256600	-0.98800200
H	4.28744400	-2.64599100	-2.69808100

H	5.68285800	-2.00647000	-1.83743900
H	4.04934600	-0.23074900	-2.20493900
H	4.19206900	-0.52245500	-0.47960500
H	1.81849700	-0.16026300	-1.51164400
H	1.95995200	-1.79039700	-2.16373100
C	2.14336700	3.98757100	2.02874200
H	2.98779000	4.22648100	2.68980300
H	1.93590100	4.86744500	1.41081700
H	1.26218000	3.81159500	2.65993700
C	4.15433100	2.73318600	0.03929000
H	4.97449400	2.90001700	0.75145300
H	4.41693400	1.86405100	-0.57610100
H	4.10553500	3.60342500	-0.62461300
C	2.91674700	1.09489600	2.25701200
H	2.03930300	0.85479900	2.86881700
H	3.27420500	0.17036100	1.79190300
H	3.70321100	1.46231400	2.93043700

1E

E = -781.3051369 a.u.

Ni	-0.96920500	-0.84446900	0.00296200
N	-0.51509300	1.06300700	0.00053600
N	0.98927200	-1.03075900	0.00396600
C	-2.77033100	-1.34245400	-0.00294200
C	-2.00258300	-2.38376900	0.00529400
H	-2.01642100	-3.46840000	0.01021900
C	-4.16907100	-0.83140800	-0.01120500
H	-4.35004900	-0.18128600	-0.87776700
H	-4.91008100	-1.64219100	-0.04302600
H	-4.37483000	-0.22858000	0.88367700
C	-1.38348100	2.10103300	0.00181900
C	-0.97633000	3.43238600	0.00214800
C	0.39529800	3.72109800	0.00137600
C	1.30088200	2.66204500	0.00022500
C	0.82502200	1.34238800	-0.00022400
C	1.68310800	0.14730900	-0.00076100
C	3.08595400	0.17337900	-0.00600100
C	3.79566600	-1.02570100	-0.00612700
C	3.08084700	-2.23150300	-0.00098700
C	1.68904200	-2.18768700	0.00379400
H	-2.43208300	1.83163000	0.00260900
H	-1.71672500	4.22377900	0.00311200
H	0.74775400	4.74650800	0.00183000
H	2.36616800	2.85853400	0.00013300
H	3.61635400	1.11792100	-0.01037700
H	4.87999900	-1.02264700	-0.01023400
H	3.59188200	-3.18716800	-0.00078200
H	1.09237300	-3.09139800	0.00770000

TS_{(1-5)E}

E = -969.8565007 a.u.

Ni	-0.84289500	-0.35055200	-0.15013700
N	0.88731900	-1.18254500	0.07579800
N	0.24385200	1.31942900	-0.18342200
C	-2.14574300	-1.56091500	-0.62170100
O	-2.22867400	0.18485300	1.86259800
O	-3.15447800	1.79464900	0.51592100
C	-2.84807100	-0.45090500	-0.52783700
C	-2.69420200	0.71069400	0.85110100
C	-2.30273500	-2.95712600	-1.10468400
H	-1.44786000	-3.28562000	-1.70810600
H	-2.37570500	-3.63931600	-0.24489000
H	-3.21834500	-3.08678600	-1.69697600
H	-3.71023100	-0.10980300	-1.09348800
C	1.11860300	-2.49824500	0.27080900
C	2.40153300	-3.02351600	0.41866000
C	3.49625900	-2.15536600	0.36122200
C	3.26481100	-0.79325200	0.16895000
C	1.95108700	-0.32610600	0.03476100
C	1.58502300	1.09455900	-0.13539400
C	2.50566300	2.14580000	-0.22770100
C	2.03408000	3.45288700	-0.36174600
C	0.65464300	3.67580300	-0.39304600
C	-0.21096300	2.58348200	-0.30107800
H	0.24187700	-3.13059900	0.30752000
H	2.53370900	-4.08718200	0.57557200

H	4.50798500	-2.52951600	0.46945400
H	4.09656800	-0.10114300	0.13213700
H	3.57067000	1.95279300	-0.19424900
H	2.73147100	4.28012000	-0.43440200
H	0.24850900	4.67595300	-0.48305100
H	-1.29046800	2.69559000	-0.29437400

TS_{(1-5)E'}

E = -969.8532711 a.u.

Ni	-0.65958600	-0.59329800	-0.09150200
N	1.18412400	-1.15151100	-0.00177800
N	0.15369900	1.23132300	-0.10786400
C	-1.68873400	-2.04520900	-0.52430800
O	-2.06398500	-0.28015900	1.91231700
O	-3.24811400	1.11062100	0.52463600
C	-2.66352600	-1.17662100	-0.45893600
C	-2.60833200	0.13255200	0.89033300
C	-3.99826200	-1.04167200	-1.13501200
H	-4.81424800	-1.21111500	-0.42168200
H	-4.12009800	-0.02144200	-1.50916500
H	-4.09976900	-1.75443700	-1.96092700
H	-1.55748200	-3.05400500	-0.90489000
C	1.61949600	-2.42524900	0.09957300
C	2.97293800	-2.75435300	0.15261600
C	3.91993700	-1.72656100	0.09592800
C	3.47647600	-0.40784500	-0.00238100
C	2.10172000	-0.14120600	-0.04406600
C	1.51545000	1.21199500	-0.11904900
C	2.26317200	2.39422100	-0.18634600
C	1.59720800	3.61987500	-0.23626800
C	0.19995000	3.63149700	-0.21419700
C	-0.48760300	2.41758700	-0.15017500
H	0.84888000	-3.18336600	0.13798500
H	3.27219700	-3.79204900	0.23650200
H	4.98086800	-1.94664400	0.13193500
H	4.19157500	0.40413500	-0.03957400
H	3.34550800	2.36299300	-0.19789700
H	2.15956800	4.54562400	-0.28745200
H	-0.35539700	4.56109400	-0.24291900
H	-1.57048400	2.36509500	-0.11426600

5E

E = -969.91904 a.u.

Ni	0.78690700	-0.11854500	-0.00672800
N	-0.87088600	-1.21948100	-0.00683900
N	-0.56081400	1.35134700	-0.00722600
C	2.26141100	-1.38253500	0.01303400
O	2.07951500	1.17648100	-0.01379400
O	4.29540900	1.53295700	-0.00824000
C	3.42947000	-0.71551300	0.01345400
C	3.34788500	0.76195700	-0.00372200
C	2.27981800	-2.89046500	0.03086700
H	1.77041300	-3.30524700	0.91308700
H	1.80260200	-3.32507600	-0.86004700
H	3.31189600	-3.26767900	0.05302600
H	4.41287300	-1.18947300	0.02561500
C	-0.96621000	-2.56513500	-0.01731800
C	-2.18319900	-3.24826800	-0.01605500
C	-3.36974100	-2.51422000	-0.00339000
C	-3.28861400	-1.12228100	0.00537700
C	-2.03565200	-0.49805200	0.00241800
C	-1.85932100	0.96593700	0.00526300
C	-2.89896500	1.90414900	0.01740100
C	-2.58134100	3.26438100	0.01558900
C	-1.23774800	3.64927800	0.00187900
C	-0.25048100	2.66077600	-0.00887400
H	-0.03489800	-3.10499500	-0.02641700
H	-2.18798700	-4.33135000	-0.02471400
H	-4.33403700	-3.00956300	-0.00128700
H	-4.19161500	-0.52559600	0.01350700
H	-3.93434200	1.58786800	0.02828500
H	-3.37056900	4.00801500	0.02475300
H	-0.95255100	4.69425500	-0.00009800
H	0.81345100	2.86948700	-0.01813000

5E'

E = -969.9261604 a.u.

Ni	0.63529100	-0.09502600	-0.00715600
N	-0.89245200	-1.30606500	-0.00476900
N	-0.79437400	1.27117400	-0.00833000
C	2.07813900	-1.31440600	0.00842800
O	1.92308100	1.21058700	-0.01192100
O	4.14584800	1.53743800	-0.00507000
C	3.27948700	-0.71370500	0.00971500
C	3.18437100	0.78315600	-0.00304800
C	4.64064200	-1.35015100	0.02229000
H	5.22283400	-1.04312100	-0.85579600
H	5.21516500	-1.02518300	0.89898700
H	4.57185600	-2.44374100	0.03321100
H	2.01265700	-2.40899200	0.01855900
C	-0.84843300	-2.65346900	-0.01103000
C	-1.99553600	-3.44777300	-0.00818100
C	-3.24697300	-2.82708400	0.00167000
C	-3.30370900	-1.43295300	0.00702600
C	-2.11627800	-0.69239900	0.00302600
C	-2.05983300	0.78292300	0.00412400
C	-3.16777800	1.63834700	0.01566500
C	-2.95374000	3.01935100	0.01345900
C	-1.64372800	3.50852500	0.00011100
C	-0.58298400	2.59911600	-0.01012700
H	0.13805700	-3.09437700	-0.01828400
H	-1.90102500	-4.52674000	-0.01350200
H	-4.15883900	-3.41337400	0.00450700
H	-4.26079000	-0.92665200	0.01351100
H	-4.17585300	1.24293600	0.02659000
H	-3.79755100	3.70042200	0.02224200
H	-1.44217000	4.57280100	-0.00184900
H	0.46200000	2.88992300	-0.01894900

DBU

E = -461.9787685 a.u.

N	-1.46246800	-1.46809700	-0.13812000
N	-0.32046700	0.62625000	-0.37358900
C	-2.72445900	-0.74332100	0.05994700
C	-2.52668100	0.62208300	0.73644000
C	-1.51078800	1.44094400	-0.06513700
C	0.90598700	1.35280400	-0.73722600
C	2.01461900	1.31317400	0.33491900
C	2.81324300	-0.00310700	0.35233600
C	1.97025800	-1.27532200	0.56419500
C	0.90182800	-1.53437500	-0.52812400
C	-0.39580700	-0.76646300	-0.34095000
H	-3.38600200	-1.37677200	0.66303900
H	-3.22421000	-0.60874100	-0.91328000
H	-2.14966300	0.46628600	1.75531700
H	-3.47193800	1.17212400	0.81456000
H	-1.97140100	1.80929100	-0.99601200
H	-1.19311200	2.32100500	0.50914700
H	1.30215700	0.97940400	-1.69208700
H	0.60969700	2.39208600	-0.91548200
H	2.70979400	2.14497500	0.15047900
H	1.55594000	1.49332400	1.31713300
H	3.35395700	-0.09690100	-0.60284500
H	3.58137800	0.05486400	1.13578300
H	1.47673200	-1.24328900	1.54554600
H	2.65140400	-2.13663400	0.58791300
H	0.61021600	-2.58701700	-0.51756600
H	1.33639400	-1.32957900	-1.51808300

CO₂

E = -188.5775705 a.u.

C	-0.46875000	0.84821400	0.00000000
O	-1.63833400	0.84821400	0.00000000
O	0.70083400	0.84821400	0.00000000