

**Computational Insight into Mechanism of Nickel-Catalyzed Reductive
Carboxylation of Styrenes Using CO₂**

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Table S1. The relative free energies of the oxidative coupling transition states **TS**₂₋₅, the metallacycle intermediates **5** and the transmetallation transition states **TS**₁₁₋₁₃, which are relevant in the oxidative coupling mechanism, and the styrene insertion transition states **TS**₁₈₋₂₀ and the reductive elimination transition states **TS**₂₀₋₁, which are relevant in the nickel-hydride mechanism, calculated for the reactions using different methods and basis sets. The free energies are given in kcal/mol.

Methods and basis sets	Oxidative coupling mechanism			Nickel-hydride mechanism	
	TS ₂₋₅ (oxidative- coupling)	5 (metallacycle intermediate)	TS ₁₁₋₁₃ (transmetallation)	TS ₁₈₋₂₀ (styrene insertion)	TS ₂₀₋₁ (reductive elimination)
B3LYP/6-31G(d,p) ^a	21.0	-9.3	24.1	19.8	19.8
B3LYP/6-311++G(d,p) ^b //B3LYP/6-31G(d,p) ^a	23.8	-5.7	27.9	18.3	21.1
B3LYP-D3/6-31G(d,p) ^a	5.7	-23.7	11.3	14.0	14.5
M06/6-31G(d,p) ^a	3.8	-22.6	13.7	14.6	9.9

^a The 6-311+G (d) basis set was used for oxygen atoms, while the 6-31G(d,p) basis set was used for Zn, C, H and N atoms.

^b All the atoms except for Nickel are described by the 6-311++G(d,p) basis set. Nickel was always described by Lanl2DZ.

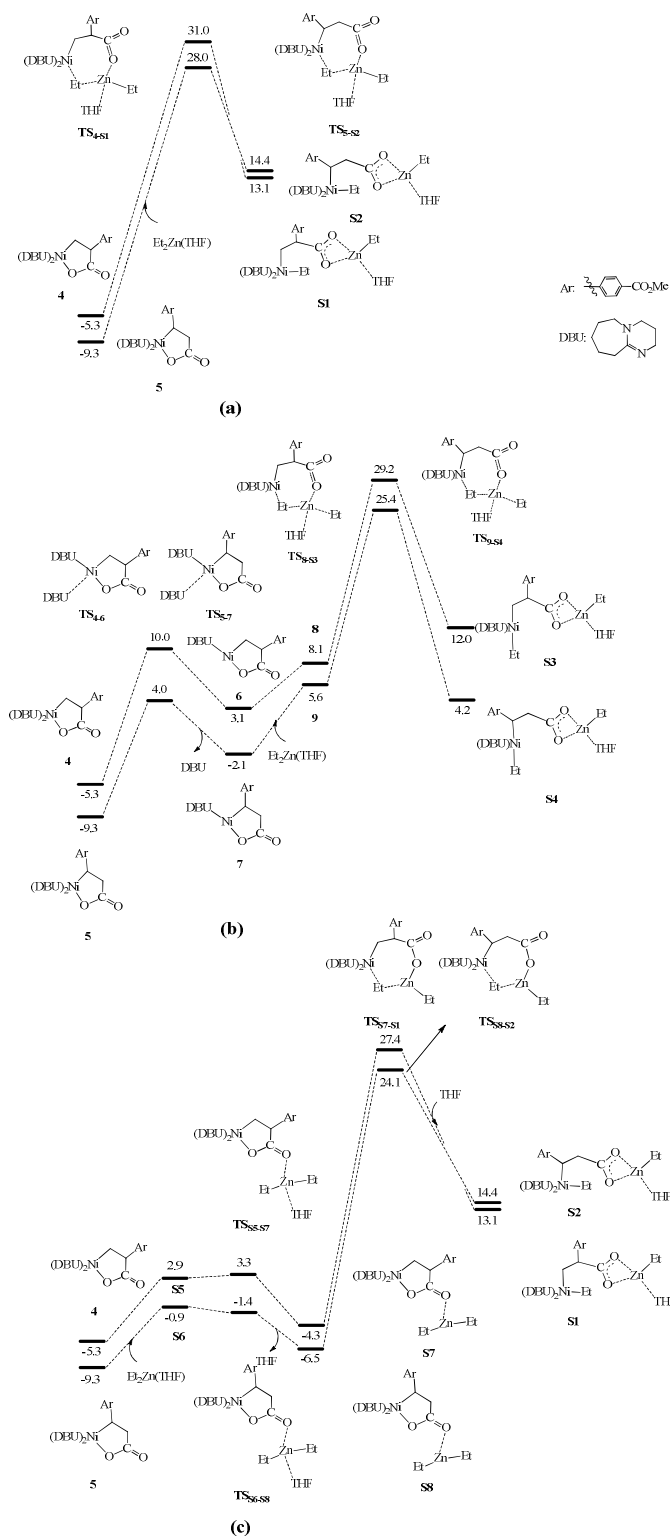


Figure S1 Free energy profiles calculated for the second step (**D** → **E**) based on the catalytic cycle shown on the right-hand side of Scheme 3, (a) without dissociation of DBU and THF, (b) only dissociation of DBU, (c) only dissociation of THF.

Cartesian coordinates and electronic energies for all of the calculated structures

CO₂

scf done: -188.63856747

C	-1.21597700	0.49785500	-2.04015700
O	-0.05327600	0.49785500	-2.04015700
O	-2.37867700	0.49785500	-2.04015700

C₂H₄

scf done: -78.59289646

C	1.90402500	1.64787200	0.00088600
C	2.62214300	2.76955400	0.00093300
H	2.37323100	0.66726200	0.00146300
H	3.70911400	2.75389900	0.00155000
H	2.15294200	3.75016700	0.00035500
H	0.81705700	1.66352900	0.00026700

THF

scf done: -232.48289361

C	0.17066200	-0.89166500	0.00000000
O	1.60517800	-0.87109800	0.00000000
C	2.12784500	0.46507400	0.00000000
C	0.93902100	1.44952300	-0.00000100
C	-0.33397400	0.56698800	-0.00000100
H	-0.16686100	-1.44154500	-0.88678600
H	-0.16686100	-1.44154500	0.88678600
H	2.76102700	0.58808100	0.88687000
H	2.76102800	0.58808100	-0.88687000
H	0.97068600	2.09728000	0.87974400
H	0.97068700	2.09727900	-0.87974700
H	-0.95154000	0.76472000	0.87976000
H	-0.95154000	0.76471900	-0.87976200

DBU

scf done: -462.10722576

C	-3.58118400	3.36459500	1.45713000
C	-3.00132000	4.31553600	0.36550200
C	-1.92319400	5.27414200	0.84207200
C	-3.40163000	3.82988900	2.91224800
C	-4.03941100	5.18487400	3.25825200
C	-3.70518900	6.29080300	2.23354600
H	-4.64508700	3.19507000	1.25088000
H	-2.54960100	3.72948200	-0.43628300
H	-2.32818900	3.87973400	3.13082100
H	-3.70099600	5.48703400	4.25707900
H	-3.09314400	2.38836600	1.36089500
H	-3.81201900	4.89552500	-0.09048000
H	-3.80887100	3.06314600	3.58204200
H	-5.13175900	5.09259400	3.31440500
H	-3.86352700	7.27836600	2.67730700
H	-4.39484100	6.22998300	1.38672200
C	-1.34898900	7.13453600	2.36969700
H	-1.62582500	7.27143400	3.42137600
H	-1.38556200	8.12696100	1.89630500
C	0.05723100	6.54963400	2.26162600
H	0.79650800	7.30094500	2.55846900
H	0.15590300	5.70071100	2.94884200
C	0.29348200	6.06530200	0.82788700
H	1.27287000	5.57737500	0.74956000
H	0.33150200	6.93295600	0.14942000
N	-2.32964200	6.24452000	1.73880200
N	-0.72842600	5.12711000	0.36765500

Et₂Zn(THF)

scf done: -2170.07372047

Zn	-1.33052600	1.41530000	0.80019700
C	-0.12132600	3.32528900	-1.12907700
H	0.86989700	3.16259600	-0.68653200
H	-0.09678300	4.32158000	-1.59614500
H	-0.22095500	2.59610000	-1.94204500
C	-1.24339500	3.17715600	-0.08581300
H	-1.11682000	3.95560300	0.68102600
H	-2.20798500	3.41211200	-0.56133500
C	-1.34442800	0.01941500	2.19786400
H	-0.42811800	-0.58568200	2.12191600
H	-2.16529400	-0.68714100	2.00191200
C	-1.47520500	0.53795100	3.64177100
H	-2.40265400	1.10573000	3.78978200
H	-1.47848000	-0.26907100	4.39038700
H	-0.65169300	1.21144900	3.91091700
C	-1.44831000	-1.34647700	-1.04711400
O	-1.49569400	0.09697600	-1.08701600
C	-2.39306800	0.45071400	-2.15481100
C	-3.54320600	-0.54592900	-2.01248600
C	-2.82338500	-1.84058900	-1.55970200
H	-0.63126800	-1.68931700	-1.69363600
H	-1.23027700	-1.63192600	-0.01757900
H	-2.67325800	1.49593900	-2.01780100
H	-1.87559300	0.33757300	-3.11782500
H	-4.23708800	-0.19879100	-1.24068000
H	-4.10398200	-0.67303200	-2.94185900
H	-3.38384600	-2.36055000	-0.77916400
H	-2.69359100	-2.53552800	-2.39354700

H₂C=CHC₆H₄-p-COOMe

scf done: -537.59515188

C	-1.78321100	0.49071300	0.00113600
C	-0.39218000	0.49803200	0.00126300
C	0.33474200	1.70293800	0.00031700
C	-0.38935400	2.91241400	-0.00075600
C	-1.77672400	2.91172500	-0.00087500
C	-2.49054200	1.70155500	0.00006500
H	-2.32219000	-0.44947400	0.00187400
H	0.14687000	-0.44527200	0.00210800
H	0.13714000	3.86119900	-0.00150300
H	-2.32617000	3.84699000	-0.00170500
C	1.80504700	1.64291900	0.00049200
C	2.65645200	2.67726500	-0.00038400
H	2.21740900	0.63487200	0.00144000
H	3.72892000	2.51207200	-0.00014900
H	2.32872700	3.71260900	-0.00136100
C	-3.97591000	1.75430200	-0.00011600
O	-4.63130700	2.78141700	-0.00091400
O	-4.54234100	0.53216100	0.00062300
C	-5.98293100	0.48523800	0.00047800
H	-6.23687900	-0.57351500	0.00130300
H	-6.37947100	0.97539500	0.89222400
H	-6.37923100	0.97393900	-0.89217600

H₃CCH(COOZn(THF)Et)C₆H₄-p-COOMe

scf done: -2817.76062975

Zn	-2.81373600	7.70161900	-0.35197300
C	-2.28445900	5.29336800	-0.68341000
O	-1.50766100	6.04991300	-0.02426800
O	-3.32706500	5.76487800	-1.22609300
C	-3.93363100	10.40740900	0.18069700
H	-2.96994400	10.87909600	-0.04739000
H	-4.47160800	11.09458200	0.85019800
H	-4.49806000	10.37649100	-0.75934900
C	-3.75673900	9.00749300	0.79120700

H	-3.21816900	9.08884000	1.74480000	H	0.89211000	4.39296200	1.34582900
H	-4.74095400	8.59189600	1.04501500	C	-3.47243100	6.32267800	-2.98047000
H	0.09152500	3.89004800	-0.10889500	O	-3.85811600	7.42440900	-3.32910500
C	-3.98023500	1.30363400	1.29506400	O	-4.21240400	5.20935700	-3.14935400
C	-3.46983500	2.01409400	0.21075100	C	-5.50397100	5.37671000	-3.76621800
C	-2.55034100	3.05544100	0.39787600	H	-5.93529300	4.37784000	-3.80794000
C	-2.15456800	3.37599800	1.70718100	H	-6.12980000	6.03944100	-3.16460800
C	-2.66343500	2.67399100	2.79431900	H	-5.39523400	5.78935100	-4.77162200
C	-3.57907200	1.62901800	2.59866600	C	2.85929300	9.24935400	4.61502000
H	-4.68858900	0.49955200	1.13298700	O	1.64212900	8.45757200	4.52968600
H	-3.78794100	1.75547700	-0.79518600	C	1.37525800	7.77445700	5.78505000
H	-1.45005000	4.18521200	1.87020700	C	2.67593000	7.89118900	6.57619300
H	-2.35818100	2.92625200	3.80417600	C	3.23522900	9.24175900	6.09647000
C	-1.97730700	3.79907000	-0.80449400	H	3.61946300	8.76875900	3.99023400
C	-0.46979200	3.53498200	-0.97609200	H	2.64364100	10.24456000	4.21764500
H	-2.50678300	3.44955100	-1.69519900	H	0.54191700	8.28334100	6.28290700
H	-0.08630600	4.04831800	-1.86332100	H	1.08375900	6.74930000	5.54810900
H	-0.28750900	2.46291500	-1.09397200	H	2.50497200	7.85684800	7.65461200
C	-4.09171600	0.90346500	3.79185000	H	3.35798600	7.07683300	6.31051100
O	-3.77241600	1.15079900	4.94099900	H	2.74224800	10.06731500	6.62017800
O	-4.96084200	-0.07565200	3.47557100	H	4.31313300	9.33745100	6.24557700
C	-5.51054500	-0.83246300	4.57213800	1			
H	-6.17456200	-1.56355500	4.11386000	scf done: -1282.22729677			
H	-4.71322800	-1.33241100	5.12621900	Ni	-2.72079800	6.91460000	1.79371100
H	-6.06773500	-0.17681000	5.24473700	C	-2.78041200	3.83260600	4.60794300
C	-0.52789700	9.03241000	-2.03684500	C	-3.72041500	4.36679900	3.48810200
O	-1.82355800	8.37260600	-2.07226600	C	-4.40942900	5.67136100	3.82323300
C	-2.43098100	8.48836100	-3.39027400	C	-3.15145100	4.24066900	6.04371100
C	-1.57344100	9.51272100	-4.13152100	C	-4.58077800	3.89576900	6.48896100
C	-0.18615600	9.30574300	-3.50008600	C	-5.66602800	4.35938900	5.49079300
H	-0.63054000	9.95641000	-1.45655700	H	-2.73972000	2.74009500	4.52642100
H	0.17290400	8.36366000	-1.53223500	H	-3.15564500	4.52558900	2.57006000
H	-2.40291600	7.50140700	-3.86310400	H	-3.00315000	5.32201100	6.14873400
H	-3.47161100	8.79384400	-3.25630900	H	-4.75843500	4.35423100	7.46879700
H	-1.58186100	9.34830100	-5.21141000	H	-1.76626100	4.19664100	4.41063500
H	-1.93514200	10.52743400	-3.93598700	H	-4.48527900	3.61876200	3.25522300
H	0.31234200	8.43785600	-3.94401600	H	-2.44169800	3.77445300	6.73651900
H	0.46967900	10.17205300	-3.61272200	H	-4.69141100	2.81324400	6.62726800
Et(THF)ZnOOCCH₂CH₂C₆H₄-p-COOMe				H	-6.61964600	4.50365700	6.00501200
scf done: -2817.76266721				H	-5.84519900	3.58588900	4.74042000
Zn	0.30122800	8.54885600	2.91298100	C	-5.96677000	6.84335600	5.35315300
C	1.08452100	6.46623200	1.81896500	H	-6.06122500	6.72594600	6.43741900
O	0.19921100	6.38117900	2.72091600	H	-6.98148500	6.95299000	4.94657900
O	1.59391900	7.59524300	1.53063700	C	-5.11751400	8.06106400	5.01659900
C	-0.99301200	10.93044900	4.13772700	H	-5.66839300	8.97645700	5.25138900
H	-1.16553100	10.37800400	5.06953700	H	-4.20336900	8.05859300	5.62087700
H	-1.75539700	11.72204100	4.09337200	C	-4.74518300	8.02224000	3.53688300
H	-0.02325900	11.43175900	4.24550500	H	-4.06581200	8.83874400	3.28927900
C	-1.02842600	10.00775200	2.90834700	H	-5.64640600	8.15028700	2.91959700
H	-2.02702800	9.56004300	2.81570400	N	-5.34968000	5.62318500	4.81237200
H	-0.89201500	10.60652600	1.99785600	N	-4.08102600	6.75968600	3.16996200
H	2.35312700	6.23051300	-0.64255200	C	-5.93559500	7.45257000	-0.99012600
C	-1.76503500	4.75749500	-1.95876600	C	-5.53726500	6.31104300	-0.00905600
C	-0.52660900	4.55490000	-1.35741800	C	-4.32500300	5.50910400	-0.43277100
C	0.34548400	5.62755800	-1.11152300	C	-5.51909500	7.25065200	-2.45658500
C	-0.05918000	6.91628100	-1.49294900	C	-6.01782400	5.95708700	-3.12000600
C	-1.29642800	7.12875900	-2.09557400	C	-5.74923000	4.69127900	-2.27539300
C	-2.16142500	6.05141200	-2.33291100	H	-7.02015300	7.60008700	-0.92584800
H	-2.42470000	3.91765300	-2.14362800	H	-5.31725900	6.72382600	0.97446800
H	-0.22809800	3.54778400	-1.07803000	H	-4.42433000	7.27586500	-2.51556800
H	0.60561100	7.75660100	-1.31720800	H	-5.53431600	5.85948700	-4.09922300
H	-1.60154300	8.12708700	-2.39051000	H	-5.47583800	8.38364400	-0.64064400
C	1.67917100	5.39522500	-0.43411700	H	-6.37946300	5.62344300	0.12254100
C	1.56155200	5.21954600	1.09596000	H	-5.86826500	8.10807800	-3.04326800
H	2.14249100	4.49017300	-0.84236700	H	-7.09694500	6.01199100	-3.30993700
H	2.55192400	4.97313500	1.49942900	H	-5.72905400	3.80461900	-2.91472400
				H	-6.56501800	4.53066700	-1.56667100

C	-3.33458600	4.04269400	-2.16958800
H	-3.42734400	4.14494800	-3.25602500
H	-3.37852100	2.96933300	-1.93913400
C	-2.02137200	4.64355000	-1.68507000
H	-1.18625800	4.00374000	-1.98556400
H	-1.86806300	5.62700700	-2.14375000
C	-2.07117600	4.79856200	-0.16670800
H	-1.16563900	5.28794800	0.20042000
H	-2.11704300	3.80604500	0.30687900
N	-4.47711300	4.72494000	-1.54369300
N	-3.22541500	5.59898500	0.26935600
C	-1.49532200	8.13326000	2.35509200
O	-1.09832900	8.92371900	3.20352100
O	-1.05155800	7.77844800	1.20369200

TS₁₋₂

scf done: -1819.81033681

Ni	-2.42630200	7.13275000	1.82906800
C	-2.91625200	3.83240700	4.33083000
C	-3.71410200	4.56623600	3.21178100
C	-4.34692600	5.87326600	3.64099600
C	-3.34296800	4.14094600	5.77514300
C	-4.81975900	3.87296200	6.10433800
C	-5.79471700	4.47547800	5.06986700
H	-2.97917600	2.75392200	4.14383500
H	-3.05499700	4.78812400	2.37277700
H	-3.12049600	5.19308700	5.98771300
H	-5.03542800	4.28027300	7.09909700
H	-1.85940700	4.10205100	4.23257700
H	-4.50114400	3.91166200	2.82219700
H	-2.71447400	3.55974900	6.45939500
H	-5.01399800	2.79465500	6.15995100
H	-6.78325900	4.61672500	5.51444700
H	-5.93613600	3.78284900	4.23680600
C	-5.97559600	6.97566700	5.14249900
H	-6.21252900	6.75246500	6.18724700
H	-6.92235900	7.20438100	4.63366500
C	-5.01468500	8.15181200	5.04777900
H	-5.52161000	9.07593900	5.34089800
H	-4.17445700	7.99934700	5.73410600
C	-4.48514500	8.26162000	3.62066600
H	-3.70654100	9.02358600	3.57387800
H	-5.29132700	8.57448600	2.94048300
N	-5.36832400	5.77908000	4.54445700
N	-3.90647000	7.00069300	3.13749700
C	-6.15169100	7.28819000	-0.92009500
C	-5.39131300	6.42488600	0.13270900
C	-4.15774700	5.70437500	-0.37388300
C	-5.92723500	6.91830800	-2.39539700
C	-6.29829000	5.47772300	-2.77769000
C	-5.72310300	4.43146700	-1.80117100
H	-7.22267200	7.25087300	-0.68803300
H	-5.06791200	7.04836100	0.96421900
H	-4.87265100	7.08589100	-2.64259400
H	-5.93807100	5.27978500	-3.79411600
H	-5.85154500	8.33434100	-0.79140000
H	-6.07136600	5.67798300	0.55783700
H	-6.49717300	7.61281200	-3.02340500
H	-7.38797200	5.35236600	-2.80291900
H	-5.67983400	3.44766900	-2.27654800
H	-6.38597000	4.32004700	-0.93945900
C	-3.25594800	4.08097700	-2.01891700
H	-3.51656500	3.98611300	-3.07851400
H	-3.13097100	3.06374300	-1.62228500
C	-1.97468700	4.88640500	-1.85160300
H	-1.11692500	4.29624800	-2.18814100
H	-2.02025200	5.79048200	-2.46780500

C	-1.81836100	5.28188400	-0.38523000
H	-0.94055500	5.91836300	-0.25131100
H	-1.65327900	4.38268900	0.22752700
N	-4.37013900	4.74464500	-1.32838100
N	-2.98971100	6.01147400	0.12768600
C	0.02408900	8.31364800	-3.17519700
C	-0.09604400	8.56051300	-1.81312700
C	-1.33941900	8.88306900	-1.22920700
C	-2.46309600	8.96394800	-2.08049300
C	-2.34774400	8.72350800	-3.44171300
C	-1.10428200	8.39101300	-4.00810200
H	0.99010800	8.06425900	-3.59877600
H	0.78484900	8.50421000	-1.17973900
H	-3.43032100	9.23621200	-1.67212200
H	-3.21649200	8.79786200	-4.08718900
C	-1.39598800	9.16062900	0.20521100
C	-2.50460000	9.35282800	0.96859900
H	-0.42741700	9.23331800	0.69387600
H	-2.40854000	9.73992200	1.97584600
H	-3.50656500	9.34155500	0.54989700
C	-1.03420300	8.14001000	-5.46810100
O	-1.98694400	8.19133600	-6.22793000
O	0.21088700	7.83861900	-5.88919400
C	0.37404800	7.57746400	-7.29649300
H	1.43206500	7.35631900	-7.42817300
H	-0.23613000	6.72351800	-7.59902700
H	0.09079800	8.45462100	-7.88248300
C	-1.13026800	7.57038500	3.06788200
O	-1.07180300	8.15517000	4.14798600
O	-0.28241700	7.00506200	2.32532900

2

scf done: -1819.82120241

Ni	-2.54217800	7.50440800	1.56712900
C	-2.63304500	3.90771700	4.11570000
C	-3.49749500	4.65763000	3.05639800
C	-4.21521000	5.89123400	3.56195000
C	-3.00084700	4.15045600	5.58827500
C	-4.43992500	3.77798200	5.97650300
C	-5.48729300	4.32541600	4.98600600
H	-2.67411200	2.83415500	3.89589400
H	-2.86510700	4.97538300	2.23179600
H	-2.83388000	5.20890100	5.82120300
H	-4.64464200	4.15650800	6.98509000
H	-1.59274000	4.21635300	3.97767000
H	-4.24569000	3.97890500	2.63194700
H	-2.30322000	3.59216200	6.22293300
H	-4.55824700	2.68814900	6.02220000
H	-6.47554600	4.36216900	5.45229100
H	-5.58265400	3.65282100	4.13039600
C	-5.85156300	6.79229000	5.19091900
H	-5.99519200	6.50976200	6.23870400
H	-6.84825200	6.95276300	4.75673500
C	-5.00651000	8.05274200	5.08303600
H	-5.57525600	8.91807800	5.43629200
H	-4.11688300	7.95824200	5.71611000
C	-4.57604500	8.24889400	3.63186700
H	-3.88903000	9.09293500	3.55860500
H	-5.45189400	8.48760300	3.01015300
N	-5.18608000	5.67842900	4.50212800
N	-3.89511800	7.06784700	3.08178600
C	-6.28709000	7.43716600	-1.04080600
C	-5.53306600	6.62021900	0.05290800
C	-4.34147200	5.81615300	-0.42913500
C	-6.08842700	6.96993600	-2.49182000
C	-6.51925700	5.52380300	-2.77995000
C	-5.98711100	4.51828700	-1.73839000

H	-7.35599900	7.44045500	-0.79665300	H	-6.40696900	7.27303100	5.77004800
H	-5.16373700	7.28691900	0.83075600	H	-6.99015200	7.63862900	4.14329000
H	-5.02998600	7.08163600	-2.75452100	C	-5.07106900	8.53054600	4.61748900
H	-6.17013500	5.24487600	-3.78123400	H	-5.55634500	9.49730900	4.78251700
H	-5.96047800	8.48141300	-0.97977200	H	-4.29921300	8.41072300	5.38637700
H	-6.22946700	5.93317500	0.54657400	C	-4.42340400	8.48322700	3.23621900
H	-6.63638100	7.64542200	-3.15881000	H	-3.63651200	9.23336000	3.16087700
H	-7.61338500	5.44323900	-2.79729200	H	-5.17157800	8.72656800	2.46637900
H	-5.99921400	3.50401400	-2.14686800	N	-5.50307600	6.14645800	4.26101000
H	-6.64543900	4.49772100	-0.86597500	N	-3.82351900	7.17259000	2.93138300
C	-3.54240000	4.02937200	-1.95225900	C	-5.48123600	6.99387300	-1.44659800
H	-3.82806700	3.85782900	-2.99550500	C	-4.98323600	6.24044600	-0.17569600
H	-3.45168400	3.04387100	-1.47428700	C	-3.76403000	5.36236800	-0.37708600
C	-2.22390800	4.78808200	-1.87583400	C	-5.09176600	6.37766700	-2.80037200
H	-1.40010300	4.13140700	-2.17190000	C	-5.55082100	4.92960900	-3.02629400
H	-2.23954500	5.63629300	-2.56803700	C	-5.22550100	4.00330100	-1.83641900
C	-2.02295700	5.30216800	-0.45159100	H	-6.57150500	7.09370800	-1.38309500
H	-1.11658900	5.90882800	-0.38846100	H	-4.72531800	6.95805500	0.60240400
H	-1.88199400	4.45122900	0.23165800	H	-4.00135700	6.42526000	-2.90228600
N	-4.61481300	4.79376400	-1.29988400	H	-5.07522100	4.54771300	-3.93761900
N	-3.15180900	6.11905000	0.01613500	H	-5.07339900	8.00960200	-1.42275900
C	0.07432400	8.12632100	-2.88848500	H	-5.79204800	5.62305700	0.23135200
C	-0.15257700	8.35917600	-1.53783400	H	-5.49353300	7.00868900	-3.60170500
C	-1.43183900	8.70062700	-1.04990100	H	-6.63356400	4.88916900	-3.19980300
C	-2.47986600	8.80727600	-1.98871600	H	-5.20878800	2.95848400	-2.15927600
C	-2.25859400	8.58132000	-3.34003500	H	-6.01321600	4.07063600	-1.08178400
C	-0.98022900	8.23422700	-3.81042200	C	-2.79458700	3.45458100	-1.62924000
H	1.06821700	7.86679900	-3.23465800	H	-2.92441400	3.20676000	-2.68828500
H	0.67458900	8.28358500	-0.83695900	H	-2.79836600	2.50766500	-1.07083100
H	-3.47341000	9.08873000	-1.65803700	C	-1.48771200	4.20316900	-1.40735200
H	-3.07155600	8.67944200	-4.05189200	H	-0.64064200	3.52286900	-1.53996400
C	-1.59417200	8.97916800	0.38481500	H	-1.38877400	5.00769200	-2.14458100
C	-2.76729700	9.41181200	1.02652500	C	-1.48578700	4.80396900	-0.00339800
H	-0.65188800	9.16279500	0.89751900	H	-0.58996500	5.40548500	0.15805700
H	-2.68440800	10.00285700	1.93281400	H	-1.45905500	4.00019200	0.74649300
H	-3.69654900	9.53118000	0.47358400	N	-3.93111100	4.28272700	-1.20659500
C	-0.79556800	8.00374100	-5.26228800	N	-2.65321800	5.66216500	0.24281400
O	-1.68294700	8.07434500	-6.09669900	C	-0.64576000	8.08133300	-3.19966000
O	0.47798200	7.69834100	-5.58810300	C	-0.40639200	7.94379200	-1.84074100
C	0.75042800	7.45698000	-6.98150400	C	-1.22503400	8.56647300	-0.86650200
H	1.81472600	7.23241300	-7.03295600	C	-2.30126100	9.35267000	-1.34825200
H	0.16292000	6.61056100	-7.34417400	C	-2.54213600	9.49646800	-2.70563000
H	0.51763800	8.34379700	-7.57513400	C	-1.72373500	8.86200500	-3.65903700
C	-1.28500200	7.78080600	2.95966300	H	0.00690000	7.59441600	-3.91599300
O	-1.13713900	8.73066200	3.71265600	H	0.44008000	7.34853000	-1.50757500
O	-0.74886700	6.68029200	2.75259000	H	-2.95048600	9.86156500	-0.64308500
				H	-3.36901900	10.10886200	-3.05101300
				C	-0.92801200	8.38517300	0.55439700
				C	-1.55476800	9.09647700	1.63080500
				H	0.05268300	7.94505100	0.74163600
				H	-0.97747400	9.29819800	2.53042400
				H	-2.27845800	9.88124800	1.40259600
				C	-2.02055300	9.04915200	-5.09025600
				O	-2.93381400	9.72774800	-5.53738500
				O	-1.16562200	8.37992400	-5.90123400
				C	-1.38324000	8.51154600	-7.31687800
				H	-0.59826300	7.92060200	-7.78712500
				H	-2.36740300	8.12467400	-7.59183800
				H	-1.30702500	9.55775800	-7.62174000
				C	-0.79674000	6.63899200	3.35177500
				O	-0.89720400	7.41285100	4.24020400
				O	-0.38426500	5.67587700	2.79593600

TS₂₋₃

scf done: -1819.8136741

Ni	-2.33114200	7.32187900	1.51308500
C	-3.21744500	4.02431700	4.48164700
C	-3.79069300	4.74468200	3.22226000
C	-4.38256900	6.11694200	3.47145600
C	-3.77118100	4.48123900	5.84113100
C	-5.29181100	4.34417200	6.00885400
C	-6.07752500	4.91247500	4.80936200
H	-3.37583000	2.94592400	4.36123600
H	-3.00928900	4.86753100	2.47651900
H	-3.49127300	5.52949300	6.00013800
H	-5.59384200	4.85523400	6.93080100
H	-2.13249500	4.17201600	4.49800200
H	-4.56067500	4.11941900	2.75688300
H	-3.27034000	3.91476800	6.63462800
H	-5.57398400	3.29074800	6.12903900
H	-7.10803000	5.13714100	5.09800900
H	-6.14316000	4.16457500	4.01601000
C	-6.09021200	7.40781400	4.73044600

3

scf done: -1631.18380753

Ni	-2.68093100	7.06304800	1.70569800
C	-2.59648100	4.42307100	5.09174500

C	-3.33269800	4.58202400	3.72687800	H	-2.24958100	9.45889200	2.59650000
C	-4.41049200	5.64554400	3.69604800	C	-1.53549300	10.84784800	-3.79661700
C	-3.36315500	4.89809100	6.33764000	O	-2.28174000	11.79563000	-4.01093700
C	-4.72794300	4.23227800	6.57040900	O	-0.73614000	10.34213200	-4.77383400
C	-5.61521400	4.21483000	5.30788700	C	-0.80871300	10.98031200	-6.05878600
H	-2.31130600	3.37095200	5.21010900	H	-0.10869200	10.43735700	-6.69310800
H	-2.61270600	4.85469600	2.95410500	H	-1.82029400	10.91442100	-6.46683000
H	-3.50725600	5.98296500	6.26637400	H	-0.51724200	12.03096100	-5.98567000
H	-5.24269300	4.76115800	7.38153300	TS _{2,4} scf done: -1819.79845268			
H	-1.66109100	4.99166400	5.04467100				
H	-3.77356200	3.62533900	3.42524400	Ni	-3.16290600	7.28855800	2.12028400
H	-2.73311200	4.73823700	7.22029800	C	-2.58167900	4.36637700	5.19769300
H	-4.59934100	3.19601500	6.90745300	C	-3.41594300	4.56226800	3.89542100
H	-6.66771200	4.10139700	5.58282300	C	-4.57998000	5.52167800	4.01176400
H	-5.37180700	3.34662200	4.69030200	C	-3.30629400	4.66876000	6.51974400
C	-6.51864700	6.47018200	4.70729000	C	-4.59035000	3.86269300	6.76974600
H	-6.80136200	6.46285900	5.76556500	C	-5.54823100	3.86376600	5.56001500
H	-7.42299400	6.23516900	4.12818800	H	-2.20034900	3.33884500	5.20853600
C	-5.96740600	7.83399900	4.30995400	H	-2.77531600	4.93784700	3.09863300
H	-6.77607600	8.57059400	4.28394300	H	-3.54911800	5.73791000	6.55036700
H	-5.23503400	8.17021200	5.05304400	H	-5.09770300	4.27473200	7.64995000
C	-5.28885800	7.72135700	2.94569900	H	-1.70307300	5.01886800	5.14824500
H	-4.82301100	8.66915800	2.66560800	H	-3.79999600	3.59651600	3.54973000
H	-6.04164100	7.49377000	2.17671600	H	-2.60991400	4.49742400	7.70482980
N	-5.50749600	5.42741600	4.49164000	H	-4.35081400	2.81921300	7.30845300
N	-4.24409300	6.68860400	2.92904000	H	-6.56899900	3.63606100	5.87877800
C	-4.89414800	7.59566700	-1.95654900	H	-5.26989300	3.07562900	4.85692800
C	-4.89568800	6.66001600	-0.70819700	C	-6.67630200	6.06877800	5.22346400
C	-3.81850100	5.59515900	-0.69093600	H	-6.85721900	5.96318500	6.29827200
C	-4.18516800	7.05224800	-3.20824800	H	-7.60060600	5.77805200	4.70628800
C	-4.74724300	5.73552500	-3.76510000	C	-6.29609300	7.50217900	4.88045900
C	-4.95824900	4.66554200	-2.67448800	H	-7.17376700	8.14991700	4.96071200
H	-5.93213700	7.85281300	-2.19992400	H	-5.54288400	7.87152700	5.58558500
H	-4.74704600	7.25432500	0.19401800	H	-5.72764800	7.53600700	3.46395400
H	-3.12317200	6.91591500	-2.97283400	H	-5.40542600	8.54336700	3.19631100
H	-4.06417500	5.35571900	-4.53462100	H	-6.50818700	7.24572900	2.74700400
H	-4.39710600	8.53055500	-1.68005300	N	-5.59450700	5.14630300	4.84714300
H	-5.87103200	6.17043600	-0.60645500	N	-4.57376800	6.63297400	3.31888900
H	-4.22139000	7.81681900	-3.99294200	C	-5.82621200	7.57492300	-1.36013400
H	-5.71119600	5.90602100	-4.26105400	C	-5.51788500	6.65673900	-1.3634300
H	-5.01380800	3.66856400	-3.12126100	C	-4.29036600	5.77844700	-0.26434500
H	-5.91700000	4.82436600	-2.17459000	C	-5.18212000	7.17199300	-2.69638300
C	-2.80376300	3.67243500	-1.88230800	C	-5.57391200	5.78185400	-3.21916900
H	-2.64534200	3.56509100	-2.96089600	C	-5.48550000	4.69354800	-2.13169100
H	-3.09942400	2.68580900	-1.49809000	H	-6.91460000	7.63831200	-1.47911900
C	-1.52863100	4.15188200	-1.19957900	H	-5.36312400	7.27861800	0.74286000
H	-0.78633900	3.34788800	-1.18916400	H	-4.09236200	7.21842900	-2.58793000
H	-1.10114100	4.99360500	-1.75621400	H	-4.92413900	5.52214700	-4.06355800
C	-1.86454500	4.60569400	0.22033900	H	-5.47617100	8.58140600	-1.11511100
H	-0.97916400	5.01084700	0.71726500	H	-6.37918700	6.01347200	-0.7836900
H	-2.19702300	3.74159900	0.81461400	H	-5.43902300	7.92417800	-3.45108900
N	-3.89365100	4.63309900	-1.66716400	H	-6.60078200	5.78853800	-3.60595800
N	-2.90392700	5.64351100	0.23917600	H	-5.43216200	3.69928900	-2.58426900
C	-0.51187200	9.06214700	-2.32807800	H	-6.39145500	4.69862600	-1.52064500
C	-0.41320100	8.43738700	-1.09756600	C	-3.12213000	4.06125200	-1.61722600
C	-1.18957100	8.84184900	0.02334900	H	-3.07652200	3.99206100	-2.70928100
C	-2.06979300	9.93996200	-0.18582700	H	-3.21622500	3.03704100	-1.22988700
C	-2.16731900	10.56946200	-1.41438700	C	-1.87087700	4.73260600	-1.06788000
C	-1.39618700	10.14593500	-2.51696700	H	-1.01296000	4.06056600	-1.16558300
H	0.10365800	8.72503000	-3.15540200	H	-1.65099100	5.64261300	-1.63561300
H	0.28465600	7.61239400	-0.97343300	C	-2.10592100	5.10152700	0.39418400
H	-2.67709500	10.29742100	0.63950300	H	-1.24664500	5.64706900	0.78941400
H	-2.84242400	11.41020100	-1.54300800	H	-2.21720100	4.18484200	0.99241500
C	-1.05566100	8.14619300	1.29119100	N	-4.31768600	4.83533500	-1.25520400
C	-1.71666900	8.50722100	2.52646800	N	-3.29585500	5.94875900	0.56742200
H	-0.16941500	7.51092800	1.35447100	C	1.37930200	6.40860500	3.20920000
H	-1.20345400	8.25240000	3.45687800				

C	0.10304500	6.93908000	3.05859000	H	-4.27864200	7.72999800	-4.14917200
C	-0.10154200	8.21345700	2.49800200	H	-6.44734400	6.65840600	-4.40133900
C	1.03504400	8.93397200	2.08624100	H	-6.90818900	4.49019400	-3.05104500
C	2.31479000	8.41303200	2.23147900	H	-7.18691800	6.01763800	-2.25006600
C	2.50389900	7.14238800	2.79672200	C	-5.00473800	3.57289700	-1.66350800
H	1.51025700	5.42562000	3.64732500	H	-4.86664500	3.30664100	-2.71688900
H	-0.75531000	6.35767300	3.37912400	H	-5.76254200	2.89145700	-1.25257400
H	0.90640300	9.91931900	1.64723700	C	-3.69158500	3.43734300	-0.90172000
H	3.18068800	8.98373800	1.91290600	H	-3.44612400	2.37909100	-0.77110100
C	-1.45587200	8.81815700	2.34634700	H	-2.87886700	3.90016700	-1.47263400
C	-2.49061200	8.54349000	3.36375300	C	-3.82122900	4.14104500	0.44813600
H	-1.37431200	9.88133600	2.11079500	H	-2.87231400	4.10741600	0.98954500
H	-2.16232800	8.05391400	4.28204100	H	-4.56234400	3.62003300	1.07276300
H	-3.18107600	9.36634700	3.55854900	N	-5.50317500	4.95416700	-1.59764900
O	-3.16718600	9.27407400	0.42170300	N	-4.20994000	5.54570000	0.29220400
C	-2.09879400	8.66548500	0.54603000	C	1.57162300	6.26411400	2.48675000
O	-1.23013300	8.26593000	-0.21693100	C	0.41022400	6.86164900	2.00542200
C	3.88631500	6.62544800	2.93935600	C	0.01617500	8.13876700	2.44088000
O	4.89330700	7.23081800	2.61338600	C	0.83318200	8.80046300	3.37221900
O	3.93239000	5.38903500	3.48016500	C	1.99394000	8.20979200	3.86123400
C	5.23882400	4.80880600	3.65508300	C	2.37498800	6.93244600	3.42463000
H	5.06345200	3.83026000	4.09961800	H	1.86226100	5.28118900	2.13372100
H	5.74292100	4.70636700	2.69151300	H	-0.19642800	6.33599400	1.27432000
H	5.84564300	5.42760400	4.31982700	H	0.55288500	9.79298300	3.71437400

4

scf done: -1819.8535933

Ni	-3.33574600	6.87610900	1.58462000
C	-1.67458300	5.22230600	5.23854800
C	-2.52114100	4.85677400	3.97902900
C	-3.96171400	5.32724300	3.98775600
C	-2.46368400	5.62303700	6.49565400
C	-3.40027400	4.53795500	7.04969400
C	-4.24464900	3.86471300	5.95141400
H	-1.01663000	4.37692100	5.47093300
H	-2.05497800	5.28629600	3.09088800
H	-3.05068500	6.52230900	6.27233600
H	-4.05593400	4.98398500	7.80692000
H	-1.01847500	6.05762400	4.97497500
H	-2.52547900	3.77063500	3.83316400
H	-1.75416100	5.91658400	7.27742000
H	-2.82379500	3.75436000	7.55683000
H	-5.10082800	3.34299900	6.38745400
H	-3.65363000	3.10146800	5.43904800
C	-6.14654200	5.28568100	5.15757700
H	-6.33201400	5.35941100	6.23404300
H	-6.85117900	4.54526300	4.75473100
C	-6.34564000	6.63779200	4.48641600
H	-7.40977800	6.89011400	4.46556800
H	-5.82983700	7.41752100	5.05802600
C	-5.77579700	6.58521300	3.07081700
H	-5.83392600	7.56894800	2.59840200
H	-6.36232900	5.89533500	2.44809700
N	-4.76988300	4.81040300	4.95981900
N	-4.36918000	6.16278400	3.06685600
C	-5.04181200	8.01318300	-2.15323300
C	-5.47356000	7.28932000	-0.84180500
C	-5.00941500	5.85427400	-0.69314500
C	-4.61090300	7.10294400	-3.31401000
C	-5.68536300	6.12644300	-3.81781600
C	-6.40349300	5.38393200	-2.67334100
H	-5.86151900	8.66567500	-2.47735700
H	-5.08254900	7.83489900	0.01810500
H	-3.72832100	6.53327300	-2.99983800
H	-5.21950900	5.40404200	-4.49888500
H	-4.19617000	8.66391900	-1.91335700
H	-6.56578900	7.29933000	-0.74831700

TS_{2,5}

scf done: -1819.81014369

Ni	-3.40938200	7.16637800	1.82073900
C	-2.32890200	5.96039200	5.79174600
C	-2.83061100	5.40056700	4.42573200
C	-4.30176100	5.61811500	4.13536700
C	-3.40179400	6.17099600	6.87284200
C	-4.19580800	4.91637000	7.26868300
C	-4.71658600	4.12315700	6.05278200
H	-1.54564000	5.29368500	6.17018300
H	-2.26751600	5.85791600	3.61010500
H	-4.10533600	6.93745100	6.52574900
H	-5.03549500	5.21751300	7.90625800
H	-1.84518100	6.92630700	5.61021700
H	-2.63193000	4.32479900	4.36889800
H	-2.92384600	6.58723400	7.76696200
H	-3.57408700	4.24078100	7.86910400
H	-5.55218600	3.48123700	6.34383600
H	-3.93765000	3.45327800	5.68035600
C	-6.63604700	5.18541200	4.84170800
H	-7.05719800	5.21311700	5.85179700
H	-7.09256600	4.33192700	4.32141900
C	-6.92955800	6.48460200	4.10354800
H	-7.99423000	6.54005100	3.85783400
H	-6.68900300	7.34079000	4.74253400
C	-6.07928400	6.54998100	2.83650400

H	-6.20585800	7.51703200	2.34382600	H	-2.07153400	5.90043700	3.88476400
H	-6.39936800	5.77909500	2.12140500	H	-3.56958200	6.01860300	7.13354300
N	-5.18650000	4.97422200	4.95346000	H	-4.02029000	3.92812300	8.21170500
N	-4.65163800	6.37309500	3.12545900	H	-1.47037800	6.57052500	5.99928300
C	-4.75385500	8.00987300	-2.22476300	H	-2.04607400	4.19936800	4.29146700
C	-5.20208800	7.34429400	-0.88670300	H	-2.17962500	5.66427000	8.13418200
C	-4.65318500	5.95811900	-0.61550100	H	-2.43668800	3.26363900	7.83326900
C	-4.18388300	7.05878500	-3.28917800	H	-4.42642100	2.42485800	6.38583200
C	-5.15535500	5.97594300	-3.78393300	H	-2.94949800	2.86220600	5.56334700
C	-5.89332000	5.26700900	-2.63187900	C	-6.01230500	4.11909800	5.40973600
H	-5.60347900	8.56558500	-2.63919200	H	-6.27790300	3.85789900	6.43891300
H	-4.89783200	7.96780200	-0.04384000	H	-6.37464500	3.30850200	4.76278300
H	-3.28759400	6.58086600	-2.87804800	C	-6.64287800	5.44746800	5.01360700
H	-4.59915700	5.24262700	-4.38016000	H	-7.72395500	5.32708500	4.89832200
H	-3.97913800	8.74680200	-1.99484400	H	-6.47471500	6.18745300	5.80337700
H	-6.29572700	7.28606500	-0.84373000	C	-6.01742600	5.94073800	3.71171800
H	-3.84320600	7.65165000	-4.14577000	H	-6.38190000	6.94333200	3.47451700
H	-5.91216100	6.41032900	-4.44929500	H	-6.30191600	5.28602300	2.87693000
H	-6.31929100	4.31895100	-2.97216900	N	-4.54768200	4.19922700	5.32040800
H	-6.73768400	5.87527000	-2.29739600	N	-4.55247400	6.00151400	3.79305400
C	-4.44306300	3.62469700	-1.42366800	C	-5.37165100	8.56102400	-1.14125700
H	-4.23828300	3.29533000	-2.44789100	C	-5.75149100	7.63276700	0.05136000
H	-5.17405900	2.92416400	-0.99651000	C	-5.09503100	6.26669800	0.04487600
C	-3.16302000	3.63601000	-0.59829900	C	-4.86636000	7.85572800	-2.41074300
H	-2.84891600	2.60973100	-0.38559600	C	-5.83133200	6.83434200	-3.03100800
H	-2.35846900	4.12073600	-1.16225900	C	-6.41351400	5.84713500	-1.99832600
C	-3.40499900	4.41055700	0.69578900	H	-6.24027500	9.18553600	-1.38206400
H	-2.48015400	4.49553500	1.26956500	H	-5.47739500	8.12118400	0.98757500
H	-4.13496200	3.87806900	1.32304900	H	-3.92036900	7.35345000	-2.17612600
N	-5.03227200	4.97004800	-1.48180600	H	-5.30317000	6.28237400	-3.81770300
N	-3.89325200	5.76880900	0.43003600	H	-4.58044000	9.23521200	-0.80150800
C	-6.07297500	10.91008500	2.57280100	H	-6.83699100	7.48614400	0.08240400
C	-4.93400200	10.21245400	2.19094000	H	-4.62170400	8.61606500	-3.16117500
C	-4.11631900	9.55577400	3.13946300	H	-6.67196800	7.34349900	-3.51872400
C	-4.50174200	9.65551900	4.49686600	H	-6.77178500	4.94084000	-2.49433200
C	-5.63646000	10.35213300	4.88372200	H	-7.28528100	6.28605200	-1.50697400
C	-6.44570000	10.98817100	3.92608000	C	-4.77331700	4.13980700	-1.18499700
H	-6.67834100	11.40456600	1.82130200	H	-4.60591800	4.01142500	-2.25957900
H	-4.66912900	10.18442000	1.13914100	H	-5.43156200	3.32272100	-0.85843100
H	-3.88430900	9.17812300	5.25252200	C	-3.45029300	4.09894600	-0.42932500
H	-5.90848000	10.41974500	5.93210700	H	-3.05902000	3.07724400	-0.42042500
C	-2.91337900	8.78741800	2.78732600	H	-2.71310800	4.73365400	-0.93346600
C	-2.22712100	8.91222600	1.50842000	C	-3.66885400	4.61146300	0.99307800
H	-2.27970000	8.56123600	3.64524700	H	-2.71941800	4.65682600	1.53295600
H	-2.69375600	9.50432800	0.72493200	H	-4.31733600	3.91608800	1.54676200
H	-1.16521900	9.14218300	1.58675400	N	-5.44950700	5.42727900	-0.97436400
O	-1.48633000	7.54817900	-0.59162100	N	-4.26434800	5.95046700	1.00283200
C	-1.51806800	7.30449700	0.60485600	C	-5.89047800	11.21549100	3.32750300
O	-0.91612700	6.55920500	1.38015200	C	-4.72660800	10.47368600	3.16961300
C	-7.64894100	11.71729000	4.38065700	C	-4.41504900	9.38800200	4.02360500
O	-8.01306900	11.80863300	5.54235200	C	-5.33751300	9.11339500	5.06318300
O	-8.33428100	12.28948200	3.36587900	C	-6.50049400	9.84965500	5.22563100
C	-9.52295900	13.02050100	3.71966200	C	-6.80191900	10.91201800	4.35449000
H	-9.91963200	13.40025400	2.77918300	H	-6.09760500	12.04118500	2.65567000
H	-10.24834300	12.36096700	4.20158400	H	-4.04537200	10.74021200	2.36825000
H	-9.27870700	13.84596000	4.39210000	H	-5.11523100	8.30640000	5.75569900
				H	-7.18736600	9.62135800	6.03446900
				C	-3.19922700	8.55969000	3.86302900
				C	-1.96747300	9.25644400	3.27858600
				H	-2.97465400	8.03955400	4.79592000
				H	-1.84623000	10.29784000	3.60596000
				H	-1.06104800	8.72680300	3.59969000
				O	-1.26605500	9.93928900	1.05692300
				C	-1.97397400	9.19876600	1.75148300
				O	-2.76350200	8.29265200	1.26327200
				C	-8.05305100	11.66937900	4.55904500
				O	-8.87302100	11.44494100	5.43657700

5
scf done: -1819.86417876

Ni	-3.70284000	7.19845900	2.50836100
C	-1.79128000	5.52370100	6.01845900
C	-2.40945200	5.17636400	4.62833800
C	-3.92479700	5.15145100	4.56764300
C	-2.71405200	5.33962500	7.23440600
C	-3.23449000	3.91015600	7.44743700
C	-3.77381100	3.27035500	6.15355200
H	-0.88129300	4.92728800	6.15026200

O	-8.22167900	12.66506400	3.65906400
C	-9.41762100	13.45543200	3.78408000
H	-9.36665900	14.18678800	2.97865200
H	-10.30525100	12.82813600	3.67392100
H	-9.44562500	13.95779100	4.75374500

TS₄₋₆

scf done: -1819.82761241

Ni	-3.17826000	6.81778000	1.74742400
C	-1.54048900	4.82937500	5.10423900
C	-2.50091700	4.60979400	3.89530600
C	-3.87326100	5.23509700	4.03415200
C	-2.21022000	5.17476100	6.44451800
C	-3.20739200	4.13108300	6.96991400
C	-4.21189000	3.66520000	5.89672100
H	-0.92226100	3.93184900	5.21867100
H	-2.04985100	5.02436400	2.99119000
H	-2.72467300	6.13819600	6.34376500
H	-3.74442800	4.55394400	7.82694300
H	-0.85586500	5.64488200	4.85054000
H	-2.63632700	3.53915700	3.70825500
H	-1.42904100	5.33185200	7.19662100
H	-2.67822000	3.24406500	7.33884800
H	-5.09949800	3.22850900	6.36108800
H	-3.77078800	2.87641900	5.28320000
C	-5.97588500	5.35715100	5.33070900
H	-6.09783900	5.35659100	6.41813400
H	-6.77534800	4.73354900	4.90961600
C	-6.05009900	6.77556100	4.78178500
H	-7.07641600	7.14684000	4.85092800
H	-5.41436500	7.43994800	5.37778100
C	-5.57394600	6.77817400	3.33154100
H	-5.53104800	7.79701100	2.93905400
H	-6.27574400	6.21867100	2.69901300
N	-4.67212500	4.75097100	5.01913900
N	-4.23197300	6.18711100	3.19989500
C	-5.24168500	7.44566600	-2.59630800
C	-5.99518800	6.71708600	-1.44061700
C	-5.76383400	5.21975000	-1.34708600
C	-4.78214800	6.55811500	-3.76522400
C	-5.89906800	5.80750000	-4.50758600
C	-6.88082100	5.09581200	-3.55376100
H	-5.87730000	8.25583600	-2.97420700
H	-5.68712700	7.13390900	-0.48034400
H	-4.05805000	5.82869500	-3.38368700
H	-5.44223800	5.07791600	-5.18751900
H	-4.34972600	7.92249100	-2.17743700
H	-7.07313300	6.89700600	-1.52791700
H	-4.23109200	7.17805100	-4.48198300
H	-6.47723500	6.49783500	-5.13527200
H	-7.43392900	4.31654700	-4.08708800
H	-7.63227400	5.80585900	-3.19781800
C	-5.89937700	3.04051100	-2.52060400
H	-5.63508400	2.82978900	-3.56338400
H	-6.78420200	2.43181300	-2.28364800
C	-4.74145600	2.67772900	-1.59534400
H	-4.64527500	1.58906500	-1.53035500
H	-3.80274000	3.06913900	-2.00486900
C	-4.98649600	3.30309600	-0.21975900
H	-4.14568300	3.09421600	0.45105400
H	-5.87259300	2.83630600	0.24054300
N	-6.23392000	4.46543700	-2.40178600
N	-5.17456800	4.75162600	-0.29089300
C	1.74129600	6.48214900	2.78286900
C	0.57273200	6.94229400	2.18160500
C	0.12910500	8.26096600	2.37669400
C	0.90108100	9.10909000	3.18605900

C	2.06848000	8.65661000	3.79266100
C	2.49876900	7.33625600	3.59980800
H	2.07188800	5.46324300	2.61709100
H	0.00328700	6.27179400	1.54488600
H	0.58124500	10.13596800	3.34007700
H	2.65914600	9.31963900	4.41571300
C	-1.17495600	8.76643000	1.78155600
C	-2.40100500	8.32268700	2.61072000
H	-1.11113600	9.86136800	1.74813000
H	-2.16059700	8.09171200	3.65097900
H	-3.19757300	9.07695100	2.57870100
O	-2.24951900	7.32958800	0.20876900
C	-1.36315900	8.27400800	0.33290900
O	-0.71673300	8.73847500	-0.60733300
C	3.74988200	6.89386300	4.26883700
O	4.43909600	7.59925400	4.98455200
O	4.05784900	5.60819900	4.00715200
C	5.26178800	5.09494300	4.61020900
H	5.19352400	5.14474900	5.69915300
H	5.33212900	4.06024800	4.27851900
H	6.12959000	5.66544800	4.27225700

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scf done: -1357.71423714

Ni	-3.30498200	6.89916700	1.73741900
C	-1.72231100	4.83924400	5.06764000
C	-2.68595500	4.64459900	3.85711800
C	-4.04512200	5.29743800	3.99691000
C	-2.38566400	5.18554500	6.41075800
C	-3.40548700	4.15878300	6.92583800
C	-4.42102500	3.72567200	5.84928700
H	-1.11936900	3.93055500	5.17427500
H	-2.22440700	5.05376900	2.95593700
H	-2.87835000	6.16127000	6.32006100
H	-3.93225600	4.58467600	7.78756900
H	-1.02435000	5.64505700	4.81961900
H	-2.84357400	3.57782500	3.66560600
H	-1.60154700	5.31780100	7.16449600
H	-2.89615300	3.25640300	7.28494500
H	-5.31985400	3.30883000	6.31005800
H	-4.00028500	2.93095800	5.22936700
C	-6.14141400	5.46649800	5.29768300
H	-6.25765900	5.46680500	6.38558900
H	-6.95660400	4.86160500	4.87981900
C	-6.18478300	6.88688400	4.75104000
H	-7.20179700	7.28183300	4.82446700
H	-5.53149200	7.53591800	5.34470700
C	-5.71444100	6.87975400	3.29896200
H	-5.65176700	7.89689100	2.90539400
H	-6.43345400	6.33497900	2.67207000
N	-4.85344100	4.82979100	4.97914600
N	-4.38449400	6.25951600	3.16225700
C	1.55732100	6.29979500	2.63833200
C	0.39658800	6.83669500	2.08818000
C	0.04686400	8.17998600	2.30466500
C	0.90257200	8.97231500	3.08531800
C	2.06313800	8.44280400	3.64144800
C	2.40101100	7.09954700	3.42510400
H	1.81540400	5.26314100	2.45509200
H	-0.24043100	6.20788700	1.47358900
H	0.65501600	10.01625700	3.25629500
H	2.71927400	9.06328100	4.24241300
C	-1.24099700	8.77278300	1.75389800
C	-2.47530100	8.37670900	2.59510500
H	-1.11738400	9.86289200	1.74470100
H	-2.23631200	8.13664200	3.63362300
H	-3.24532700	9.15770300	2.56571900

O	-2.39963200	7.40045500	0.18613200
C	-1.48507400	8.32196400	0.30031600
O	-0.85870900	8.78862200	-0.65046800
C	3.65020100	6.57457200	4.03656400
O	4.41148900	7.22937700	4.72655500
O	3.86641600	5.27541400	3.75158400
C	5.06214500	4.68252700	4.29513700
H	5.04513300	4.72287000	5.38645000
H	5.05417800	3.64964300	3.95067400
H	5.94740100	5.20328800	3.92380700

TS₅₋₇

scf done: -1819.8363211

Ni	-3.86629900	7.48186500	2.75200000
C	-1.75555000	5.48998100	5.84838300
C	-2.56883900	5.23265100	4.54372500
C	-4.07178700	5.36671100	4.67933700
C	-2.52334700	5.30887700	7.16787200
C	-3.14247100	3.92000300	7.38511700
C	-3.93383100	3.40971600	6.16331200
H	-0.87459600	4.83835000	5.83644500
H	-2.24887900	5.92971300	3.76638100
H	-3.31912100	6.06221800	7.21853900
H	-3.79812800	3.96053700	8.26266200
H	-1.37689800	6.51745400	5.82120900
H	-2.35617800	4.23026400	4.15803100
H	-1.84778400	5.53245800	8.00095500
H	-2.36352100	3.18156800	7.61006300
H	-4.64980300	2.64078300	6.46326400
H	-3.26120900	2.93394300	5.44590700
C	-6.13676900	4.54171200	5.76087100
H	-6.29137900	4.26396900	6.80776700
H	-6.66635600	3.80466000	5.14313700
C	-6.65831700	5.94703300	5.49374500
H	-7.75145100	5.95018100	5.52515700
H	-6.30182000	6.63045800	6.27223900
C	-6.16045700	6.41986100	4.13068700
H	-6.43883600	7.46309800	3.96330500
H	-6.62439300	5.82519400	3.33268600
N	-4.69523400	4.46467000	5.47814800
N	-4.69610900	6.31839800	4.01744800
C	-6.90986500	7.46223700	-0.81157600
C	-6.75371300	6.01739800	-0.24910000
C	-5.47557200	5.30136400	-0.64796200
C	-6.10890700	7.77194300	-2.08702300
C	-6.40752900	6.87088200	-3.29505700
C	-6.38672000	5.36510900	-2.95062000
H	-7.97531200	7.65954400	-0.98213200
H	-6.76654300	6.04042000	0.84162400
H	-5.04062300	7.70331100	-1.85063900
H	-5.67141500	7.08377800	-4.07972200
H	-6.58537600	8.17009000	-0.04085200
H	-7.60897100	5.40471400	-0.55586500
H	-6.28609100	8.81629200	-2.36956600
H	-7.39161900	7.10768100	-3.71967000
H	-6.22168500	4.77178200	-3.85493600
H	-7.36345800	5.05761200	-2.56653500
C	-4.09370900	4.45350200	-2.52091300
H	-3.88715400	4.94083800	-3.48051200
H	-4.20577200	3.37813700	-2.72324200
C	-2.94596000	4.69419500	-1.54446700
H	-2.06874300	4.11661000	-1.85374500
H	-2.66591700	5.75379500	-1.55569100
C	-3.39929000	4.31070400	-0.13390700
H	-2.60946400	4.52735400	0.59366700
H	-3.57249900	3.22324500	-0.08799300
N	-5.35155200	4.98961000	-1.98559900

N	-4.61311600	5.01656100	0.27830400
C	-5.95486800	11.60649700	3.57333500
C	-4.84768700	10.81197800	3.30189400
C	-4.45375400	9.77548900	4.17691300
C	-5.22567800	9.58655300	5.34497500
C	-6.33291300	10.37654900	5.62123300
C	-6.71544200	11.39769600	4.73641400
H	-6.23285300	12.39668200	2.88519300
H	-4.28025600	11.00094400	2.39662500
H	-4.93368200	8.80979200	6.04630400
H	-6.90845900	10.22124100	6.52781700
C	-3.27069000	8.91509200	3.92031100
C	-2.10073600	9.55280200	3.15684100
H	-2.94985900	8.42421700	4.84161700
H	-1.95343900	10.61249900	3.39925200
H	-1.16852000	9.04013000	3.42421600
O	-1.65654700	10.05670900	0.82364600
C	-2.26998500	9.37621900	1.64860200
O	-3.09982700	8.42484000	1.33176700
C	-7.89985500	12.22315500	5.07132600
O	-8.59413600	12.07344600	6.06332500
O	-8.14764600	13.18186200	4.15500800
C	-9.28141500	14.03568900	4.39936500
H	-9.30832700	14.72734200	3.55875400
H	-10.20071500	13.44724100	4.44033100
H	-9.15403800	14.57955400	5.33801900

7

scf done: -1357.72339955

Ni	-3.54116100	7.25280800	2.71710600
C	-1.75590800	5.33787200	6.07772000
C	-2.37298000	5.05978900	4.67342700
C	-3.88535800	5.11764000	4.60685200
C	-2.68009300	5.09546500	7.28232000
C	-3.25079700	3.67431700	7.40167800
C	-3.85134100	3.15010100	6.08162500
H	-0.84750500	4.73332400	6.17653500
H	-1.98746500	5.78475100	3.95325000
H	-3.51233100	5.80858600	7.23749800
H	-4.01346700	3.66629000	8.18877600
H	-1.43333800	6.38403200	6.11034800
H	-2.05870700	4.07518400	4.31160600
H	-2.13085500	5.33687300	8.19904700
H	-2.47032300	2.97075000	7.71539600
H	-4.56384400	2.34459200	6.27457400
H	-3.06899300	2.71966300	5.45277200
C	-6.03227600	4.20389100	5.42730700
H	-6.29532200	3.92362800	6.45171200
H	-6.45650800	3.44358900	4.75881300
C	-6.57429800	5.58613700	5.09044300
H	-7.66237200	5.54401500	4.99072500
H	-6.34150900	6.28656500	5.90005500
C	-5.93534000	6.07565100	3.79404100
H	-6.23667600	7.10432400	3.58244900
H	-6.26956800	5.45621600	2.95092100
N	-4.56493200	4.18253700	5.31417700
N	-4.46345600	6.04277600	3.86633400
C	-5.98323700	11.21238600	3.23371200
C	-4.79773600	10.50276900	3.08435400
C	-4.40685500	9.52082300	4.02072900
C	-5.26292400	9.29678200	5.12166100
C	-6.44811800	10.00239200	5.27613700
C	-6.82689800	10.96915100	4.33083500
H	-6.25959800	11.96177700	2.50082600
H	-4.16692700	10.71429500	2.22715800
H	-4.97655100	8.56088100	5.86792500
H	-7.08945600	9.82170800	6.13239500

C	-3.14672100	8.74551900	3.89160200
C	-1.95746500	9.44558000	3.21712600
H	-2.87681300	8.29304000	4.84834200
H	-1.91489000	10.52092100	3.42862600
H	-1.02142400	9.01750400	3.59609700
O	-1.30593300	9.89381400	0.92149900
C	-1.95602600	9.20500000	1.70854100
O	-2.68461700	8.18499000	1.34981200
C	-8.09992600	11.70173300	4.53394500
O	-8.86524100	11.51954900	5.46623100
O	-8.34152600	12.61139300	3.56809200
C	-9.55968500	13.37168600	3.68249300
H	-9.56488500	14.03944100	2.82243100
H	-10.42704100	12.70822200	3.65705400
H	-9.56539400	13.94501600	4.61214300

8

scf done: -3527.80161882

Ni	-3.64677500	7.54159000	2.25105000
Zn	-3.50825100	6.75358000	-0.20838600
C	-2.60837700	3.91328400	4.09825600
C	-3.76827400	4.52854400	3.25791400
C	-4.67421300	5.48244500	4.00704200
C	-2.81240700	3.90629700	5.62212400
C	-4.05728200	3.15401400	6.11779400
C	-5.33959200	3.52529100	5.34465800
H	-2.42838600	2.89301000	3.74092400
H	-3.35725100	5.07845100	2.40930700
H	-2.86238500	4.94403700	5.97358000
H	-4.19203500	3.36193600	7.18576200
H	-1.69431800	4.47868900	3.88765200
H	-4.39061400	3.73218500	2.83597600
H	-1.92318200	3.47384500	6.09435700
H	-3.91410400	2.07036200	6.02607500
H	-6.22698200	3.27617500	5.93193700
H	-5.41048400	2.93720300	4.42654500
C	-6.26440000	5.79709900	5.87564500
H	-6.20084600	5.40617700	6.89577500
H	-7.31367800	5.72033300	5.56015100
C	-5.79086800	7.24411000	5.82692200
H	-6.52135500	7.89146500	6.32045400
H	-4.84118400	7.34224900	6.36477600
C	-5.59613200	7.66491900	4.37182100
H	-5.15814100	8.66461100	4.31682700
H	-6.56515400	7.70892900	3.85548100
N	-5.42984100	4.95241800	5.00891700
N	-4.70689400	6.74336800	3.65199000
C	2.23618500	8.30050500	3.77671100
C	0.97641900	8.22547300	3.19320000
C	0.00319200	9.20972400	3.43724100
C	0.33509800	10.27296600	4.29033900
C	1.59187900	10.35463000	4.88314800
C	2.55595900	9.36872300	4.63152900
H	2.97671800	7.53634300	3.57035600
H	0.74615900	7.39649300	2.53057600
H	-0.40147800	11.04672500	4.49007900
H	1.83929800	11.18169200	5.54013300
C	-1.38500900	9.10139400	2.84458500
C	-2.26091800	8.01897000	3.50548300
H	-1.88790000	10.06915400	2.98323700
H	-1.69052300	7.09474600	3.66585800
H	-2.66255000	8.35065200	4.46764500
O	-2.54505000	8.35037200	0.92579300
C	-1.41615700	8.88943100	1.32100500
O	-0.52677400	9.23867900	0.55515500
C	3.88696400	9.49600700	5.27877700
O	4.21060600	10.40074400	6.02868700

O	4.72648400	8.49282500	4.95257800
C	6.04558100	8.53809700	5.52988200
H	5.98616700	8.50170400	6.61991200
H	6.55911200	7.65803600	5.14588000
H	6.56462300	9.44865300	5.22260800
C	-5.84953100	8.73292200	0.65129900
H	-5.61265100	9.24001800	1.59500200
H	-6.93726200	8.81882500	0.50994700
H	-5.36810600	9.31671700	-0.14051100
C	-5.36067500	7.27317200	0.65039100
H	-5.83640000	6.70939900	1.45737200
H	-5.77884400	6.78154200	-0.24862900
C	-2.37344200	5.23335000	-0.82818100
H	-2.25623500	5.31577000	-1.91887400
H	-2.92564700	4.29469200	-0.66990400
C	-0.98235200	5.10595400	-0.18317200
H	-1.04864300	4.97074600	0.90437800
H	-0.40335000	4.25380000	-0.57141000
H	-0.37497200	6.00398300	-0.34883600
C	-4.91064900	7.96847300	-2.88341400
O	-3.76117700	8.02265300	-2.00495700
C	-2.61559800	8.58559700	-2.69939700
C	-3.03088400	8.67286600	-4.16871800
C	-4.55333500	8.86172500	-4.07048500
H	-5.06898900	6.92767500	-3.19412900
H	-5.78219100	8.30825400	-2.31932500
H	-2.40993000	9.57022200	-2.26674100
H	-1.75715200	7.93334100	-2.52163100
H	-2.52760600	9.49064100	-4.69009400
H	-2.79503800	7.73907200	-4.69044700
H	-4.79694700	9.90626300	-3.84846800
H	-5.08522300	8.57211900	-4.98009000

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scf done: -3527.80714115

Ni	-3.80837300	7.25879000	2.51623300
Zn	-2.62930100	6.03890300	0.48324000
C	-1.91507300	5.33493700	5.83489500
C	-2.67744800	5.06801400	4.50032000
C	-4.18072100	5.25314100	4.55419600
C	-2.75773500	5.27573900	7.11920800
C	-3.44903500	3.92997200	7.38486800
C	-4.17430200	3.37277500	6.14442100
H	-1.08335600	4.62482200	5.90385700
H	-2.29718800	5.73126500	3.72166900
H	-3.51817100	6.06525100	7.07866100
H	-4.16021600	4.05272200	8.21007100
H	-1.46270100	6.33081500	5.77863100
H	-2.47985900	4.04921400	4.15030400
H	-2.11618600	5.52281000	7.97238900
H	-2.71796000	3.17968600	7.70988100
H	-4.92243700	2.63150400	6.43582300
H	-3.46719700	2.85049200	5.49542700
C	-6.32155400	4.53022000	5.56241500
H	-6.54231200	4.30114600	6.60941000
H	-6.83913700	3.78267200	4.94658100
C	-6.78671700	5.93622600	5.21010900
H	-7.87945300	5.97062000	5.18036000
H	-6.45383500	6.64155500	5.97924300
C	-6.20503700	6.33897100	3.85766000
H	-6.43754000	7.38447100	3.64107800
H	-6.65161200	5.73299600	3.05813800
N	-4.87025600	4.40533700	5.36408000
N	-4.74287000	6.18376900	3.81728400
C	-5.72440700	11.44313400	3.25868400
C	-4.64413700	10.59167100	3.06229200
C	-4.34882600	9.55014200	3.97169300

C	-5.19390100	9.42149900	5.09757400	H	-4.28380700	1.98187500	5.88504100
C	-6.27452000	10.26811200	5.29894000	H	-6.50097200	3.37228000	5.84412900
C	-6.55865700	11.29160100	4.37965400	H	-5.69139900	3.05160200	4.33062400
H	-5.92449000	12.23435900	2.54491800	C	-6.33915200	5.88507400	5.92672300
H	-4.01776000	10.73912800	2.18838300	H	-6.31266700	5.44048400	6.92618200
H	-4.97900700	8.64602800	5.82759100	H	-7.38748300	5.89785600	5.60045900
H	-6.90521500	10.15675800	6.17490500	C	-5.76431300	7.29517300	5.95095400
C	-3.20148400	8.62754500	3.78755100	H	-6.45064200	7.96783300	6.47289500
C	-1.94401000	9.22621700	3.14467000	H	-4.81342400	7.30032500	6.49546900
H	-2.97655300	8.11098800	4.72183700	C	-5.53365400	7.76999700	4.51847400
H	-1.77370500	10.27564600	3.41544900	H	-5.02724100	8.73867200	4.50996300
H	-1.05985100	8.67260700	3.48498400	H	-6.49487300	7.90447400	4.00274800
O	-1.23654900	9.74012500	0.87953600	N	-5.55714700	5.02607400	5.02490400
C	-1.95935100	9.08854500	1.62634300	N	-4.70539700	6.82287800	3.75705300
O	-2.81024800	8.18355900	1.19810100	C	2.30791900	8.39068500	3.53640800
C	-7.71675400	12.17721100	4.63756200	C	1.01975300	8.30722500	3.01880400
O	-8.47530500	12.07308100	5.58795700	C	0.03542000	9.24633500	3.37072300
O	-7.86321200	13.13887600	3.70141300	C	0.38465600	10.27495100	4.25839700
C	-8.96756800	14.04694000	3.87311500	C	1.66978800	10.36416600	4.78511600
H	-8.90762100	14.73681500	3.03267800	C	2.64395100	9.42131100	4.43001400
H	-9.91516400	13.50381800	3.85488200	H	3.05683900	7.66114500	3.25058700
H	-8.87488300	14.58666000	4.81818300	H	0.77546300	7.50717600	2.32612600
C	-5.24046900	5.65713700	-0.68907200	H	-0.36114700	11.01385600	4.53919300
H	-5.16604500	6.60258000	-1.23526100	H	1.93136800	11.16248800	5.47127600
H	-6.30237800	5.37171400	-0.67889500	C	-1.38402900	9.12440800	2.85941100
H	-4.71476500	4.90639500	-1.29132600	C	-2.17065900	7.96590300	3.50069500
C	-4.65585800	5.77541800	0.73832500	H	-1.90936200	10.05908100	3.10099200
H	-5.31368800	6.49823500	1.25122800	H	-1.58624900	7.03698900	3.50179500
H	-4.81481400	4.83071600	1.27326800	H	-2.48344400	8.19008900	4.52387900
C	-0.83207400	5.22586400	0.78428800	O	-2.64819700	8.43188300	0.98288600
H	-0.45761800	4.82666500	-0.17040900	C	-1.52027500	9.00883000	1.33052700
H	-0.95507900	4.33997100	1.42639100	O	-0.71072100	9.45517300	0.52929400
C	0.25359700	6.12783800	1.39773900	C	4.00292000	9.55222700	5.01748600
H	-0.04869500	6.52042800	2.37750700	O	4.33691100	10.42106800	5.80409400
H	1.21145000	5.60684000	1.55125100	O	4.85228700	8.59711200	4.59065700
H	0.46543700	6.99897700	0.76666500	C	6.19685600	8.64778700	5.10602400
C	-1.99425700	6.05345200	-2.70548400	H	6.19277900	8.53588400	6.19254100
O	-2.46685300	6.83420500	-1.58513700	H	6.71681200	7.81321000	4.63838900
C	-2.76572800	8.19608600	-2.00137800	H	6.67183100	9.59395600	4.83779200
C	-2.61191500	8.20042800	-3.52451700	C	-6.18987300	8.04215900	-0.44471000
C	-1.58922100	7.07767700	-3.76320900	H	-5.70713400	9.00806800	-0.62617500
H	-1.17212100	5.42564900	-2.35392600	H	-7.22436700	8.24941300	-0.13609200
H	-2.80976700	5.40805700	-3.05828900	H	-6.23950500	7.53138400	-1.41284700
H	-3.77627500	8.44111800	-1.66424800	C	-5.41945800	7.21205700	0.60705800
H	-2.06023500	8.86140100	-1.49716600	H	-5.53432900	7.76766000	1.55581800
H	-3.56322200	7.95536300	-4.00937000	H	-5.95128000	6.26996400	0.79781400
H	-2.28057700	9.17185300	-3.89984900	C	-2.32056100	5.49152400	-1.00985700
H	-1.62594400	6.66650100	-4.77517300	H	-2.43148500	5.57853800	-2.09911100
H	-0.57192600	7.43710100	-3.57470600	H	-2.62700700	4.46088300	-0.77387900
TS₈₋₁₀				C	-0.83917800	5.66930700	-0.63639900
scf done: -3527.7961018				H	-0.67279000	5.54672800	0.44187100
Ni	-3.66307600	7.61870800	2.35793600	H	-0.18140400	4.94547600	-1.14112400
Zn	-3.61005100	6.71577300	-0.15053500	H	-0.47329700	6.66964200	-0.89481500
C	-2.80590700	3.83934200	4.10312800	C	-2.37318900	8.20796400	-3.52677700
C	-3.90822300	4.56610500	3.27460100	O	-3.45475400	8.49387700	-2.62556700
C	-4.75967500	5.54563000	4.05394300	C	-3.39049100	9.88571100	-2.23065300
C	-3.04579800	3.75541400	5.61956000	C	-2.26183100	10.53147800	-3.05682100
C	-4.35010300	3.06466000	6.04632200	C	-2.06780900	9.53725400	-4.21496600
C	-5.58723000	3.57919100	5.28153000	H	-1.50153400	7.84473800	-2.96441100
H	-2.67518400	2.83324400	3.68913000	H	-2.70536500	7.41816800	-4.20639700
H	-3.44527700	5.11974900	2.45619000	H	-4.36731500	10.33411500	-2.44562700
H	-3.03167400	4.77045400	6.03444800	H	-3.20277300	9.93550800	-1.15387600
H	-4.48943400	3.21246900	7.12355500	H	-2.52151600	11.53834300	-3.39422800
H	-1.85683400	4.36287200	3.94569000	H	-1.34590300	10.60086000	-2.46181000
H	-4.57486700	3.83282800	2.80875600	H	-2.79297900	9.72366400	-5.01510300
H	-2.19928900	3.23375900	6.07981900	H	-1.06371900	9.56946800	-4.64663100

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scf done: -3295.30783278

Ni	-3.60558900	7.64482400	2.49263800
Zn	-3.43667000	6.85499000	-0.05111200
C	-2.81324400	3.80026500	4.12972600
C	-3.90530000	4.55955300	3.31677200
C	-4.74470700	5.53155500	4.11816700
C	-3.05545700	3.68682500	5.64383300
C	-4.36848300	3.00305000	6.05479900
C	-5.59859900	3.54966500	5.30114000
H	-2.69581500	2.80167000	3.69432000
H	-3.43413400	5.12588900	2.51159400
H	-3.02901900	4.69230700	6.08088400
H	-4.50677900	3.12893700	7.13488100
H	-1.85715000	4.31411900	3.98382500
H	-4.58121800	3.84543400	2.83461100
H	-2.21584000	3.14482800	6.09298800
H	-4.31558000	1.92337100	5.86984000
H	-6.51527700	3.34264400	5.85883100
H	-5.70916300	3.04498900	4.33863100
C	-6.31768800	5.85039800	5.99981900
H	-6.29503100	5.38233200	6.98854500
H	-7.36628300	5.88454000	5.67623800
C	-5.72392800	7.25158600	6.05539200
H	-6.40047700	7.92111900	6.59379400
H	-4.77222300	7.23194800	6.59814100
C	-5.48938300	7.75583600	4.63375200
H	-4.97083100	8.71790100	4.64570900
H	-6.44945100	7.91366800	4.12273200
N	-5.54932400	5.00152900	5.07641300
N	-4.67291600	6.81489600	3.85041200
C	2.36619100	8.31410100	3.66654100
C	1.06667400	8.26796100	3.17371300
C	0.10379800	9.20766300	3.57927200
C	0.48512100	10.19698800	4.49749600
C	1.78239300	10.24898200	4.99945700
C	2.73551700	9.30724600	4.58871900
H	3.09844900	7.58553700	3.33839500
H	0.79720200	7.49687000	2.45789000
H	-0.24357400	10.93583000	4.82010100
H	2.06995900	11.01810700	5.70818300
C	-1.32311500	9.12940200	3.07943000
C	-2.11749700	7.94209900	3.65547400
H	-1.83663000	10.05349400	3.37910900
H	-1.53879000	7.01100000	3.60618400
H	-2.43318000	8.11081700	4.68807400
O	-2.59865800	8.54718200	1.17412000
C	-1.47013900	9.10416000	1.54796600
O	-0.66651000	9.59203700	0.76455400
C	4.10993400	9.40085100	5.14714300
O	4.47526200	10.24123900	5.95036800
O	4.93443400	8.44688400	4.67187300
C	6.29300600	8.46595800	5.15172400
H	6.31624400	8.33280700	6.23555100
H	6.78653000	7.63287700	4.65374300
H	6.77584100	9.40970200	4.88888700
C	-5.78434200	8.56309800	-0.26379100
H	-5.17038000	9.45236500	-0.08062400
H	-6.82414200	8.83156800	-0.02992200
H	-5.74144900	8.36847500	-1.34240200
C	-5.28318900	7.35699400	0.55567900
H	-5.50463500	7.56847800	1.61640100
H	-5.90732600	6.47412800	0.35766200
C	-1.94634900	5.94531400	-0.96321100
H	-1.16321700	6.68885000	-1.16539600
H	-2.27710000	5.59596600	-1.95173900
C	-1.33342600	4.76088100	-0.19411500

H	-2.06712400	3.96532300	-0.01227500
H	-0.49148000	4.29702800	-0.72916200
H	-0.95053800	5.06570500	0.78824900

TS₉₋₁₁

scf done: -3527.80275726

Ni	-4.09919800	7.23202700	2.35307300
Zn	-3.20903300	5.72665300	0.41649900
C	-1.72745100	5.50002900	5.45923200
C	-2.65065800	5.14780500	4.25267900
C	-4.13734000	5.30989100	4.50090800
C	-2.38228700	5.45060200	6.84917700
C	-2.98915100	4.09512100	7.24199900
C	-3.87620800	3.48822100	6.13643100
H	-0.85945400	4.83171400	5.43184700
H	-2.39186900	5.77549800	3.39778900
H	-3.16606300	6.21668300	6.89629900
H	-3.57296800	4.22309300	8.16083100
H	-1.33815000	6.51293200	5.31056400
H	-2.47416500	4.11517300	3.93384100
H	-1.63737300	5.73956900	7.59883500
H	-2.19830100	3.37074300	7.47148800
H	-4.56431100	2.75071500	6.55667600
H	-3.26200500	2.95052700	5.41054100
C	-6.10008600	4.60710600	5.83235000
H	-6.16114300	4.41869000	6.90840900
H	-6.69182300	3.83148300	5.32847400
C	-6.63042900	5.99468100	5.49847300
H	-7.71585700	6.02011700	5.62929300
H	-6.19645000	6.73282100	6.18149100
C	-6.25899000	6.34691500	4.06092900
H	-6.53402300	7.38127400	3.83998700
H	-6.80883000	5.70533600	3.35935200
N	-4.69149500	4.48545300	5.42852000
N	-4.81520400	6.20311900	3.81513800
C	-5.93302800	11.40215900	3.13559200
C	-4.87094600	10.55842900	2.83353800
C	-4.42758800	9.57501100	3.74675000
C	-5.09746700	9.50051900	4.98892200
C	-6.15806700	10.34070000	5.29652700
C	-6.59606000	11.30166300	4.37062800
H	-6.25187100	12.14648500	2.41467600
H	-4.38062700	10.66326700	1.87113300
H	-4.76223100	8.77204700	5.72198300
H	-6.65507600	10.27079100	6.25857600
C	-3.30684600	8.64776000	3.44822100
C	-2.16109400	9.20177900	2.59453100
H	-2.94787300	8.17800100	4.36505000
H	-1.93931100	10.25697900	2.79567000
H	-1.24280000	8.64240100	2.81357600
O	-1.83975000	9.64292000	0.22997500
C	-2.41980900	9.00664700	1.10403200
O	-3.30788600	8.07388500	0.85146000
C	-7.73379700	12.17614700	4.73884800
O	-8.33918700	12.12110100	5.79684700
O	-8.05095300	13.06232400	3.77200300
C	-9.15185300	13.95046200	4.04328400
H	-9.24606400	14.57335000	3.15510500
H	-10.06899000	13.38110200	4.21025300
H	-8.93919700	14.56509200	4.92082200
C	-5.89018100	5.88594900	-0.68926400
H	-5.71324600	6.88858200	-1.09124400
H	-6.97876200	5.74875200	-0.62498100
H	-5.51683600	5.17856200	-1.43744000
C	-5.20379600	5.69959800	0.68239900
H	-5.71572400	6.39808800	1.36593000
H	-5.44161200	4.70964900	1.09442500

C	-1.35684900	5.07850600	0.27308500
H	-1.22402900	4.62228000	-0.71776700
H	-1.24002800	4.24671100	0.98430600
C	-0.23392900	6.10082900	0.51320600
H	-0.28515400	6.53301500	1.52066900
H	0.76938400	5.66150400	0.40980700
H	-0.29011600	6.94075300	-0.18800700
C	-1.79409500	6.34655200	-3.35231200
O	-3.03335900	6.54880000	-2.65105500
C	-3.41303200	7.94717900	-2.72364400
C	-2.36472600	8.63801000	-3.60790800
C	-1.13934600	7.72494900	-3.44542300
H	-1.20502700	5.61429900	-2.79331100
H	-1.99960000	5.93916200	-4.35369700
H	-4.42498500	8.01261400	-3.13829000
H	-3.41359800	8.34609400	-1.70494200
H	-2.68906100	8.65446800	-4.65453200
H	-2.17778600	9.66800500	-3.29369100
H	-0.42985100	7.79833400	-4.27436100
H	-0.60903600	7.95725500	-2.51583800

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scf done: -3295.31532838

Ni	-3.87050400	7.48066600	2.48747000
Zn	-2.69501000	6.33020400	0.51587200
C	-1.88929200	5.36508600	5.61318000
C	-2.66630500	5.16910000	4.27529800
C	-4.17111200	5.32069500	4.36884000
C	-2.70770900	5.17814300	6.90111600
C	-3.36019000	3.79779700	7.07007100
C	-4.10359700	3.32296000	5.80565800
H	-1.03074400	4.68418100	5.61480900
H	-2.31508300	5.89197700	3.53528900
H	-3.48986000	5.94666700	6.93580700
H	-4.05424700	3.83659600	7.91765700
H	-1.47567900	6.37917400	5.62536900
H	-2.45442200	4.17882700	3.85824700
H	-2.05838800	5.37427800	7.76146300
H	-2.60495500	3.04202900	7.31751000
H	-4.83423200	2.55021100	6.05652400
H	-3.40380900	2.86168400	5.10467000
C	-6.28110900	4.48551000	5.35211700
H	-6.47827000	4.16899300	6.38062900
H	-6.79933900	3.78240900	4.68668200
C	-6.77261900	5.90841500	5.12366900
H	-7.86600800	5.92867800	5.11791700
H	-6.43297600	6.55447300	5.94028000
C	-6.22401200	6.42765600	3.79764200
H	-6.47572100	7.48332700	3.67029800
H	-6.67675900	5.87976100	2.96044400
N	-4.83176600	4.39938800	5.11866100
N	-4.76057700	6.29916500	3.72026500
C	-5.87292200	11.53651100	3.56573500
C	-4.77522500	10.73505900	3.27609400
C	-4.41548600	9.64917200	4.10581900
C	-5.21408400	9.41946000	5.24884800
C	-6.31169700	10.21568500	5.54311600
C	-6.65955200	11.28623500	4.70304500
H	-6.12331500	12.36410000	2.91173500
H	-4.18803500	10.95684100	2.39071600
H	-4.94919300	8.60494200	5.91711400
H	-6.90650800	10.02768100	6.43096000
C	-3.24915700	8.77567400	3.82243900
C	-2.03170400	9.44982900	3.17630400
H	-2.97638300	8.20541600	4.71176100
H	-1.88285200	10.48510000	3.50650900

H	-1.12144600	8.90407500	3.45520500
O	-1.41577600	10.12357200	0.92478700
C	-2.09242100	9.40651400	1.65277400
O	-2.92562900	8.49763400	1.19500200
C	-7.83493600	12.11564500	5.05694300
O	-8.55356200	11.92711700	6.02488900
O	-8.04534000	13.12693500	4.18862300
C	-9.17031400	13.98600700	4.45401800
H	-9.16372400	14.72552400	3.65475200
H	-10.10027600	13.41326800	4.43738800
H	-9.05855900	14.47214500	5.42570300
C	-5.09332700	6.33158400	-0.88755400
H	-4.86146600	7.34580300	-1.23289200
H	-6.16761500	6.17488200	-1.05442400
H	-4.56326900	5.63911500	-1.55265200
C	-4.70064600	6.13173100	0.59637100
H	-5.37003000	6.78776600	1.17484200
H	-4.94770100	5.11576400	0.92571300
C	-0.81934800	5.98015000	0.04530700
H	-0.53953900	6.64800100	-0.78093800
H	-0.72321300	4.96123500	-0.35483100
C	0.17716300	6.16363400	1.20390400
H	-0.03734700	5.48751500	2.04113900
H	1.21675000	5.97077200	0.90140300
H	0.15137400	7.18415700	1.60445000

TS₁₀₋₁₂

scf done: -3295.27139405

Ni	-3.51478900	5.95653300	2.05006100
Zn	-1.22310700	6.25111400	0.68476500
C	-4.41220200	3.59720800	5.50179400
C	-4.58913900	3.69277500	3.95432300
C	-5.63685500	4.67781200	3.47798600
C	-5.59256200	4.09371500	6.35248300
C	-6.92697300	3.37217600	6.10986100
C	-7.27017300	3.23174800	4.61414900
H	-4.18238200	2.55630300	5.75433800
H	-3.63772600	3.97591800	3.50004600
H	-5.73118100	5.16679100	6.17239000
H	-7.72464600	3.91800900	6.62685500
H	-3.52965500	4.18172200	5.78052400
H	-4.84327600	2.71059400	3.54174000
H	-5.32395800	4.00154000	7.41051400
H	-6.90464500	2.36482800	6.54268800
H	-8.33969700	3.05616500	4.47612600
H	-6.76182600	2.36383100	4.18806200
C	-8.01092400	5.36227900	3.51147400
H	-8.70480700	5.36848500	4.35707700
H	-8.56294600	4.99954500	2.63449800
C	-7.45485300	6.75775300	3.26262100
H	-8.23985500	7.40501900	2.86207300
H	-7.11040100	7.19548000	4.20609100
C	-6.28693700	6.66912500	2.28343200
H	-5.80356500	7.64266300	2.17263200
H	-6.64449700	6.37071400	1.28858100
N	-6.92281800	4.42321400	3.82448600
N	-5.27299900	5.70620400	2.74149900
C	-0.70079100	10.40025700	5.88768300
C	-0.89324000	9.57065300	4.78517000
C	-1.35593200	8.25457000	4.93505900
C	-1.62515800	7.78825600	6.23408900
C	-1.43511300	8.60859400	7.33952800
C	-0.97343600	9.92450400	7.17835700
H	-0.34064700	11.41331300	5.75025500
H	-0.67805900	9.95037800	3.78983000
H	-1.97220500	6.77142400	6.37731400
H	-1.63975300	8.24088000	8.33934800

C	-1.59292700	7.38844200	3.71333300	H	3.37674100	7.41771000	3.76172300
C	-3.09776800	7.06452100	3.56454800	H	1.28068600	6.90703800	2.56955400
H	-1.26729500	7.96223700	2.83564600	H	-0.27900500	10.76526200	3.64977200
H	-3.46588800	6.54556300	4.45355600	H	1.82302500	11.26998200	4.86027400
H	-3.68477300	7.98117900	3.42979900	C	-0.98028000	8.46170900	2.36328300
O	-0.83986300	5.48213400	2.51592000	C	-1.86298500	7.45914600	3.13942300
C	-0.79401800	6.05994800	3.66905800	H	-1.55018200	9.39749100	2.25752000
O	-0.21628800	5.60352000	4.65781600	H	-1.23510900	6.63641200	3.51713900
C	-3.72703700	6.37842700	-1.04141500	H	-2.31073000	7.94952100	4.01242700
H	-4.32274100	7.16632900	-0.56876900	O	-1.82879000	7.22118300	0.50251400
H	-4.39614100	5.80848000	-1.70021800	C	-0.86210500	7.96141400	0.93611500
H	-2.99378800	6.87772600	-1.68466100	O	0.07417900	8.24311500	0.14841600
C	-3.03067700	5.48382200	-0.00223800	C	3.97716500	9.72844000	5.13730700
H	-3.81096400	4.87428700	0.52869200	O	4.16225100	10.77917300	5.72760500
H	-2.50736000	4.67029600	-0.53123600	O	4.90634000	8.75048200	5.09756900
C	0.21724000	7.34832600	-0.12363300	C	6.14268100	9.00471900	5.79137600
H	-0.15431000	8.37497000	-0.25848200	H	5.95704100	9.16343100	6.85603100
H	0.42001100	6.98575700	-1.14159500	H	6.74836800	8.11270900	5.63879500
C	1.53389500	7.38616500	0.66952300	H	6.64130500	9.88195000	5.37324300
H	1.97827100	6.38849300	0.76807900	C	-4.08748600	5.80487700	-0.97991000
H	2.29549700	8.02854800	0.20208400	H	-3.86242200	6.79452500	-1.39708200
H	1.38748000	7.76125700	1.68975600	H	-4.88106800	5.37385600	-1.61345400
C	-0.79372300	10.76503500	8.39049300	H	-3.19491900	5.18491800	-1.14364000
O	-1.03908800	10.40236900	9.52782700	C	-4.45939700	5.88127400	0.50345000
O	-0.32479200	11.99739900	8.11036300	H	-5.37597600	6.48656600	0.61491100
C	-0.11826600	12.88068300	9.22983700	H	-4.72488700	4.87542200	0.86757400
H	0.25940200	13.80736600	8.80061900	C	-1.37978500	7.73537000	-3.28293100
H	-1.05978700	13.05711500	9.75462700	H	-1.94298100	6.92020500	-3.75553000
H	0.61093000	12.45393500	9.92194700	H	-0.47634100	7.86589800	-3.89413200

12

scf done: -3527.7947753

Ni	-3.16387000	6.66148600	1.82491900
Zn	-0.83469500	7.16510300	-1.47137900
C	-2.53103400	3.59988900	4.65321700
C	-3.53055000	3.97574500	3.51872200
C	-4.49707400	5.08901800	3.86245800
C	-2.97443800	3.95345300	6.08234300
C	-4.30675700	3.33620600	6.53677100
C	-5.44457900	3.51597100	5.50890200
H	-2.31657500	2.52684900	4.58396800
H	-2.98311700	4.30018100	2.63182800
H	-3.04652200	5.04453900	6.16500000
H	-4.59393900	3.78997700	7.49282500
H	-1.58456100	4.11778800	4.46282100
H	-4.11050900	3.09493300	3.22308100
H	-2.18581700	3.65222100	6.78148800
H	-4.18967100	2.26139400	6.72425900
H	-6.41753300	3.41838300	5.99756000
H	-5.40361800	2.71915800	4.76152100
C	-6.36106900	5.84541100	5.30238600
H	-6.51621000	5.70241200	6.37641300
H	-7.33647000	5.71718700	4.81171900
C	-5.80195000	7.23533400	5.02294400
H	-6.56646100	7.99239400	5.22130100
H	-4.95582900	7.43329600	5.69090500
C	-5.33278600	7.31267600	3.57111000
H	-4.81719100	8.25844000	3.38516200
H	-6.19279000	7.27526500	2.88823300
N	-5.42826000	4.81555100	4.83019800
N	-4.40529100	6.22823500	3.23358700
C	2.57593300	8.14806500	3.74036100
C	1.39369300	7.86645600	3.06653600
C	0.34169800	8.79920100	3.01936900
C	0.51935500	10.02817200	3.67442800
C	1.69676700	10.31708900	4.35713400
C	2.73892000	9.37984900	4.39828500

TS₁₁₋₁₃

scf done: -3295.27928653

Ni	-2.77962600	6.65840300	1.92012800
Zn	-1.16061200	6.31331500	-0.21010600
C	-2.08605200	4.32395800	5.45725600
C	-2.84683100	4.38004700	4.09653000
C	-4.07058900	5.27157700	4.07337900
C	-2.89526100	4.72349100	6.70121300
C	-4.15526300	3.88442000	6.96447500
C	-5.03165600	3.70374800	5.70904200
H	-1.68566000	3.31186200	5.58181700
H	-2.16866000	4.71699700	3.31045500
H	-3.18487700	5.77784600	6.61154700
H	-4.73817600	4.36139000	7.76083100
H	-1.21918300	4.98850000	5.39202700
H	-3.16784400	3.37428000	3.80474800
H	-2.24044100	4.66830600	7.57784200
H	-3.88427000	2.88610400	7.32844500
H	-6.05588900	3.44325100	5.98651600
H	-4.66092300	2.87409100	5.10290700

C	-6.31466700	5.74031000	5.00529500	H	-2.23997600	5.63825400	8.51175100
H	-6.62943600	5.71387600	6.05293100	H	-2.69859500	3.25313000	8.34065800
H	-7.12304600	5.29912400	4.40767400	H	-4.74159500	2.51620600	6.90413900
C	-6.03449100	7.17005500	4.56464700	H	-3.21160800	2.74516300	6.09534400
H	-6.97321700	7.72515700	4.48389100	C	-6.12947000	4.26599600	5.74193500
H	-5.41241800	7.67505900	5.31176000	H	-6.46478900	4.05769900	6.76270000
C	-5.30737500	7.15268300	3.22267300	H	-6.53611900	3.47491000	5.09645400
H	-5.01095000	8.16416800	2.93656500	C	-6.61856400	5.63452200	5.28639900
H	-5.97262700	6.77147300	2.43528600	H	-7.70202200	5.61299000	5.13649800
N	-5.10609100	4.91193200	4.87297000	H	-6.40624000	6.37953700	6.06064700
N	-4.09668200	6.31964900	3.27608400	C	-5.90945900	6.02661400	3.99210500
C	-3.51088300	10.89761900	4.00139000	H	-6.16001300	7.05355900	3.71805900
C	-2.98574400	9.61259500	4.05818800	H	-6.24124200	5.38039000	3.16855300
C	-2.18845500	9.09058700	3.01593100	N	-4.66230200	4.21539900	5.72048900
C	-1.94445800	9.92817500	1.90436000	N	-4.44846200	5.93646500	4.11234700
C	-2.47237300	11.21118700	1.83848800	C	-5.70076400	11.13786000	3.30802500
C	-3.26011400	11.71405200	2.88633600	C	-4.52406100	10.40642500	3.29023000
H	-4.10714600	11.27731600	4.82318500	C	-4.25103400	9.38870600	4.24920800
H	-3.17411700	8.99694200	4.93315200	C	-5.25323200	9.18958300	5.24279200
H	-1.33113500	9.57037200	1.08343800	C	-6.42745500	9.91677200	5.26233100
H	-2.27439200	11.84214400	0.97848100	C	-6.68473200	10.90830100	4.29096200
C	-1.64529500	7.71123300	3.11005100	H	-5.86675600	11.90364100	2.55756200
C	-0.16301400	7.54044400	2.74087200	H	-3.79407600	10.62661200	2.51680900
H	-1.82447400	7.30416100	4.10731000	H	-5.07252100	8.44700500	6.01566500
H	0.09020800	8.09819500	1.83187500	H	-7.16456100	9.74244200	6.04036000
H	0.45771200	7.95014300	3.54675000	C	-3.04283600	8.58154700	4.23251000
O	1.00455000	5.48545700	3.23922400	C	-1.78296300	9.23409800	3.66692900
C	0.20158600	6.06995700	2.50320200	H	-2.86328900	8.09836300	5.19377900
O	-0.41780000	5.51844300	1.51270600	H	-1.67380700	10.30687900	3.88321700
C	-3.78629700	13.09829200	2.78099700	H	-0.89196300	8.74878400	4.08845100
O	-3.58950100	13.84478400	1.83804700	O	-0.94973800	9.75851400	1.43507100
O	-4.51832100	13.46220100	3.85313200	C	-1.67852300	9.04115900	2.17689000
C	-5.06032300	14.79744400	3.84543100	O	-2.34973400	8.08758300	1.64356300
H	-5.60329500	14.89379100	4.78432800	C	-7.94209800	11.65938900	4.35299500
H	-4.25580100	15.53404400	3.79100400	O	-8.82801100	11.49520400	5.18358100
H	-5.73519700	14.92975900	2.99702200	O	-8.05616600	12.59538400	3.37357600
C	-4.00051900	7.36687700	-0.85428500	C	-9.26540600	13.37087000	3.36270600
H	-4.12365500	8.23591500	-0.19996500	H	-9.16581500	14.05268900	2.51869800
H	-5.00014600	7.05918300	-1.18955800	H	-10.13691300	12.72549100	3.22801000
H	-3.45812300	7.71371200	-1.74127700	H	-9.37303000	13.93280300	4.29374000
C	-3.23662800	6.22712500	-0.16041600	C	-3.13224000	5.72532900	0.12072600
H	-3.88358100	5.78558900	0.64372800	H	-3.54531900	6.60789900	-0.38221700
H	-3.19914800	5.36525000	-0.84698600	H	-3.34407800	4.86149800	-0.53051700
C	0.20054400	6.78794700	-1.57067800	H	-2.04282800	5.84677300	0.13693500
H	0.09866000	7.85458600	-1.81931300	C	-3.70528700	5.55421900	1.52720000
H	-0.02532900	6.25856000	-2.50768800	H	-4.79348600	5.40870800	1.46314400
C	1.65568300	6.49927700	-1.16617200	H	-3.29664700	4.64397100	1.99210700
H	1.82166900	5.43199900	-0.97731000	C	-2.31588200	9.38974800	-2.05283300
H	2.38037300	6.80275800	-1.93682100	H	-2.26228500	10.48451000	-2.12600000
H	1.93648400	7.02388200	-0.24463700	H	-3.38383900	9.15086600	-1.97060100
				C	-1.74586500	8.76277100	-3.33554100
				H	-1.83528900	7.66968700	-3.33089300
				H	-2.26324700	9.11650200	-4.23905600
				H	-0.68208500	8.99371300	-3.47012400
				C	1.65407900	8.46718000	-0.05786900
				O	0.38200000	7.83468300	-0.39853100
				C	0.60601700	6.55540300	-1.05807400
				C	2.08231900	6.56455900	-1.44317300
				C	2.70968800	7.39215400	-0.30966400
				H	1.78371000	9.33515500	-0.71351700
				H	1.59136400	8.80368000	0.97783000
				H	0.37249200	5.75993900	-0.34240600
				H	-0.07828900	6.49130400	-1.90661800
				H	2.49272000	5.55484900	-1.51667000
				H	2.22279200	7.06427600	-2.40734200
				H	2.84772700	6.77475700	0.58404700
				H	3.67581700	7.82555700	-0.57820500

13
scf done: -3527.80973215

Ni	-3.42379300	7.00138000	2.86073100
Zn	-1.43117500	8.87849100	-0.36846900
C	-1.81188100	5.33730300	6.41959400
C	-2.42295700	4.94681000	5.03907600
C	-3.93024600	5.06414500	4.93685500
C	-2.77689800	5.30611200	7.61591800
C	-3.42768700	3.94335300	7.89817900
C	-4.00299400	3.27478100	6.63278900
H	-0.95480100	4.68292500	6.61709300
H	-2.00388700	5.58152100	4.25538600
H	-3.56711800	6.04804000	7.44820500
H	-4.22185900	4.07869200	8.64195300
H	-1.41095400	6.35372700	6.34274200
H	-2.14631600	3.91826800	4.78312600

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scf done: -3452.30626192

Ni	-3.80967100	4.84558800	1.91871100
Zn	-0.50655600	3.66641900	-0.02108300
C	-6.04126700	3.38606400	5.11600700
C	-6.33445300	4.02446600	3.72658900
C	-6.05603500	5.50985700	3.64707600
C	-6.14981600	4.33226300	6.32305700
C	-7.49160700	5.06469700	6.47770000
C	-7.96887300	5.75832700	5.18190600
H	-6.71464300	2.53120100	5.24755600
H	-5.73251200	3.53940700	2.95871000
H	-5.34788500	5.07711500	6.25621600
H	-7.39249500	5.80582700	7.27949800
H	-5.02369700	2.98070000	5.10132900
H	-7.38070200	3.85428200	3.45187100
H	-5.94977400	3.76142800	7.23691800
H	-8.27739700	4.36760200	6.79375100
H	-8.64836500	6.58087900	5.41909400
H	-8.54555300	5.06179300	4.56877800
C	-6.62117500	7.76194400	4.51180900
H	-6.84534900	8.05054600	5.54354100
H	-7.30577800	8.32109800	3.85943400
C	-5.17196800	8.07720900	4.16932800
H	-5.03478600	9.15944800	4.08913200
H	-4.51244500	7.71602700	4.96622100
C	-4.80357400	7.39054000	2.85687400
H	-3.74548900	7.53013600	2.63174600
H	-5.37361100	7.83555800	2.02838800
N	-6.87893700	6.32103700	4.37365300
N	-5.06657500	5.94177600	2.90224000
C	-5.73465000	6.37428100	-1.62256200
C	-6.21279800	5.52681900	-0.40575400
C	-5.71410900	4.09702500	-0.38583100
C	-5.35359300	5.58265900	-2.88484100
C	-6.45033800	4.66966500	-3.45605200
C	-7.12000900	3.77841000	-2.38835000
H	-6.51571400	7.10560300	-1.86150900
H	-5.88395800	5.99039400	0.52322400
H	-4.46837600	4.97539800	-2.66116900
H	-6.00953600	4.04341800	-4.24068600
H	-4.85467300	6.95024800	-1.31627300
H	-7.30769400	5.50785900	-0.37308100
H	-5.03978100	6.28945700	-3.66149700
H	-7.23612300	5.26489400	-3.93771400
H	-7.58725700	2.90770900	-2.85654000
H	-7.92828500	4.32394400	-1.89567000
C	-5.64005500	1.92848100	-1.58914000
H	-5.51331100	1.78124400	-2.66695200
H	-6.36441300	1.17918400	-1.24147300
C	-4.31013600	1.76727400	-0.86466200
H	-4.02151400	0.71211100	-0.84808300
H	-3.52358900	2.31864300	-1.39214300
C	-4.44370400	2.31924600	0.55234100
H	-3.48620000	2.26710300	1.07550900
H	-5.16143700	1.71095400	1.12334900
N	-6.18974400	3.27559400	-1.37068100
N	-4.88524900	3.72311500	0.55456300
C	-2.15777100	5.18840300	2.58561900
O	-1.93387100	4.31398500	1.65958800
O	-1.42477200	5.78488300	3.35981700
C	0.69500400	0.92757000	-0.41886900
H	0.22294600	0.83619900	-1.40633700
H	0.86726200	-0.10015000	-0.05923900
H	1.68814800	1.36374400	-0.59312400
C	-0.14766800	1.78621800	0.54147800

H	-1.11065900	1.27954200	0.71260800
H	0.34065100	1.79657500	1.52803800
C	-0.95684400	5.00270700	-1.43216400
H	-1.19050700	5.96749700	-0.95518700
H	-1.89436700	4.70252900	-1.92774300
C	0.11828400	5.22767900	-2.51014300
H	0.34273300	4.30493900	-3.06210100
H	-0.16111200	5.98166800	-3.26399200
H	1.06786200	5.56195600	-2.07143500
C	2.38835800	4.05722700	1.63009900
O	1.28722400	4.72927100	0.98405000
C	1.37425800	6.16117500	1.19370300
C	2.56497000	6.37446500	2.13587000
C	3.44032200	5.14188800	1.85523000
H	2.04306700	3.62768300	2.57934400
H	2.71586800	3.24530700	0.97620100
H	1.53171100	6.63513100	0.21798400
H	0.42627900	6.50264400	1.61593300
H	3.07744200	7.32116500	1.94621200
H	2.23104800	6.37186600	3.17873500
H	4.03546300	5.29003900	0.94716500
H	4.12130000	4.89890500	2.67506700

TS₁₄₋₁₅

scf done: -3452.30370896

Ni	-3.82689400	4.86759600	1.74677600
Zn	-0.50932800	3.77079200	-0.28537900
C	-5.69900300	3.37389700	5.12926400
C	-6.15321300	3.97487000	3.76633700
C	-5.94914500	5.46888900	3.64140300
C	-5.71625300	4.34049500	6.32503700
C	-7.06260900	5.02359200	6.61157500
C	-7.70397800	5.66541000	5.36108500
H	-6.32532000	2.50025600	5.34405900
H	-5.60672800	3.50399500	2.94914400
H	-4.95769300	5.11488900	6.15932200
H	-6.90845700	5.78701000	7.38329900
H	-4.67505500	3.00104900	5.01798100
H	-7.21274600	3.75626100	3.59582000
H	-5.39584700	3.79732200	7.22125700
H	-7.78023500	4.30425200	7.02486000
H	-8.39479800	6.46113000	5.65136200
H	-8.30432600	4.92818500	4.82339600
C	-6.50677500	7.70868600	4.54440200
H	-6.62455900	7.99279400	5.59488800
H	-7.27934300	8.24084200	3.97298600
C	-5.11676700	8.07453900	4.04238400
H	-5.03201600	9.16022900	3.93960200
H	-4.35911800	7.74797300	4.76335600
C	-4.87029500	7.38621200	2.70295900
H	-3.85364100	7.57077300	2.35353700
H	-5.55390700	7.79177600	1.94289800
N	-6.72977200	6.25848200	4.43485200
N	-5.05774300	5.92845100	2.79652600
C	-6.02385100	6.32395200	-1.65958700
C	-6.39445200	5.45453600	-0.42066100
C	-5.83806700	4.04622400	-0.43994700
C	-5.67363800	5.54817700	-2.94009600
C	-6.76329900	4.59618000	-3.45770500
C	-7.34563300	3.68143400	-2.35895600
H	-6.85126400	7.01566300	-1.85688000
H	-6.02845000	5.92682800	0.48948700
H	-4.75784100	4.97230600	-2.75985000
H	-6.34092500	3.98599700	-4.26476400
H	-5.15854800	6.94343500	-1.39981900
H	-7.48352000	5.39115800	-0.32212700
H	-5.42358200	6.26565800	-3.72987700

H	-7.59331700	5.16293500	-3.89757300	H	-7.48557300	8.31390000	3.68051000
H	-7.80837900	2.79656200	-2.80420200	C	-5.31675700	8.26326600	3.74116300
H	-8.14373100	4.19908400	-1.82163200	H	-5.28800700	9.34674500	3.59406400
C	-5.77194900	1.87510700	-1.63531500	H	-4.53948800	8.00494900	4.46891200
H	-5.72692900	1.71219600	-2.71713100	C	-5.04240900	7.53463800	2.42860400
H	-6.44031800	1.10944200	-1.21830300	H	-4.03742300	7.75556400	2.06676100
C	-4.38369800	1.76922600	-1.01821300	H	-5.74823400	7.87529500	1.65697300
H	-4.05490800	0.72573700	-1.01868800	N	-6.82918200	6.38460200	4.22183200
H	-3.66364200	2.34348400	-1.61271200	N	-5.15634800	6.07419200	2.58035900
C	-4.42288300	2.32651500	0.40271700	C	-6.25246600	6.15084900	-1.90391500
H	-3.42226800	2.32709100	0.84144600	C	-6.53766400	5.39329600	-0.57370700
H	-5.05619100	1.68767100	1.03641400	C	-5.94975600	3.99964300	-0.50426100
N	-6.34520300	3.20798700	-1.39419800	C	-6.02652400	5.26657700	-3.14178000
N	-4.93192900	3.70733800	0.44095000	C	-7.15490900	4.27609500	-3.46715700
C	-2.15521600	5.26259500	2.32902700	C	-7.59372000	3.42600800	-2.25336800
O	-1.95002900	4.39913900	1.38598000	H	-7.07987200	6.84640200	-2.08721200
O	-1.40157400	5.87473900	3.06950400	H	-6.13252200	5.95169300	0.26875000
C	0.92230400	1.14598900	-0.50435700	H	-5.09488200	4.70457200	-3.00430300
H	0.65659900	1.05494000	-1.56588400	H	-6.81808300	3.61962900	-4.27812000
H	1.08262800	0.12109800	-0.13364100	H	-5.35618700	6.76580500	-1.76666500
H	1.89845700	1.64636900	-0.47037200	H	-7.61828600	5.32302400	-0.41023600
C	-0.14308700	1.91945500	0.29223600	H	-5.85920900	5.91309400	-4.01079000
H	-1.08613800	1.35039000	0.27112100	H	-8.03779300	4.80718800	-3.84387400
H	0.14891900	1.93475300	1.35261100	H	-8.04761300	2.48976900	-2.58885200
C	-0.69197100	5.36037800	-1.44104000	H	-8.36862400	3.94752900	-1.68656700
H	-0.49494400	6.26106700	-0.84013300	C	-5.89592300	1.73950300	-1.52190400
H	-1.74957300	5.44815000	-1.73682300	H	-5.91742400	1.49136000	-2.58822800
C	0.18614000	5.40322000	-2.70389800	H	-6.50943700	0.99174300	-1.00099800
H	-0.00777700	4.55030300	-3.36760600	C	-4.46640200	1.72251600	-0.99610300
H	0.03451700	6.31101500	-3.30908500	H	-4.10436800	0.69184200	-0.93621900
H	1.25508900	5.36685600	-2.45722600	H	-3.80804800	2.26605500	-1.68368200
C	1.98622100	4.38732400	2.53576400	C	-4.42882100	2.39332200	0.37526900
O	2.18834300	4.70059700	1.15018800	H	-3.40237800	2.45524500	0.74510100
C	2.32591400	6.12494600	1.09338600	H	-4.99822100	1.79131300	1.09933100
C	3.13916400	6.51885500	2.34520400	N	-6.49380900	3.07156400	-1.34814800
C	2.95288400	5.30802100	3.30226900	N	-4.97786800	3.75828000	0.33772400
H	0.94199000	4.59447100	2.80873900	C	-2.22958500	5.53043600	2.07619500
H	2.18595900	3.32134500	2.66574800	O	-2.00932800	4.63772200	1.16415200
H	2.81438800	6.37329700	0.14809300	O	-1.48286500	6.19929100	2.77328200
H	1.33015900	6.59116500	1.10753600	C	1.12653700	1.17817900	0.57057700
H	4.19466900	6.66100000	2.09771900	H	0.97431000	0.80356800	-0.45010100
H	2.77141300	7.45288600	2.77820000	H	1.24433900	0.29269900	1.21483000
H	3.90781100	4.80417000	3.47700700	H	2.09529900	1.69421300	0.57057000
H	2.54596000	5.59881000	4.27435700	C	-0.01579700	2.10597000	1.01895400

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scf done: -3219.81548918

Ni	-3.89398200	5.03347100	1.54835800
Zn	-0.32864700	3.72322100	-0.06721500
C	-5.64827400	3.58876800	5.02392600
C	-6.14168000	4.10842600	3.64174700
C	-6.01578300	5.60441500	3.45256500
C	-5.72200100	4.59646800	6.18283600
C	-7.10431800	5.21427800	6.44318100
C	-7.77436600	5.78096700	5.17096200
H	-6.21957000	2.68704200	5.27325700
H	-5.57684400	3.63151700	2.84115900
H	-5.00712300	5.40496200	5.98895600
H	-6.99447900	6.00911400	7.19018200
H	-4.60359200	3.27568100	4.92167500
H	-7.18937700	3.82809900	3.48972800
H	-5.37430700	4.10524200	7.09865800
H	-7.78392300	4.47076900	6.87740900
H	-8.50047600	6.55429500	5.43422400
H	-8.34074300	4.99857400	4.66063100
C	-6.68321400	7.84760900	4.26826300
H	-6.81067600	8.16949400	5.30660200

TS₁₅₋₁₆

scf done: -3219.79798118

Ni	-3.64480800	5.27402900	1.80737000
Zn	-1.08628600	4.24181500	1.11101200
C	-5.25615000	3.85362800	5.44957000
C	-5.64913700	4.00952800	3.94905700
C	-5.98270900	5.42333800	3.52520600
C	-5.81737800	4.91224500	6.41345300
C	-7.34584300	5.06405900	6.41907600
C	-7.94447900	5.20902200	5.00353700
H	-5.55794300	2.85195100	5.77720900
H	-4.81955600	3.67597300	3.32563100
H	-5.36949100	5.88194300	6.16735300

H	-7.60825600	5.93883800	7.02549700	C	-3.81586400	3.99730300	5.30151400
H	-4.16402100	3.88736700	5.52077800	C	-4.45876800	3.84982400	3.88806800
H	-6.49973900	3.36134500	3.71266300	C	-5.41290800	4.95612600	3.48449500
H	-5.47814400	4.67579300	7.42827500	C	-4.54190500	4.93175400	6.28347000
H	-7.81962900	4.19839800	6.89826800	C	-5.98911600	4.53954400	6.61952300
H	-8.91333300	5.71345600	5.04715600	C	-6.81663700	4.19254400	5.36606400
H	-8.13809100	4.22387600	4.57254000	H	-3.71611200	2.99938300	5.74569100
C	-7.43121500	7.39528100	3.88223300	H	-3.66930100	3.83637400	3.13436000
H	-7.84682600	7.78205200	4.81791800	H	-4.53691200	5.94600500	5.86625000
H	-8.21100100	7.48975200	3.11365800	H	-6.46436400	5.36332400	7.16592900
C	-6.18452000	8.17348100	3.48352500	H	-2.80410600	4.38805300	5.16174400
H	-6.45782500	9.18860300	3.18099000	H	-4.98935300	2.89361600	3.81191800
H	-5.50287600	8.24888100	4.33741200	H	-3.96165800	4.98774600	7.21196200
C	-5.48016400	7.44625800	2.34167800	H	-6.00826900	3.66928000	7.28792500
H	-4.52322200	7.92347300	2.12245900	H	-7.88702700	4.24561500	5.58479200
H	-6.09272100	7.49369300	1.43055000	H	-6.62070700	3.16027500	5.06452400
N	-7.10025200	5.97748100	4.08027800	C	-7.48321600	6.20225600	4.02686900
N	-5.20656900	6.03950000	2.67004900	H	-7.84163000	6.53474600	5.00689700
C	-4.72649600	6.10769700	-2.40631400	H	-8.36084200	5.86149300	3.45894700
C	-5.37488400	5.67120200	-1.05634700	C	-6.78365600	7.34264800	3.29702800
C	-5.15931500	4.22613700	-0.65384100	H	-7.51731600	8.09326700	2.98746800
C	-4.40481300	4.98032400	-3.40112500	H	-6.07166700	7.83235300	3.97098000
C	-5.60536800	4.13166200	-3.84640100	C	-6.03309100	6.78420400	2.08909200
C	-6.47801000	3.66487200	-2.66421400	H	-5.44279400	7.56934500	1.60996200
H	-5.38292100	6.84605400	-2.88150600	H	-6.74835100	6.41434500	1.33971800
H	-4.98057500	6.28703900	-0.24853700	N	-6.55790900	5.08055800	4.22917900
H	-3.65224600	4.32116500	-2.95154800	N	-5.11463200	5.70397800	2.45897500
H	-5.23716600	3.26418100	-4.40682300	C	-4.58040800	6.55176000	-2.90406900
H	-3.78904600	6.62490200	-2.17968100	C	-5.21097400	6.27283300	-1.50438900
H	-6.45484600	5.85558900	-1.08427000	C	-5.32322000	4.81210400	-1.11241500
H	-3.92803400	5.41798100	-4.28560400	C	-4.58065900	5.37432100	-3.89286700
H	-6.24519900	4.69832100	-4.53410600	C	-5.96850000	4.82874700	-4.26108300
H	-7.08142900	2.79892700	-2.95062800	C	-6.86756600	4.60354900	-3.02901500
H	-7.18732200	4.44839700	-2.38778100	H	-5.09274500	7.41122000	-3.35268900
C	-5.39940400	1.84954800	-1.33170300	H	-4.60982800	6.75243000	-0.72994000
H	-5.19471500	1.43866100	-2.32643700	H	-3.98016700	4.56065600	-3.46844000
H	-6.28292800	1.32761200	-0.93975200	H	-5.84562500	3.88835100	-4.81183900
C	-4.20394500	1.64767300	-0.40993500	H	-3.54002100	6.85831200	-2.75362600
H	-4.12989100	0.59496900	-0.12186700	H	-6.20973500	6.72032600	-1.44883500
H	-3.27688600	1.91646400	-0.92886300	H	-4.06282400	5.68198200	-4.80872100
C	-4.37528500	2.54058100	0.81678300	H	-6.48830100	5.52055500	-4.93587100
H	-3.52216400	2.43619600	1.49297600	H	-7.68795500	3.92272900	-3.27322800
H	-5.26733500	2.22582000	1.37808100	H	-7.33660000	5.54521000	-2.73214200
N	-5.70472800	3.28068200	-1.47786800	C	-6.24997100	2.58536300	-1.68056500
N	-4.50462800	3.95878500	0.44728200	H	-6.31622700	2.10602800	-2.66312800
C	-2.48927200	5.96324300	3.09349100	H	-7.17525200	2.34367500	-1.13831600
O	-1.61089300	5.02402800	3.04328600	C	-5.03456500	2.07384800	-0.91662700
O	-2.50361300	6.97097400	3.79702400	H	-5.19849500	1.03749700	-0.60586200
C	0.77937500	2.03511600	0.30662100	H	-4.15382400	2.08933000	-1.56889300
H	0.24500500	1.89577600	-0.64225300	C	-4.78414500	2.97218300	0.29375800
H	1.26707700	1.07447600	0.53525900	H	-3.86337400	2.67521500	0.80389600
H	1.58432200	2.75394600	0.10684700	H	-5.60096100	2.85879000	1.02152900
C	-0.15494500	2.52389700	1.42692300	N	-6.15721000	4.03700500	-1.87887400
H	-0.90857700	1.74716700	1.62946500	N	-4.65741000	4.38421000	-0.07682500
H	0.41887000	2.60967000	2.36150100	C	-2.49900200	6.56112900	2.37678100
C	-1.70586200	5.75991900	-0.04141400	O	-1.76952300	6.08972200	3.33123800
H	-2.66183700	6.24613400	0.22923700	O	-2.58130800	7.85227000	2.33344100
H	-1.89470200	5.35056000	-1.04296300	C	-1.05058200	10.42154600	5.79734200
C	-0.63349900	6.86587400	-0.11167900	H	-0.01456000	10.52691600	5.45133300
H	0.32678200	6.47909000	-0.47550500	H	-1.10161700	10.89827900	6.78846100
H	-0.91596300	7.69362200	-0.77931400	H	-1.66805600	11.03002100	5.12451400
H	-0.44045200	7.30354100	0.87476100	C	-1.50137500	8.95089400	5.81494900
				H	-0.89278800	8.39722800	6.54507800
				H	-2.52997300	8.89470600	6.19827000
				C	-1.98275200	5.28650800	-0.01948900
				H	-2.36396200	5.66240900	-0.98127600
				H	-1.92864000	4.18947700	-0.12470600

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scf done: -3452.31663975

Ni	-3.50369300	5.50487600	1.20074000
Zn	-1.42334900	8.01031700	4.07313400

C	-0.57064400	5.83725700	0.20901000
H	-0.13788900	5.47199900	1.14702900
H	0.12439000	5.55666000	-0.59963300
H	-0.56780500	6.93239200	0.26532200
C	0.79135800	9.47701100	2.24372400
O	0.50285700	8.37869700	3.14510100
C	1.68926000	7.58359300	3.39055600
C	2.84808900	8.41464500	2.83984300
C	2.18242900	9.17924900	1.68310000
H	0.00544500	9.50638700	1.48530600
H	0.76933700	10.40922700	2.82056300
H	1.75254900	7.39347700	4.46545800
H	1.57881400	6.62894800	2.86433800
H	3.21381100	9.11298800	3.60027100
H	3.68548400	7.79104200	2.51774200
H	2.71793700	10.08983800	1.40379300
H	2.10625800	8.54062500	0.79692700

TS₁₆₋₁₇

scf done: -3452.29831609

Ni	-3.11457500	5.71245000	2.15130100
Zn	0.34508000	7.75658200	3.71162500
C	-3.39685500	4.08368300	6.06712400
C	-4.25842800	4.27010100	4.78171500
C	-4.80172300	5.66804400	4.56786800
C	-3.63852400	5.10154900	7.19401900
C	-5.07827900	5.17202200	7.72571400
C	-6.13280000	5.27618100	6.60384100
H	-3.55450900	3.06629200	6.44408100
H	-3.65801500	4.02629900	3.90168800
H	-3.34519700	6.09565500	6.83579700
H	-5.16305500	6.03343200	8.39895300
H	-2.34188400	4.14936700	5.78151300
H	-5.10139600	3.57078500	4.78554000
H	-2.96238500	4.87285000	8.02578700
H	-5.31231300	4.28344800	8.32518000
H	-7.06508400	5.69560100	6.99144600
H	-6.38252800	4.28101800	6.22803600
C	-6.19059600	7.50919200	5.46561400
H	-6.25978300	7.85614800	6.50184300
H	-7.20345200	7.54302700	5.04140000
C	-5.24245800	8.39333600	4.66482300
H	-5.69912500	9.37361100	4.49910200
H	-4.31475500	8.54940400	5.22715000
C	-4.92072100	7.71104000	3.33677200
H	-4.17505700	8.28054200	2.77708200
H	-5.82615700	7.65884100	2.71468400
N	-5.71188200	6.11914300	5.47895900
N	-4.38849400	6.35590600	3.53303500
C	-5.96699000	6.47858800	-1.48823900
C	-6.62193800	5.75591100	-0.27100500
C	-6.31902800	4.27257400	-0.15134500
C	-5.53923700	5.57223000	-2.65472400
C	-6.66694600	4.75736600	-3.30839100
C	-7.56410200	4.03783200	-2.27938700
H	-6.65430000	7.25210000	-1.85200500
H	-6.27698800	6.21155400	0.65832500
H	-4.76883700	4.88122900	-2.29219800
H	-6.22086200	4.02489300	-3.99233700
H	-5.07289900	7.00435000	-1.13553000
H	-7.70951200	5.88929000	-0.30020900
H	-5.05362900	6.18783900	-3.42107800
H	-7.30640100	5.40624700	-3.92063700
H	-8.11490000	3.22321000	-2.75917500
H	-8.32223300	4.72975300	-1.90181100
C	-6.47513700	2.04469300	-1.22100900
H	-6.30762300	1.77856600	-2.27076900

H	-7.31784700	1.43388500	-0.86491400
C	-5.22530500	1.75805800	-0.39319900
H	-5.08617100	0.67676400	-0.29211500
H	-4.34317000	2.15842800	-0.90690600
C	-5.35929500	2.43453900	0.97360100
H	-4.43999700	2.30225400	1.55502900
H	-6.16247000	1.94554900	1.54788200
N	-6.82827000	3.46751300	-1.15003000
N	-5.63350100	3.86699100	0.87128800
C	-1.60932200	6.57101100	2.75325100
O	-0.75811400	5.98274500	3.51473500
O	-1.40927300	7.80837600	2.48871600
C	2.58722400	9.26959000	4.97119900
H	3.25984600	8.41101400	4.85247600
H	2.97775000	9.86258400	5.81205100
H	2.70500300	9.88449700	4.07033800
C	1.12858100	8.82972000	5.17770100
H	1.05150000	8.25332400	6.11024200
H	0.50021000	9.71775800	5.33407700
C	-2.13442900	4.99071800	0.66671600
H	-2.91874100	4.30112700	0.30217800
H	-1.28387600	4.37484300	0.98992500
C	-1.70338800	5.93565200	-0.46005100
H	-0.93025100	6.63427500	-0.12098400
H	-1.29701500	5.39938600	-1.33272200
H	-2.54149700	6.54379300	-0.82310700
C	2.64231300	6.37274800	1.99114900
O	1.66750800	7.44496500	2.07256900
C	1.81509800	8.36836500	0.96293500
C	2.73081700	7.65042600	-0.02733000
C	3.62111800	6.80505000	0.89946500
H	3.10061700	6.25714400	2.97698500
H	2.11207400	5.45027800	1.73172700
H	0.81754400	8.58390000	0.57420100
H	2.26399400	9.29422200	1.34215500
H	2.14405600	7.00439200	-0.68871800
H	3.29709500	8.35047600	-0.64625400
H	4.07718200	5.94997000	0.39501100
H	4.42222600	7.41890800	1.32457000

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scf done: -2990.18707422

Ni	-3.39073300	5.54153200	1.71930200
Zn	-1.11865600	8.24969700	4.18180200
C	-4.21891700	3.74215000	5.48857400
C	-4.70674200	3.68235900	4.00830900
C	-5.58552700	4.83354100	3.56260100
C	-5.03987800	4.63626700	6.43217700
C	-6.52202400	4.25709600	6.57469600
C	-7.21121600	4.00872800	5.21762200
H	-4.18301200	2.71987000	5.88278800
H	-3.84323100	3.66962500	3.33891600
H	-4.97077700	5.67269600	6.08049800
H	-7.04182700	5.05575900	7.11708200
H	-3.18930000	4.11271200	5.49061600
H	-5.25379300	2.75004900	3.82869600
H	-4.57194600	4.62562700	7.42311000
H	-6.63181600	3.34710900	7.17740200
H	-8.29707000	4.08937100	5.31581300
H	-7.01204800	2.99075300	4.87461600
C	-7.66850100	6.11699300	3.94424100
H	-8.09612100	6.41598700	4.90678600
H	-8.50293700	5.82270700	3.29347100
C	-6.88053000	7.26477600	3.32591300
H	-7.56810100	8.03971800	2.97466200
H	-6.22527200	7.71755600	4.07865200
C	-6.03327300	6.72581200	2.17566900

H	-5.40236800	7.51193400	1.75404300	O	-2.08247200	6.30800700	3.03199400
H	-6.68629800	6.36658200	1.36706200	O	-3.28726100	7.45610700	1.61702000
N	-6.79716100	4.95352800	4.17252700	C	-1.67811900	11.27407700	3.76080800
N	-5.15391600	5.63074600	2.61299800	H	-0.67604300	11.28976300	3.31448500
C	-2.37024900	6.68742700	2.71730800	H	-1.69267100	12.05922300	4.53219200
O	-1.66357300	6.27116700	3.70116000	H	-2.37425600	11.59292700	2.97482400
O	-2.41027100	7.94913900	2.49975000	C	-2.03599300	9.88471400	4.31419800
C	0.20121200	10.34074100	5.83560600	H	-1.34974600	9.63521000	5.13631500
H	1.15645000	9.80379300	5.78497500	H	-3.03287800	9.92533800	4.77489100
H	0.22910800	10.94939100	6.75194000	C	-4.64038400	2.97446000	0.80543100
H	0.19223000	11.04160000	4.99162900	H	-5.56099000	3.22136900	0.28423400
C	-0.99781100	9.37930800	5.79593000	H	-4.72683700	2.27132000	1.62865300
H	-0.96863500	8.72599700	6.67925100	C	-3.39975600	3.19450800	0.19050400
H	-1.92893800	9.95451600	5.89319100	H	-2.53247800	2.61404700	0.49511500
C	-1.96094200	5.24226100	0.49081300	H	-3.35782100	3.54868800	-0.83639100
H	-1.62743000	6.16295700	-0.00676100	H	-2.68791300	4.60216700	0.72781400
H	-2.57137600	4.68505300	-0.25443700	C	1.01471200	8.64031300	2.01102200
C	-0.75588200	4.39748300	0.91275500	O	-0.37883100	8.68063500	1.61145300
H	-1.06199800	3.45260500	1.37862100	C	-0.50080700	8.86961000	0.17610300
H	-0.10300100	4.13880700	0.06436300	C	0.90887100	8.65476200	-0.37382300
H	-0.13948600	4.92826800	1.64617100	C	1.79437400	9.12904400	0.79081100
C	1.85215300	7.57893900	3.31082500	H	1.12933600	9.27263700	2.89537400
O	0.64060800	8.30949800	2.99108600	H	1.26819600	7.60660200	2.27308200
C	0.83537400	9.16136300	1.83197300	H	-1.24115500	8.15710100	-0.19182400
C	2.34544600	9.17018100	1.59663800	H	-0.86171300	9.88911300	-0.00361000
C	2.76745500	7.78025300	2.10350900	H	1.08146100	7.59260800	-0.57728700
H	2.27734500	8.00396300	4.22763300	H	1.07947700	9.21188700	-1.29820700
H	1.57807000	6.53663700	3.49109900	H	2.80664200	8.71912800	0.75797900
H	0.28599900	8.72531600	0.99115800	H	1.86716800	10.22183700	0.79615800
H	0.41594200	10.14415400	2.06225400				
H	2.59639000	9.33845600	0.54671100				
H	2.82137900	9.95574600	2.19300200				
H	2.56709500	7.01863400	1.34284100				
H	3.82441000	7.72393800	2.37430400				

TS₁₇₋₁₈

scf done: -2990.16286782

Ni	-3.89313900	4.72181500	1.56902200
Zn	-2.00899300	8.41732600	2.98610700
C	-3.89601400	4.68644900	5.81878200
C	-4.59128300	3.95553700	4.63099700
C	-5.66070900	4.75700500	3.92014400
C	-4.69399000	5.83210200	6.46410300
C	-6.07349100	5.45079000	7.02339700
C	-6.92236300	4.62471500	6.03408800
H	-3.63438400	3.94039800	6.57839300
H	-3.84346300	3.69102400	3.88062400
H	-4.82216300	6.62904600	5.72165200
H	-6.60808900	6.36832700	7.29710300
H	-2.95663800	5.10673200	5.44792600
H	-5.03821000	3.01589600	4.97429700
H	-4.09206700	6.26922900	7.26912300
H	-5.96769000	4.86488300	7.94499800
H	-7.98289300	4.69260200	6.29110000
H	-6.66237900	3.56568400	6.10961300
C	-7.83258300	5.93039600	4.09465100
H	-8.20124000	6.56769500	4.90492600
H	-8.67937300	5.32164600	3.74773700
C	-7.28007800	6.77818500	2.95523400
H	-8.09887700	7.28852600	2.43951600
H	-6.60812600	7.54616300	3.35474900
C	-6.50606200	5.88460300	1.98851000
H	-6.01470200	6.48754600	1.22121000
H	-7.19177400	5.19595500	1.47387700
N	-6.78608400	5.05446700	4.63806100
N	-5.46886000	5.10751200	2.67709700
C	-2.97592600	6.30511600	2.10683100

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scf done: -2911.55583387

Ni	-3.54741900	5.18728800	1.59304500
Zn	-1.33049200	8.78869900	2.36268500
C	-3.89638200	4.65104800	5.78027100
C	-4.43017800	4.05679600	4.44234200
C	-5.49429000	4.88345400	3.75089400
C	-4.83479800	5.62573500	6.51159200
C	-6.22101600	5.07015900	6.87266200
C	-6.91723700	4.36383700	5.69082500
H	-3.63194400	3.81930400	6.44332700
H	-3.60219500	3.94410100	3.73713200
H	-4.96367200	6.52084100	5.89134400
H	-6.84670300	5.89460800	7.23409200
H	-2.96559100	5.18596800	5.56667000
H	-4.83294800	3.05206400	4.60924600
H	-4.33915700	5.96773100	7.42714900
H	-6.14648500	4.34988600	7.69653900
H	-7.99904100	4.33284200	5.84397300
H	-6.59031100	3.32352300	5.62502100
C	-7.72987200	5.93185700	3.91208100
H	-8.16173100	6.44245600	4.77882300
H	-8.53192700	5.34625200	3.44348000
C	-7.14882300	6.93821600	2.92756100
H	-7.95842000	7.47708900	2.42700000
H	-6.53889300	7.67512600	3.46207300
C	-6.27868300	6.19958200	1.91368300
H	-5.79046700	6.90051200	1.23295600
H	-6.90170600	5.53305800	1.30044900
N	-6.68235100	5.01896200	4.39695300
N	-5.22810700	5.40881200	2.57524800
C	-2.57630100	6.70175200	1.86495100
O	-1.71690700	6.76752300	2.81054100
O	-2.79424800	7.73609000	1.15385200
C	-0.24964300	11.52682200	2.81516900
H	0.77192100	11.13625100	2.90004800
H	-0.27221800	12.47619100	3.37101400

H	-0.40153400	11.77657300	1.75782700
C	-1.29229800	10.51706400	3.32194600
H	-1.12341200	10.32409800	4.39029500
H	-2.29370100	10.96482400	3.26193100
H	-2.38425100	4.85902200	0.73798000
C	0.18258500	8.67257800	-0.42449000
O	0.25159100	8.45797900	1.01150300
C	1.57352400	8.00594900	1.40784400
C	2.27651000	7.64549700	0.09997000
C	1.63332900	8.62001800	-0.90131300
H	-0.42735300	7.87439100	-0.85914300
H	-0.30792800	9.63399100	-0.59593500
H	2.07322100	8.82827300	1.93284900
H	1.44965000	7.16241600	2.09107000
H	3.36090200	7.75721700	0.17238100
H	2.05560600	6.60975200	-0.17768800
H	2.09828500	9.60875100	-0.82641800
H	1.71140500	8.28319700	-1.93766200

TS₁₈₋₁₉

scf done: -3449.15738503

Ni	-3.43053600	5.71933000	1.74347100
Zn	-2.62693100	9.52322600	3.79122100
C	-4.59208500	4.72121500	5.74591100
C	-4.77492500	4.22913300	4.27741500
C	-5.73454700	5.04355000	3.43511300
C	-5.73050100	5.58481400	6.31355700
C	-7.11716200	4.92382900	6.32877300
C	-7.48597400	4.26274600	4.98469800
H	-4.43507300	3.84528300	6.38620900
H	-3.81112000	4.24714700	3.76501200
H	-5.78728800	6.51365800	5.73357200
H	-7.86601900	5.68106100	6.58992800
H	-3.67226500	5.31213200	5.79462800
H	-5.11283600	3.18699000	4.26925300
H	-5.46767300	5.88584400	7.33410700
H	-7.16822000	4.15262500	7.10755000
H	-8.56916100	4.13922600	4.90341700
H	-7.06409300	3.25549000	4.93246600
C	-8.04925800	5.86611000	3.13882300
H	-8.74480700	6.24305100	3.89546700
H	-8.63150300	5.25256900	2.43706900
C	-7.37346100	7.02058300	2.40916200
H	-8.09760900	7.53042000	1.76697900
H	-7.00126600	7.75161900	3.13553900
C	-6.20488800	6.48614000	1.58375100
H	-5.63782700	7.31092400	1.14586300
H	-6.57730900	5.86469100	0.75662200
N	-7.04828600	5.02834800	3.81228800
N	-5.27570700	5.69462700	2.39984300
C	-2.99551100	7.36452900	2.61566600
O	-2.39668100	7.41738100	3.75150900
O	-3.36631300	8.49278200	2.11643400
C	-2.41056500	12.17770900	5.15587100
H	-1.36412900	11.97623000	5.41679900
H	-2.78955600	12.89412900	5.90063100
H	-2.39568600	12.70388900	4.19316300
C	-3.24312600	10.88669800	5.09068400
H	-3.27332100	10.42621600	6.08856400
H	-4.28763200	11.14151500	4.86205900
H	-2.03575400	5.87773000	1.26371400
C	-0.34743400	5.32148700	-2.77297300
C	-0.68095600	4.84290300	-1.50854500
C	-1.93383100	5.11588700	-0.93884400
C	-2.84467500	5.90183500	-1.66561200
C	-2.51839200	6.38111500	-2.92790000
C	-1.26727600	6.09395100	-3.49646000

H	0.62311900	5.09718100	-3.20001100
H	0.03806100	4.24247200	-0.95796700
H	-3.80905600	6.14577900	-1.23111600
H	-3.22377300	6.98797400	-3.48528700
C	-2.26948700	4.54099300	0.40110300
C	-3.54901900	4.00047600	0.68049500
H	-1.41958700	4.06647100	0.88855400
H	-3.63059400	3.17917300	1.38658700
H	-4.34316400	4.07495400	-0.05690100
C	-0.96504800	6.62753900	-4.85059200
O	-1.73550500	7.29306800	-5.51972300
O	0.26861000	6.29730500	-5.27984500
C	0.64832400	6.77179900	-6.58665700
H	1.66150800	6.40524200	-6.74349400
H	-0.02599800	6.37214200	-7.34718100
H	0.62660300	7.86333400	-6.61590400
C	-0.44717100	10.81435400	1.83936900
O	-0.69301800	9.98094400	3.00162900
C	0.54314700	9.68579200	3.70030600
C	1.57579100	10.64009000	3.10158600
C	1.07088700	10.80635200	1.65834600
H	-0.99662700	10.38764700	0.99726000
H	-0.83257900	11.81891800	2.04985600
H	0.36946700	9.83333800	4.76963200
H	0.79679200	8.63521700	3.52043300
H	1.55771200	11.60111300	3.62639100
H	2.59002200	10.23792900	3.15887000
H	1.43260900	11.71878000	1.17838500
H	1.37672200	9.95218400	1.04525500

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scf done: -3449.18175207

Ni	-2.40895700	5.40605800	1.93453800
Zn	-1.01491400	9.06651800	3.71980400
C	-4.39636700	4.36646600	5.53751700
C	-4.39236300	4.01569700	4.01861600
C	-5.06676600	5.02919200	3.11636100
C	-5.48695300	5.34610300	6.00144600
C	-6.93282900	4.90617100	5.72512500
C	-7.15104400	4.42064800	4.27718900
H	-4.46818400	3.43222800	6.10632200
H	-3.35967100	3.92161800	3.67275900
H	-5.31316900	6.31646400	5.52084000
H	-7.60396300	5.74541600	5.94243100
H	-3.42581900	4.80763200	5.78680200
H	-4.86579800	3.04155700	3.85387100
H	-5.36716600	5.52079500	7.07667600
H	-7.22373800	4.09099600	6.39906300
H	-8.20908000	4.47726700	4.00798900
H	-6.87162200	3.36834900	4.18495100
C	-7.14143200	6.26540100	2.57937000
H	-7.85937200	6.70099000	3.28177100
H	-7.71662700	5.82741700	1.75248100
C	-6.17878800	7.32794000	2.06408500
H	-6.70375900	8.00538200	1.38436000
H	-5.79946200	7.92478800	2.90135500
C	-5.00990200	6.64701000	1.35603000
H	-4.25925100	7.37914500	1.05041400
H	-5.36528900	6.14186100	0.44669000
N	-6.40734000	5.20041100	3.27977200
N	-4.34245900	5.66737800	2.22698500
C	-1.73324400	6.93497000	2.68467900
O	-1.26476600	6.95648400	3.87381100
O	-1.79632200	8.04138000	2.04051000
C	-1.62645200	11.96527200	4.03731100
H	-0.73293100	12.23460600	3.46018400
H	-1.84867200	12.82166600	4.69167700

H	-2.45328300	11.89329700	3.32011500	C	-4.54306200	6.85791500	0.83383400
C	-1.43039900	10.65509600	4.82001300	H	-3.70027700	7.48304000	0.53326900
H	-0.62344600	10.79001900	5.55430300	H	-4.81483300	6.24600200	-0.03796400
H	-2.33245200	10.44797000	5.41138500	N	-6.31762900	5.79926300	2.69003700
H	0.09358100	6.41066200	0.18949100	N	-4.08578000	5.97557600	1.92179700
C	-1.63696400	3.50721400	-2.85043400	C	-0.90631500	6.62577100	2.76961200
C	-0.81250800	3.81512300	-1.77153200	O	-0.80367500	6.53650500	4.06821500
C	-0.93745600	5.03055900	-1.07893300	O	-0.59486800	7.76859500	2.23884100
C	-1.91938200	5.93876100	-1.51122500	C	-0.30789500	10.92991400	6.01855700
C	-2.74698500	5.64275900	-2.58971400	H	0.10123400	10.30198500	6.81984500
C	-2.61649200	4.42185100	-3.27000900	H	-0.78834500	11.79119400	6.50720700
H	-1.52202300	2.56440900	-3.37301000	H	0.55135700	11.32322400	5.46122300
H	-0.05161800	3.10324300	-1.46133400	C	-1.26845200	10.14605000	5.10963800
H	-2.02680700	6.88814000	-0.99463900	H	-2.12636000	9.80001800	5.70339300
H	-3.49721700	6.35342400	-2.92069200	H	-1.69566600	10.82917600	4.36167500
C	-0.06137500	5.32790700	0.11599100	H	0.92345800	6.55718400	0.68546900
C	-0.65627900	4.80723300	1.44305200	C	-1.23473200	4.23683100	-2.55761700
H	0.92799800	4.87925000	-0.06404600	C	-0.44205800	4.30396600	-1.41442800
H	0.08922800	4.91217500	2.24041700	C	-0.34455700	5.48673800	-0.66527400
H	-0.86904500	3.72251400	1.34259200	C	-1.06298100	6.61292000	-1.10158800
C	-3.51908900	4.14758800	-4.41604700	C	-1.85345100	6.55735800	-2.24485900
O	-4.39559200	4.89980000	-4.80644800	C	-1.94937400	5.36744600	-2.98372900
O	-3.27630800	2.95763200	-5.00383900	H	-1.29604200	3.31520300	-3.12500300
C	-4.10979700	2.60718700	-6.12500700	H	0.11666600	3.42600500	-1.10002200
H	-3.75472500	1.63214800	-6.45521000	H	-0.99445600	7.53189200	-0.52801900
H	-5.15662800	2.54922700	-5.81849700	H	-2.40133600	7.43176100	-2.58021000
H	-4.00381900	3.34394900	-6.92429700	C	0.51686500	5.54704500	0.57659200
C	1.48765900	9.66385000	1.85903800	C	-0.20976800	5.17973100	1.87998500
O	1.00726000	8.99278700	3.05269200	H	1.36820100	4.86604200	0.44636800
C	2.11527000	8.54359700	3.87764900	H	0.50515800	4.96029300	2.67365700
C	3.36156800	9.17311900	3.25344400	H	-0.79444800	4.24065300	1.76415900
C	2.96729700	9.29536800	1.77187700	C	-2.80249200	5.35445500	-4.19938500
H	0.88729000	9.31357400	1.01681100	O	-3.46097800	6.30076200	-4.59540900
H	1.34079000	10.74350000	1.98401100	O	-2.78227900	4.16939700	-4.84301400
H	1.92722900	8.86611100	4.90519000	C	-3.58650300	4.06454900	-6.03355900
H	2.13911400	7.44941900	3.84352200	H	-3.43346400	3.04949200	-6.39683600
H	3.54499300	10.16408600	3.68199500	H	-4.63992700	4.23197200	-5.79827600
H	4.25313400	8.56215600	3.41237800	H	-3.25937000	4.79157500	-6.78013400
H	3.54822100	10.04764500	1.23314900	C	2.58591800	9.31046700	3.67561900
H	3.09079600	8.33476800	1.26089300	O	1.64752200	8.49641100	4.42389800

TS₁₉₋₁

scf done: -3449.15942459

Ni	-2.20460900	5.60903400	1.99482900
Zn	-0.49391500	8.58922800	4.17133500
C	-4.70494000	5.19168400	5.31034000
C	-4.55008000	4.59448200	3.88040000
C	-4.98770000	5.51226100	2.75871200
C	-5.78664100	6.27263400	5.47414600
C	-7.20652600	5.86598800	5.05077700
C	-7.26434300	5.21695900	3.65038300
H	-4.89085500	4.36652000	6.00768200
H	-3.50047100	4.35016500	3.69650700
H	-5.48770800	7.15604900	4.89731700
H	-7.84658900	6.75585400	5.07486400
H	-3.74621300	5.63463200	5.60020600
H	-5.11158000	3.65753100	3.80028600
H	-5.80661500	6.59434000	6.52164700
H	-7.63482700	5.15486700	5.76781900
H	-8.26377100	5.32295800	3.22053000
H	-7.07993000	4.14285000	3.72385600
C	-6.84859200	6.80524500	1.75776500
H	-7.61514700	7.38438800	2.28274200
H	-7.34026800	6.29878000	0.91619900
C	-5.73207300	7.71451100	1.26156500
H	-6.09189300	8.32356800	0.42723700
H	-5.42156900	8.39618700	2.06166000

TS₁₈₋₂₀

scf done: -3449.16515323

Ni	-3.66573000	4.73356200	1.90507500
Zn	-2.56386000	8.96619600	1.87224200
C	-4.29682700	6.27359100	5.86915800
C	-4.63350800	5.04159800	4.97517500
C	-5.72264200	5.25802300	3.94611000
C	-5.38093000	7.35936200	5.96790100
C	-6.73487000	6.89224800	5.62367000
C	-7.23287000	5.58999200	5.86525300
H	-4.04112200	5.91294300	6.87257800
H	-3.73942700	4.73801600	4.42830900
H	-5.53629600	7.78952700	4.97122900
H	-7.47294100	7.69050400	6.38003900
H	-3.39793800	6.74185500	5.45879900

H	-4.92001300	4.18592600	5.59623900	C	-3.78939000	5.48349500	5.35266300
H	-5.00267300	8.17817700	6.59074700	C	-4.47107000	4.44165600	4.41425300
H	-6.66918300	6.71794800	7.60495700	C	-5.53402300	4.99865400	3.48985200
H	-8.31098900	5.47452300	6.00617800	C	-4.58591200	6.77019900	5.62415000
H	-6.77039200	4.72514300	6.34749000	C	-5.97397000	6.57193800	6.25289400
C	-8.07977100	5.88951200	3.52577800	C	-6.80963900	5.48955400	5.53944300
H	-8.66530100	6.68065100	4.00535300	H	-3.54825600	4.98760300	6.30007000
H	-8.74549900	5.02503800	3.39469300	H	-3.71529100	3.96774700	3.78393500
C	-7.54224900	6.36138900	2.18031600	H	-4.69997900	7.31657600	4.68034400
H	-8.36198700	6.44755900	1.46104600	H	-6.50898900	7.52885900	6.23554400
H	-7.08795000	7.35287500	2.28697600	H	-2.83647300	5.77415700	4.90003100
C	-6.48917200	5.37277900	1.68407000	H	-4.92454900	3.63997800	5.00680400
H	-6.02372600	5.73878100	0.76540100	H	-3.99008900	7.42080600	6.27447800
H	-6.96004300	4.40771200	1.44555100	H	-5.88330700	6.28402200	7.30762800
N	-6.97419300	5.52790300	4.42225400	H	-7.87359800	5.62077800	5.75412000
N	-5.42739100	5.16157900	2.67573600	H	-6.54465700	4.49948200	5.91804700
C	-3.09947200	6.54197800	1.90645600	C	-7.68741100	6.20914200	3.30651700
O	-2.51620900	7.10100600	2.89900900	H	-8.01368900	7.07627800	3.88995900
O	-3.36979900	7.28078000	0.89078500	H	-8.56032900	5.55487400	3.17739400
C	-2.00569900	11.86033100	2.30456500	C	-7.13786600	6.64717500	1.95490200
H	-1.28687800	11.62377600	3.09892200	H	-7.95654500	6.98690300	1.31382300
H	-2.37030300	12.87987000	2.50167800	H	-6.44722000	7.48777900	2.08606800
H	-1.43290700	11.90531600	1.36993000	C	-6.39395500	5.47830600	1.31255000
C	-3.13945800	10.82439900	2.23054900	H	-5.92280600	5.78647700	0.37660500
H	-3.70607900	10.83794500	3.17198900	H	-7.09961200	4.66959300	1.07287800
H	-3.85815700	11.12795300	1.45634600	N	-6.65689100	5.49978700	4.07931600
H	-2.32525900	4.68530200	1.31854300	N	-5.34123600	4.95549200	2.19447900
C	-5.53971900	0.89005900	4.62256500	C	-2.92464700	5.90289800	0.98639300
C	-5.40696100	1.54480300	3.40529700	O	-2.20068800	6.48034500	1.86870900
C	-4.15161900	1.99055900	2.93844600	O	-3.13794300	6.53482000	-0.11079100
C	-3.02718900	1.74800600	3.75904900	C	-3.75618500	10.63249900	0.50793500
C	-3.15504300	1.09335300	4.97517700	H	-4.19845300	10.31109900	-0.44298900
C	-4.41170900	0.65494500	5.42729400	H	-3.84566600	11.72878400	0.54509600
H	-6.51579800	0.55386300	4.95362800	H	-4.40013600	10.23626800	1.30278100
H	-6.28736400	1.71500500	2.79159600	C	-2.30326600	10.15051300	0.65555700
H	-2.04298700	2.07645500	3.44127400	H	-1.68665200	10.60864300	-0.13079200
H	-2.28135700	0.91120700	5.59220100	H	-1.89248200	10.53116300	1.60172300
C	-4.07163400	2.67378400	1.64357400	H	-0.51942900	3.66922100	1.41405100
C	-2.88307400	3.01367800	0.98337600	C	-5.04566300	1.04308700	1.67921700
H	-4.99432700	2.69189300	1.06896000	C	-4.34540300	1.92577400	0.85210000
H	-2.91054300	3.18721400	-0.08810600	C	-2.95783600	2.19871500	1.05632600
H	-1.92152700	2.67202000	1.35367200	C	-2.32444900	1.52392200	2.14558400
C	-4.49443600	-0.04521800	6.72919700	C	-3.02264000	0.64858100	2.94992400
O	-3.54300700	-0.28142100	7.45540300	C	-4.39951800	0.39702400	2.73767600
O	-5.75423600	-0.41143100	7.05085900	H	-6.09418700	0.84511000	1.48630400
C	-5.92591600	-1.10985500	8.29849900	H	-4.84589600	2.34364800	-0.01858500
H	-6.99196100	-1.32154300	8.36689900	H	-1.26842500	1.69142100	2.32844800
H	-5.35096700	-2.03854600	8.29822500	H	-2.51950700	0.13218900	3.76107000
H	-5.60624000	-0.48357200	9.13442000	C	-2.34628600	3.26745800	0.28942900
C	-0.13460400	9.03835500	-0.18121300	C	-0.85694400	3.53305200	0.38153100
O	-0.55181400	8.80810300	1.18947800	H	-2.73484300	3.34937000	-0.72988300
C	0.57074100	8.39636600	2.01370700	H	-0.60216400	4.44642100	-0.16318600
C	1.68129000	8.05432300	1.02207300	H	-0.26445600	2.71416200	-0.05364900
C	1.39360700	9.01821700	-0.14183500	C	-5.09274500	-0.55338200	3.63169300
H	-0.54280600	8.23360700	-0.80283400	O	-4.56713800	-1.14848300	4.55931200
H	-0.55788900	9.99240200	-0.50672700	O	-6.39970200	-0.71243200	3.32413100
H	0.84353200	9.23557100	2.66448700	C	-7.14821600	-1.63083900	4.14168900
H	0.24026800	7.55564300	2.62677200	H	-8.16220300	-1.61117200	3.74478200
H	2.67553800	8.18840500	1.45482600	H	-6.72927100	-2.63700100	4.06806400
H	1.58869300	7.01483700	0.69014900	H	-7.13991900	-1.30880300	5.18543100
H	1.78382500	10.01644700	0.08307300	C	1.04037600	7.36528000	0.70076200
H	1.82443200	8.68874500	-1.09023300	O	-0.11517400	7.62986900	-0.13972400
				C	0.28273600	7.80527400	-1.52502300
				C	1.72386700	7.30353400	-1.58889000
				C	2.25246300	7.64869500	-0.18650000
				H	0.97523400	8.01105900	1.58025100
				H	0.99455000	6.31907700	1.02014900

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scf done: -3449.19626467

Ni	-3.74419000	4.25641500	1.29426700
Zn	-2.03635500	8.19329800	0.60067900

H	-0.41523800	7.24031700	-2.14746000
H	0.20666000	8.87035700	-1.77408200
H	1.74396700	6.22070100	-1.75054900
H	2.29038900	7.78032900	-2.39225100
H	3.12184200	7.05421700	0.10404700
H	2.52762500	8.70733500	-0.13208900

TS₂₀₋₁

scf done: -3449.16656691

Ni	-4.87379600	4.55959600	-0.27118300
Zn	-3.10457000	8.23909900	-0.15682100
C	-3.88631200	4.32953300	3.83273500
C	-4.97436800	3.83937100	2.82997600
C	-5.96986400	4.89464800	2.39513400
C	-4.24982300	5.56869600	4.66699900
C	-5.51918500	5.44362300	5.52360800
C	-6.72828300	4.89147500	4.73940700
H	-3.62793800	3.49547000	4.49550300
H	-4.49358600	3.46539000	1.92274800
H	-4.36298000	6.42411300	3.99025200
H	-5.76191900	6.42971800	5.93709900
H	-2.98089800	4.56692000	3.26429200
H	-5.52887000	2.99687300	3.25728600
H	-3.40353200	5.81424000	5.31876300
H	-5.34348500	4.78066600	6.37986400
H	-7.66341300	5.16861400	5.23316500
H	-6.70494700	3.79899900	4.73052000
C	-7.71469200	6.50544000	3.09225200
H	-7.73142600	7.14657500	3.97935800
H	-8.73491000	6.12587800	2.94346300
C	-7.24898600	7.28685900	1.87080200
H	-8.01936100	8.00368700	1.57160000
H	-6.34364600	7.85461700	2.11477300
C	-6.94734100	6.31334800	0.73394700
H	-6.51767200	6.83768600	-0.12242300
H	-7.87588400	5.83267600	0.39429100
N	-6.80633400	5.38052300	3.35760400
N	-5.98586000	5.27537500	1.14019100
C	-3.67196500	5.92775600	-0.77312500
O	-2.73074700	6.16969400	0.07805100
O	-4.20364900	6.94776500	-1.37905300
C	-3.19326600	11.17818000	0.30480000
H	-2.17802600	11.27487200	-0.09975200
H	-3.34425600	12.02822300	0.98712500
H	-3.88188900	11.32458800	-0.53678800
C	-3.40774000	9.81831800	0.99039600
H	-2.74520200	9.74660000	1.86489500
H	-4.42745200	9.77369900	1.39694800
H	-1.57830800	3.91543400	-0.84501000
C	-6.36932100	2.13611600	-2.26748600
C	-5.54124900	3.24342500	-2.39045000
C	-4.27295500	3.30770700	-1.73121300
C	-3.91000200	2.18445100	-0.92502700
C	-4.74528200	1.08099900	-0.81263900
C	-5.98101000	1.02923500	-1.48489100
H	-7.31897000	2.11577600	-2.79047800
H	-5.83577700	4.06311200	-3.03973400
H	-2.94893200	2.17396100	-0.42262000
H	-4.44420900	0.23400700	-0.20453700
C	-3.39543300	4.50209100	-1.90132300
C	-1.89436900	4.24163500	-1.83815500
H	-3.68008600	5.02751900	-2.81181000
H	-1.33944400	5.15429900	-2.06906400
H	-1.61218300	3.46830100	-2.56325900
C	-6.81771200	-0.17360600	-1.33896500
O	-6.52954600	-1.15476800	-0.66796500
O	-7.97750900	-0.10081600	-2.03621000

C	-8.85777100	-1.23455500	-1.94440000
H	-9.71645800	-0.98580700	-2.56672700
H	-8.36493400	-2.13520100	-2.31779000
H	-9.17090300	-1.39480600	-0.91000100
C	-0.07385600	8.46526000	-1.11517000
O	-1.46606700	8.59314300	-1.50294700
C	-1.58809900	9.29562800	-2.76793200
C	-0.20271100	9.88352700	-3.03358800
C	0.72347000	8.85829800	-2.35877100
H	0.11389000	9.14424400	-0.27483200
H	0.09020700	7.43594900	-0.78838000
H	-1.88301400	8.57074300	-3.53465300
H	-2.37529500	10.04670200	-2.66343500
H	-0.00525900	10.00491500	-4.10129100
H	-0.10417300	10.86298700	-2.55359000
H	0.86910400	7.98895000	-3.00853800
H	1.70555000	9.26518100	-2.10651800

TS_{2-5_H}

scf done: -1591.87072585

Ni	-3.39126800	7.15932600	1.82232900
C	-2.32281400	5.94834100	5.79134400
C	-2.82474800	5.38579400	4.42666200
C	-4.29489200	5.60838900	4.13504000
C	-3.39551600	6.16048500	6.87237500
C	-4.19135000	4.90720200	7.26890900
C	-4.71580100	4.11526300	6.05343500
H	-1.53879300	5.28306300	6.17092900
H	-2.26085400	5.84064800	3.61015000
H	-4.09775200	6.92773300	6.52438700
H	-5.02952700	5.20984000	7.90793200
H	-1.84053700	6.91461400	5.60782800
H	-2.62865500	4.30937000	4.37310000
H	-2.91715900	6.57660000	7.76644400
H	-3.57008100	4.23036500	7.86849600
H	-5.55349200	3.47651900	6.34570000
H	-3.93937100	3.44190300	5.68188200
C	-6.63081900	5.18245500	4.83891300
H	-7.05541000	5.20513500	5.84779900
H	-7.08915700	4.33385900	4.31190300
C	-6.91766200	6.48702800	4.10743000
H	-7.98212400	6.54927300	3.86191200
H	-6.67229600	7.33898000	4.75027900
C	-6.06690400	6.55568000	2.84082800
H	-6.18491700	7.52847800	2.35756300
H	-6.39369500	5.79353300	2.11929000
N	-5.18266400	4.96671500	4.95372900
N	-4.64052200	6.36522500	3.12625700
C	-4.76894700	8.00687900	-2.21690800
C	-5.20416600	7.33604200	-0.87716200
C	-4.64960500	5.95027900	-0.61480900
C	-4.20378400	7.06085700	-3.28843900
C	-5.17585300	5.97693300	-3.77976300
C	-5.90341200	5.26221800	-2.62453900
H	-5.62381200	8.56034700	-2.62373800
H	-4.89357500	7.95720400	-0.03474100
H	-3.30338400	6.58369400	-2.88542000
H	-4.62204500	5.24712500	-4.38255600
H	-3.99546700	8.74647000	-1.99109800
H	-6.29738500	7.27546700	-0.82542000
H	-3.87065400	7.65724800	-4.14561800
H	-5.93861200	6.41152800	-4.43825900
H	-6.33002100	4.31453500	-2.96534000
H	-6.74662400	5.86771400	-2.28207200
C	-4.43971800	3.61997800	-1.43303900
H	-4.24146300	3.29434100	-2.45986700
H	-5.16475300	2.91500400	-1.00269700

C	-3.15331300	3.63252100	-0.61730700
H	-2.83459000	2.60642300	-0.41030100
H	-2.35454400	4.12104900	-1.18617500
C	-3.38691900	4.40327500	0.68066900
H	-2.45757700	4.49008800	1.24696600
H	-4.10977700	3.86651100	1.31271700
N	-5.03386800	4.96328300	-1.48191200
N	-3.88140800	5.76049700	0.42357200
C	-6.06891300	10.93247600	2.54927600
C	-4.93195300	10.21189100	2.18128300
C	-4.13573600	9.55664700	3.14394000
C	-4.53332100	9.67169600	4.49244800
C	-5.66827900	10.39231400	4.86167200
C	-6.44866000	11.02715000	3.89077100
H	-6.65738300	11.42908700	1.78199000
H	-4.65571000	10.16796600	1.13212300
H	-3.93040900	9.19081400	5.25880500
H	-5.94005000	10.46521700	5.91168300
C	-2.92870500	8.76907000	2.80944400
C	-2.20749900	8.91301800	1.55381700
H	-2.31518800	8.53866800	3.68146600
H	-2.65139600	9.52207900	0.77010300
H	-1.14454300	9.12604300	1.65951300
O	-1.48730900	7.57947800	-0.57261500
C	-1.52188000	7.32016800	0.62363000
O	-0.90515700	6.55898900	1.37685300
H	-7.33085400	11.59315200	4.17533400

TS₂₋₅_NH₂

scf done: -1647.22792278

Ni	-3.33902200	7.16836000	1.84487100
C	-2.30945700	5.90027400	5.80227100
C	-2.80235900	5.35285900	4.42817900
C	-4.27014400	5.58025800	4.12839000
C	-3.39037000	6.10876600	6.87576600
C	-4.19358600	4.85527500	7.25689300
C	-4.70625500	4.07126600	6.03126100
H	-1.53222400	5.22775700	6.18322000
H	-2.23309500	5.81658300	3.62034300
H	-4.08719500	6.88069000	6.52710900
H	-5.03825900	5.15620300	7.88823600
H	-1.82065500	6.86566400	5.63158700
H	-2.60659600	4.27686200	4.36428500
H	-2.91830500	6.51724100	7.77672700
H	-3.58044700	4.17376800	7.85964200
H	-5.54519600	3.42886400	6.31193800
H	-3.92517300	3.40206300	5.66190100
C	-6.61157800	5.15040000	4.81288500
H	-7.04215100	5.16422500	5.81948100
H	-7.06920700	4.30815100	4.27501700
C	-6.89124900	6.46286000	4.09276800
H	-7.95380900	6.52912400	3.83996300
H	-6.65026900	7.30821500	4.74583800
C	-6.03082100	6.54422300	2.83335100
H	-6.14397200	7.52259400	2.36049600
H	-6.35435800	5.79046200	2.10142200
N	-5.16478800	4.92976600	4.93391400
N	-4.60661600	6.34825100	3.12558800
C	-4.80700800	8.01803800	-2.19471100
C	-5.18851600	7.34838900	-0.83838700
C	-4.62006100	5.96499700	-0.59385400
C	-4.29204800	7.07371000	-3.29318100
C	-5.28428200	5.98866000	-3.73960400
C	-5.95070300	5.26699800	-2.55181800
H	-5.67568700	8.57609600	-2.56416200
H	-4.84807200	7.97207500	-0.00928800
H	-3.37313000	6.59355600	-2.93790200

H	-4.75870200	5.26344500	-4.37232600
H	-4.02250100	8.75591200	-2.00092500
H	-6.27887400	7.28568800	-0.74585700
H	-4.00051100	7.67205900	-4.16402000
H	-6.08029400	6.42340100	-4.35740300
H	-6.38297000	4.31519500	-2.87349600
H	-6.78366700	5.86412300	-2.17162000
C	-4.43171300	3.63413100	-1.41747000
H	-4.26667100	3.30617700	-2.44959100
H	-5.14109500	2.92877400	-0.96200000
C	-3.11944900	3.65034400	-0.64369200
H	-2.79290500	2.62501800	-0.44492300
H	-2.34021700	4.13779400	-1.23988000
C	-3.31217200	4.42336600	0.65970000
H	-2.36590200	4.51215300	1.19706400
H	-4.01400600	3.88608400	1.31467200
N	-5.02854600	4.97642800	-1.44932900
N	-3.81743900	5.77950000	0.41860900
C	-6.06400300	10.93664000	2.53309400
C	-4.91767100	10.21791600	2.20223600
C	-4.14856800	9.55018600	3.17634200
C	-4.59734400	9.65835800	4.50752800
C	-5.74017000	10.37502300	4.85128000
C	-6.50167300	11.02834200	3.86593100
H	-6.62686200	11.44109000	1.75083400
H	-4.61213900	10.19040700	1.16036300
H	-4.02439800	9.17455800	5.29517800
H	-6.04560800	10.43867700	5.89337900
C	-2.92864600	8.76821700	2.87348400
C	-2.16193900	8.93485400	1.65063000
H	-2.34754400	8.52303100	3.76389900
H	-2.57658200	9.55814900	0.86211900
H	-1.10184100	9.13684300	1.79658100
O	-1.38511000	7.64305000	-0.48372700
C	-1.45945300	7.35689100	0.70663100
O	-0.85190200	6.58144700	1.45605200
N	-7.68678900	11.69936800	4.19336400
H	-7.72036300	12.04404600	5.14473100
H	-7.94480100	12.42944200	3.54102000

TS₂₋₅_OMe

scf done: -1706.41913493

Ni	-3.27876800	7.17956400	1.87219600
C	-2.25775800	5.79161200	5.80235700
C	-2.78495100	5.29872600	4.42015600
C	-4.24454400	5.59648100	4.14213300
C	-3.32069200	6.01768300	6.89039500
C	-4.17103700	4.78901600	7.24870500
C	-4.72662300	4.05818300	6.00947900
H	-1.50623600	5.07814300	6.15959500
H	-2.20334100	5.75637200	3.61765900
H	-3.98852100	6.82520500	6.56632500
H	-4.99705100	5.10814300	7.89539900
H	-1.73041200	6.73974300	5.65084700
H	-2.63653100	4.21721600	4.32888100
H	-2.82522000	6.38501200	7.79641100
H	-3.58100300	4.06806000	7.82802800
H	-5.58913500	3.44424100	6.28211000
H	-3.97782100	3.36677600	5.61511400
C	-6.59582400	5.24833200	4.83668300
H	-7.01789300	5.24890000	5.84684400
H	-7.09249100	4.44366400	4.27651700
C	-6.82447000	6.59370700	4.16044200
H	-7.88549600	6.71409500	3.92165400
H	-6.54032500	7.40586800	4.83794600
C	-5.97353400	6.67704100	2.89474700
H	-6.04490100	7.67466300	2.45469000

H	-6.33789100	5.96400900	2.14150200	H	-1.84961600	6.92945600	5.61418100
N	-5.15869300	4.96288800	4.93820900	H	-2.62902900	4.32867500	4.36765400
N	-4.55729400	6.40727400	3.16516100	H	-2.93078600	6.58647500	7.76880600
C	-4.51211300	8.11131100	-2.19266900	H	-3.57524900	4.23858800	7.86865000
C	-5.04737000	7.52714500	-0.85178800	H	-5.54797300	3.47355300	6.33982000
C	-4.64542400	6.09481100	-0.56727400	H	-3.93249400	3.45208100	5.67832900
C	-4.19826800	7.08741700	-3.29660500	C	-6.63621700	5.17282300	4.83545100
C	-5.35826500	6.16832000	-3.70556700	H	-7.06083800	5.19517300	5.84419200
C	-6.06443700	5.50944400	-2.50117900	H	-7.08660400	4.31857700	4.31115600
H	-5.23702100	8.84750100	-2.56061200	C	-6.93415400	6.47253500	4.09996500
H	-4.68207100	8.12878700	-0.01707900	H	-7.99854500	6.52416000	3.85236300
H	-3.35763300	6.46721700	-2.96514000	H	-6.69858200	7.32794900	4.74201900
H	-4.97081800	5.39435700	-4.37885500	C	-6.08170100	6.54451300	2.83471800
H	-3.58654600	8.65278700	-1.97784300	H	-6.21132900	7.51202700	2.34363200
H	-6.14082200	7.59153500	-0.82346800	H	-6.39768900	5.77426300	2.11722300
H	-3.84126600	7.62582900	-4.18220500	N	-5.18596100	4.96927400	4.95128000
H	-6.11283800	6.72614800	-4.27422800	N	-4.65383300	6.37240900	3.12556000
H	-6.57802100	4.59601300	-2.81359200	C	-4.75882000	8.00585000	-2.22442400
H	-6.84183800	6.17258500	-2.11268900	C	-5.20506000	7.33896000	-0.88635000
C	-4.73560700	3.73875500	-1.32449300	C	-4.65252500	5.95415100	-0.61538200
H	-4.63807600	3.34843600	-2.34299700	C	-4.18781400	7.05612300	-3.28952200
H	-5.51548000	3.14824000	-0.82287500	C	-5.15731400	5.97120500	-3.78358200
C	-3.41297200	3.62488600	-0.57613900	C	-5.89210500	5.25980800	-2.63100100
H	-3.20223000	2.57482600	-0.35157500	H	-5.60975200	8.56008400	-2.63813100
H	-2.59726800	3.99958300	-1.20400900	H	-4.90194100	7.96303500	-0.04342700
C	-3.48527800	4.44921500	0.70754200	H	-3.29008300	6.58004100	-2.87939700
H	-2.51610300	4.45839500	1.21119200	H	-4.60005200	5.23961200	-4.38091700
H	-4.21035100	4.00098800	1.40242900	H	-3.98530800	8.74416700	-1.99478300
N	-5.15780500	5.14285600	-1.40760400	H	-6.29853400	7.27809300	-0.84305300
N	-3.86325800	5.84268900	0.44692400	H	-3.84926200	7.64989500	-4.14632100
C	-5.78581500	11.04783600	2.76871600	H	-5.91600100	6.40408100	-4.44776400
C	-4.67825500	10.29232500	2.37059800	H	-6.31549500	4.31053400	-2.97110700
C	-3.90059100	9.56216900	3.28654600	H	-6.73804100	5.86540400	-2.29567100
C	-4.28575600	9.63986500	4.64290700	C	-4.43570300	3.62167200	-1.42448800
C	-5.38205000	10.38525000	5.05734400	H	-4.22962300	3.29377800	-2.44892900
C	-6.14646700	11.09439800	4.11948500	H	-5.16462100	2.91851900	-0.99810000
H	-6.34779900	11.59515000	2.02083500	C	-3.15589300	3.63635200	-0.59881300
H	-4.41925500	10.28683200	1.31619400	H	-2.83885600	2.61089100	-0.38652100
H	-3.70208200	9.10369800	5.38679400	H	-2.35259400	4.12369000	-1.16229900
H	-5.65785900	10.43711600	6.10648000	C	-3.40037100	4.40972100	0.69550400
C	-2.73543900	8.73236900	2.90554000	H	-2.47599000	4.49677200	1.26971300
C	-2.02435400	8.88619800	1.64557100	H	-4.12936600	3.87513700	1.32214600
H	-2.11947900	8.44567600	3.75942400	N	-5.02918600	4.96521400	-1.48168900
H	-2.45451100	9.53400500	0.88535900	N	-3.89184100	5.76687500	0.43000600
H	-0.95244400	9.05403700	1.74151800	C	-6.06810200	10.92839700	2.55987900
O	-1.36670700	7.58021000	-0.51583400	C	-4.93003800	10.22311100	2.18413800
C	-1.41776600	7.29049000	0.67373900	C	-4.12306900	9.56086900	3.13585700
O	-0.83594700	6.47959300	1.40395800	C	-4.51508400	9.66049200	4.48957900
O	-7.21198400	11.80232400	4.61840000	C	-5.64932600	10.36357900	4.87535800
C	-8.01781900	12.54232700	3.70612200	C	-6.44135800	10.99695800	3.90804500
H	-8.48237800	11.88563300	2.96080900	H	-6.66599300	11.42715400	1.80391300
H	-8.79526100	13.01443200	4.30718700	H	-4.66200900	10.19426300	1.13351100
H	-7.43346500	13.31596700	3.19410700	H	-3.90758900	9.17679400	5.24876200
TS₂₋₅_CF₃				H	-5.91886300	10.42247500	5.92501200
scf done: -1929.01975				C	-2.92126700	8.78423100	2.78829900
Ni	-3.41168000	7.16611200	1.82110800	C	-2.22764900	8.91307400	1.51349900
C	-2.33203900	5.96252100	5.79378700	H	-2.29155800	8.56041000	3.64976800
C	-2.83101000	5.40371900	4.42637600	H	-2.68956100	9.50798000	0.72928900
C	-4.30256600	5.61711900	4.13490600	H	-1.16604700	9.14228200	1.59798900
C	-3.40661800	6.16971800	6.87380200	O	-1.48747700	7.55544200	-0.58983100
C	-4.19791900	4.91272400	7.26761400	C	-1.51908100	7.30937800	0.60623100
C	-4.71436700	4.11873300	6.05036600	O	-0.91721900	6.56175000	1.37946400
H	-1.54819000	5.29668600	6.17246600	C	-7.63800200	11.79531000	4.31894800
H	-2.26858600	5.86420700	3.61209200	F	-7.33691100	13.09872800	4.59607500
H	-4.11187600	6.93456200	6.52642400	F	-8.23204000	11.31356900	5.43907700
H	-5.03948300	5.21109600	7.90406400	F	-8.59555400	11.83878700	3.35997700

TS₂₋₅_CN

scf done: -1684.11696503

Ni	-3.14473800	7.27304000	1.85908600
C	-2.21657200	5.83229500	5.88126800
C	-2.65394500	5.38189800	4.45345700
C	-4.12663600	5.55024200	4.13026400
C	-3.33605100	5.93194300	6.93065100
C	-4.09234600	4.62343900	7.20608000
C	-4.51840600	3.89236400	5.91695900
H	-1.43639400	5.14948300	6.23652000
H	-2.09664000	5.94302100	3.70015200
H	-4.05450000	6.69583800	6.60842100
H	-4.97429500	4.84578200	7.81867800
H	-1.74393300	6.81784200	5.80429200
H	-2.39267500	4.32961500	4.29795800
H	-2.90757500	6.30183700	7.86899800
H	-3.46997400	3.93599900	7.79226100
H	-5.32199600	3.18165800	6.12756900
H	-3.68612200	3.29974300	5.52854100
C	-6.45400200	4.94287900	4.72348300
H	-6.90379200	4.87898100	5.71979300
H	-6.85370300	4.10718900	4.13234700
C	-6.79359700	6.27509500	4.06715500
H	-7.85032400	6.29076500	3.78379000
H	-6.62920200	7.09344200	4.77674600
C	-5.90159800	6.47755200	2.84358400
H	-6.07267300	7.46415100	2.40548600
H	-6.15280600	5.73759200	2.07063700
N	-4.99940100	4.79363100	4.86370500
N	-4.47707600	6.36698700	3.17233800
C	-4.88049900	8.05481600	-2.11907100
C	-5.14658200	7.46587400	-0.70043600
C	-4.60415300	6.07509400	-0.44692700
C	-4.57879500	7.03993300	-3.23449800
C	-5.67119700	5.99168900	-3.49085000
C	-6.18038400	5.33212800	-2.19392300
H	-5.74091400	8.67295300	-2.40282100
H	-4.69648200	8.11685800	0.05038000
H	-3.64263100	6.52396500	-2.99203100
H	-5.27626400	5.22662500	-4.17008300
H	-4.01709100	8.72019900	-2.04021300
H	-6.22328200	7.44842700	-0.49462500
H	-4.38486500	7.58813300	-4.16368500
H	-6.53230900	6.44463700	-3.99796700
H	-6.66434800	4.37597900	-2.41229200
H	-6.94593400	5.95930200	-1.73043500
C	-4.56271500	3.70934800	-1.19060900
H	-4.51220500	3.34176600	-2.22128300
H	-5.24171200	3.04267100	-0.64067300
C	-3.18023500	3.71352300	-0.55172400
H	-2.86109400	2.68680600	-0.34902200
H	-2.45123000	4.15928900	-1.23743700
C	-3.22524900	4.53196700	0.73672900
H	-2.22752700	4.61251700	1.17182000
H	-3.87454700	4.03897900	1.47458100
N	-5.12220200	5.06768800	-1.21313500
N	-3.71529300	5.89304100	0.49490000
C	-5.68928800	11.18887000	1.96221200
C	-4.54213700	10.40780300	1.98794400
C	-4.19320000	9.65968300	3.13204800
C	-5.04393500	9.73241200	4.25275800
C	-6.19475400	10.51024100	4.24149400
C	-6.52961800	11.24556600	3.09046400
H	-5.94198200	11.75844400	1.07404800
H	-3.90939700	10.37417700	1.10741900
H	-4.78816400	9.17412300	5.14843800
H	-6.83445100	10.55684500	5.11657000

C	-2.97401500	8.83147400	3.20426300
C	-1.89402300	8.94848900	2.33418100
H	-2.81866200	8.34100400	4.16077600
H	-1.87524800	9.70838500	1.56244600
H	-0.92693500	8.56285200	2.63655600
O	-1.89978000	8.20142900	-0.52782800
C	-1.68994100	7.47239800	0.44056100
O	-0.81417500	6.65304400	0.74115800
C	-7.71494600	12.04662100	3.06673800
N	-8.68121500	12.69665500	3.04759400

5_H

scf done: -1591.88076885

Ni	-3.73564800	7.19002200	2.48727200
C	-1.79261100	5.47606700	5.97566900
C	-2.44518800	5.14113100	4.59813700
C	-3.96158900	5.15218800	4.56362800
C	-2.70077600	5.33404600	7.20796300
C	-3.25832700	3.92254000	7.44564800
C	-3.83061000	3.28272200	6.16597700
H	-0.90228900	4.84871000	6.09850800
H	-2.10691900	5.85783500	3.84751500
H	-3.53753900	6.03670600	7.11214600
H	-4.03382400	3.97133000	8.21919900
H	-1.43553700	6.51074300	5.94266800
H	-2.11057500	4.15561500	4.25578100
H	-2.14287900	5.65316800	8.09547200
H	-2.47380800	3.25893300	7.82996800
H	-4.49788700	2.45372400	6.41592500
H	-3.02367000	2.85116900	5.56826900
C	-6.05929000	4.17902600	5.44928200
H	-6.31475600	3.92880500	6.48384600
H	-6.45458000	3.37608200	4.81185100
C	-6.66108400	5.52209800	5.05778200
H	-7.74723600	5.43091100	4.96445100
H	-6.45609100	6.26206900	5.83879400
C	-6.04738100	5.99183900	3.74150300
H	-6.38588800	7.00462800	3.50895100
H	-6.36760100	5.34348700	2.91469300
N	-4.59521200	4.22053300	5.33537600
N	-4.58024000	6.01011600	3.79249900
C	-5.50704300	8.51201900	-1.14867600
C	-5.83234300	7.54775800	0.03386300
C	-5.11455000	6.21244600	0.01347400
C	-4.86440200	7.86496500	-2.38545600
C	-5.71784900	6.79114600	-3.07959900
C	-6.33683300	5.78898800	-2.08627700
H	-6.42736100	9.03320300	-1.43822900
H	-5.57462100	8.03197500	0.97692000
H	-3.90598200	7.42431200	-2.08648900
H	-5.09783500	6.25886500	-3.81101700
H	-4.81532900	9.27376100	-0.77840200
H	-6.90962300	7.34798900	0.07078700
H	-4.61993300	8.65063900	-3.10923200
H	-6.53768800	7.25429700	-3.64313900
H	-6.66511000	4.88365800	-2.60476600
H	-7.23197800	6.21817800	-1.62943900
C	-4.66687100	4.12656300	-1.24894400
H	-4.46036500	4.03618700	-2.32072900
H	-5.29493700	3.27054900	-0.96560900
C	-3.36717700	4.12608600	-0.45329600
H	-2.93250100	3.12198000	-0.45304600
H	-2.64303400	4.80277400	-0.92030800
C	-3.65197800	4.59948900	0.97103500
H	-2.72413000	4.66729800	1.54484500
H	-4.29277300	3.86853200	1.48688200
N	-5.41199000	5.37391600	-1.02597300

N	-4.29633600	5.91538800	0.98685900	C	-4.67283900	4.11384000	-1.25971100
C	-5.89709100	11.24774700	3.44499700	H	-4.46461200	4.02092600	-2.33101700
C	-4.75712500	10.47626300	3.21240900	H	-5.30500600	3.26071900	-0.97650400
C	-4.41291900	9.39570000	4.05405200	C	-3.37453900	4.10831200	-0.46154300
C	-5.26855700	9.14696500	5.14936900	H	-2.94486600	3.10200300	-0.45876000
C	-6.40853900	9.91486600	5.38299500	H	-2.64613400	4.78042100	-0.92862400
C	-6.73554600	10.97208100	4.52842500	C	-3.65963500	4.58634000	0.96130600
H	-6.12711000	12.07444500	2.77727100	H	-2.73282600	4.64995300	1.53739000
H	-4.12440400	10.71967800	2.36404800	H	-4.30555600	3.85974700	1.47710000
H	-5.01863800	8.33857600	5.83212200	N	-5.41278300	5.36459400	-1.03959000
H	-7.03805400	9.69509700	6.24199300	N	-4.29664400	5.90564700	0.97393600
C	-3.21196200	8.54083200	3.82566200	C	-5.89867300	11.25179000	3.41116700
C	-1.99308300	9.24631800	3.22025900	C	-4.76746400	10.46913900	3.18468400
H	-2.95435800	8.02043400	4.75106800	C	-4.41131800	9.40100100	4.03459000
H	-1.86631500	10.28537000	3.55366300	C	-5.26205600	9.18125100	5.13726000
H	-1.07753100	8.71527600	3.51356900	C	-6.39633600	9.95420300	5.37394400
O	-1.35277400	9.95461900	0.98621200	C	-6.74039200	11.00726300	4.50917000
C	-2.03456400	9.19989900	1.69393500	H	-6.13183500	12.06895800	2.73161200
O	-2.82154500	8.28525100	1.21941500	H	-4.14538500	10.70363600	2.32556600
H	-7.61986900	11.57624300	4.70994000	H	-5.01504700	8.38607300	5.83689300
				H	-7.01895800	9.75039300	6.24282800
				C	-3.21172600	8.53812800	3.80983600
				C	-1.98801500	9.24207400	3.21102100
				H	-2.95734600	8.02377500	4.74005800
				H	-1.86166200	10.28104900	3.54553200
				H	-1.07395400	8.70957000	3.50725300
				O	-1.33987400	9.95353400	0.97964900
				C	-2.02288600	9.19588400	1.68449100
				O	-2.80424900	8.27884000	1.20701600
				N	-7.91446300	11.75281200	4.70497700
				H	-8.21542600	11.79586900	5.67113000
				H	-7.87785400	12.68433300	4.30903800

5_NH₂

scf done: -1647.28011668

Ni	-3.72573100	7.18575300	2.47706800
C	-1.78842600	5.47586800	5.97204500
C	-2.44519500	5.13592200	4.59772400
C	-3.96154200	5.15630800	4.56500200
C	-2.69739900	5.35343500	7.20582600
C	-3.26537200	3.94849500	7.45756200
C	-3.84122000	3.29992700	6.18379500
H	-0.90432100	4.84078600	6.10037300
H	-2.10526000	5.84659100	3.84199100
H	-3.52885100	6.06133800	7.10260900
H	-4.04114300	4.01059800	8.22995700
H	-1.42129000	6.50668800	5.92994500
H	-2.11674000	4.14634000	4.26100000
H	-2.13716400	5.67728300	8.09020000
H	-2.48584700	3.28327300	7.84930100
H	-4.51270000	2.47668100	6.44158700
H	-3.03629900	2.85861900	5.59040600
C	-6.06458700	4.20383900	5.46045500
H	-6.32097500	3.96173600	6.49678700
H	-6.46697500	3.40011100	4.82834100
C	-6.65694100	5.54891500	5.06135400
H	-7.74398700	5.46559500	4.97077400
H	-6.44466900	6.29248000	5.83706300
C	-6.04196900	6.00571200	3.74098800
H	-6.37231200	7.01993300	3.50308200
H	-6.36937800	5.35517900	2.91863100
N	-4.60055900	4.23393500	5.34470100
N	-4.57470200	6.01236400	3.78835400
C	-5.49202500	8.50363200	-1.16643900
C	-5.82370800	7.54249500	0.01671900
C	-5.11214600	6.20382400	-0.00075000
C	-4.85017000	7.85173800	-2.40114900
C	-5.70725100	6.78089900	-3.09554100
C	-6.33316300	5.78304800	-2.10209000
H	-6.40923900	9.02898300	-1.45841400
H	-5.56439000	8.02580000	0.95984800
H	-3.89454900	7.40692700	-2.09935800
H	-5.08806300	6.24456300	-3.82475000
H	-4.79715900	9.26248100	-0.79605100
H	-6.90207200	7.34833400	0.05235400
H	-4.60033700	8.63510300	-3.12565500
H	-6.52356100	7.24714200	-3.66171900
H	-6.66522700	4.87892700	-2.62038600
H	-7.22701900	6.21751800	-1.64765900

5_OMe

scf done: -1706.47212085

Ni	-3.64983300	7.20140800	2.55477000
C	-1.71127800	5.34841200	5.97058000
C	-2.38624500	5.06395500	4.59250700
C	-3.90220800	5.10948000	4.57576100
C	-2.60999900	5.19743100	7.20871100
C	-3.19790200	3.79383800	7.41864300
C	-3.79664100	3.19817300	6.12988700
H	-0.83535700	4.69678200	6.06819400
H	-2.04138800	5.79219800	3.85592500
H	-3.43093100	5.92151300	7.13896300
H	-3.96460000	3.84204300	8.20097900
H	-1.32934300	6.37464100	5.95942200
H	-2.07771600	4.08034000	4.22125100
H	-2.03585300	5.48189800	8.09766700
H	-2.42533200	3.10353200	7.77950700
H	-4.47921100	2.37773400	6.36649100
H	-3.00507000	2.76462900	5.51340400
C	-6.01207400	4.16075500	5.46015000
H	-6.26198700	3.89227800	6.49151100
H	-6.43166000	3.38140900	4.80913900
C	-6.58864900	5.52520400	5.10590400
H	-7.67724800	5.45896200	5.02041700
H	-6.36186200	6.24200600	5.90240200
C	-5.97647200	6.01265600	3.79534300
H	-6.29639600	7.03663200	3.58781500
H	-6.31749500	5.38999100	2.95704800
N	-4.54868800	4.17270400	5.33072900
N	-4.50896500	6.00023200	3.83304600
C	-5.32674100	8.66199100	-1.07628700
C	-5.72545500	7.73454000	0.11049100
C	-5.11764100	6.34687800	0.07948700
C	-4.87184900	7.95382800	-2.36343700

C	-5.88476800	6.97645000	-2.97871400	H	-6.31604100	3.90198100	6.46161900
C	-6.48167300	5.99575200	-1.94795300	H	-6.43787100	3.34954300	4.78808000
H	-6.17232400	9.32514600	-1.29526300	C	-6.67345600	5.49253600	5.03556600
H	-5.42113800	8.19913700	1.04939000	H	-7.75743600	5.38755700	4.93331000
H	-3.94187000	7.41277900	-2.15249900	H	-6.48484200	6.23257700	5.82072000
H	-5.39122100	6.41764100	-3.78293100	C	-6.05575300	5.97208300	3.72478800
H	-4.50212500	9.29736300	-0.74117700	H	-6.40865900	6.97904600	3.48771500
H	-6.81512500	7.62620700	0.15307800	H	-6.35901200	5.31884100	2.89562000
H	-4.61162300	8.71367800	-3.10921700	N	-4.59290800	4.21633300	5.32457100
H	-6.71554400	7.52211300	-3.44340400	N	-4.58927500	6.01188700	3.78944400
H	-6.87775000	5.10809300	-2.44912300	C	-5.52151500	8.50537000	-1.14272500
H	-7.33083600	6.45709400	-1.43775400	C	-5.83905400	7.54098000	0.04182000
C	-4.88122400	4.22949000	-1.18818000	C	-5.11113200	6.21126000	0.02331500
H	-4.72754500	4.11689500	-2.26677300	C	-4.87951900	7.86010600	-2.38071600
H	-5.56055200	3.42579900	-0.87134700	C	-5.72827800	6.77918800	-3.06931400
C	-3.55349400	4.13361400	-0.44594800	C	-6.33497300	5.77344100	-2.07209100
H	-3.19555300	3.09968300	-0.45695200	H	-6.44537200	9.02153800	-1.42959800
H	-2.80032400	4.75209500	-0.94675900	H	-5.58560600	8.03008800	0.98346300
C	-3.74333300	4.63132800	0.98588800	H	-3.91676100	7.42660700	-2.08527200
H	-2.79002800	4.62957800	1.52079000	H	-5.10793500	6.25093300	-3.80328100
H	-4.41562100	3.95208900	1.53142700	H	-4.83249400	9.27093400	-0.77537100
N	-5.51615300	5.53198100	-0.94548600	H	-6.91460500	7.33287400	0.07969400
N	-4.28575600	5.99240700	1.02170900	H	-4.64369100	8.64614400	-3.10688600
C	-5.73297400	11.27364300	3.63415800	H	-6.55446700	7.23542700	-3.62905100
C	-4.60970900	10.47729600	3.38377900	H	-6.65596000	4.86373900	-2.58726700
C	-4.27442100	9.37202800	4.18789600	H	-7.23273400	6.19483500	-1.61327200
C	-5.13062900	9.11613100	5.28250300	C	-4.65014600	4.12550100	-1.23345800
C	-6.25186300	9.89308400	5.54655200	H	-4.44690000	4.03239600	-2.30551100
C	-6.56531200	10.98006400	4.71868000	H	-5.27190900	3.26694300	-0.94437000
H	-5.93858600	12.11543300	2.98267400	C	-3.34792400	4.13748600	-0.44241400
H	-3.98383900	10.73540000	2.53482000	H	-2.90524600	3.13696600	-0.44098500
H	-4.89749900	8.28773000	5.94655600	H	-2.63095500	4.81887700	-0.91352900
H	-6.89070100	9.68103800	6.39917900	C	-3.63132100	4.61134600	0.98189600
C	-3.09177200	8.49730700	3.92838100	H	-2.70141000	4.69014500	1.55088600
C	-1.86138700	9.19768300	3.34074200	H	-4.26263500	3.87583000	1.50266300
H	-2.84088000	7.94860300	4.83935500	N	-5.40275200	5.36911600	-1.01336200
H	-1.71306800	10.22314500	3.70636600	N	-4.28857500	5.92112000	0.99619200
H	-0.95478100	8.63990800	3.61166800	C	-5.87400000	11.26235300	3.40487400
O	-1.21888700	9.96551900	1.12734600	C	-4.73272600	10.49535900	3.19915300
C	-1.91218300	9.20137900	1.81403100	C	-4.41293100	9.39983400	4.03543800
O	-2.72068000	8.31939100	1.31514400	C	-5.30147200	9.13627100	5.10342700
O	-7.69150700	11.69461500	5.05657900	C	-6.44574700	9.89459400	5.31704000
C	-8.04234500	12.81628900	4.25309600	C	-6.74108400	10.96755700	4.46555700
H	-8.24181900	12.51887500	3.21646000	H	-6.08634600	12.09847100	2.74565000
H	-8.95127500	13.22869200	4.69213500	H	-4.07645400	10.75512700	2.37536300
H	-7.25436800	13.57878800	4.26512600	H	-5.07187200	8.32172600	5.78406300

5_CF3

scf done: -1929.07388586

Ni	-3.74514100	7.19381700	2.48817400
C	-1.80975900	5.50166200	5.98805000
C	-2.44888200	5.16172300	4.60552500
C	-3.96506000	5.15687800	4.56113600
C	-2.72243400	5.33867200	7.21443500
C	-3.26280300	3.91852200	7.43964000
C	-3.82318300	3.28061500	6.15381800
H	-0.90982800	4.88864500	6.11240400
H	-2.11015800	5.88101700	3.85773500
H	-3.56806800	6.03083500	7.11940500
H	-4.04117200	3.95205600	8.21098500
H	-1.46935400	6.54216800	5.96191400
H	-2.10247800	4.17979200	4.26504700
H	-2.17329800	5.65891300	8.10690300
H	-2.47131500	3.26196700	7.82152100
H	-4.48443600	2.44463100	6.39590500
H	-3.01013200	2.85948000	5.55712900
C	-6.05743900	4.15660000	5.42902600

5_CN

scf done: -1684.17013888

Ni	-3.74846700	7.19680200	2.49208400
C	-1.80817100	5.50110900	5.98872900
C	-2.44855400	5.16324200	4.60625800
C	-3.96476700	5.15793700	4.56342500
C	-2.71947100	5.33545200	7.21578200

C	-3.25907000	3.91469200	7.43891500	O	-2.84143500	8.29087200	1.22433800
C	-3.82056100	3.27897900	6.15253100	C	-7.92012900	11.74366400	4.68288000
H	-0.90783100	4.88829700	6.11093700	N	-8.88133300	12.37941700	4.85899100
H	-2.11036300	5.88353900	3.85920000	TS_{II-13_H}			
H	-3.56548600	6.02748400	7.12308800	scf done: -1591.9216751			
H	-4.03657900	3.94650600	8.21118000	Ni	-2.78403600	6.75758900	1.96320700
H	-1.46816900	6.54179200	5.96415500	Zn	-1.34310700	6.49290900	-0.30749600
H	-2.10233200	4.18190900	4.26393000	C	-2.25350900	3.98429300	5.19302100
H	-2.16944000	5.65420000	8.10821500	C	-3.04924500	4.25596800	3.87891200
H	-2.46693500	3.25771700	7.81867500	C	-4.16906600	5.26785100	3.99849100
H	-4.48140400	2.44242000	6.39366600	C	-2.97565900	4.32915100	6.50590100
H	-3.00808700	2.85922500	5.55412300	C	-4.30985900	3.60208500	6.73515200
C	-6.05591700	4.15570900	5.43211600	C	-5.23819800	3.64203100	5.50558700
H	-6.31298100	3.90022200	6.46485800	H	-1.95321200	2.93069100	5.19795700
H	-6.43662500	3.34890000	4.79108400	H	-2.36755100	4.60024600	3.09945300
C	-6.67310300	5.49162000	5.04046700	H	-3.15251800	5.41149200	6.53748600
H	-7.75707600	5.38597700	4.93897500	H	-4.81405800	4.05159000	7.59857500
H	-6.48439400	6.23106600	5.82614700	H	-1.32668900	4.56492600	5.15771900
C	-6.05679300	5.97260200	3.72959900	H	-3.48503700	3.32285400	3.50620400
H	-6.41111500	6.97916700	3.49302200	H	-2.30313800	4.11314600	7.34341300
H	-6.35964600	5.31936000	2.90031400	H	-4.13585000	2.54908100	6.98741500
N	-4.59145300	4.21613400	5.32579900	H	-6.27456100	3.45610500	5.79797100
N	-4.59028000	6.01410400	3.79374100	H	-4.97363500	2.84726200	4.80472300
C	-5.52654900	8.51418500	-1.13596800	C	-6.31206700	5.86733800	5.08396800
C	-5.84323900	7.54986100	0.04896700	H	-6.58639900	5.75658500	6.13757200
C	-5.11701000	6.21916000	0.02940700	H	-7.18969100	5.58973100	4.48535700
C	-4.88439000	7.86907000	-2.37393900	C	-5.88553300	7.29803100	4.78753800
C	-5.73374600	6.78885000	-3.06289900	H	-6.75629300	7.95918600	4.81455500
C	-6.34208700	5.78416800	-2.06574100	H	-5.18133200	7.64332500	5.55261600
H	-6.45085000	9.02952700	-1.42287300	C	-5.21409800	7.35258600	3.41772300
H	-5.58810400	8.03880600	0.99022100	H	-4.81544000	8.35174100	3.22977500
H	-3.92188500	7.43506200	-2.07842300	H	-5.94687900	7.13669900	2.62724100
H	-5.11351700	6.25969100	-3.79628900	N	-5.21379900	4.93126800	4.79893200
H	-4.83811800	9.28041700	-0.76891900	N	-4.10326300	6.39427700	3.32058300
H	-6.91892500	7.34266100	0.08837000	C	-3.04340500	10.83465500	4.36672000
H	-4.64809400	8.65522300	-3.09980700	C	-2.62781800	9.50480200	4.32649800
H	-6.55911600	7.24580200	-3.62323900	C	-1.91186900	8.98900900	3.22502800
H	-6.66481500	4.87505700	-2.58082500	C	-1.62410900	9.87722600	2.16538000
H	-7.23890700	6.20711300	-1.60651600	C	-2.04498400	11.20629600	2.20204000
C	-4.66016700	4.13290900	-1.22790400	C	-2.75814100	11.69327300	3.30096600
H	-4.45790600	4.03940400	-2.30008000	H	-3.58475000	11.20387800	5.23346700
H	-5.28355500	3.27574400	-0.93829200	H	-2.84528600	8.84717400	5.16421200
C	-3.35737100	4.14239700	-0.43783300	H	-1.06192000	9.52906500	1.30428400
H	-2.91651600	3.14108800	-0.43680600	H	-1.80896900	11.86619700	1.37184800
H	-2.63950400	4.82254200	-0.90935700	C	-1.51418200	7.55511700	3.19700300
C	-3.63883700	4.61627400	0.98682000	C	-0.08706100	7.24547300	2.71680000
H	-2.70818300	4.69379900	1.55472600	H	-1.69225300	7.08753900	4.16788900
H	-4.27054100	3.88151000	1.50810500	H	0.17957800	7.86108900	1.84994100
N	-5.41004500	5.37812900	-1.00741600	H	0.62779400	7.48936300	3.51202600
N	-4.29449700	5.92692800	1.00193000	O	0.84283100	5.02192800	2.90655400
C	-5.87052800	11.25812300	3.40593300	C	0.07327100	5.77763800	2.30276200
C	-4.72923400	10.49437500	3.20283400	O	-0.67591200	5.41867000	1.31098000
C	-4.40653100	9.39890300	4.04021200	C	-3.98736800	8.08042900	-0.61733700
C	-5.29503900	9.13151100	5.11005700	H	-3.92405500	8.84051400	0.16770100
C	-6.43855000	9.88464400	5.32527000	H	-5.04062700	8.00155500	-0.91973700
C	-6.74529800	10.96057400	4.46841900	H	-3.43545100	8.47141100	-1.48011500
H	-6.08990100	12.09353600	2.74842300	C	-3.40186200	6.73374000	-0.16073300
H	-4.07376400	10.75378300	2.37833500	H	-4.07921500	6.28064500	0.60694800
H	-5.06258900	8.31603000	5.78855000	H	-3.54078200	6.00111200	-0.97350900
H	-7.09543600	9.65805400	6.15931700	C	0.07724000	6.91434600	-1.62471400
C	-3.20791100	8.55571500	3.83507500	H	0.16841300	8.00729300	-1.71089800
C	-1.98675500	9.24528500	3.21936100	H	-0.24486400	6.58135400	-2.62221900
H	-2.96082500	8.02916700	4.75861300	C	1.45902600	6.31448700	-1.31590900
H	-1.84710100	10.28387400	3.54812200	H	1.42968500	5.21875500	-1.28571200
H	-1.07675800	8.70589800	3.51270200	H	2.22081300	6.59255500	-2.06002500
O	-1.34848200	9.93664200	0.98125100	H	1.83796900	6.64011200	-0.33943800
C	-2.03670900	9.19426200	1.69283000				

H -3.07939100 12.73020800 3.33038500

H -2.66706000 13.68887500 2.55850500

TS₁₁₋₁₃_NH₂

scf done: -3122.70247433

Ni	-2.77519100	6.79208200	1.98760600
Zn	-1.35812200	6.50810400	-0.28866100
C	-2.25505400	3.95890700	5.18401600
C	-3.05344100	4.25029700	3.87590400
C	-4.17028700	5.26307000	4.01199700
C	-2.97308800	4.28680500	6.50352400
C	-4.30812700	3.55923000	6.72663100
C	-5.23968400	3.61842100	5.50000500
H	-1.95601000	2.90487700	5.17424600
H	-2.37376900	4.60752100	3.10060600
H	-3.14806600	5.36888300	6.55005500
H	-4.80894300	3.99774800	7.59777100
H	-1.32769000	4.53895600	5.15416600
H	-3.49068100	3.32290200	3.49048100
H	-2.29877200	4.05835800	7.33639800
H	-4.13554000	2.50245200	6.96401400
H	-6.27554500	3.42967300	5.79291700
H	-4.97815400	2.83255400	4.78799700
C	-6.30636200	5.85327200	5.11800800
H	-6.57384100	5.72879800	6.17200200
H	-7.19038600	5.58980400	4.52214000
C	-5.87438400	7.28605300	4.83908100
H	-6.74147800	7.95138200	4.88097700
H	-5.16398300	7.61631300	5.60530900
C	-5.20982900	7.35527400	3.46634000
H	-4.81152200	8.35610600	3.28613500
H	-5.94837400	7.14952300	2.67819800
N	-5.21518700	4.91644500	4.81093600
N	-4.10056200	6.39760400	3.35072600
C	-3.03804100	10.89402800	4.26585200
C	-2.62786600	9.56749800	4.26024600
C	-1.88345300	9.01258500	3.19517700
C	-1.56783800	9.88586800	2.12922000
C	-1.97818200	11.21354800	2.11966300
C	-2.72534900	11.74694600	3.18802600
H	-3.60015200	11.28490500	5.11047300
H	-2.87204000	8.93747900	5.11200600
H	-0.98105200	9.52566000	1.28943200
H	-1.71440600	11.85421600	1.28193600
C	-1.49571600	7.58156000	3.21002300
C	-0.07318800	7.24121000	2.73527000
H	-1.68386000	7.13537100	4.18931600
H	0.20912200	7.85270900	1.87011800
H	0.64350100	7.47035000	3.53317700
O	0.82243900	5.00379100	2.92265400
C	0.06504800	5.77222300	2.31789800
O	-0.68415700	5.42571900	1.32231200
C	-3.98149800	8.09687900	-0.63290800
H	-3.90223500	8.87325300	0.13474500
H	-5.03820000	8.02758600	-0.92633500
H	-3.43062000	8.46163100	-1.50792800
C	-3.41294800	6.75212100	-0.14822900
H	-4.09198300	6.33072000	0.63333700
H	-3.56537600	6.00230800	-0.94288600
C	0.06928100	6.92881500	-1.59996200
H	0.19285000	8.02093600	-1.65205800
H	-0.26642400	6.63809900	-2.60626400
C	1.43414600	6.27907100	-1.31842600
H	1.37208400	5.18426200	-1.32354100
H	2.20135500	6.55806500	-2.05679000
H	1.82613100	6.56090500	-0.33359800
N	-3.18250200	13.05827000	3.15790400
H	-3.39007900	13.47197600	4.05697400

TS₁₁₋₁₃_OMe

scf done: -3181.89203122

Ni	-2.69933900	6.73265900	2.08253200
Zn	-1.19762100	6.46340700	-0.13300300
C	-2.17217000	4.04428600	5.41424700
C	-2.93589200	4.25587700	4.07074200
C	-4.09302800	5.23070100	4.12682200
C	-2.94055800	4.40981400	6.69449900
C	-4.25859600	3.64917800	6.91048100
C	-5.14946100	3.61362100	5.65355600
H	-1.84675200	2.99914000	5.46100200
H	-2.24422200	4.60264200	3.30168300
H	-3.14979800	5.48689200	6.68606600
H	-4.80333800	4.11375300	7.74067800
H	-1.25850500	4.64591300	5.38715600
H	-3.32932700	3.29907700	3.71064700
H	-2.28633500	4.24109700	7.55704700
H	-4.05968500	2.61233900	7.20748400
H	-6.18659600	3.39849100	5.92238800
H	-4.83564400	2.80613800	4.98819100
C	-6.29532400	5.77724100	5.11854200
H	-6.60538400	5.68872600	6.16433200
H	-7.13804500	5.44573200	4.49755400
C	-5.91490400	7.21395500	4.79061200
H	-6.81104000	7.84039000	4.76567100
H	-5.25297500	7.61030700	5.56867800
C	-5.19729500	7.25069200	3.44387000
H	-4.83537000	8.25923300	3.23236100
H	-5.89271600	6.97714800	2.63748900
N	-5.15065700	4.87887300	4.90475500
N	-4.04473900	6.33779300	3.41709400
C	-3.15503600	10.86506000	4.19916300
C	-2.70757300	9.55391100	4.25965300
C	-1.88275100	8.99644900	3.25426700
C	-1.52189900	9.84683800	2.19029500
C	-1.96764200	11.16752400	2.11012000
C	-2.79398000	11.68326600	3.11621200
H	-3.78087700	11.27998700	4.98325000
H	-2.98934000	8.93766000	5.10924000
H	-0.87452400	9.48057300	1.39924400
H	-1.66100400	11.77951800	1.27039300
C	-1.46816700	7.57221200	3.32596300
C	-0.02269500	7.24499900	2.91844600
H	-1.68773100	7.15293900	4.31008900
H	0.28820100	7.84901200	2.05827200
H	0.65594100	7.49351000	3.74321800
O	0.91024900	5.02725800	3.15621800
C	0.15580800	5.77419500	2.52256900
O	-0.55660600	5.40454800	1.50854600
C	-3.84453500	8.00065000	-0.56701300
H	-3.81809900	8.78141400	0.19969500
H	-4.88551500	7.90166300	-0.90424800
H	-3.26697200	8.37631800	-1.41978300
C	-3.26167800	6.67237700	-0.05558900
H	-3.95976000	6.23506000	0.70180300
H	-3.36937300	5.91796200	-0.85285200
C	0.25051200	6.87843900	-1.42287100
H	0.13708600	7.91626600	-1.76892400
H	0.10743200	6.26572400	-2.32521300
C	1.68278100	6.67490400	-0.90103300
H	1.85685000	5.64091300	-0.58157100
H	2.44878000	6.91002500	-1.65553200
H	1.89588900	7.30850900	-0.03074900
O	-3.28506000	12.95785000	3.13795900
C	-2.97361400	13.82825800	2.05049300

H	-3.34580900	13.42495000	1.10177900
H	-3.47820100	14.76928500	2.26867900
H	-1.89406600	14.00128200	1.97683000

C	-3.72109600	13.00882500	2.56792700
F	-3.90430900	13.63592700	3.75426900
F	-2.93578400	13.81455800	1.81647200
F	-4.94193700	13.00466400	1.95888100

TS_{II-13}_CF₃

scf done: -3404.48912632

Ni	-2.81028000	6.57389000	1.91815500
Zn	-1.15968100	6.57850300	-0.18393100
C	-2.08832100	4.33974300	5.50106700
C	-2.87381900	4.32263600	4.15363200
C	-4.09802900	5.21217800	4.10638400
C	-2.88022000	4.80427100	6.73376500
C	-4.13306900	3.97780300	7.06070500
C	-5.03089100	3.72695000	5.83238200
H	-1.68440500	3.33609400	5.67309200
H	-2.21266700	4.61820000	3.33737700
H	-3.17397400	5.85177100	6.59129600
H	-4.70434400	4.49490500	7.84032200
H	-1.22381000	5.00018400	5.38479300
H	-3.19872500	3.30305700	3.92122200
H	-2.21294500	4.79819000	7.60265600
H	-3.85284200	3.00106300	7.47296100
H	-6.04916400	3.48031300	6.14227800
H	-4.66869800	2.86605000	5.26595600
C	-6.33267300	5.71975500	5.03922900
H	-6.63997600	5.73637700	6.08912500
H	-7.14447800	5.25298900	4.46627900
C	-6.05817400	7.13043000	4.53720400
H	-6.99822200	7.68089400	4.44175500
H	-5.43072600	7.66610700	5.25799300
C	-5.34290500	7.05815600	3.19070900
H	-5.04740500	8.05675800	2.86050600
H	-6.01571900	6.64766300	2.42502700
N	-5.12375600	4.88794000	4.93299500
N	-4.13264900	6.22488000	3.26497900
C	-3.47914200	10.86440400	3.85287500
C	-2.98689800	9.56951800	3.97471300
C	-2.16303300	8.99446200	2.98367200
C	-1.85004000	9.78877600	1.85920900
C	-2.34152100	11.08268400	1.72486300
C	-3.15617600	11.62785600	2.72462000
H	-4.09955200	11.28466200	4.63753300
H	-3.22611400	8.99171900	4.86249400
H	-1.21531100	9.38759700	1.07578600
H	-2.08437500	11.66988900	0.84967200
C	-1.66834800	7.60045200	3.13272400
C	-0.17966600	7.36604500	2.81459200
H	-1.89769200	7.22202900	4.13018400
H	0.14170400	7.97533600	1.96227900
H	0.42486900	7.67845200	3.67425200
O	0.86857400	5.21678200	3.17750300
C	0.12542000	5.90278700	2.46705000
O	-0.47397700	5.47749300	1.40454800
C	-4.07405800	7.41109100	-0.81553000
H	-4.29193100	8.20571100	-0.09453000
H	-5.03375600	7.03963300	-1.19950500
H	-3.55307500	7.88042900	-1.65791500
C	-3.21895200	6.29350600	-0.19897000
H	-3.83379100	5.72952000	0.55363300
H	-3.08705100	5.49652000	-0.95023300
C	0.28105500	7.36392000	-1.29342600
H	0.49126400	8.37928700	-0.92555900
H	-0.07405500	7.50279600	-2.32413100
C	1.58672100	6.55124500	-1.31213600
H	1.43709600	5.55214300	-1.73982100
H	2.37982300	7.03310000	-1.90323300
H	1.98795600	6.39959300	-0.30313200

TS_{II-13}_CN

scf done: -3159.58458575

Ni	-2.77835400	6.66479600	1.93126500
Zn	-1.16613100	6.33003100	-0.20419000
C	-2.08767000	4.30900500	5.45700600
C	-2.84743100	4.37945400	4.09640400
C	-4.06926000	5.27371300	4.07946400
C	-2.89559300	4.70080300	6.70422300
C	-4.15868400	3.86393100	6.95995000
C	-5.03448000	3.69573200	5.70256100
H	-1.69125200	3.29433500	5.57293900
H	-2.16759300	4.72088600	3.31380500
H	-3.18123900	5.75703100	6.62391600
H	-4.74069900	4.33657900	7.75950600
H	-1.21810300	4.97058000	5.39767300
H	-3.17094500	3.37718400	3.79539000
H	-2.24106300	4.63542200	7.58034400
H	-3.89129300	2.86192500	7.31631000
H	-6.05959400	3.43565700	5.97709800
H	-4.66552300	2.87029000	5.08965200
C	-6.31209900	5.74106300	5.01571500
H	-6.62421000	5.71013800	6.06399900
H	-7.12258200	5.30397200	4.41805800
C	-6.03059900	7.17238700	4.58127500
H	-6.96868700	7.72901200	4.50415000
H	-5.40715300	7.67301000	5.33026200
C	-5.30526300	7.15928400	3.23824000
H	-5.01076100	8.17162400	2.95318000
H	-5.97136300	6.77928000	2.45102200
N	-5.10525800	4.91108100	4.87637000
N	-4.09385400	6.32708600	3.28838900
C	-3.51733600	10.91708900	3.95532900
C	-2.98797300	9.63607500	4.03181900
C	-2.17908900	9.10333600	3.00345500
C	-1.92018100	9.92852800	1.88612300
C	-2.44713900	11.20972500	1.79224900
C	-3.25275600	11.71715000	2.82853400
H	-4.12593900	11.30826700	4.76390300
H	-3.18489900	9.03156800	4.91221700
H	-1.29573300	9.56271200	1.07765200
H	-2.23509900	11.82564300	0.92465800
C	-1.64141500	7.72340800	3.11551900
C	-0.15851800	7.54114500	2.75451000
H	-1.82765100	7.32785200	4.11593000
H	0.10508500	8.09838300	1.84809500
H	0.46177600	7.94232400	3.56483500
O	0.99757800	5.47628100	3.24004200
C	0.19531900	6.06894100	2.51053400
O	-0.43213600	5.52684000	1.51970000
C	-4.01163100	7.38499000	-0.83205900
H	-4.13060200	8.25099100	-0.17287900
H	-5.01340900	7.07836300	-1.16165200
H	-3.47570500	7.73603000	-1.72133400
C	-3.24199500	6.24245900	-0.14933700
H	-3.88377200	5.79400300	0.65548300
H	-3.20623200	5.38518400	-0.84163700
C	0.19674900	6.80595900	-1.56197200
H	0.09615200	7.87269000	-1.81071500
H	-0.02934900	6.27683000	-2.49903100
C	1.65126200	6.51556200	-1.15648500
H	1.81541500	5.44835100	-0.96590300
H	2.37643300	6.81663900	-1.92755200

H	1.93277700	7.04134700	-0.23582100
C	-3.79148200	13.03988100	2.74259300
N	-4.23187500	14.11585800	2.67438600

TS_{18-20_H}

scf done: -3221.22446516

Ni	-3.68045500	4.74374700	1.90357000
Zn	-2.54517200	8.97380800	1.87579500
C	-4.32644900	6.26223200	5.87186100
C	-4.65953500	5.03222200	4.97419200
C	-5.74400100	5.25252300	3.94140900
C	-5.41324600	7.34511300	5.97292500
C	-6.76748400	6.87273600	6.52338200
C	-7.26255600	5.57324400	5.85666100
H	-4.07065500	5.89946500	6.87464200
H	-3.76417200	4.72812900	4.43008600
H	-5.56738200	7.77886100	4.97762600
H	-7.50638800	7.67080200	6.38274400
H	-3.42817300	6.73434000	5.46430200
H	-4.94912500	4.17522900	5.59165100
H	-5.03846500	8.16242200	6.59993500
H	-6.70367000	6.69277500	7.60393200
H	-8.34114700	5.45688400	5.99360700
H	-6.80151900	4.70650300	6.33687800
C	-8.10122700	5.88219800	3.51579100
H	-8.69129800	6.66863800	3.99769600
H	-8.76443800	5.01712800	3.37530700
C	-7.55880000	6.36454500	2.17592300
H	-8.37550300	6.45386800	1.45350800
H	-7.10738100	7.35637700	2.29161000
C	-6.50081300	5.38201400	1.67782500
H	-6.03175800	5.75576600	0.76408400
H	-6.96790400	4.41740400	1.43011500
N	-6.99895000	5.51744400	4.41462400
N	-5.44303000	5.16618600	2.67236900
C	-3.09642800	6.55172300	1.90806800
O	-2.50427400	7.11136800	2.89854700
O	-3.35674600	7.30023200	0.89326800
C	-1.97069600	11.86409000	2.32807200
H	-1.25911700	11.61741100	3.12594800
H	-2.32999400	12.88475800	2.52960400
H	-1.39053500	11.91191800	1.39809600
C	-3.10988900	10.83539500	2.23813900
H	-3.68511700	10.84815600	3.17450200
H	-3.81991700	11.14844900	1.45955500
H	-2.35148600	4.61829900	1.29012300
C	-5.50106600	0.89092100	4.66011700
C	-5.38665200	1.54697600	3.43507600
C	-4.14048100	2.00065500	2.95919300
C	-3.00925500	1.76699100	3.76788500
C	-3.12356800	1.11079700	4.99233800
C	-4.36921800	0.66919000	5.44933800
H	-6.47599000	0.54890700	4.99748200
H	-6.27352200	1.71134200	2.82773500
H	-2.03001300	2.10264600	3.43962600
H	-2.23390200	0.94284300	5.59346900
C	-4.07520700	2.68967400	1.65912200
C	-2.89266900	3.01812700	0.97886000
H	-5.00183900	2.69624400	1.08999800
H	-2.93450000	3.17612300	-0.09498400
H	-1.93074800	2.66007100	1.33430100
C	-0.12438800	9.06113000	-0.18756800
O	-0.53067300	8.82156100	1.18447500
C	0.59497100	8.38865500	1.99280600
C	1.69274200	8.04597500	0.98707600
C	1.40389700	9.02509100	-0.16373400
H	-0.54678600	8.26701900	-0.81347600

H	-0.54099200	10.02266700	-0.49949900
H	0.88316900	9.21730800	2.65053100
H	0.26162900	7.54444500	2.59953700
H	2.69240300	8.16526300	1.41168800
H	1.58636500	7.01112500	0.64493700
H	1.80648700	10.01687500	0.06792500
H	1.82211000	8.70149800	-1.11979700
H	-4.45465900	0.15584600	6.40258200

TS_{18-20_NH₂}

scf done: -3276.58390726

Ni	-3.70031200	4.75103100	1.90170100
Zn	-2.53300700	8.97709600	1.89380900
C	-4.37829400	6.24308500	5.86767900
C	-4.71065400	5.01715400	4.96423300
C	-5.78419800	5.24788700	3.92241700
C	-5.46112700	7.33051100	5.96358700
C	-6.82206700	6.86285100	6.50139000
C	-7.31881100	5.56849000	5.82554700
H	-4.13148900	5.87670600	6.87150100
H	-3.81296200	4.70760600	4.42708400
H	-5.60526200	7.76797500	4.96844300
H	-7.55562800	7.66536200	6.35801500
H	-3.47482200	6.71263500	5.46862300
H	-5.01153900	4.16052800	5.57680600
H	-5.08782400	8.14426500	6.59611700
H	-6.76787200	6.67858100	7.58180200
H	-8.39921300	5.45799700	5.95311700
H	-6.86690800	4.69767200	6.30719300
C	-8.13455300	5.89243200	3.47888300
H	-8.72519400	6.67888000	3.96016000
H	-8.80130900	5.03216500	3.32568100
C	-7.57646200	6.38091600	2.14759100
H	-8.38554500	6.47940900	1.41777700
H	-7.12122000	7.36962900	2.27460300
C	-6.51823700	5.39652900	1.65349000
H	-6.03814400	5.77395300	0.74703000
H	-6.98738000	4.43581400	1.39463700
N	-7.04320800	5.51544500	4.38592800
N	-5.47122300	5.16889100	2.65641300
C	-3.10019200	6.55765100	1.91851700
O	-2.50617700	7.11399400	2.91208400
O	-3.34787500	7.31567200	0.90509600
C	-1.93960900	11.86321400	2.35848400
H	-1.23064700	11.60783000	3.15600400
H	-2.29234200	12.88531000	2.56469400
H	-1.35770100	11.91201100	1.42962900
C	-3.08500300	10.84206500	2.26154400
H	-3.66261300	10.85533400	3.19653900
H	-3.79116300	11.16321700	1.48263600
H	-2.37590800	4.57748400	1.28347100
C	-5.49943300	0.86625900	4.65415200
C	-5.38819600	1.53676500	3.43960400
C	-4.15078100	1.99596200	2.94970800
C	-3.02068700	1.74781000	3.75419500
C	-3.11984500	1.07856500	4.96969200
C	-4.36293100	0.62139000	5.44541800
H	-6.47256700	0.51886500	4.99354900
H	-6.28547000	1.70919800	2.84955900
H	-2.04043100	2.08614400	3.43054400
H	-2.22456500	0.90072000	5.56092200
C	-4.09275400	2.69787000	1.65635000
C	-2.91283500	3.02591600	0.96687300
H	-5.02169600	2.70573300	1.09058700
H	-2.96391400	3.18284500	-0.10699600
H	-1.95226000	2.65015300	1.30909700
C	-0.11154100	9.07016000	-0.17008900

O	-0.51528700	8.82389800	1.20126900	H	-2.31963200	0.99906700	5.71849600
C	0.60823800	8.37106400	2.00120400	C	-4.03147600	2.71757900	1.69941000
C	1.69865700	8.02498100	0.98857400	C	-2.82804000	3.03991300	1.05096600
C	1.41639200	9.01697500	-0.15276800	H	-4.93896700	2.71252100	1.10005600
H	-0.54507800	8.28615900	-0.80116700	H	-2.83798300	3.17910700	-0.02633800
H	-0.51851000	10.03885900	-0.47248800	H	-1.87824100	2.68185300	1.43846400
H	0.90828400	9.19035600	2.66540200	C	-0.07960200	9.20671800	-0.11144200
H	0.26789500	7.52507800	2.60156900	O	-0.48661400	8.85107400	1.23571300
H	2.70112500	8.12957600	1.41048200	C	0.60218400	8.21276400	1.95490500
H	1.57965400	6.99434500	0.63798400	C	1.62487900	7.85298700	0.87959400
H	1.83089100	10.00224300	0.08569300	C	1.43283000	8.98157500	-0.14794500
H	1.82731200	8.69693300	-1.11319400	H	-0.61144200	8.55363800	-0.81239600
N	-4.45311700	-0.11426600	6.63144600	H	-0.37739400	10.24317000	-0.29145500
H	-3.71260100	0.06778600	7.29691400	H	1.00274600	8.93298600	2.67832500
H	-5.35962600	-0.08083400	7.08028000	H	0.18685800	7.35620500	2.48881100
				H	2.64134400	7.80322900	1.27742600
				H	1.38273600	6.88269800	0.43323300
				H	1.96212600	9.88477300	0.17368600
				H	1.78437700	8.71820300	-1.14831900
				O	-4.47749700	0.08183900	6.70923000
				C	-5.73246700	-0.40456000	7.17672800
				H	-6.14868700	-1.15459200	6.49384700
				H	-5.53379600	-0.86594300	8.14419900
				H	-6.45403500	0.41129100	7.30346400

TS_{18-20_}OMe

scf done: -3335.7750482

Ni	-3.64975000	4.77324300	1.93277400
Zn	-2.50459400	9.00422300	1.92383500
C	-4.40943100	6.32670100	5.86118300
C	-4.72172800	5.08639100	4.97005300
C	-5.77423500	5.29811000	3.90320000
C	-5.49266200	7.41712200	5.91210400
C	-6.86612900	6.96089400	6.42769200
C	-7.34742700	5.65275700	5.76779700
H	-4.18828900	5.97665900	6.87660700
H	-3.81240800	4.77136500	4.45631300
H	-5.61393200	7.83599800	4.90593700
H	-7.59591800	7.75998200	6.24998600
H	-3.49530500	6.78772300	5.47681900
H	-5.03249900	4.23852000	5.59004500
H	-5.13254600	8.24216800	6.53754700
H	-6.83742900	6.79924900	7.51261900
H	-8.43008700	5.54291600	5.87531500
H	-6.90410200	4.79218000	6.27500800
C	-8.11444700	5.93610200	3.39978200
H	-8.71062200	6.73416500	3.85441900
H	-8.78181200	5.07556300	3.25125500
C	-7.52952000	6.39626200	2.06986000
H	-8.32399000	6.48001600	1.32237800
H	-7.07561800	7.38700500	2.18497500
C	-6.46284800	5.40099300	1.61749300
H	-5.96569900	5.75822500	0.71212400
H	-6.92768900	4.43485500	1.37142600
N	-7.04239000	5.57241800	4.33515600
N	-5.43559900	5.19587500	2.64511700
C	-3.06291000	6.58238900	1.94653700
O	-2.47590500	7.14092800	2.94223500
O	-3.31290100	7.33544800	0.93185700
C	-1.92802400	11.88693400	2.43297500
H	-1.24600200	11.62497300	3.25146100
H	-2.28922800	12.90656200	2.63641500
H	-1.31532000	11.94557200	1.52471100
C	-3.06837700	10.86582600	2.28827000
H	-3.67620000	10.86918900	3.20396800
H	-3.74921500	11.19408300	1.49001100
H	-2.30812800	4.62230600	1.34966900
C	-5.54913900	0.92152200	4.66871700
C	-5.38605900	1.57506200	3.44458500
C	-4.13590500	2.03653000	3.00116500
C	-3.03273300	1.81362200	3.85368400
C	-3.17677400	1.16604500	5.07326200
C	-4.43723000	0.71362400	5.49216800
H	-6.53494500	0.57970900	4.96157100
H	-6.25856500	1.72606000	2.81368800
H	-2.04360100	2.15365900	3.56200000

TS_{18-20_}CF₃

scf done: -3558.37491555

Ni	-3.66618700	4.73092500	1.89937600
Zn	-2.56486700	8.96455400	1.87089900
C	-4.29229500	6.27680800	5.86520600
C	-4.62716000	5.04364100	4.97205000
C	-5.71908600	5.25585400	3.94497400
C	-5.37814100	7.36079200	5.96394700
C	-6.73037200	6.89178000	6.52219500
C	-7.22617200	5.58730200	5.86670500
H	-4.03554800	5.91722700	6.86875300
H	-3.73325300	4.74357300	4.42301000
H	-5.53552300	7.78943300	4.96693800
H	-7.47039800	7.68811900	6.37809800
H	-3.39446100	6.74630000	5.45396000
H	-4.90946200	4.18718000	5.59410600
H	-5.00045600	8.18099900	6.58529200
H	-6.66297900	6.71941700	7.60366900
H	-8.30367700	5.46909700	6.00991400
H	-6.76046400	4.72437700	6.34927600
C	-8.07816500	5.88206500	3.52836000
H	-8.66410600	6.67289500	4.00791800
H	-8.74262100	5.01622300	3.39999800
C	-7.54408900	6.35277200	2.18113200
H	-8.36539600	6.43655100	1.46339000
H	-7.09115900	7.34513700	2.28538400
C	-6.49041600	5.36514300	1.68420100
H	-6.02739800	5.73055300	0.76405700
H	-6.96013100	4.39895800	1.44796100
N	-6.97013800	5.52378800	4.42321200
N	-5.42622600	5.15728700	2.67412300
C	-3.09987300	6.53984100	1.90267400
O	-2.51587500	7.09742600	2.89573900
O	-3.37069600	7.28060600	0.88846600
C	-2.00446900	11.85578300	2.31897500
H	-1.29123700	11.61409500	3.11682700
H	-2.36848100	12.87503700	2.51859900
H	-1.42557200	11.90416600	1.38827700
C	-3.13962500	10.82232000	2.23261900
H	-3.71300300	10.83311400	3.16998300
H	-3.85220000	11.13041900	1.45456100
H	-2.32747900	4.67984900	1.30802400

C	-5.53032000	0.90023000	4.63421500	C	-2.01167800	11.84874300	2.32380300
C	-5.39790600	1.54268800	3.40889500	H	-1.29921000	11.60719600	3.12236300
C	-4.14559300	1.99422000	2.94286400	H	-2.37703200	12.86742900	2.52373000
C	-3.02277100	1.76844000	3.76777700	H	-1.43175900	11.89839200	1.39381800
C	-3.14581000	1.12717700	4.99412700	C	-3.14581700	10.81434400	2.23536700
C	-4.40247400	0.69453500	5.43858600	H	-3.72034100	10.82382200	3.17201000
H	-6.50644400	0.56175700	4.96591500	H	-3.85765900	11.12209900	1.45654400
H	-6.27885700	1.70019900	2.79326800	H	-2.32338500	4.68891500	1.31785900
H	-2.04031000	2.10269800	3.45168200	C	-5.53845300	0.89769500	4.63058900
H	-2.26627600	0.96788700	5.60919700	C	-5.40394200	1.54178900	3.40918800
C	-4.06729400	2.67297600	1.64383100	C	-4.14862700	1.98664700	2.94035500
C	-2.87882300	3.01096100	0.98260000	C	-3.02305500	1.75293600	3.76173800
H	-4.98926300	2.68231400	1.06801500	C	-3.14349200	1.11002700	4.98470800
H	-2.90645000	3.17831900	-0.08986000	C	-4.40524900	0.67555800	5.43560800
H	-1.91674400	2.67167200	1.35393400	H	-6.51334800	0.56107800	4.96798300
C	-0.13774200	9.04270200	-0.18365600	H	-6.28457300	1.70474900	2.79452900
O	-0.55315500	8.80664700	1.18668100	H	-2.03990700	2.08062700	3.44106300
C	0.57107700	8.39477900	2.00833400	H	-2.26549200	0.93931300	5.59903900
C	1.68007600	8.05518700	1.01418900	C	-4.07018700	2.66394600	1.64287200
C	1.39058000	9.02218200	-0.14669400	C	-2.88256600	3.00563600	0.98239100
H	-0.54715900	8.24068100	-0.80796300	H	-4.99331000	2.67866700	1.06911100
H	-0.56124000	9.99821900	-0.50460700	H	-2.91107900	3.17868900	-0.08907000
H	0.84458100	9.23313000	2.65993200	H	-1.91951000	2.66807800	1.35239600
H	0.24223900	7.55290100	2.62070500	C	-0.14040600	9.03702100	-0.17937500
H	2.67501900	8.18814200	1.44569900	O	-0.55736000	8.79903100	1.19027500
H	1.58688900	7.01656500	0.67970000	C	0.56700900	8.39130400	2.01389700
H	1.78135700	10.01972300	0.08025300	C	1.67831800	8.05448600	1.02146200
H	1.81983400	8.69522500	-1.09667100	C	1.38791500	9.02047200	-0.14004600
C	-4.52936800	-0.03873000	6.73814500	H	-0.54686400	8.23427400	-0.80464400
F	-3.60238700	0.34290000	7.64978300	H	-0.56585100	9.99163400	-0.50043500
F	-5.74155700	0.13221200	7.32054800	H	0.83701500	9.23097500	2.66523700
F	-4.37513700	-1.38843000	6.59918000	H	0.23985300	7.54887500	2.62640100

TS₁₈₋₂₀_CN

scf done: -3313.47077439

Ni	-3.66445500	4.72414500	1.90229300
Zn	-2.56831000	8.95770900	1.87317800
C	-4.28857300	6.27552500	5.86558200
C	-4.62548600	5.04196000	4.97370900
C	-5.71731200	5.25473300	3.94656900
C	-5.37297500	7.36102000	5.96375000
C	-6.72578600	6.89431200	6.52256800
C	-7.22366500	5.59019700	5.86804100
H	-4.03202100	5.91643900	6.86934400
H	-3.73200000	4.74001400	4.42490100
H	-5.52994400	7.78922900	4.96649100
H	-7.46464200	7.69165300	6.37813100
H	-3.39027200	6.74338600	5.45354000
H	-4.90915000	4.18669800	5.59669900
H	-4.99403800	8.18109200	6.58448800
H	-6.65843200	6.72248500	7.60411300
H	-8.30135900	5.47382800	6.01123400
H	-6.75935000	4.72687700	6.35119400
C	-8.07529100	5.88404300	3.52930200
H	-8.66009700	6.67614900	4.00808500
H	-8.74085200	5.01891400	3.40197300
C	-7.54059400	6.35255800	2.18157700
H	-8.36182000	6.43690200	1.46382700
H	-7.08609900	7.34430500	2.28480400
C	-6.48859800	5.36272900	1.68550300
H	-6.02494800	5.72658300	0.76506600
H	-6.96004000	4.39719800	1.45002900
N	-6.96766900	5.52526100	4.42453200
N	-5.42479300	5.15385600	2.67569200
C	-3.10005400	6.53256300	1.90469000
O	-2.51797200	7.08947700	2.89849200
O	-3.37233800	7.27141000	0.89029300

20_H

scf done: -3221.25525478

Ni	-3.71405000	4.27641800	1.29866800
Zn	-2.02699900	8.21647300	0.57206400
C	-3.76981000	5.51000600	5.35165600
C	-4.44155600	4.45216500	4.42453600
C	-5.51859100	4.98925100	3.50484100
C	-4.58957300	6.78072600	5.62972300
C	-5.96821600	6.55620000	6.27024500
C	-6.79219000	5.46151300	5.56103000
H	-3.50642300	5.02216500	6.29748500
H	-3.68406800	3.98711400	3.78956900
H	-4.72280000	7.32368500	4.68654100
H	-6.51963200	7.50392500	6.26036000
H	-2.82887200	5.81943500	4.88635100
H	-4.87758900	3.64690800	5.02518900
H	-4.00123800	7.44382000	6.27434200
H	-5.86312800	6.26753500	7.32353700
H	-7.85666400	5.57786700	5.78211300
H	-6.51130000	4.47566900	5.93955600
C	-7.69214500	6.16503700	3.33170400
H	-8.03048700	7.02716100	3.91589800
H	-8.55561600	5.49764700	3.20469700
C	-7.15393200	6.61206000	1.97815800
H	-7.97998200	6.93924100	1.33987900
H	-6.47650800	7.46360000	2.10793300
C	-6.39249800	5.45578800	1.33312600
H	-5.92927500	5.77174500	0.39569200

H	-7.08584000	4.63609700	1.09432000	C	-7.19918400	6.44225000	2.05280100
N	-6.64818100	5.47189200	4.10060600	H	-8.05760200	6.68943500	1.42117700
N	-5.32865700	4.94956200	2.21028500	H	-6.58439500	7.34448900	2.14705000
C	-2.90532000	5.92389300	0.96567100	C	-6.36481000	5.32649200	1.42664400
O	-2.18252700	6.51734800	1.84354100	H	-5.94014300	5.64856000	0.47280400
O	-3.11394600	6.55505000	-0.13648200	H	-6.99971500	4.45247600	1.22031300
C	-3.73773200	10.66164600	0.47675500	N	-6.57328200	5.41227300	4.19830400
H	-4.18393000	10.33881100	-0.47191200	N	-5.25382300	4.92215400	2.29781900
H	-3.82489200	11.75834000	0.51124500	C	-2.85153700	5.96383200	0.97362600
H	-4.38045100	10.26905200	1.27444500	O	-2.13695300	6.60337500	1.82884800
C	-2.28566800	10.17557300	0.62122100	O	-3.07826000	6.56226900	-0.14554500
H	-1.67039200	10.63094100	-0.16793900	C	-3.74174400	10.69921700	0.36297100
H	-1.87137500	10.55874200	1.56502300	H	-4.17885700	10.36201900	-0.58500600
H	-0.55189800	3.63751300	1.55998100	H	-3.83294500	11.79605900	0.38154600
C	-5.10075800	1.02317600	1.60779300	H	-4.39034000	10.31551600	1.16022000
C	-4.36297800	1.92480500	0.82365400	C	-2.28955400	10.21941900	0.52654500
C	-2.98706400	2.17779900	1.08400900	H	-1.66903800	10.66634900	-0.26345300
C	-2.40023900	1.48320300	2.17958200	H	-1.88465200	10.61751500	1.46839700
C	-3.13724300	0.58916800	2.94113500	H	-0.57386900	3.61056000	1.85805300
C	-4.49699300	0.35546500	2.66655500	C	-5.10076300	0.91253600	1.33157700
H	-6.14439700	0.83804100	1.36767900	C	-4.29392600	1.84749000	0.67945300
H	-4.82753100	2.37382900	-0.05196300	C	-2.99218800	2.17523100	1.13960200
H	-1.35098400	1.64338900	2.40640200	C	-2.56297400	1.51115800	2.32055000
H	-2.65531800	0.05836100	3.75824500	C	-3.35854000	0.57984200	2.96815600
C	-2.33125600	3.26505100	0.35135700	C	-4.64989700	0.26295900	2.48956200
C	-0.84042000	3.49514700	0.51338600	H	-6.08514600	0.67895200	0.93321800
H	-2.65100900	3.32307200	-0.69431500	H	-4.65172800	2.29645500	-0.24432700
H	-0.53720600	4.39602700	-0.02802900	H	-1.57316100	1.71924200	2.71543300
H	-0.24383900	2.65788400	0.11908600	H	-2.98801500	0.08158000	3.86122200
C	1.06246200	7.41652200	0.66652000	C	-2.24528400	3.27111000	0.48864400
O	-0.09759600	7.66221500	-0.17239800	C	-0.76696400	3.44755500	0.79229700
C	0.29472200	7.83424500	-1.55901300	H	-2.44777800	3.32552700	-0.58634800
C	1.73998700	7.34467400	-1.62494600	H	-0.37796900	4.32314800	0.26393200
C	2.26998200	7.70314900	-0.22639600	H	-0.16643700	2.57940700	0.47786300
H	0.99426900	8.06960800	1.54048800	C	1.07946900	7.49517700	0.60048600
H	1.02748300	6.37303000	0.99619400	O	-0.08797000	7.71507700	-0.23461500
H	-0.40006800	7.26017200	-2.17666100	C	0.29254300	7.85721700	-1.62737400
H	0.20888500	8.89738600	-1.81371700	C	1.74302200	7.38247600	-1.69296300
H	1.76874100	6.26105300	-1.77996900	C	2.27832200	7.77585600	-0.30585300
H	2.29986000	7.82126600	-2.43312500	H	1.01092800	8.16335800	1.46293300
H	3.14495200	7.11757400	0.06553500	H	1.05717900	6.45758200	0.94990900
H	2.53705400	8.76426500	-0.18001200	H	-0.39967900	7.26004300	-2.22577900
H	-5.06284900	-0.34918100	3.26868700	H	0.19223200	8.91269000	-1.90757800

20_NH₂

scf done: -3276.6152408

Ni	-3.61649600	4.31045900	1.37170700
Zn	-2.02273000	8.26067900	0.51063700
C	-3.68685000	5.67143000	5.40387800
C	-4.29549100	4.55317600	4.50454400
C	-5.42377100	4.99022900	3.59377700
C	-4.58318700	6.89411300	5.66047000
C	-5.93382900	6.59521400	6.32861000
C	-6.69235800	5.42965400	5.66047600
H	-3.38724000	5.22325200	6.35863900
H	-3.51663900	4.13716100	3.86142400
H	-4.76550800	7.39973300	4.70485600
H	-6.54828500	7.50317500	6.30442700
H	-2.76978700	6.02862300	4.92505900
H	-4.65939900	3.72637300	5.12431400
H	-4.03090300	7.61205100	6.27769000
H	-5.79365900	6.34154100	7.38686500
H	-7.75847000	5.47971100	5.89804200
H	-6.33959500	4.47459100	6.05773900
C	-7.68025400	5.99688700	3.42856500
H	-8.07685600	6.84787500	3.99220100
H	-8.49084100	5.26073200	3.33624000

20_OME

scf done: -3335.80533586

Ni	-3.66337000	4.35661100	1.28539400
Zn	-2.00450500	8.30552100	0.56631400
C	-3.71782900	5.50054600	5.36412200
C	-4.33545200	4.42392200	4.42248800
C	-5.46434800	4.91293700	3.53916100
C	-4.63024500	6.68456800	5.72563800
C	-5.96765000	6.31736700	6.38578700
C	-6.73543100	5.21225800	5.62893900
H	-3.37341200	5.00159100	6.27767400
H	-3.56075400	4.03095500	3.75972800
H	-4.83320700	7.25923700	4.81412600
H	-6.58535700	7.22082600	6.45260700
H	-2.82739300	5.90772100	4.87496300
H	-4.70164100	3.57488600	5.00968700

H	-4.07990100	7.36188400	6.38873700	C	-4.58026900	6.77569500	5.62944600
H	-5.80844300	5.97168000	7.41472900	C	-5.96694500	6.57333400	6.25992100
H	-7.80206500	5.25726800	5.86484900	C	-6.79941100	5.48700100	5.54878700
H	-6.39651200	4.22599400	5.95538100	H	-3.53608200	4.99749300	6.30664900
C	-7.71326400	5.94450000	3.44044300	H	-3.70145800	3.97514700	3.79099800
H	-8.10036200	6.76081200	4.05927100	H	-4.69718100	7.32045500	4.68506000
H	-8.53088400	5.22379000	3.30195000	H	-6.50537200	7.52831500	6.24184000
C	-7.22842000	6.47366400	2.09618000	H	-2.82797800	5.78473300	4.90507300
H	-8.08469700	6.76871900	1.48255500	H	-4.90806400	3.64313000	5.01589300
H	-6.60568500	7.36251900	2.24794100	H	-3.98594300	7.42913400	6.27829500
C	-6.40408900	5.39377200	1.39816000	H	-5.87416800	6.28717300	7.31494400
H	-5.97761300	5.77243400	0.46624800	H	-7.86359200	5.61445800	5.76449900
H	-7.04586400	4.53954700	1.13760800	H	-6.53042300	4.49834500	5.92825000
N	-6.61129500	5.30012200	4.16943900	C	-7.68213400	6.20098200	3.31583400
N	-5.29496900	4.92687100	2.24075700	H	-8.01135100	7.06720600	3.89893700
C	-2.88062600	6.01342600	0.96486700	H	-8.55255700	5.54323800	3.18773700
O	-2.16457700	6.61352700	1.84480900	C	-7.13502200	6.64033400	1.96364500
O	-3.09472500	6.64574700	-0.13608500	H	-7.95530400	6.97687000	1.32294300
C	-3.61627500	10.78769500	0.15789900	H	-6.44729500	7.48344700	2.09405500
H	-3.84862500	10.49333100	-0.87302800	C	-6.38737600	5.47387000	1.32127200
H	-3.68992500	11.88520500	0.19805900	H	-5.91761800	5.78342600	0.38505500
H	-4.42571400	10.39422100	0.78503900	H	-7.09054100	4.66288100	1.08191700
C	-2.23965900	10.26799100	0.60640400	N	-6.64831700	5.49614000	4.08844500
H	-1.45869800	10.72560300	-0.01757500	N	-5.33243500	4.95471400	2.20274700
H	-2.03743600	10.62359700	1.62698600	C	-2.91320300	5.90023900	0.98528300
H	-0.62632200	3.61661700	1.73923300	O	-2.18896700	6.48099300	1.86553800
C	-5.13682700	0.96058800	0.98617100	O	-3.12703600	6.52973900	-0.11351500
C	-4.33464200	1.94465200	0.41051400	C	-3.76216000	10.62653400	0.50084900
C	-3.02670800	2.22661800	0.89126000	H	-4.20502300	10.30193600	-0.44871700
C	-2.59111600	1.46555000	2.00434000	H	-3.85511700	11.72258700	0.53610200
C	-3.38177900	0.47645000	2.58208800	H	-4.40348900	10.22973300	1.29752900
C	-4.66679100	0.21960500	2.07469700	C	-2.30740200	10.14950100	0.64692600
H	-6.12607700	0.74838500	0.59225900	H	-1.69369900	10.60838900	-0.14127200
H	-4.69967500	2.47668200	-0.46465100	H	-1.89637000	10.53340500	1.59167600
H	-1.59958800	1.63975600	2.41031200	H	-0.52675800	3.63592000	1.45201900
H	-2.99270100	-0.08919000	3.42079500	C	-5.07625300	1.04863200	1.67324800
C	-2.28546200	3.37623900	0.33546500	C	-4.36069700	1.92958200	0.85236400
C	-0.80995000	3.53364100	0.66274000	C	-2.97353800	2.18535200	1.06302300
H	-2.48310400	3.51639500	-0.73241500	C	-2.35053100	1.49870800	2.14964300
H	-0.41977100	4.44753400	0.20518000	C	-3.05908600	0.62605600	2.95014300
H	-0.20455000	2.69293200	0.28912900	C	-4.43539800	0.40131600	2.72466800
C	1.08342700	7.48961500	0.66020900	H	-6.12672100	0.86501200	1.47504900
O	-0.07709200	7.73509100	-0.17769300	H	-4.85535100	2.35692900	-0.01654600
C	0.31318900	7.89720900	-1.56565100	H	-1.29393000	1.65387000	2.33813400
C	1.75300700	7.39218200	-1.63296800	H	-2.55437200	0.10678400	3.75958100
C	2.29116600	7.75611800	-0.23897100	C	-2.34530800	3.25633600	0.30646300
H	1.02346400	8.15272200	1.52726800	C	-0.85332000	3.50178400	0.41567100
H	1.04112900	6.45010700	1.00152500	H	-2.71790600	3.33679500	-0.71895600
H	-0.38928600	7.32768300	-2.17873800	H	-0.58036300	4.41096100	-0.12709100
H	0.23819900	8.96009500	-1.82510900	H	-0.26551000	2.67503600	-0.01108000
H	1.76977400	6.30712600	-1.77959800	C	1.04943900	7.38997900	0.69301900
H	2.31515700	7.85656100	-2.44665900	O	-0.11044700	7.63663400	-0.14686700
H	3.16072200	7.16355100	0.05509300	C	0.28309500	7.80900000	-1.53373700
H	2.56990500	8.81459400	-0.20208500	C	1.72804200	7.31871100	-1.59820700
O	-5.51763500	-0.73225700	2.57188300	C	2.25715700	7.67692100	-0.19927100
C	-5.08318400	-1.52840300	3.67179300	H	0.98072000	8.04261000	1.56720700
H	-4.87513000	-0.91115500	4.55366100	H	1.01370100	6.34626000	1.02166000
H	-5.90664000	-2.20793600	3.89175100	H	-0.41164700	7.23549100	-2.15192200
H	-4.19020600	-2.10996500	3.41505100	H	0.19790200	8.87225500	-1.78773300
				H	1.75653600	6.23510600	-1.75333800
				H	2.28872900	7.79518800	-2.40583900
				H	3.13188700	7.09120000	0.09297800
				H	2.52418900	8.73798700	-0.15242500
				C	-5.16552200	-0.56546400	3.60181700
				F	-6.50077500	-0.57177500	3.39203600
				F	-4.74721800	-1.85248700	3.42742200
				F	-4.98402500	-0.30849100	4.92677000
20_CF3							
scf done: -3558.40562727							
Ni	-3.73485400	4.25612200	1.30060300				
Zn	-2.03386200	8.19324000	0.59463800				
C	-3.77958600	5.49137900	5.35878600				
C	-4.45848500	4.44612100	4.42208200				
C	-5.52448000	4.99835500	3.49823300				

20_CN

scf done: -3313.50174559

Ni	-3.73891900	4.25325400	1.30453000
Zn	-2.03496800	8.18854500	0.60018400
C	-3.78435500	5.49357000	5.36117600
C	-4.46236600	4.44839900	4.42367100
C	-5.52707300	5.00015400	3.49804800
C	-4.58349700	6.77959500	5.62812100
C	-5.97157700	6.58011300	6.25641700
C	-6.80356400	5.49286700	5.54632800
H	-3.54461000	5.00028800	6.31029200
H	-3.70455300	3.97675900	3.79403000
H	-4.69779600	7.32300100	4.68261600
H	-6.50913000	7.53549800	6.23510800
H	-2.83084600	5.78456300	4.91000300
H	-4.91333300	3.64583300	5.01691400
H	-3.98939500	7.43315300	6.27702500
H	-5.88105800	6.29622600	7.31222700
H	-7.86795800	5.62091400	5.76047200
H	-6.53524300	4.50470800	5.92748100
C	-7.68394400	6.20321000	3.31123400
H	-8.01310300	7.07075400	3.89234600
H	-8.55433100	5.54524400	3.18442400
C	-7.13607300	6.63930400	1.95835900
H	-7.95592000	6.97475300	1.31657100
H	-6.44795100	7.48234300	2.08714000
C	-6.38892200	5.47095800	1.31893600
H	-5.91862200	5.77804400	0.38219800
H	-7.09227300	4.65964000	1.08142500
N	-6.65062500	5.49986400	4.08602100
N	-5.33460300	4.95336000	2.20232000
C	-2.91681800	5.89673500	0.99205600
O	-2.19234400	6.47486200	1.87254600
O	-3.13242500	6.52445000	-0.10640100
C	-3.76613800	10.61971700	0.50519400
H	-4.20789300	10.29476700	-0.44474300
H	-3.85997300	11.71566000	0.54043600
H	-4.40768200	10.22231700	1.30138200
C	-2.31102000	10.14428200	0.65240900
H	-1.69710300	10.60352100	-0.13536900
H	-1.90098300	10.52832200	1.59748500
H	-0.52075400	3.65203100	1.43467700
C	-5.05447300	1.03366900	1.66662300
C	-4.34792900	1.91522000	0.84622600
C	-2.96194600	2.18898100	1.06061900
C	-2.33266900	1.51172300	2.15066500
C	-3.02989000	0.63531900	2.95468200
C	-4.40872200	0.38960300	2.72965000
H	-6.10292400	0.83333600	1.47017600
H	-4.84446200	2.33591300	-0.02484500
H	-1.27757200	1.67812700	2.33813000
H	-2.52483200	0.12127500	3.76644400
C	-2.34385200	3.25896200	0.30057400
C	-0.85362800	3.51701000	0.40049700
H	-2.72718200	3.34457000	-0.72026700
H	-0.59206300	4.42924000	-0.14269000
H	-0.26270000	2.69557900	-0.03189000
C	1.04467600	7.37625500	0.69876900
O	-0.11466300	7.62718000	-0.14086300
C	0.27951900	7.80101400	-1.52758900
C	1.72385400	7.30899800	-1.59231400
C	2.25290300	7.66382400	-0.19249900
H	0.97661700	8.02653300	1.57472500
H	1.00714600	6.33161500	1.02426100
H	-0.41582300	7.22929000	-2.14674200
H	0.19570200	8.86474300	-1.77989000

H	1.75111500	6.22567100	-1.74955000
H	2.28542000	7.78637100	-2.39879200
H	3.12690900	7.07656800	0.09881400
H	2.52099300	8.72451100	-0.14335100
C	-5.12535700	-0.51496900	3.57077300
N	-5.70825700	-1.25312500	4.25943500

TS₂₀₋₁_H

scf done: -3221.22353838

Ni	-4.80432200	4.78620600	-0.22855700
Zn	-3.03241000	8.46935200	-0.48277500
C	-4.40415200	3.85658500	3.82040000
C	-5.46825100	3.72932500	2.69115700
C	-6.16277400	5.02071800	2.31477200
C	-4.59306300	5.03672000	4.78824500
C	-5.94552500	5.09043500	5.51578500
C	-7.15556500	4.92918600	4.56903900
H	-4.38013100	2.91386100	4.37953200
H	-4.99633000	3.34136600	1.78514200
H	-4.45640000	5.97051100	4.22977300
H	-6.01640500	6.04433100	6.05180700
H	-3.41943600	3.96515700	3.35316100
H	-6.23365500	3.00003400	2.97761300
H	-3.78912400	5.01378900	5.53281400
H	-6.00678800	4.30135600	6.27549900
H	-8.05316900	5.36057200	5.02031900
H	-7.37516400	3.87001100	4.41575600
C	-7.56069300	6.91405500	3.10210300
H	-7.46071300	7.44710000	4.05370500
H	-8.63496700	6.81830300	2.89334200
C	-6.86183000	7.67412900	1.98234900
H	-7.44024800	8.56573300	1.72232100
H	-5.87139700	8.00621800	2.31424000
C	-6.70685100	6.75393800	0.77348500
H	-6.16464000	7.24681400	-0.03498800
H	-7.69870700	6.48000300	0.38427400
N	-6.97583700	5.57425400	3.26311100
N	-5.97276400	5.52620700	1.11965100
C	-3.70118200	6.14330000	-0.89473300
O	-2.68100400	6.44151100	-0.14389900
O	-4.25558000	7.13274200	-1.53526200
C	-2.81738300	9.99557000	2.08269600
H	-3.31760100	9.18417200	2.62594100
H	-3.00039000	10.91909900	2.65313100
H	-1.74067100	9.79428600	2.14674500
C	-3.29754400	10.08978200	0.62386100
H	-4.36609200	10.34758200	0.61371800
H	-2.79114100	10.93286700	0.13234800
H	-1.40604300	4.53627300	-1.37985500
C	-5.81163400	1.64549600	-1.38453300
C	-5.32378700	2.88324400	-1.81983100
C	-4.01663700	3.32578000	-1.46662500
C	-3.24611700	2.46603400	-0.63499100
C	-3.74242700	1.23410100	-0.21483900
C	-5.02510500	0.81142100	-0.58839800
H	-6.80621200	1.32971300	-1.68868700
H	-5.92065800	3.48728100	-2.49801100
H	-2.24479200	2.76509000	-0.34318900
H	-3.12103100	0.59384700	0.40603600
C	-3.50715800	4.64902200	-1.95932700
C	-2.01296700	4.67787900	-2.27624400
H	-4.09587000	4.97114600	-2.81860800
H	-1.73291900	5.64193800	-2.70961500
H	-1.76329000	3.88673000	-2.99449100
C	-0.16381100	8.66720000	-1.89431200
O	-1.59831200	8.81832800	-2.04644100
C	-1.92084500	9.47836100	-3.29801100

C	-0.58622100	10.00045600	-3.83120100
C	0.41657900	8.97622400	-3.27377100
H	0.18118200	9.37931400	-1.13509300
H	0.03109500	7.64986400	-1.54720200
H	-2.37498900	8.73849000	-3.96613000
H	-2.65008100	10.26557500	-3.08804100
H	-0.57542900	10.06394400	-4.92184500
H	-0.37790900	10.99705400	-3.42797500
H	0.42824200	8.07391900	-3.89432800
H	1.43699800	9.36226900	-3.21395300
H	-5.40082200	-0.15500100	-0.26559400

TS₂₀₋₁_NH₂

scf done: -3276.58207753

Ni	-4.79957400	4.81414600	-0.21994300
Zn	-3.02296700	8.48696000	-0.49118600
C	-4.42079800	3.85760900	3.83196400
C	-5.48026500	3.73167100	2.69818300
C	-6.17298000	5.02359700	2.32075400
C	-4.61384900	5.03643400	4.80067100
C	-5.96919500	5.08925400	5.52289700
C	-7.17540500	4.92935700	4.57094900
H	-4.39845400	2.91417900	4.39013500
H	-5.00455800	3.34666100	1.79294800
H	-4.47519800	5.97083000	4.24378800
H	-6.04217500	6.04250200	6.05980000
H	-3.43430300	3.96747800	3.36878800
H	-6.24679800	3.00187800	2.98102200
H	-3.81281500	5.01282000	5.54836000
H	-6.03359100	4.29934600	6.28154500
H	-8.07487600	5.35994000	5.01940600
H	-7.39427400	3.87030500	4.41558000
C	-7.56948900	6.91870800	3.10797600
H	-7.46942400	7.44901700	4.06117000
H	-8.64374800	6.82822100	2.89657900
C	-6.86513600	7.67885100	1.99170700
H	-7.44015600	8.57268400	1.73176200
H	-5.87451900	8.00733700	2.32666800
C	-6.70937200	6.76033900	0.78166900
H	-6.16456900	7.25337500	-0.02496500
H	-7.70097900	6.48847300	0.39032500
N	-6.99080600	5.57595300	3.26670600
N	-5.97740900	5.53082000	1.12749200
C	-3.69689300	6.16051100	-0.88162500
O	-2.67150800	6.46699400	-0.13647200
O	-4.24214800	7.15020100	-1.53569400
C	-2.81115300	10.02574600	2.06769400
H	-3.31639100	9.21862900	2.61273800
H	-2.99242400	10.95239600	2.63380600
H	-1.73545400	9.82043100	2.13652700
C	-3.28571800	10.11490600	0.60667100
H	-4.35341500	10.37646600	0.59209000
H	-2.77503800	10.95457500	0.11358100
H	-1.42147800	4.48830700	-1.32173200
C	-5.82621300	1.61541600	-1.51920700
C	-5.32567200	2.86327000	-1.89402300
C	-4.04687000	3.31690000	-1.47308200
C	-3.31833100	2.43990300	-0.62663800
C	-3.81732100	1.19496000	-0.25584000
C	-5.07949600	0.75449400	-0.69837800
H	-6.80150200	1.29831000	-1.88128600
H	-5.90728300	3.48149500	-2.57297600
H	-2.33501300	2.73393500	-0.27370200
H	-3.22038700	0.54654800	0.38164600
C	-3.51130700	4.65038700	-1.93153700
C	-2.01179200	4.64968000	-2.22624300
H	-4.07702100	4.98139700	-2.80322300

H	-1.70222100	5.61001100	-2.64805500
H	-1.76749200	3.85776300	-2.94579800
C	-0.14753800	8.69384000	-1.89875700
O	-1.58159300	8.84137200	-2.05454200
C	-1.90273000	9.49381000	-3.31004900
C	-0.56746500	10.01171200	-3.84625600
C	0.43485300	8.99196300	-3.27980700
H	0.19557000	9.41287800	-1.14511100
H	0.04849300	7.67982800	-1.54260100
H	-2.35721600	8.75036700	-3.97396900
H	-2.63141800	10.28303600	-3.10560500
H	-0.55567600	10.06663800	-4.93737200
H	-0.35936700	11.01149100	-3.45079500
H	0.44710800	8.08475000	-3.89316200
H	1.45522800	9.37847600	-3.22186700
N	-5.54336800	-0.53003600	-0.38672200
H	-5.16359200	-0.91440400	0.46932800
H	-6.55114800	-0.62458000	-0.40458200

TS₂₀₋₁_OMe

scf done: -3335.77368143

Ni	-4.80831600	4.88362400	-0.34782800
Zn	-2.89423100	8.54177000	-0.24282600
C	-5.00417300	3.44402300	3.57059500
C	-5.90399200	3.53147900	2.30178700
C	-6.47763300	4.90228700	2.00863600
C	-5.24844500	4.51907900	4.64214800
C	-6.67938600	4.58808100	5.19747100
C	-7.75906000	4.60923300	4.09401300
H	-5.12145400	2.44585100	4.00852600
H	-5.32800900	3.22797700	1.42432200
H	-4.98553300	5.49685700	4.22122700
H	-6.76946500	5.48316300	5.82431100
H	-3.95826500	3.52192600	3.25468900
H	-6.73705300	2.82468400	2.38427700
H	-4.55177300	4.35422200	5.47206700
H	-6.88244100	3.72930300	5.84924200
H	-8.68933400	5.03664700	4.47811400
H	-8.00141400	3.58988100	3.78459800
C	-7.87282800	6.77511200	2.84913400
H	-7.87395700	7.18441500	3.86524600
H	-8.91347400	6.77380000	2.49712000
C	-6.99638600	7.61602600	1.93048300
H	-7.49068900	8.56821600	1.71594300
H	-6.04299800	7.84030600	2.42243400
C	-6.73039000	6.83878500	0.64335900
H	-6.06384000	7.38777600	-0.02343400
H	-7.67496500	6.67935200	0.10234000
N	-7.37972000	5.39087000	2.91156800
N	-6.11040600	5.53248900	0.91827400
C	-3.61223900	6.24968200	-0.79506900
O	-2.68245400	6.47388200	0.08631900
O	-4.06121100	7.29389800	-1.43591800
C	-2.14291300	11.28525900	0.68656800
H	-1.12570700	10.95336600	0.92930500
H	-2.34884600	12.16019500	1.32185900
H	-2.11363000	11.64768800	-0.34857100
C	-3.17172200	10.15722800	0.86873500
H	-3.18973500	9.85233900	1.92474900
H	-4.17807500	10.55096200	0.66666200
H	-1.29829000	4.64607700	-1.16603600
C	-5.67574100	1.78149900	-1.81450000
C	-5.14160000	3.04751100	-2.09754000
C	-3.89208000	3.47191700	-1.57620700
C	-3.21527500	2.55382300	-0.72493700
C	-3.73956300	1.29989500	-0.44482500
C	-4.97223700	0.90119700	-0.98952800

H	-6.62525900	1.50108400	-2.25520100
H	-5.67027000	3.69168900	-2.79476100
H	-2.25644100	2.82761100	-0.29753400
H	-3.20464200	0.60729100	0.19820300
C	-3.33636100	4.82649100	-1.92510400
C	-1.81854700	4.85485100	-2.10309700
H	-3.83746100	5.20375100	-2.81703600
H	-1.49175200	5.84166700	-2.44337500
H	-1.51061800	4.10868200	-2.84643600
C	0.14810000	8.49711100	-1.23160300
O	-1.23031800	8.78138500	-1.57974000
C	-1.31878600	9.40132700	-2.88804300
C	0.12062300	9.75869600	-3.26018000
C	0.92933800	8.67061500	-2.53340500
H	0.46513400	9.21270300	-0.46358000
H	0.18668700	7.48656400	-0.81903700
H	-1.75810200	8.67535800	-3.58122300
H	-1.98335100	10.26602800	-2.80911200
H	0.27727700	9.76177200	-4.34144600
H	0.38031100	10.74976000	-2.87352300
H	0.92331700	7.73928400	-3.10963100
H	1.96919600	8.95473800	-2.35508100
O	-5.39371400	-0.36305400	-0.65827400
C	-6.63989000	-0.81621400	-1.17805400
H	-6.77742300	-1.82608000	-0.79095300
H	-7.46752100	-0.18072600	-0.84057100
H	-6.62863600	-0.84512700	-2.27412700

TS₂₀₋₁_CF₃

scf done: -3558.37545606

Ni	-4.79144000	4.73258000	-0.24752900
Zn	-3.02430700	8.44186600	-0.44015800
C	-4.29831800	3.95870500	3.84395000
C	-5.36297200	3.76560900	2.72441700
C	-6.10591200	5.02050600	2.31723300
C	-4.51876700	5.15843900	4.78073200
C	-5.86816900	5.18937000	5.51528400
C	-7.07647400	4.95788100	4.58176700
H	-4.24188200	3.03291800	4.42827300
H	-4.88121700	3.36908900	1.82743700
H	-4.41409300	6.08080800	4.19686600
H	-5.96868900	6.15677300	6.02139100
H	-3.31963600	4.08508800	3.36863400
H	-6.10076800	3.01721800	3.03306600
H	-3.71026500	5.18019300	5.52031500
H	-5.89860500	4.42271800	6.29929000
H	-7.98675300	5.36906300	5.02619900
H	-7.25828600	3.88769800	4.45862600
C	-7.56943200	6.88109200	3.05969200
H	-7.48633600	7.44685200	3.99380300
H	-8.63983200	6.73345200	2.86189100
C	-6.90963900	7.63476800	1.91241300
H	-7.52521500	8.49429400	1.63071700
H	-5.93145900	8.01635000	2.22694300
C	-6.72636600	6.68700400	0.72904500
H	-6.20372200	7.17763400	-0.09371900
H	-7.70902400	6.36791800	0.35137600
N	-6.92689100	5.57308100	3.25735400
N	-5.94799900	5.49550800	1.10447400
C	-3.68247400	6.11682600	-0.89743000
O	-2.67958300	6.39667100	-0.12663300
O	-4.25045100	7.10636100	-1.51338300
C	-2.94588300	9.89273400	2.17665900
H	-3.53929900	9.10285900	2.65385200
H	-3.12349600	10.81407000	2.75191100
H	-1.89285200	9.62456100	2.32770200
C	-3.29030600	10.04715800	0.68519400

H	-4.33757300	10.36684100	0.58903300
H	-2.69567100	10.86882800	0.26138900
H	-1.38335400	4.51000700	-1.36770200
C	-5.86917700	1.72903000	-1.41796900
C	-5.33934800	2.94529200	-1.85325300
C	-4.00939200	3.34127500	-1.51233100
C	-3.25901800	2.44567900	-0.69185400
C	-3.79024000	1.23632900	-0.26996600
C	-5.09974800	0.86687000	-0.63037200
H	-6.87731100	1.45135000	-1.70648600
H	-5.92155600	3.56518800	-2.52847900
H	-2.24566000	2.70500900	-0.40686200
H	-3.19003300	0.57246900	0.34494200
C	-3.46943900	4.64515000	-1.99220500
C	-1.96920100	4.67013100	-2.27473300
H	-4.04435700	4.99469900	-2.84912800
H	-1.67537200	5.64014700	-2.68451100
H	-1.70952200	3.89037200	-3.00138300
C	-0.17589100	8.65665300	-1.85853900
O	-1.61433300	8.76297300	-2.01705200
C	-1.95100700	9.41174700	-3.27224600
C	-0.62685800	9.95399500	-3.81175500
C	0.39732900	8.95813500	-3.24198400
H	0.14683300	9.39220200	-1.11195400
H	0.04612300	7.65168000	-1.49243400
H	-2.39392500	8.65976200	-3.93384500
H	-2.69310400	10.18762900	-3.06528100
H	-0.61768200	10.00369900	-4.90308500
H	-0.43874100	10.95973400	-3.42163100
H	0.42726800	8.04776500	-3.85002100
H	1.40943500	9.36618000	-3.18809800
C	-5.63210400	-0.45933000	-0.19757800
F	-5.09001700	-1.50480700	-0.89387500
F	-5.36710000	-0.73175300	1.10980000
F	-6.97216600	-0.57103900	-0.34934600

TS₂₀₋₁_CN

scf done: -3313.47225538

Ni	-4.89140300	4.55523000	-0.29255400
Zn	-3.15417100	8.25122200	-0.18700300
C	-3.96983900	4.34615600	3.84396800
C	-5.03915900	3.85876600	2.81947200
C	-6.02195000	4.91529000	2.35920000
C	-4.33819600	5.59689900	4.65846300
C	-5.62436800	5.48977100	5.49199300
C	-6.82031100	4.93535100	4.69013000
H	-3.73718400	3.51554800	4.52044900
H	-4.54109000	3.47926500	1.92393000
H	-4.43133000	6.44640600	3.97129300
H	-5.86939100	6.48187300	5.88939600
H	-3.04784500	4.56723800	3.29611900
H	-5.60671300	3.02021200	3.23754800
H	-3.50218600	5.84172900	5.32358000
H	-5.46929300	4.83558700	6.35884000
H	-7.76373800	5.21881700	5.16420600
H	-6.80006700	3.84282200	4.68953300
C	-7.76339400	6.54718200	3.01813700
H	-7.77802800	7.19921400	3.89739900
H	-8.78699900	6.17781000	2.86759800
C	-7.28088600	7.30801400	1.79025300
H	-8.04348000	8.02586400	1.47406900
H	-6.37343700	7.87268200	2.03345500
C	-6.97602900	6.31573300	0.67060900
H	-6.54064200	6.82455000	-0.19210900
H	-7.90403000	5.83061900	0.33549500
N	-6.87079500	5.41442500	3.30355200
N	-6.01869200	5.28295900	1.10020700

C	-3.72772000	5.94465400	-0.82451400
O	-2.76275700	6.17953400	0.00175700
O	-4.27867300	6.96530100	-1.40600900
C	-2.48736200	10.95021000	0.89113400
H	-1.46898400	10.62923800	1.14289500
H	-2.72767800	11.78995300	1.56044300
H	-2.44392300	11.35999000	-0.12554400
C	-3.49503900	9.79428200	0.99984900
H	-3.52669200	9.43729400	2.03882600
H	-4.50598500	10.17477900	0.79620800
H	-1.54415500	4.09254300	-1.07543200
C	-6.29686400	1.95134500	-2.05207400
C	-5.56315400	3.11171900	-2.26256100
C	-4.24999300	3.27689900	-1.71658800
C	-3.73734900	2.19908800	-0.92989600
C	-4.47076600	1.03930400	-0.72718700
C	-5.75691800	0.89389100	-1.29081100
H	-7.28529200	1.84908600	-2.48873000
H	-5.96785800	3.88814100	-2.90506200
H	-2.74148000	2.27175500	-0.50740400
H	-4.05183200	0.23104200	-0.13601600
C	-3.48076800	4.52596400	-1.97958100
C	-1.96473900	4.37264200	-2.04337200
H	-3.87911000	5.01813000	-2.86541900
H	-1.49876300	5.31708200	-2.33582500
H	-1.69068700	3.60580200	-2.77838100
C	-0.16549800	8.48221600	-1.27681600
O	-1.57566900	8.65229400	-1.57451600
C	-1.76008400	9.39697300	-2.80739900
C	-0.37584700	9.94453300	-3.15531200
C	0.56078600	8.87882300	-2.56171600
H	0.09224100	9.14047000	-0.43880000
H	-0.00910900	7.44290700	-0.97957000
H	-2.13676300	8.70604700	-3.56935400
H	-2.50988600	10.17208200	-2.62663000
H	-0.24618900	10.07924800	-4.23172500
H	-0.21267000	10.91128900	-2.66750800
H	0.64027100	8.01956300	-3.23593600
H	1.56822000	9.25342900	-2.36569000
C	-6.50315400	-0.30376400	-1.08677300
N	-7.11300400	-1.28417900	-0.91974100

1_COD

scf done: -670.01848374

Ni	-2.60038400	7.06921900	1.88322100
C	-1.41593500	8.41818500	2.31427400
O	-1.12414300	9.22813400	3.16349400
O	-1.02737500	8.03995200	1.17541000
C	-3.41471200	6.31185200	3.63732800
C	-4.34554900	7.14856100	3.04561200
H	-2.77856100	6.75057400	4.40438500
H	-4.34748700	8.18496300	3.37850700
C	-3.33040000	4.80411200	3.53073700
H	-2.29281000	4.51739900	3.73498300
H	-3.92994500	4.34570200	4.33048000
C	-5.53974500	6.71519400	2.20985200
H	-6.33950600	7.45005500	2.34251000
H	-5.93170800	5.76926300	2.59094800
C	-3.76068600	4.20534900	2.16461500
H	-3.37060300	3.18448900	2.10508300
H	-4.84794200	4.12040500	2.11319400
C	-5.24163300	6.60177300	0.69030400
H	-6.04510100	6.02757100	0.20817800
H	-5.28227300	7.60193100	0.24610000
C	-3.24641400	4.99230300	0.97841500
H	-2.29693600	4.66610000	0.55584800
C	-3.89529900	6.00284300	0.33978600

H	-3.43614900	6.38849500	-0.56977800
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1_bipyridine

scf done: -853.39227243

Ni	-2.78129300	6.95303600	1.52856200
C	-2.45702700	5.32977600	-0.84113700
C	-2.77905200	4.29536900	-1.71563600
C	-3.86060100	3.47197800	-1.40863600
C	-4.58427400	3.70721900	-0.24091800
C	-4.21116200	4.76114400	0.59449200
N	-3.15399600	5.55827100	0.28533500
H	-4.14027900	2.65615100	-2.06678100
H	-1.62696400	6.00069900	-1.02904400
H	-2.18998400	4.14711400	-2.61323000
H	-5.42701400	3.07565800	0.01187700
C	-4.90028800	5.10988200	1.85903200
C	-6.00651400	4.42626800	2.36865000
N	-4.36717000	6.17133300	2.51002800
C	-6.56684100	4.85009500	3.57297500
H	-6.42780200	3.57909500	1.84156400
C	-4.90833500	6.57522800	3.66692700
C	-6.01126400	5.94240100	4.23701200
H	-7.42630200	4.33129700	3.98455300
H	-4.43794300	7.43027300	4.14188100
H	-6.41812100	6.30185800	5.17519600
C	-1.37635400	8.02636500	1.12299500
O	-1.83398300	8.48364300	2.23217100
O	-0.46010200	8.32827900	0.37701100

1_pyridine

scf done: -854.58380671

Ni	-2.68634600	7.12291600	1.79881200
C	-4.90343800	7.85333700	3.58366300
C	-5.93652700	7.73076600	4.50798000
C	-6.38550600	6.45490100	4.84943600
C	-5.78185500	5.34930300	4.25027600
C	-4.75723700	5.56034400	3.33210300
N	-4.31930800	6.78947400	2.99726600
H	-7.18768000	6.32481900	5.56895600
H	-4.51469000	8.82618700	3.30001800
H	-6.37285700	8.62027000	4.94872800
H	-6.09395700	4.33800100	4.48664900
H	-4.26428900	4.72676900	2.84212300
C	-1.92200000	5.12607300	-0.09487000
C	-2.07430900	4.18458000	-1.10710500
C	-3.34744800	3.94198000	-1.62215400
C	-4.42634700	4.65389900	-1.09831400
C	-4.19707500	5.57237100	-0.07967800
N	-2.96605100	5.81058100	0.42211400
H	-3.49531000	3.21719800	-2.41623000
H	-0.94839900	5.36078600	0.31722000
H	-1.20280900	3.66083400	-1.48349500
H	-5.43495200	4.50595700	-1.46774900
H	-5.00909700	6.14053600	0.35924400
C	-1.14604300	8.03897100	1.49460000
O	-1.63557000	8.57674300	2.54997100
O	-0.14391400	8.21437700	0.82132600

1_Cs2CO3

scf done: -894.3061371

Ni	-2.06271300	-1.36073000	1.84132900
Cs	-0.02680600	3.54969500	-1.15249400
Cs	-1.29965400	1.47011800	4.64112900
C	-0.61349200	0.96948100	1.20001700
O	0.12308500	1.94954900	1.58197000
O	-1.24653700	0.96356300	0.09283300
O	-0.70442200	-0.06660500	2.03020200

C	-3.39562600	-1.11123400	3.02331900
O	-3.87291000	-0.45104200	3.94590700
O	-3.77399200	-2.17645300	2.41670900
C	0.31006000	-2.59498100	0.22226700
O	-1.13207200	-2.58495900	0.39147100
C	-1.79268100	-2.87692100	-0.87034400
C	-0.68976800	-2.83808000	-1.92954000
C	0.55011300	-3.26759400	-1.12864800
H	0.66311600	-1.55972000	0.24343400
H	0.73949100	-3.13642300	1.06924300
H	-2.25104600	-3.86960200	-0.79092000
H	-2.57621200	-2.13146900	-1.02482800
H	-0.90732600	-3.49582100	-2.77493400
H	-0.56342800	-1.81910200	-2.31006500
H	0.57616700	-4.35718300	-1.01784700
H	1.49000400	-2.94831800	-1.58641000

1_KHMDs

scf done: -2063.7971781

Ni	-2.41924100	0.34574100	-0.48898200
N	-4.23142500	0.45421400	0.18141600
Si	-4.51697600	-0.65535900	1.48548300
Si	-4.89236800	2.05005200	0.00431900
C	-4.12080900	0.01191200	3.22411400
H	-4.22101600	-0.77911800	3.97767000
H	-3.09837600	0.40133400	3.27778600
H	-4.79618000	0.82622800	3.50846800
C	-3.49209500	-2.24449300	1.26981500
H	-3.72481300	-2.76749900	0.33449500
H	-2.41651000	-2.03700400	1.26607200
H	-3.69718100	-2.93962200	2.09387300
C	-6.33697700	-1.23179100	1.56483700
H	-6.66571800	-1.71682000	0.63639100
H	-6.46289400	-1.96561800	2.37072500
H	-7.02633400	-0.40454600	1.76429200
C	-4.53255600	3.23292500	1.45169200
H	-4.87776600	4.24889400	1.22310300
H	-5.03340700	2.91347200	2.37226300
H	-3.45870900	3.27934400	1.66239900
C	-4.22048400	2.89841200	-1.56226000
H	-3.13489200	3.03801400	-1.51521300
H	-4.43234200	2.32578900	-2.47295400
H	-4.68030400	3.88768800	-1.68225100
C	-6.79197500	2.03750200	-0.20261200
H	-7.11309000	1.47348800	-1.08829000
H	-7.30410700	1.60659400	0.66410800
H	-7.16170000	3.06308100	-0.32649200
K	-5.30458300	-0.97530800	-2.10751600
C	-2.23908900	-0.51087300	-2.06768500
O	-2.78203000	-1.11206500	-2.99949300
O	-1.03005000	-0.19432100	-1.82003800
C	-0.55050400	2.57558400	0.60430900
O	-1.24870700	1.39064600	1.04089600
C	-0.28393700	0.61522600	1.78615800
C	0.57733900	1.64574400	2.54386400
C	0.30157500	2.98752400	1.81039200
H	0.07061700	2.32804000	-0.26744000
H	-1.30272000	3.30975300	0.31140600
H	-0.84326700	-0.06258400	2.43295000
H	0.31856600	0.02502800	1.08348200
H	0.28348400	1.70840300	3.59433300
H	1.63353700	1.36732100	2.51004500
H	-0.25893200	3.67048500	2.45428100
H	1.21852600	3.49456700	1.50013400

TS₂₋₅_COD

scf done: -1207.59603396

Ni	-3.13963400	7.23257800	1.31263800
C	-2.04453800	8.23490100	-3.51880700
C	-1.73153300	7.68498700	-2.28130200
C	-1.94048800	8.40164300	-1.08437700
C	-2.47173300	9.70553600	-1.17795300
C	-2.78348900	10.25774000	-2.41353800
C	-2.57792800	9.53064900	-3.59734500
H	-1.87091400	7.66673800	-4.42524300
H	-1.30310200	6.68719100	-2.23657400
H	-2.65976400	10.27377900	-0.27392200
H	-3.19310800	11.26030000	-2.47610100
C	-1.60423000	7.75938900	0.19970200
C	-1.30779700	8.47861300	1.42721100
H	-1.06776400	6.81803900	0.08390900
H	-0.63578000	7.97283100	2.11452600
H	-1.04407300	9.52896200	1.30046700
C	-2.93248600	10.16467100	-4.89359600
O	-3.38911800	11.28777200	-5.01307800
O	-2.69824700	9.36075600	-5.94967100
C	-3.01410200	9.89233600	-7.25154800
H	-2.75225700	9.10446700	-7.95600800
H	-4.07851100	10.12773700	-7.31833400
H	-2.42749500	10.79242000	-7.44741400
C	-4.52706700	6.22563800	0.01325400
C	-3.45396600	5.39436400	0.26318600
H	-4.45672600	6.85306900	-0.87309500
H	-2.66082900	5.38855300	-0.47920600
C	-5.89877900	6.13341600	0.65979300
H	-6.64237500	6.47057900	-0.06862300
H	-6.13106300	5.08635900	0.86894500
C	-3.34807800	4.29611200	1.29612500
H	-2.28402300	4.15270100	1.51530700
H	-3.69335700	3.34765700	0.85968600
C	-6.06063500	6.98674900	1.94294600
H	-6.26742400	8.02283300	1.65757800
H	-6.94516200	6.64377300	2.49786800
C	-4.10665600	4.56371700	2.61716400
H	-5.16132000	4.30157900	2.50882600
H	-3.70339800	3.89613500	3.38508200
C	-4.85562200	7.00573700	2.85260200
H	-4.73079900	7.91815400	3.42812700
C	-3.98377900	5.99131100	3.10911800
H	-3.19757900	6.19018100	3.83547400
C	-2.72423200	9.12919100	2.52880100
O	-3.60041400	9.68897600	1.87183600
O	-2.36708700	9.08288700	3.69336500

TS₂₋₅_bipyridine

scf done: -1390.9724716

Ni	-3.40472200	7.04083800	2.14836600
C	-6.05375400	10.79053700	2.25504600
C	-4.92304600	9.99475400	2.13130600
C	-4.24043000	9.50680500	3.26861700
C	-4.74686800	9.86999000	4.53547500
C	-5.87850900	10.66523800	4.66410800
C	-6.54936900	11.13492900	3.52539600
H	-6.55913200	11.15134200	1.36649100
H	-4.56511700	9.74297500	1.13808500
H	-4.22675200	9.53504300	5.42915500
H	-6.24970600	10.93801300	5.64632400
C	-3.04683200	8.64452200	3.18438900
C	-2.10961800	8.71082900	2.06135700
H	-2.59098700	8.43484200	4.15290800
H	-2.41242500	9.26267000	1.17366300
H	-1.09592100	8.99010100	2.35037200
O	-0.91223500	7.19831600	0.36113300
C	-1.25740100	7.09571000	1.53336700

O	-0.92985500	6.39726800	2.49317200
C	-7.75145200	11.98379700	3.70833900
O	-8.21721800	12.30436000	4.78874000
O	-8.29752200	12.37901500	2.54006700
C	-9.47040000	13.21166100	2.62237700
H	-9.74975900	13.41955000	1.59066200
H	-10.27623700	12.68528700	3.13869200
H	-9.24242400	14.13940600	3.15167400
C	-3.41950600	5.72020100	-0.58869900
C	-3.96466000	4.90026600	-1.57519600
C	-5.06888100	4.11363400	-1.25871500
C	-5.59267700	4.17360700	0.03103900
C	-4.99533200	5.01609000	0.97103700
N	-3.91734100	5.77851700	0.65758700
H	-5.52220700	3.46554500	-2.00145300
H	-2.55317400	6.34338400	-0.77716300
H	-3.52453300	4.88718000	-2.56571500
H	-6.46042900	3.58074200	0.29225400
C	-5.47842900	5.16616600	2.35973600
C	-6.46435400	4.35911800	2.93225400
N	-4.87659100	6.15434200	3.07083600
C	-6.83568000	4.56933000	4.25785800
H	-6.92783400	3.56721800	2.35755100
C	-5.23591900	6.34929300	4.35046900
C	-6.20922100	5.58107900	4.98222100
H	-7.59775600	3.94791500	4.71604100
H	-4.73147400	7.15073400	4.87342800
H	-6.46209000	5.77925700	6.01731900

TS₂₋₅_pyridine

scf done: -1392.16383741

Ni	-3.35037500	7.00525300	1.92190600
C	-6.06697100	10.70321900	2.46262100
C	-4.90808700	9.99338700	2.17426500
C	-4.14997100	9.37755900	3.19507600
C	-4.61636900	9.51501900	4.52130300
C	-5.77386700	10.22185900	4.81391900
C	-6.51757700	10.82738900	3.78794500
H	-6.62743100	11.16903200	1.65997200
H	-4.58442000	9.92080000	1.14105100
H	-4.04897600	9.05998600	5.32861600
H	-6.11283300	10.32028400	5.83985100
C	-2.92841800	8.59401500	2.93848100
C	-2.12215600	8.75269600	1.72389100
H	-2.37063800	8.35077400	3.84397000
H	-2.53954600	9.35125700	0.91763800
H	-1.09163100	9.04933000	1.92277500
O	-1.22027600	7.44501700	-0.28261000
C	-1.33649000	7.23534500	0.91860100
O	-0.81505600	6.46935200	1.73429100
C	-7.74400400	11.57754300	4.14545700
O	-8.17448800	11.70739200	5.27941000
O	-8.36052300	12.11883100	3.07348000
C	-9.56087400	12.87277400	3.32920500
H	-9.89784500	13.21909300	2.35332500
H	-10.31920500	12.23793300	3.79290100
H	-9.34637200	13.72125600	3.98276300
C	-3.57743500	4.35520400	0.63579900
C	-3.85374800	3.41274800	-0.35002000
C	-4.30496300	3.85323800	-1.59420300
C	-4.45757300	5.22336300	-1.80473900
C	-4.15116500	6.10016100	-0.76836500
N	-3.72267000	5.67891600	0.43678400
H	-4.53017900	3.14365000	-2.38399800
H	-3.22545600	4.05341500	1.61633100
H	-3.71411700	2.35816100	-0.14010900
H	-4.80134100	5.61482900	-2.75567100

H	-4.23667500	7.17313100	-0.89864200
C	-4.29093900	5.52976800	4.20713800
C	-5.19827000	4.92288200	5.06994400
C	-6.56308500	5.04621100	4.81054300
C	-6.96902000	5.77480100	3.69268500
C	-6.00109600	6.34961200	2.87532400
N	-4.68203000	6.22988500	3.12276800
H	-7.29494800	4.58636200	5.46673900
H	-3.22194300	5.46336800	4.37642600
H	-4.83292900	4.36904600	5.92744800
H	-8.01833400	5.90139500	3.45079900
H	-6.27517100	6.92681800	1.99947400

TS₂₋₅_Cs₂CO₃

scf done: -1203.94664927

Ni	-4.13414000	7.22992800	2.21448800
C	-4.67345200	11.93839500	1.72051600
C	-3.99693900	10.72150300	1.80115000
C	-3.95414200	9.99338100	3.00914800
C	-4.61780600	10.54274800	4.12559500
C	-5.29616800	11.75821300	4.04264300
C	-5.32893500	12.46573800	2.83773800
H	-4.69004200	12.47928300	0.77757100
H	-3.51265300	10.31505100	0.91856200
H	-4.59306800	10.00389700	5.06988000
H	-5.79557400	12.15662100	4.92209500
C	-3.27082500	8.69237000	3.13773500
C	-2.21779000	8.24031700	2.23762400
H	-3.19257900	8.33725700	4.16742500
H	-1.73764400	9.01017600	1.63282000
H	-1.49300300	7.56037700	2.67685300
O	-3.27821000	8.05287300	-0.20184200
C	-2.63629800	7.35790800	0.60245200
O	-1.84891700	6.41665500	0.43564500
Cs	-1.16382100	3.38482200	1.07035000
Cs	-4.81623100	5.77075200	-1.90019000
C	-4.35128100	4.49272900	1.42123200
O	-4.43719600	3.63156000	0.47106100
O	-3.80383400	4.22707500	2.54647500
O	-4.82944200	5.70643900	1.19184400
H	-5.85354100	13.41458400	2.77087000
C	-5.72455000	6.23942500	4.49478900
O	-5.75463700	7.20337800	3.39944600
C	-7.06150300	7.18171400	2.74918600
C	-7.86587500	6.09400100	3.46760300
C	-7.19165500	6.01960900	4.84749100
H	-5.23305400	5.32975900	4.13426000
H	-5.13392200	6.68975600	5.29676000
H	-7.49690100	8.17861700	2.87644200
H	-6.90630300	6.96996900	1.69080100
H	-8.92978900	6.33912800	3.52101200
H	-7.75843600	5.13892800	2.94396000
H	-7.55722200	6.81917500	5.50131800
H	-7.35271900	5.06275700	5.35087300

TS₂₋₅_KHMDs

scf done: -2373.42334161

Ni	-3.85616400	7.45021100	1.62371200
C	-4.11485200	12.21523300	2.38052500
C	-3.59955500	10.93112600	2.20844800
C	-3.71398200	9.96358400	3.22918700
C	-4.36285500	10.34198100	4.42206400
C	-4.87811200	11.62755900	4.59163200
C	-4.75792300	12.57294600	3.57023900
H	-4.01594600	12.94264100	1.57887900
H	-3.12371400	10.65760200	1.27139200
H	-4.45202000	9.61692300	5.22794700

H	-5.36886600	11.89200900	5.52453600
C	-3.18037600	8.59363600	3.08937400
C	-1.98933600	8.29213100	2.33256600
H	-3.35338100	7.96251200	3.96271600
H	-1.37124500	9.14078300	2.04162500
H	-1.39886100	7.44516700	2.66778600
O	-2.61393400	8.86316500	-0.23249300
C	-2.11949200	7.94240000	0.44584100
O	-1.26089000	7.09826700	0.15242400
N	-4.29548200	6.05037500	0.19814700
Si	-5.74697700	6.30337400	-0.69737200
Si	-3.59516700	4.49856100	0.49520200
K	-2.50940700	6.92235200	-2.24804100
C	-6.06044600	8.15187600	-1.02756400
H	-5.20662500	8.63040500	-1.51932700
H	-6.93805200	8.27860000	-1.67400700
H	-6.24436200	8.71090000	-0.10493700
C	-7.36095800	5.60474000	0.04615900
H	-7.35454200	4.50972700	0.06284300
H	-7.52299800	5.94803500	1.07168500
H	-8.22484300	5.91909500	-0.55336200
C	-5.69610500	5.49535100	-2.44209400
H	-5.40656300	4.43892600	-2.40238700
H	-6.69299800	5.54137200	-2.89848100
H	-5.01742000	5.99442400	-3.14705000
C	-2.56462700	4.44076000	2.09212200
H	-2.13478900	3.44026400	2.23027100
H	-1.74077400	5.15953800	2.05138300
H	-3.17178400	4.66397000	2.97697600
C	-4.86206900	3.07504500	0.65550800
H	-5.57888600	3.25441600	1.46497900
H	-5.43943800	2.92231800	-0.26359100
H	-4.34458300	2.13281400	0.87600600
C	-2.41139600	3.90833300	-0.89296100
H	-2.06696100	2.88608800	-0.69227000
H	-2.90181700	3.88904500	-1.87544100
H	-1.51672100	4.53914500	-0.95369400
H	-5.15641100	13.57507800	3.69945200
C	-5.85136700	6.20537800	3.56517500
O	-5.67872800	7.24604900	2.56882900
C	-6.70814700	8.26561700	2.70949100
C	-7.38286200	7.97444800	4.04840800
C	-7.23441600	6.44914500	4.16880700
H	-5.74861100	5.24207800	3.06215900
H	-5.05667700	6.30544200	4.31448200
H	-6.22852100	9.24357600	2.66074700
H	-7.40439600	8.15777500	1.87093200
H	-6.84898500	8.47912700	4.86031100
H	-8.42366300	8.30743500	4.06333400
H	-7.30069400	6.08940800	5.19857200
H	-8.00457300	5.94129600	3.57884800

5_COD

scf done: -1207.64305564

Ni	-4.08330200	7.11856000	2.59782400
C	-6.09789200	11.22329300	3.36743900
C	-5.04294700	10.35580600	3.10815700
C	-4.57731700	9.45159500	4.08756000
C	-5.21993600	9.47230600	5.34489100
C	-6.27719000	10.33406100	5.60853100
C	-6.73236800	11.21972900	4.62041200
H	-6.43465800	11.90728600	2.59689200
H	-4.58187000	10.37569400	2.12703900
H	-4.86487900	8.81276800	6.13282900
H	-6.75365200	10.33844400	6.58320900
C	-3.44479600	8.51347500	3.84373000
C	-2.22175800	9.10824200	3.13300200

H	-3.16405800	8.01169200	4.77255800
H	-1.99703500	10.13246900	3.45323900
H	-1.33401900	8.50541000	3.36115200
O	-1.76109300	9.74694600	0.83402300
C	-2.40584100	9.05693700	1.62058800
O	-3.30301900	8.18399600	1.24593100
C	-7.86532900	12.12364200	4.94209800
O	-8.45278100	12.14449600	6.01002100
O	-8.19273000	12.93729800	3.91907000
C	-9.28529300	13.85064800	4.14000600
H	-9.38442600	14.41138700	3.21196500
H	-10.20391400	13.30029000	4.35500600
H	-9.05818500	14.52187500	4.97100400
C	-5.35471500	5.82362500	1.06531300
C	-4.06733200	5.38583300	1.06997000
H	-5.59772700	6.63160600	0.37722100
H	-3.38856200	5.85989400	0.36632300
C	-6.50823000	5.23161300	1.84459300
H	-7.42604100	5.35234600	1.26105000
H	-6.36598800	4.15670000	1.97320200
C	-3.47233400	4.26386900	1.88990000
H	-2.39184800	4.43254500	1.94330500
H	-3.60079100	3.30654700	1.36627800
C	-6.71134800	5.92118000	3.21387800
H	-7.22429800	6.87725500	3.06114300
H	-7.38588500	5.31777900	3.83833900
C	-4.03476800	4.14209200	3.32705500
H	-4.95953000	3.56055300	3.32604600
H	-3.31851800	3.57411900	3.92811700
C	-5.44466100	6.20727700	3.98842600
H	-5.54910300	6.99097400	4.73221700
C	-4.27883500	5.47494800	4.01635600
H	-3.53923000	5.76207800	4.76017500

5_bipyridine

scf done: -1391.02541535

Ni	-3.98024200	7.13101500	2.46871000
C	-5.81964400	11.27211000	3.30545700
C	-4.73272700	10.41473400	3.19985200
C	-4.59009000	9.29138500	4.04831300
C	-5.59716300	9.09898600	5.02221300
C	-6.68852900	9.95024700	5.13067000
C	-6.81910100	11.05082900	4.26660200
H	-5.90604400	12.12749900	2.64337100
H	-3.98270200	10.62169300	2.44418600
H	-5.51215900	8.26934400	5.71741700
H	-7.43883100	9.77264900	5.89300700
C	-3.44901000	8.34221900	3.93321500
C	-2.11110100	8.94209500	3.48224100
H	-3.32826900	7.77888000	4.86135400
H	-1.91487200	9.94280000	3.88798200
H	-1.28890400	8.30203100	3.82607000
O	-1.19847300	9.65869100	1.34670400
C	-2.01965400	8.97646700	1.96113700
O	-2.88371100	8.19411400	1.37393700
C	-7.96179100	11.98887900	4.33699400
O	-8.11056500	12.96300900	3.61775200
O	-8.85521700	11.65971100	5.29602600
C	-10.00140200	12.52017500	5.43376700
H	-10.58279500	12.53339300	4.50905200
H	-10.58758600	12.09333000	6.24631800
H	-9.68863200	13.53696900	5.68144200
C	-4.43893200	6.43058400	-0.38977000
C	-5.07737500	5.76577400	-1.43504000
C	-6.00709400	4.77383700	-1.12786200
C	-6.26692400	4.47061400	0.20794900
C	-5.58514800	5.17343200	1.20349700

N	-4.69072200	6.13851300	0.89332200
H	-6.52686400	4.23963000	-1.91631700
H	-3.70985700	7.21642600	-0.55162300
H	-4.84770100	6.02726400	-2.46157000
H	-6.98870000	3.70399000	0.46130400
C	-5.73358200	4.94265900	2.65425100
C	-6.51400200	3.92017800	3.19668600
N	-5.01177800	5.78366300	3.44772300
C	-6.54384000	3.73655500	4.57636900
H	-7.08286900	3.26566400	2.54839800
C	-5.03078100	5.58234200	4.77594300
C	-5.77864600	4.57660100	5.38077700
H	-7.14468000	2.94436300	5.01005500
H	-4.42200600	6.24808200	5.37122900
H	-5.75273800	4.46479300	6.45840300

5_pyridine

scf done: -1392.21794075

Ni	-3.77842200	7.09768600	2.50577000
C	-5.96346100	11.14622400	3.31945600
C	-4.81914600	10.38423200	3.12380600
C	-4.47441900	9.33137000	4.00306500
C	-5.33981600	9.10202300	5.09742800
C	-6.48498000	9.86018300	5.29856000
C	-6.81701100	10.89493600	4.40642400
H	-6.20803800	11.95050000	2.63317400
H	-4.18050700	10.61040300	2.27597300
H	-5.09141100	8.31816600	5.80770400
H	-7.12217700	9.66364300	6.15358500
C	-3.26591200	8.48992000	3.80997500
C	-2.04599300	9.18304200	3.19014200
H	-3.00882600	7.98335200	4.74394800
H	-1.94409100	10.23695900	3.47822000
H	-1.12982200	8.68177700	3.52733200
O	-1.37780500	9.77916900	0.93217300
C	-2.05926100	9.06302600	1.66948100
O	-2.83539200	8.11346400	1.22893700
C	-6.04392900	5.93386500	3.81967500
C	-6.74855400	5.15593000	4.73230500
C	-6.04231200	4.45272500	5.70820700
C	-4.65161500	4.55711500	5.73495900
C	-4.01837800	5.36036000	4.79189300
N	-4.69991700	6.03724500	3.84535700
H	-6.56466400	3.83722200	6.43337200
H	-6.55397600	6.49229600	3.04317700
H	-7.82995900	5.10879100	4.67226100
H	-4.05840200	4.03060700	6.47398500
H	-2.94063300	5.47744300	4.78335300
C	-4.66433700	6.30177800	-0.17183200
C	-5.00243200	5.49764100	-1.25655900
C	-4.93774700	4.11193000	-1.11556900
C	-4.53833100	3.58192600	0.11131500
C	-4.22838900	4.45471100	1.14982200
N	-4.28905700	5.79310900	1.01806100
H	-5.18984100	3.45846900	-1.94476200
H	-4.66908600	7.38279000	-0.24255000
H	-5.30386500	5.95733800	-2.19119100
H	-4.46561200	2.51146900	0.26850500
H	-3.92090200	4.07898200	2.11963500
C	-8.02270200	11.73539800	4.57662900
O	-8.34735900	12.65069900	3.83788100
O	-8.75823500	11.38852500	5.65664700
C	-9.94792000	12.16087400	5.90353300
H	-10.63884100	12.07974400	5.06133400
H	-10.39012100	11.73189300	6.80161800
H	-9.69502300	13.21090600	6.06682500

5_Cs2CO3 scf done: -1203.99790817

Ni	-4.33927200	7.11628900	2.22844200
C	-4.34635800	11.72527300	1.30319700
C	-3.67096800	10.54653000	1.62573900
C	-3.99234800	9.80381700	2.78392400
C	-5.01632600	10.32299400	3.60839000
C	-5.69203400	11.49871900	3.28660500
C	-5.36547100	12.20999600	2.12701300
H	-4.06609900	12.27328000	0.40660300
H	-2.87678900	10.20279100	0.96880900
H	-5.27390300	9.78599600	4.51771800
H	-6.46894900	11.87005700	3.95055800
C	-3.31598400	8.52674100	3.13612200
C	-1.87423500	8.35584000	2.64619600
H	-3.40806000	8.33049300	4.20832700
H	-1.29655500	9.28943100	2.59908900
H	-1.32626400	7.69588500	3.33142700
O	-2.94923100	7.11600700	0.92377100
C	-1.82976800	7.67064400	1.28393400
O	-0.80079000	7.60218200	0.59529700
Cs	-1.46447500	4.22296100	0.15094800
Cs	-5.03232700	7.07148300	-1.66080400
C	-4.76319600	4.65707400	0.91543600
O	-4.82012000	4.20043500	-0.28313500
O	-4.13378100	4.06202300	1.85411900
O	-5.36338200	5.81916200	1.16209000
H	-5.88504700	13.13105100	1.87885900
C	-5.65323100	5.89300900	4.50290900
O	-5.72820000	7.06208300	3.63247000
C	-7.11290000	7.27422900	3.20807800
C	-7.94616800	6.22176800	3.95144800
C	-7.04158100	5.80792800	5.12507900
H	-5.40695300	5.02144400	3.88803800
H	-4.84909500	6.08408700	5.21737100
H	-7.36705500	8.29994600	3.48943900
H	-7.15601400	7.15640800	2.12494600
H	-8.90999400	6.62153400	4.27675000
H	-8.13504100	5.36299400	3.30065000
H	-7.13425600	6.51390500	5.95763500
H	-7.26307800	4.80498200	5.49859300

5_KHMDs

scf done: -2373.47795694

Ni	-3.92521300	7.37817400	1.67847500
C	-3.82345500	12.11352600	1.68520900
C	-3.32879700	10.81703700	1.82570700
C	-3.71173800	9.99167300	2.90694600
C	-4.60021100	10.55470600	3.84782200
C	-5.10204100	11.85013800	3.70719200
C	-4.72014100	12.63968700	2.62047300
H	-3.50442300	12.71886400	0.84020500
H	-2.63680700	10.43770800	1.07974100
H	-4.88731100	9.96403200	4.71517400
H	-5.78281000	12.24655300	4.45642400
C	-3.19767600	8.59967900	3.07810800
C	-1.67219500	8.46630500	2.93922900
H	-3.53163400	8.20503600	4.04371500
H	-1.10886400	9.33076100	3.31458600
H	-1.32351000	7.59461400	3.50947800
O	-2.26648800	7.68900200	0.78995100
C	-1.29328300	8.19847500	1.49125500
O	-0.17167300	8.41642400	1.02070800
N	-4.47398500	6.06040900	0.19495000
Si	-5.93393200	6.39455200	-0.65259300
Si	-3.75369700	4.50032300	0.35240800
K	-2.55461100	7.25726400	-1.73983600
C	-6.22119400	8.27522700	-0.78819400

H	-5.42692700	8.77213400	-1.35982200
H	-7.16720800	8.48402200	-1.30345100
H	-6.26183600	8.76245800	0.19130100
C	-7.52477800	5.63131800	0.07523300
H	-7.53652800	4.54474200	-0.06452400
H	-7.61480200	5.82146000	1.14881700
H	-8.41881400	6.03594600	-0.41555000
C	-5.90946600	5.76632000	-2.46366000
H	-5.74175800	4.68444200	-2.51929400
H	-6.87232900	5.97261300	-2.94811100
H	-5.13744400	6.24761000	-3.07863200
C	-2.61564200	4.35696900	1.87042000
H	-2.13405600	3.37087500	1.88483300
H	-1.82740700	5.11633100	1.84660200
H	-3.16053600	4.47104000	2.81372700
C	-4.99515400	3.05550700	0.48266600
H	-5.68081300	3.18638800	1.32778700
H	-5.60740800	2.95293500	-0.42065300
H	-4.46557400	2.10585000	0.62887600
C	-2.62477100	4.03266000	-1.12949300
H	-2.33469300	2.97644000	-1.06609000
H	-3.12239500	4.17011000	-2.09781800
H	-1.68776000	4.60556800	-1.13458100
H	-5.10360100	13.64979900	2.50939800
C	-5.63713300	5.98531400	3.70429400
O	-5.60612300	7.06047100	2.72814700
C	-6.71346100	7.98332200	2.94168000
C	-7.28156300	7.61038000	4.30880000
C	-7.00075500	6.10104500	4.38396900
H	-5.48656300	5.04606900	3.16937400
H	-4.81218200	6.13692800	4.40999900
H	-6.32395600	8.99934000	2.88436700
H	-7.44253200	7.82441900	2.14078300
H	-6.74695300	8.14016500	5.10455800
H	-8.34367000	7.85413800	4.38973400
H	-6.98043900	5.71716700	5.40668300
H	-7.75713000	5.54231600	3.82304600

TS₁₁₋₁₃_COD

scf done: -3145.19327334

Ni	-3.08479500	6.52981700	1.65182000
Zn	-1.11742200	5.64848500	0.21055400
C	-3.88715200	11.19397000	3.47502500
C	-3.53143400	9.85418200	3.57400100
C	-2.54225800	9.28137000	2.74342700
C	-1.89966300	10.13790000	1.82555300
C	-2.25019900	11.47854800	1.71991700
C	-3.25266400	12.02227900	2.53658900
H	-4.64621900	11.60385300	4.13107700
H	-4.01034800	9.23932400	4.33119700
H	-1.10955900	9.75722100	1.19159200
H	-1.74505000	12.12120000	1.00671200
C	-2.19078900	7.84384500	2.90861800
C	-0.69874600	7.50559400	2.93441900
H	-2.62657900	7.49172900	3.84479800
H	-0.18890000	7.84062200	2.02512700
H	-0.21790000	8.02321700	3.77315700
O	0.21378100	5.54006200	3.99886800
C	-0.48406600	5.99493100	3.09217200
O	-1.10994800	5.26276800	2.21750400
C	-3.59257400	13.46129300	2.38735600
O	-3.07103800	14.21545600	1.58525700
O	-4.55431500	13.86117500	3.24153400
C	-4.94894400	15.24585900	3.17275700
H	-5.71804900	15.36453100	3.93424600
H	-4.09655100	15.89487700	3.38439900
H	-5.34953500	15.47833400	2.18370100

C	-0.95818900	8.11114300	-0.88190500
H	-0.19125400	8.35311800	-0.13682600
H	-1.22922500	9.05530300	-1.37085900
H	-0.46612300	7.49141400	-1.63995700
C	-2.20097300	7.40101100	-0.28179400
H	-2.81576100	8.16660000	0.20443700
H	-2.81229900	7.02547600	-1.10856500
C	-0.21453800	4.35968100	-0.98834100
H	-0.27647700	3.36839400	-0.51801600
H	0.85827500	4.59699700	-1.01389400
C	-0.75034200	4.27777500	-2.42763700
H	-0.66436000	5.23766700	-2.95195200
H	-0.21226900	3.53631500	-3.03617400
H	-1.81076600	3.99738800	-2.45562100
C	-4.57055000	5.07920700	0.08670400
C	-3.77235800	4.27653300	0.83326400
H	-4.19091400	5.37829200	-0.88665400
H	-2.84632400	3.93951500	0.36831600
C	-5.97804500	5.52351500	0.40361100
H	-6.51816200	5.66242400	-0.53799600
H	-6.51029500	4.74315200	0.95018300
C	-4.04964100	3.64642500	2.17395900
H	-3.08203900	3.48303500	2.65692100
H	-4.49266000	2.65179000	2.02400300
C	-6.01863600	6.85491600	1.18407500
H	-5.81158400	7.68213600	0.49596200
H	-7.03761700	7.02868600	1.56015800
C	-4.94428100	4.47970200	3.11450900
H	-5.99787000	4.36244000	2.85010200
H	-4.84010600	4.07486700	4.12554900
C	-5.05431300	6.96448000	2.34271800
H	-4.91457500	7.98292500	2.69031400
C	-4.57949400	5.95357600	3.15986400
H	-4.08630900	6.26316600	4.07574700

TS₁₁₋₁₃_bipyridine

scf done: -3328.56589375

Ni	-3.09061500	6.31605400	1.62832200
Zn	-1.06922000	6.22348800	-0.03335300
C	-2.91365900	10.98846200	2.17771500
C	-2.95768000	9.62609400	2.43390600
C	-1.78501200	8.83956900	2.51659000
C	-0.55816900	9.50842400	2.32537100
C	-0.50509100	10.87551900	2.06654800
C	-1.67924800	11.63508500	1.98855400
H	-3.83378200	11.55878700	2.11907200
H	-3.92504800	9.14941600	2.55649300
H	0.37620300	8.96371600	2.39676400
H	0.45220700	11.36761200	1.92969300
C	-1.88777900	7.38036600	2.81938000
C	-0.57412400	6.60969600	3.03891500
H	-2.47589000	7.25424900	3.72970000
H	0.21952300	6.94419400	2.35843600
H	-0.18956500	6.75325500	4.05480700
O	-0.40502800	4.24445000	3.55377800
C	-0.75793800	5.11439200	2.75397800
O	-1.30763900	4.87531700	1.60101300
C	-1.57413800	13.08852700	1.71412200
O	-0.52847800	13.68895600	1.53375200
O	-2.77495900	13.70348800	1.68278900
C	-2.77002200	15.11994100	1.42086600
H	-3.81647000	15.42063300	1.43858000
H	-2.20672300	15.64855600	2.19303700
H	-2.32950800	15.32509600	0.44271400
C	-2.06517300	8.64389300	-1.03465800
H	-1.54127800	9.22839400	-0.27341500
H	-2.80775100	9.30953300	-1.49530000

H	-1.33336800	8.39264000	-1.81011100
C	-2.73309200	7.38586900	-0.43836800
H	-3.56701100	7.74217900	0.18494900
H	-3.21857600	6.81298100	-1.23884400
C	0.72238200	5.85325800	-0.79149700
H	0.76088100	4.77892000	-1.02301500
H	1.45270300	5.99193200	0.01939200
C	1.17803500	6.65274300	-2.02284100
H	1.20952300	7.73074400	-1.82324700
H	2.18338000	6.36625900	-2.36675900
H	0.50314600	6.51109600	-2.87640300
C	-3.90512000	4.24279400	-0.40467900
C	-4.66120800	3.18646700	-0.90246500
C	-5.82478000	2.82672600	-0.22677500
C	-6.18299800	3.53244000	0.91749700
C	-5.37200300	4.58362400	1.35826400
N	-4.24531100	4.93307900	0.69506800
H	-6.44202100	2.00680900	-0.57832400
H	-2.99862000	4.55084700	-0.90681000
H	-4.33594900	2.66460100	-1.79484000
H	-7.07502200	3.25487300	1.46424400
C	-5.65664600	5.37750500	2.56886600
C	-6.85145000	5.25868700	3.28559100
N	-4.67970800	6.24475900	2.94650400
C	-7.05664100	6.03738300	4.41950000
H	-7.61981700	4.57067400	2.95771200
C	-4.89360200	6.99069900	4.04442600
C	-6.05480700	6.92207600	4.80769900
H	-7.97999600	5.95443500	4.98269300
H	-4.10671700	7.67614200	4.33023900
H	-6.15883200	7.55483400	5.68148500

TS_{II-13}_pyridine

scf done: -3081.45125137

Ni	-2.79674800	6.68937600	2.06577900
Zn	-1.31121000	6.65903300	-0.15291400
C	-3.48602400	10.87700200	3.85289000
C	-2.96407300	9.60177900	4.02416200
C	-2.08925000	9.02606800	3.07372300
C	-1.76167900	9.80118400	1.93674500
C	-2.28737300	11.07444400	1.75911100
C	-3.15432100	11.62897100	2.71305000
H	-4.14299900	11.29985800	4.60422600
H	-3.21779500	9.03748100	4.91696100
H	-1.08970500	9.40257400	1.18382600
H	-2.02702200	11.65730500	0.88214900
C	-1.58590400	7.64683100	3.26940600
C	-0.12848800	7.33553500	2.90190500
H	-1.80321900	7.28769100	4.27643100
H	0.21553200	7.95907300	2.06981500
H	0.51539200	7.55942100	3.75979000
O	0.75828300	5.09701100	3.14065600
C	0.05427400	5.86854100	2.48104600
O	-0.60327500	5.53793100	1.41867500
C	-3.67792900	13.00020500	2.48322700
O	-3.41161300	13.68780300	1.51339900
O	-4.49241100	13.42109800	3.47045700
C	-5.04176200	14.74702000	3.33557800
H	-5.65502800	14.89668000	4.22267700
H	-4.24039500	15.48780000	3.29392100
H	-5.65110700	14.81608700	2.43188900
C	-4.19762700	7.72623800	-0.52082700
H	-4.25451200	8.53110200	0.21855700
H	-5.22498400	7.44826300	-0.79216400
H	-3.73547500	8.15441200	-1.41778100
C	-3.38046200	6.52989900	-0.01055700
H	-3.97610000	5.98647800	0.77533500

H	-3.37860600	5.74794100	-0.78764600
C	0.10316800	7.32366200	-1.37211000
H	0.21229000	8.40872200	-1.22939700
H	-0.22341200	7.20613800	-2.41494300
C	1.47143900	6.64629700	-1.19000500
H	1.42239100	5.56962700	-1.39258900
H	2.24306800	7.06063200	-1.85600000
H	1.84650500	6.75101600	-0.16495600
C	-3.64280500	5.01821600	4.22576300
C	-4.50518600	4.49874500	5.18507100
C	-5.70537400	5.16033900	5.44495400
C	-6.00101400	6.32298800	4.73320700
C	-5.09113600	6.78321100	3.78771700
N	-3.93207100	6.14132200	3.53522800
H	-6.39640700	4.77816700	6.18917700
H	-2.69827400	4.53854700	3.99523000
H	-4.23147200	3.59346700	5.71475300
H	-6.92020200	6.87223100	4.90234400
H	-5.27753400	7.68514900	3.21599400

TS_{II-13}_C_sCO₃

scf done: -2909.05903134

Ni	-2.92290200	7.00047200	2.23598700
Zn	-1.27288000	6.49764700	0.21852800
C	-2.87573800	11.47959700	3.12604600
C	-2.72665900	10.17284700	3.58228300
C	-1.80137200	9.28436800	2.98845500
C	-1.02298000	9.78168600	1.91915200
C	-1.17633200	11.09067200	1.45954100
C	-2.10296500	11.94798400	2.05701500
H	-3.59164400	12.13966300	3.60906800
H	-3.33154300	9.81715100	4.41187500
H	-0.29106800	9.13954500	1.43832200
H	-0.56225900	11.44371900	0.63524600
C	-1.71439200	7.88130100	3.46633600
C	-0.34032200	7.19440200	3.46860100
H	-2.20946000	7.76622600	4.43157000
H	0.31967800	7.62484300	2.70729400
H	0.15710600	7.32686600	4.43650700
O	-0.02008300	4.83150700	3.90260600
C	-0.45822000	5.70363600	3.13984100
O	-1.06050400	5.45950300	2.02159100
C	-3.74878200	7.67188900	-0.97432300
H	-3.70715900	8.65388400	-0.49152500
H	-4.77868200	7.52992900	-1.33121400
H	-3.10749900	7.72416300	-1.86273000
C	-3.29452300	6.55600200	-0.01695300
H	-4.07884200	6.46591500	0.77073500
H	-3.38782900	5.58201900	-0.52652600
C	0.50183300	6.79865700	-0.60718400
H	0.93120800	5.82416700	-0.88444700
H	1.17013100	7.18362400	0.17820800
C	0.56464300	7.73923100	-1.82290800
H	0.18590200	8.74136400	-1.58481100
H	1.58601800	7.87331300	-2.21132600
H	-0.04217300	7.36687400	-2.65805800
H	-2.21576100	12.96856600	1.70284100
Cs	-8.92856400	7.93182400	2.69201700
Cs	-4.33673300	4.84529300	5.82742800
C	-5.55437900	7.07187700	3.28242600
O	-6.38030800	6.77141900	4.21633600
O	-5.90562600	7.45871100	2.12493300
O	-4.25896300	6.95056000	3.58504500

TS_{11-13_KHMSD}

scf done: -4078.53502363

Ni	-3.20158100	7.08474400	1.74359900
Zn	-1.25281700	6.79080600	-0.22989400
C	-2.53922200	11.13431800	4.31894800
C	-2.54261400	9.74125900	4.26124500
C	-1.91453000	9.04397900	3.20809600
C	-1.26258000	9.81548100	2.22218800
C	-1.26347700	11.20948200	2.27413300
C	-1.90458200	11.87871000	3.32039900
H	-3.02727100	11.63985300	5.14792200
H	-3.03149900	9.17259600	5.04759800
H	-0.74959500	9.32195700	1.40278800
H	-0.75460500	11.77507200	1.49812700
C	-1.96103800	7.55264500	3.16437800
C	-0.60124500	6.85912700	2.92805600
H	-2.40708500	7.17320200	4.08200900
H	0.00461900	7.42566000	2.21048100
H	-0.03885000	6.84116500	3.86991900
O	-0.36465000	4.45743900	3.05717700
C	-0.72707200	5.43044300	2.38445900
O	-1.24152500	5.34636500	1.20116800
C	-3.02128000	8.87009200	-1.34612200
H	-2.81452600	9.65247100	-0.60861700
H	-3.93648500	9.15977900	-1.88162900
H	-2.20344000	8.89418000	-2.07553200
C	-3.13393400	7.48962200	-0.67248400
H	-4.05497300	7.51454000	-0.05878200
H	-3.35874800	6.72910700	-1.44057800
C	0.55194900	7.11978600	-0.99618000
H	0.88407300	8.12002100	-0.67823900
H	0.48145800	7.18600600	-2.09214000
C	1.63378800	6.09103300	-0.62783800
H	1.38574200	5.08907900	-0.99943000
H	2.62419100	6.34409900	-1.03625100
H	1.75469000	5.99508500	0.45805300
H	-1.89891000	12.96392700	3.36331600
N	-4.81213500	6.63288500	2.65179500
Si	-4.82014300	5.22910400	3.70411700
Si	-5.96195700	7.94968200	2.80623600
K	-5.74854600	5.08927800	0.15605900
C	-4.00123700	3.73665600	2.85935400
H	-3.05480900	4.00052800	2.37882600
H	-3.79025200	2.96195100	3.60643200
H	-4.65209000	3.26464600	2.11015400
C	-6.59753700	4.66119900	4.10531900
H	-7.16997800	5.40012100	4.67556900
H	-7.17663500	4.41723800	3.20656200
H	-6.54564100	3.74905400	4.71264300
C	-3.96474100	5.46504000	5.38451000
H	-4.26152300	6.40262100	5.86639500
H	-4.24235700	4.64284700	6.05527800
H	-2.87382900	5.45805100	5.29833300
C	-6.26818200	8.51645300	4.59440600
H	-7.01715800	9.31757400	4.61363600
H	-6.63521200	7.70782300	5.23527900
H	-5.35353800	8.91139600	5.04808300
C	-5.45754000	9.48251600	1.81139600
H	-4.51077100	9.90808800	2.15552900
H	-5.36332300	9.26479100	0.74184500
H	-6.23204300	10.25267000	1.92119200
C	-7.66286400	7.44887900	2.09367100
H	-8.39453800	8.24084200	2.29613200
H	-7.63080600	7.33240700	1.00194200
H	-8.05344400	6.52333200	2.52721900

TS_{18-20_COD}

scf done: -3299.06424939

Ni	-5.34221500	5.73123900	2.51414100
Zn	-1.71849800	8.24765400	3.10169600
C	-3.63838500	6.73567300	2.66975100
O	-2.58588300	6.25450700	3.18927700
O	-3.66884300	7.97464700	2.35468800
C	-0.08276500	8.81671300	5.54120900
H	-0.79293200	8.27567200	6.17789500
H	0.42433000	9.55114700	6.18446800
H	0.67816900	8.08961700	5.23213000
C	-0.77624700	9.47117900	4.33415100
H	-1.49553700	10.22080700	4.69112900
H	-0.03381900	10.03294300	3.75022100
H	-4.25227300	5.83476400	1.50962400
C	-1.00423400	8.72032200	0.03715300
O	-0.78283700	7.91618500	1.22855800
C	0.38618400	7.06828900	1.07142000
C	0.69297200	7.09816700	-0.42401800
C	0.24341400	8.51428700	-0.82190300
H	-1.91219900	8.35427600	-0.45311800
H	-1.15783300	9.75667000	0.34906200
H	1.20413500	7.49091100	1.66673400
H	0.13175800	6.07879200	1.45748400
H	1.74861700	6.90844900	-0.63140900
H	0.09832000	6.34423100	-0.95043400
H	1.01345500	9.24722500	-0.55958600
H	0.02710900	8.61305900	-1.88815300
C	-4.83418600	3.42657800	5.11719900
C	-4.24805700	4.38605800	5.84197300
H	-4.18627000	2.64191400	4.72464600
H	-3.16635100	4.33323200	5.95895900
C	-6.28664100	3.23991100	4.75535400
H	-6.31130200	2.79816300	3.75561700
H	-6.71789800	2.46955800	5.41382100
C	-4.91645700	5.57031800	6.49210600
H	-4.30979200	5.89061400	7.34729400
H	-5.88911400	5.29407300	6.90631800
C	-7.25475700	4.44323200	4.76398500
H	-8.19410400	4.07435000	4.33947900
H	-7.49719700	4.72144700	5.79561100
C	-5.07145400	6.79298400	5.56638200
H	-5.50752500	7.61006000	6.16144100
H	-4.07882500	7.14556800	5.26938800
C	-6.89008600	5.71382300	3.99974800
H	-7.67512700	6.05673000	3.32930100
C	-5.94932300	6.67311600	4.33465500
H	-6.07673700	7.63505200	3.83641300
C	-8.63061300	1.70076800	1.60526900
C	-8.23222600	3.02322800	1.46065400
C	-6.88222100	3.36863300	1.23537500
C	-5.94416000	2.31480600	1.15761100
C	-6.33891000	0.99202600	1.29687100
C	-7.68622800	0.66377400	1.52392800
H	-9.67496700	1.46512500	1.77531100
H	-8.97654900	3.81318700	1.51523600
H	-4.89427400	2.53287600	0.99077400
H	-5.60711500	0.19367000	1.23179100
C	-6.52705500	4.78257000	1.05692600
C	-5.29993100	5.22889200	0.49605500
H	-7.37735000	5.45485600	0.96898500
H	-5.31651200	6.14509800	-0.09088700
H	-4.57745600	4.49688700	0.14113700
C	-8.05798900	-0.76357200	1.66104500
O	-7.27516900	-1.69655400	1.59270100
O	-9.37888400	-0.94376900	1.87329700
C	-9.83211700	-2.30321300	2.01706300

H	-10.90791500	-2.23423100	2.17111400
H	-9.61104300	-2.87684900	1.11419900
H	-9.35248700	-2.77657100	2.87671800

TS₁₈₋₂₀_bipyridine

scf done: -3482.43626991

Ni	-3.63548500	4.78753700	2.41511000
Zn	-2.56780300	8.99514000	1.77908500
C	-3.05485100	6.58599100	2.14567600
O	-2.48256300	7.30334800	3.03898700
O	-3.31804700	7.14904300	1.02239700
C	-2.12694200	11.94266300	1.65346800
H	-1.34495200	11.87708200	2.42006300
H	-2.53098100	12.96526600	1.70030200
H	-1.62155800	11.84830100	0.68434400
C	-3.20766200	10.86564000	1.84229500
H	-3.71450200	11.02513800	2.80431800
H	-3.98850800	10.99765800	1.08014800
H	-2.25580600	4.62975400	1.96813600
C	-5.55208500	0.54252200	4.65799300
C	-5.41809900	1.39951000	3.57444800
C	-4.15287600	1.85009400	3.13772600
C	-3.01934800	1.38953500	3.84504100
C	-3.14840700	0.53196100	4.92667200
C	-4.41517200	0.09516000	5.35312900
H	-6.53668200	0.21164100	4.96860600
H	-6.30637800	1.73127800	3.04334900
H	-2.02677200	1.70808400	3.54330700
H	-2.26760000	0.18460800	5.45670400
C	-4.07581300	2.74009500	1.97802900
C	-2.89346700	3.13990600	1.33191100
H	-5.00998700	2.87170100	1.43768200
H	-2.94327500	3.45444100	0.29392900
H	-1.93885400	2.70536400	1.61422600
C	-4.49945800	-0.82004400	6.51162300
O	-3.54244500	-1.23256700	7.14732400
O	-5.76905600	-1.17048500	6.81567100
C	-5.94410800	-2.06015900	7.93386300
H	-7.01869500	-2.21946800	8.01114700
H	-5.42977200	-3.00688100	7.75396200
H	-5.55888500	-1.60471900	8.84901100
C	-0.13379100	8.91651700	-0.27656900
O	-0.54413100	8.82294000	1.11190200
C	0.59456700	8.56711600	1.97588600
C	1.73570800	8.19979300	1.02782200
C	1.39133900	9.00653000	-0.23577500
H	-0.48134400	8.01768800	-0.79837100
H	-0.61905600	9.79355800	-0.71289100
H	0.80563000	9.48227800	2.54149400
H	0.31465100	7.77117800	2.66890600
H	2.71389300	8.45158900	1.44433800
H	1.72131200	7.12627800	0.81210300
H	1.71015900	10.04823300	-0.12377200
H	1.85113100	8.60419000	-1.14154900
C	-2.78147100	4.51386500	5.67859300
C	-2.90918100	4.85605700	7.02451200
C	-4.10583700	5.43452300	7.44568500
C	-5.12159500	5.63977900	6.51564600
C	-4.91189100	5.25435500	5.18348300
N	-3.75164600	4.70514300	4.77919100
H	-4.24643200	5.72886700	8.48092200
H	-1.86584200	4.06407000	5.30456800
H	-2.09222500	4.67711900	7.71519100
H	-6.04826300	6.10884000	6.82369700
C	-5.93827800	5.44678100	4.12521000
C	-7.27424200	5.75382600	4.41825200
N	-5.52105900	5.31639800	2.84290400

C	-8.18238900	5.94926900	3.38333300
H	-7.60458400	5.82671900	5.44691000
C	-6.40209100	5.51622200	1.84610200
C	-7.73749300	5.83443400	2.06647300
H	-9.21863500	6.18555700	3.60229500
H	-6.00723400	5.42288000	0.84058700
H	-8.40381400	5.98565600	1.22479400

TS₁₈₋₂₀_pyridine

scf done: -3235.3427117

Ni	-3.77154100	4.60564600	1.90037300
Zn	-2.63841600	8.83647600	1.92843300
C	-3.18258300	6.40950000	1.92399100
O	-2.60760500	6.93460300	2.93647500
O	-3.43897600	7.16998100	0.92268700
C	-2.14711300	11.77117400	2.13534600
H	-1.27164600	11.60214000	2.77449800
H	-2.51825600	12.78052800	2.36858600
H	-1.77804900	11.80209000	1.10267500
C	-3.21707100	10.68427400	2.32921400
H	-3.58449400	10.71673200	3.36433600
H	-4.09063200	10.91860800	1.70497600
H	-2.45780100	4.56804800	1.26380900
C	-5.51597600	0.66155500	4.62475800
C	-5.42832100	1.31773500	3.40338400
C	-4.21689900	1.88651900	2.95699700
C	-3.09261900	1.78282400	3.80659600
C	-3.17706100	1.12952300	5.02813200
C	-4.38717700	0.55653100	5.45402000
H	-6.45728900	0.22534700	4.93898700
H	-6.30816800	1.38579900	2.76939300
H	-2.14461100	2.21820500	3.50751900
H	-2.30473100	1.05367500	5.66862100
C	-4.17581100	2.55780700	1.65248200
C	-3.00152700	2.89708800	0.96422200
H	-5.10742800	2.54686000	1.09130700
H	-3.05222300	3.05572000	-0.10869000
H	-2.03187200	2.56342800	1.32097500
C	-4.42176500	-0.14057800	6.76167700
O	-3.46755600	-0.25954000	7.51170500
O	-5.63777900	-0.64747700	7.05414100
C	-5.76211700	-1.35078700	8.30503300
H	-6.79977900	-1.67781900	8.35056200
H	-5.08880600	-2.21051400	8.32750800
H	-5.53318800	-0.68614700	9.14098900
C	-0.24944500	8.79858500	-0.17215200
O	-0.64310400	8.66567100	1.21917100
C	0.51703600	8.49468700	2.07487900
C	1.67146600	8.19932700	1.11870800
C	1.26740700	8.98475800	-0.14072200
H	-0.54394900	7.88429300	-0.69868600
H	-0.79195400	9.64715800	-0.59731300
H	0.67169000	9.42544100	2.63326300
H	0.29780400	7.68579500	2.77515000
H	2.63493000	8.51138200	1.52856900
H	1.72194100	7.12717800	0.90182000
H	1.52105300	10.04418500	-0.02887000
H	1.74505800	8.61353000	-1.05045400
C	-5.59347300	4.82380900	4.14315800
C	-6.75098400	5.16511900	4.83672600
C	-7.81088300	5.74368700	4.14001400
C	-7.66956200	5.96039000	2.76889200
C	-6.47889900	5.59744100	2.14823300
N	-5.45294400	5.03484800	2.81934000
H	-8.72574800	6.02163200	4.65350900
H	-4.74918300	4.36891500	4.64843400
H	-6.80995200	4.97776100	5.90308800

H	-8.46376100	6.40884300	2.18250700
H	-6.32326100	5.76408000	1.08831800

TS₁₈₋₂₀_Cs₂CO₃

scf done: -3062.93272329

Ni	-3.44570400	5.13311100	2.31333900
Zn	-2.07857200	9.28674700	1.90497100
C	-2.82238300	6.92563500	2.16917400
O	-2.15080900	7.55380700	3.06630300
O	-3.11162200	7.60951000	1.10817800
C	-3.86018200	11.69252700	1.74547100
H	-4.28016900	11.35147400	0.78990700
H	-3.97251600	12.78741200	1.76467300
H	-4.50926900	11.29613700	2.53652900
C	-2.40169700	11.23730700	1.92455500
H	-1.77981200	11.70403100	1.14693900
H	-2.01908100	11.63774300	2.87467500
H	-2.04488300	4.90202600	1.93934300
C	-5.85168800	1.38309800	4.98210700
C	-5.50075500	1.95639700	3.75985500
C	-4.21272600	2.48408600	3.53924400
C	-3.29139300	2.41955600	4.60477900
C	-3.64099800	1.84498700	5.82522600
C	-4.92283000	1.32132000	6.02472400
H	-6.85097300	0.97677400	5.11734600
H	-6.22991100	1.99408300	2.95418600
H	-2.29450800	2.83198900	4.48004600
H	-2.90903500	1.80919600	6.62795100
C	-3.88588600	3.05827500	2.22476300
C	-2.59023400	3.27692900	1.74054300
H	-4.69987600	3.05645600	1.50383600
H	-2.42939300	3.31364000	0.66705700
H	-1.72635000	2.93907100	2.30647700
C	0.40873600	9.04741100	-0.11029300
O	-0.07280300	8.88039600	1.24638900
C	0.99604200	8.44427000	2.12773500
C	2.13492100	8.03486400	1.19455100
C	1.93234700	8.97492100	-0.00587500
H	-0.00166000	8.23585600	-0.72236300
H	0.03522300	10.00370400	-0.48651600
H	1.27487900	9.28817200	2.77016200
H	0.60452500	7.63458900	2.74612100
H	3.11407600	8.14548600	1.66670500
H	2.01876700	6.99030700	0.88672600
H	2.34774200	9.96514900	0.20961200
H	2.39102600	8.60473600	-0.92588300
Cs	-6.31733100	7.84250000	0.77726000
Cs	-7.45866800	6.04388600	6.84531500
C	-5.77244500	6.10672400	3.79277500
O	-6.96228400	6.61122500	3.74940600
O	-5.28206800	5.64697100	2.65560300
O	-5.09648700	6.04625900	4.87192900
H	-5.19071900	0.86962100	6.97575200

TS₁₈₋₂₀_KHMDs

scf done: -4232.41709253

Ni	-4.56978400	5.39458200	2.54934000
Zn	-1.38159400	8.40349800	2.94362500
C	-3.20276300	6.71414500	2.66118200
O	-2.52241200	6.87036300	3.74061600
O	-2.87888200	7.50840900	1.68803100
C	0.59730400	10.63674200	2.99790100
H	1.31370600	10.01619700	3.55004900
H	0.84050100	11.68408700	3.23143200
H	0.81676600	10.49206300	1.93252800
C	-0.85659200	10.27074300	3.33996900
H	-1.03761300	10.46593200	4.40627900

H	-1.53569400	10.95071700	2.80502600
H	-3.29765600	4.73109600	2.23910400
C	-7.25517200	2.54299500	5.91644500
C	-7.04864000	2.93563000	4.59439000
C	-5.75028800	3.05218800	4.05962900
C	-4.66461400	2.76189500	4.91127500
C	-4.87166900	2.36755700	6.23206200
C	-6.16742100	2.25547800	6.74501900
H	-8.26871300	2.45973300	6.29968500
H	-7.90318700	3.15486300	3.96128500
H	-3.64824300	2.85593000	4.54148800
H	-4.01587500	2.15070000	6.86584100
C	-5.57194200	3.45579100	2.65386000
C	-4.37869700	3.32530500	1.94993500
H	-6.48004800	3.63963600	2.09379300
H	-4.38983900	3.38735700	0.86548700
H	-3.54751200	2.75968700	2.35849900
N	-6.23123300	6.56095500	2.74019100
Si	-6.43767800	7.29013100	4.29655800
Si	-7.47609200	6.37607400	1.56378400
K	-5.04182800	8.82985800	1.12935400
C	-5.39391200	6.49460200	5.66239000
H	-4.33153800	6.50847700	5.40107400
H	-5.52740700	7.04027900	6.60579200
H	-5.68866000	5.45377700	5.82884300
C	-8.23356500	7.26689500	4.94608700
H	-8.95164700	7.73466200	4.26356100
H	-8.57010500	6.23990900	5.12838300
H	-8.29347000	7.80374400	5.90131900
C	-5.93620200	9.14324500	4.29279200
H	-6.54335400	9.73960200	3.59820300
H	-6.07752800	9.57976000	5.28933500
H	-4.87601500	9.27889900	4.04118200
C	-6.77922000	5.77761800	-0.10941000
H	-7.58020300	5.74716800	-0.85890100
H	-5.98798400	6.42496500	-0.50706700
H	-6.35717100	4.76930700	-0.03943800
C	-8.91746800	5.18566300	1.95662700
H	-8.60025500	4.13974400	2.01843200
H	-9.40734100	5.43861300	2.90242000
H	-9.67501400	5.24654400	1.16504200
C	-8.37969800	8.02469400	1.15627600
H	-9.24569300	7.81477600	0.51618100
H	-8.75442400	8.52572700	2.05552600
H	-7.77112400	8.75683600	0.60892700
H	-6.32613800	1.94938000	7.77496800
C	0.60349900	7.12558500	0.81647800
O	0.22378800	7.21671700	2.21406300
C	1.17838500	6.52211700	3.05919900
C	2.04830800	5.71627200	2.09517000
C	2.03417900	6.58817000	0.82812600
H	-0.09213500	6.44269900	0.31696500
H	0.50777900	8.12162300	0.37569400
H	1.75708300	7.27258800	3.61017700
H	0.61580900	5.90923100	3.76722600
H	3.05294000	5.54860100	2.49036500
H	1.59179100	4.74154700	1.89409400
H	2.75118000	7.41058400	0.92134200
H	2.27055000	6.02927500	-0.08037100

20_COD

scf done: -3299.111053

Ni	-4.45161200	5.08029400	0.80425100
Zn	-3.38120900	9.04781700	-0.63325400
C	-3.91184800	6.72174000	0.06694300
O	-2.84938300	7.29589500	0.47912500
O	-4.64954500	7.33764400	-0.77555200

C	-3.03435900	11.46353900	1.09287000	Zn	-3.61821600	8.81483600	-0.37859500
H	-3.51253800	10.95953200	1.94151400	C	-4.25546900	6.59244800	0.55316500
H	-3.17918000	12.54381000	1.24304400	O	-3.20539500	7.22847300	0.93230800
H	-1.95767600	11.27373900	1.18207800	O	-4.97571100	7.15100300	-0.35033000
C	-3.59396300	10.97549800	-0.25443400	C	-3.14972200	11.53217800	-1.51082400
H	-4.66236500	11.22468300	-0.31454400	H	-2.08074300	11.32194600	-1.63932800
H	-3.11701700	11.53643400	-1.07025200	H	-3.24812200	12.62474100	-1.42471500
H	-1.95972700	3.28753700	0.45289100	H	-3.63982100	11.24458400	-2.44923100
C	-6.25692500	2.43682300	-2.57620700	C	-3.73863100	10.78445700	-0.30293400
C	-5.45006000	3.44972200	-2.08356800	H	-3.24176900	11.12990600	0.61448100
C	-4.28731400	3.17819800	-1.32079700	H	-4.79485000	11.06340400	-0.18338800
C	-3.96887700	1.81824900	-1.10580000	H	-2.55695500	2.75854600	1.44743900
C	-4.77578900	0.79674400	-1.59630000	C	-5.97320300	3.05196600	-2.64714900
C	-5.93395300	1.08658300	-2.33277600	C	-5.25282500	3.82526500	-1.75156700
H	-7.14015600	2.68040700	-3.15627100	C	-4.23814600	3.27088800	-0.93091100
H	-5.71342600	4.48603000	-2.27809100	C	-3.97810500	1.89064900	-1.08677400
H	-3.06842600	1.55597000	-0.56002000	C	-4.70201300	1.10749700	-1.98185200
H	-4.51102700	-0.24097200	-1.42018800	C	-5.71334800	1.67121200	-2.77167600
C	-3.46871700	4.30142200	-0.79973100	H	-6.74523600	3.50766300	-3.25752700
C	-2.02976500	3.98364300	-0.39052800	H	-5.46883400	4.88609800	-1.65613400
H	-3.46219000	5.08140900	-1.56343800	H	-3.18117200	1.42619400	-0.51387000
H	-1.51579600	4.90126700	-0.09234000	H	-4.48199400	0.04943900	-2.08419300
H	-1.46109500	3.53400700	-1.21940600	C	-3.48685900	4.15296800	0.00661700
C	-6.76111100	-0.03336400	-2.82975700	C	-2.28553400	3.54384500	0.73331300
O	-6.52231200	-1.21629900	-2.64413600	H	-3.11565700	4.98817400	-0.59270300
O	-7.84235700	0.37925600	-3.52898100	H	-1.76481400	4.32265900	1.29920500
C	-8.70703400	-0.64786100	-4.04797400	H	-1.55370300	3.10367000	0.03699900
H	-9.50801300	-0.11900400	-4.56264700	C	-6.45780100	0.80053200	-3.70472700
H	-8.16360900	-1.28956000	-4.74533100	O	-6.27487300	-0.39922900	-3.84323800
H	-9.11105900	-1.25483300	-3.23462600	O	-7.39343400	1.46862900	-4.41769000
C	-0.74865400	8.54930600	-2.34123900	C	-8.17140800	0.69476700	-5.34857000
O	-2.19983400	8.58907300	-2.33990500	H	-8.85982700	1.40225300	-5.80879600
C	-2.72521000	8.48032400	-3.69084600	H	-7.52600700	0.24320300	-6.10561500
C	-1.50678700	8.61273300	-4.60498000	H	-8.72363600	-0.09024000	-4.82673400
C	-0.37245500	8.04688000	-3.73364700	C	-1.04160300	7.98639800	-2.05046700
H	-0.37384200	9.56269300	-2.15477600	O	-2.49114700	8.04325100	-2.01788900
H	-0.43284000	7.89203500	-1.52810300	C	-3.05601100	7.66338100	-3.30100100
H	-3.21383000	7.50499400	-3.78546100	C	-1.86880600	7.62774800	-4.26298200
H	-3.46919400	9.26934100	-3.82941600	C	-0.70462100	7.23480900	-3.33754900
H	-1.63846000	8.07045900	-5.54411200	H	-0.65645400	9.01286600	-2.05994600
H	-1.31838500	9.66531400	-4.84090300	H	-0.70535300	7.48371600	-1.14060800
H	-0.37918800	6.95220800	-3.75806500	H	-3.52886900	6.68211800	-3.18825200
H	0.61772900	8.39074100	-4.04170500	H	-3.81916900	8.40025100	-3.56467800
C	-5.74374400	3.22093100	1.64040200	H	-2.02472500	6.92046200	-5.08089800
C	-4.46876400	3.17157200	2.10907200	H	-1.69605000	8.61902600	-4.69515800
H	-5.93769900	2.72891000	0.69147100	H	-0.70501000	6.15445500	-3.15909200
H	-3.75767400	2.59611300	1.52315700	H	0.27377900	7.51601100	-3.73416500
C	-6.95561400	3.77521700	2.35711900	C	-5.10756000	2.03395700	2.16605200
H	-7.83672200	3.21020400	2.03623700	C	-5.47369600	1.00199200	3.02698000
H	-6.86669000	3.61471000	3.43334300	C	-6.13961000	1.32287300	4.20631400
C	-3.93969200	3.68887200	3.42727400	C	-6.43163800	2.65883000	4.46623300
H	-2.86609400	3.87054100	3.30654700	C	-6.04124900	3.63932100	3.54923500
H	-4.02564400	2.90680300	4.19532300	N	-5.36466600	3.32758100	2.41358700
C	-7.20453200	5.27084500	2.05293800	H	-6.43686800	0.55093800	4.90848900
H	-7.65672800	5.36159300	1.05908400	H	-4.60240600	1.81965100	1.23506700
H	-7.94942900	5.66951300	2.75706700	H	-5.23767400	-0.02384500	2.76771900
C	-4.61424900	4.98568700	3.93892900	H	-6.96301900	2.92956500	5.36974400
H	-5.55209500	4.75088800	4.44710600	C	-6.36484400	5.07185000	3.71277100
H	-3.96210900	5.43165400	4.69655200	C	-7.08429600	5.58316800	4.79732700
C	-5.97185700	6.14373700	2.07248100	N	-5.94219100	5.87041100	2.70188200
H	-6.05599600	7.05130200	1.47999400	C	-7.39407300	6.93973000	4.83366800
C	-4.85376300	6.01377000	2.85058900	H	-7.40478600	4.93445600	5.60262200
H	-4.11562400	6.80858000	2.78091800	C	-6.26172800	7.17616600	2.73623300
				C	-6.98565400	7.75032500	3.77721600
				H	-7.95131100	7.35080100	5.66895200
				H	-5.93118100	7.76943400	1.89366400
				H	-7.21600000	8.80926800	3.75142900

20_bipyridine
scf done: -3482.48462928
Ni -4.76273200 4.97117100 1.34421000

20_pyridine

scf done: -3235.37246608

Ni	-4.95793800	5.05559200	-1.05965400
Zn	-3.04280000	8.78705200	0.08725700
C	-4.03550700	6.63249100	-0.65298300
O	-3.05556800	6.65310900	0.16473300
O	-4.44553300	7.75520100	-1.12402700
C	-1.96866400	11.32271400	1.23662000
H	-0.96190300	10.89124500	1.29621800
H	-2.01968400	12.11396800	1.99954600
H	-2.03796400	11.82031800	0.26135500
C	-3.06018300	10.25469400	1.41412400
H	-2.97548400	9.81100700	2.41582100
H	-4.04768500	10.73614400	1.39281600
H	-1.77378400	4.46916400	-1.45608500
C	-6.42515000	2.08422100	-1.73695400
C	-5.72238400	3.16946300	-2.27602100
C	-4.30555900	3.28759000	-2.12300800
C	-3.64444500	2.24425900	-1.40120100
C	-4.34659500	1.17954800	-0.88172200
C	-5.75378400	1.08639000	-1.02855200
H	-7.49697600	2.01307800	-1.88416100
H	-6.25008700	3.87688000	-2.91197200
H	-2.56811600	2.29012300	-1.27492200
H	-3.82734800	0.39003000	-0.34820800
C	-3.68551000	4.54280700	-2.49848500
C	-2.18311800	4.71913000	-2.43898600
H	-4.14464700	5.01616900	-3.37122100
H	-1.91650200	5.76001000	-2.64110400
H	-1.66921500	4.09611700	-3.18579600
C	-6.45157700	-0.07912800	-0.44172800
O	-5.90024000	-0.99241600	0.15041000
O	-7.78946400	-0.04006400	-0.62238700
C	-8.54597200	-1.14264000	-0.08698800
H	-9.58425500	-0.92830600	-0.33578500
H	-8.22901800	-2.08187200	-0.54569100
H	-8.41697700	-1.20419100	0.99595200
C	-0.16965800	8.30476400	-1.16880300
O	-1.47829800	8.90752000	-1.34522500
C	-1.53200100	9.68885600	-2.56825000
C	-0.08648500	9.75743800	-3.06333200
C	0.51226800	8.44527900	-2.52799600
H	0.36110600	8.85567300	-0.38328500
H	-0.32159100	7.27250400	-0.84654300
H	-2.18886400	9.16926500	-3.27417300
H	-1.96393600	10.66422500	-2.32862400
H	-0.02929900	9.84373500	-4.15089900
H	0.42775100	10.61889900	-2.62454500
H	0.24228500	7.60681700	-3.17867200
H	1.60097800	8.47428000	-2.44130200
C	-6.73266400	4.34865900	1.12062000
C	-7.77314200	4.47700300	2.03483600
C	-8.52076500	5.65502300	2.04502400
C	-8.19212200	6.66367700	1.14013800
C	-7.13145000	6.46365900	0.26112800
N	-6.41273000	5.32228400	0.24332900
H	-9.33963100	5.78442000	2.74559300
H	-6.13451700	3.44503600	1.07481500
H	-7.98656100	3.66536600	2.72148000
H	-8.74096200	7.59849700	1.11253100
H	-6.81914100	7.22833300	-0.44145400

20_Cs₂CO₃

scf done: -3062.96718099

Ni	-4.68997300	4.62536700	-0.41045600
Zn	-2.83655300	8.52672900	-0.01135300

C	-3.85767800	6.27429100	-0.29680900
O	-2.74587400	6.45032100	0.33150100
O	-4.40982500	7.33897200	-0.77507500
C	-2.33521000	11.44767800	0.27657500
H	-1.41729000	11.35750000	-0.31714600
H	-2.21211400	12.33248300	0.91877600
H	-3.14242500	11.68110300	-0.42910100
C	-2.62531900	10.16611400	1.07645700
H	-1.81787100	10.00692900	1.80602100
H	-3.53268100	10.31126700	1.67937300
H	-2.18271900	2.97740800	-0.84900600
C	-6.87021500	2.37507400	-3.15966100
C	-5.81287300	3.27238600	-3.07153000
C	-4.73736500	3.06858400	-2.16772300
C	-4.80008800	1.91570000	-1.34735300
C	-5.86814300	1.01639400	-1.43622800
C	-6.90626400	1.23777200	-2.33931500
H	-7.67078700	2.55420200	-3.87291100
H	-5.79216800	4.14996500	-3.71383500
H	-3.99661800	1.71292700	-0.64601200
H	-5.88126900	0.13889500	-0.79532100
C	-3.68798800	4.09805100	-1.98779300
C	-2.25677800	3.64528300	-1.71375300
H	-3.71892100	4.83449000	-2.79664100
H	-1.62312000	4.51101300	-1.50059900
H	-1.81971700	3.11315900	-2.57386700
C	-0.23922800	8.32661500	-1.81426000
O	-1.66961100	8.56797800	-1.79030800
C	-2.13689900	9.05481600	-3.07643500
C	-0.86851400	9.42014500	-3.84587600
C	0.15538800	8.41657100	-3.28849700
H	0.24887100	9.09955400	-1.20881300
H	-0.05719100	7.34725800	-1.36531400
H	-2.69923100	8.25053900	-3.56278600
H	-2.80449400	9.90086700	-2.89376900
H	-1.00575500	9.33766700	-4.92657100
H	-0.56410800	10.44665300	-3.61609300
H	0.03955100	7.44234100	-3.77459800
H	1.19017900	8.74219700	-3.41775500
H	-7.73190100	0.53576800	-2.41130800
Cs	-7.36425800	7.40000900	0.64945900
Cs	-2.43467900	5.66418600	3.42992300
C	-5.52245900	4.75738100	2.30944900
O	-5.77362000	5.84457800	2.94270900
O	-5.94992900	4.66367200	1.04423000
O	-4.87996700	3.78745300	2.82892600

20_KHMDs

scf done: -4232.45888622

Ni	-4.39382300	4.95008400	0.21737200
Zn	-3.42317900	9.12774700	-0.47508900
C	-3.92026700	6.70421900	-0.10151500
O	-2.91053700	7.30067900	0.41082100
O	-4.69246400	7.43739600	-0.84691200
C	-3.41613100	11.28758300	1.58871500
H	-3.97335300	10.65115800	2.28758800
H	-3.63056300	12.32970000	1.86901500
H	-2.35222900	11.11773500	1.79400900
C	-3.77202000	10.98319000	0.12267500
H	-4.83298800	11.21682900	-0.04790100
H	-3.21752400	11.66941000	-0.53276900
H	-1.90926300	3.66793100	1.16950500
C	-4.29270500	1.99456200	-3.23560900
C	-3.77206600	3.14574900	-2.65160700
C	-3.28939400	3.15359200	-1.32066200
C	-3.36660400	1.93599900	-0.60763300
C	-3.88981400	0.78001200	-1.19357600

C	-4.35709600	0.79900900	-2.50876300	H	-1.87278900	3.45117600	0.53640200
H	-4.64287200	2.02403500	-4.26449700	C	-6.18974000	2.79110000	-2.35396900
H	-3.71963100	4.06628800	-3.22907000	C	-5.26114200	3.76133400	-1.99878900
H	-2.99763400	1.88992800	0.41252000	C	-4.04828000	3.41468800	-1.35276800
H	-3.92406300	-0.14209600	-0.61867000	C	-3.79828000	2.04148200	-1.12499600
C	-2.76037100	4.40717400	-0.72002200	C	-4.72296300	1.07264800	-1.49113100
C	-1.62606100	4.26567700	0.29565400	C	-5.93625300	1.43096300	-2.10310000
H	-2.46119900	5.09447500	-1.51672600	H	-7.11390300	3.08295200	-2.84018200
H	-1.33714200	5.25423800	0.66148700	H	-5.45509100	4.80744900	-2.20949300
H	-0.73602800	3.78771700	-0.14543900	H	-2.86766300	1.73006900	-0.66426000
C	-0.76332300	8.86809600	-2.15961300	H	-4.51228100	0.02286500	-1.31486100
O	-2.21441300	8.92076200	-2.19707200	C	-3.02763400	4.47832400	-1.02921500
C	-2.69548100	9.07952900	-3.55858900	C	-1.72125100	4.01693500	-0.38710200
C	-1.44729400	9.37399300	-4.39153600	H	-2.78809400	4.97514900	-1.97308800
C	-0.34360300	8.64066800	-3.61031600	H	-1.11440100	4.89017300	-0.14291000
H	-0.39314200	9.82315600	-1.76837800	H	-1.14977300	3.38324900	-1.07685700
H	-0.47769400	8.06316300	-1.47925100	C	-6.88760800	0.36050400	-2.47649400
H	-3.18322500	8.14516500	-3.85552300	O	-6.70644200	-0.83130900	-2.28571000
H	-3.43119500	9.88838700	-3.56675000	O	-8.00787500	0.83343600	-3.06464400
H	-1.54983300	9.02375400	-5.42121700	C	-8.99003800	-0.14139100	-3.46270800
H	-1.24812600	10.45053100	-4.41431400	H	-9.79970800	0.43115100	-3.91279000
H	-0.35197200	7.57130200	-3.84551600	H	-8.56467400	-0.83785700	-4.18870200
H	0.65692600	9.02887900	-3.81464300	H	-9.35131400	-0.69644000	-2.59401600
N	-6.00468000	4.69120300	1.30874800	C	-0.66061000	8.56899000	-2.31878900
Si	-5.76990200	4.95583800	3.00947300	O	-2.10130200	8.47731300	-2.45912000
Si	-7.28902300	3.74163500	0.63125200	C	-2.49924600	8.66263500	-3.84407900
K	-7.07604900	7.27503900	0.25656100	C	-1.21774800	9.04991400	-4.58661100
C	-6.66293400	6.54041500	3.60849100	C	-0.12093600	8.38812000	-3.73506600
H	-7.73849600	6.51325800	3.39153900	H	-0.40946300	9.55483900	-1.90859100
H	-6.55642200	6.65593800	4.69428100	H	-0.34842400	7.79567700	-1.61397100
H	-6.24043300	7.44799700	3.15665600	H	-2.91883100	7.71653800	-4.20166400
C	-3.94624300	5.17793200	3.48526900	H	-3.27426200	9.43340100	-3.87760200
H	-3.37326900	4.26611000	3.28042100	H	-1.22490500	8.70445000	-5.62298400
H	-3.47549500	5.99409100	2.92837700	H	-1.09164100	10.13760400	-4.59053100
H	-3.85526400	5.39474100	4.55764100	H	-0.03508000	7.32338600	-3.97668000
C	-6.41875500	3.55025100	4.12277500	H	0.86078500	8.84963300	-3.86556900
H	-5.89649700	2.60902300	3.91683900	C	-5.58304500	2.96073300	1.71807900
H	-6.24472100	3.79872900	5.17710100	C	-4.34081700	3.14308900	2.24460800
H	-7.49182000	3.36560200	4.00330700	H	-5.67205100	2.27662000	0.87794300
C	-7.13170000	1.87139300	0.93223600	H	-3.53528100	2.54453900	1.82210800
H	-7.95444500	1.32743000	0.45177100	C	-6.87626400	3.53059700	2.25586800
H	-6.19181100	1.48846000	0.52035400	H	-7.68878300	2.83058300	2.03400600
H	-7.15268700	1.63188500	2.00030900	H	-6.83127300	3.60736700	3.34449200
C	-9.01248800	4.23753300	1.30384800	C	-3.96962200	3.96909800	3.45853700
H	-9.07978200	4.12826600	2.39185100	H	-2.90129400	4.20075800	3.38706200
H	-9.28357700	5.27502300	1.06735600	H	-4.08667700	3.37160700	4.37445400
H	-9.78813500	3.59976000	0.86160400	C	-7.24264600	4.90641600	1.63743300
C	-7.40066300	3.97222400	-1.25631800	H	-7.69351600	4.74351600	0.65208100
H	-8.20514100	3.34254900	-1.65737000	H	-8.02651700	5.37475300	2.25177300
H	-7.62425100	5.00225700	-1.56287900	C	-4.75906700	5.29761800	3.61222300
H	-6.46883500	3.68038300	-1.75149000	H	-5.71113600	5.11282100	4.11653500
H	-4.75703500	-0.10194000	-2.96501600	H	-4.18870700	5.95346300	4.27822600

TS₂₀₋₁_COD

scf done: -3299.08705579

Ni	-4.45852700	4.77538800	0.65890900
Zn	-3.47370000	8.49827600	-0.81486900
C	-3.60043600	6.07102400	-0.44641100
O	-2.67545500	6.76849100	0.12777800
O	-4.37783200	6.69205100	-1.28931500
C	-3.45400400	10.75604100	1.14053200
H	-3.76774000	10.08547100	1.94990600
H	-3.78308200	11.76770300	1.42198400
H	-2.35706700	10.76685900	1.15151100
C	-4.01043400	10.30926400	-0.22284200
H	-5.10786900	10.35913300	-0.19888100
H	-3.70256200	11.03099000	-0.99258600

TS₂₀₋₁_bipyridine

scf done: -3482.44905776

Ni	-4.87334900	4.48508300	0.36154000
Zn	-3.42904400	8.31366400	-0.30571700
C	-3.88835900	5.89406400	-0.41862900
O	-3.01328300	6.39048600	0.40898400
O	-4.48587800	6.75538100	-1.20621000
C	-3.04558600	11.27553500	-0.23273200
H	-1.96167700	11.15910200	-0.11040300
H	-3.30812200	12.25452000	0.19593300

H	-3.23218600	11.34418800	-1.31168900
C	-3.82190100	10.11465300	0.41078500
H	-3.63177700	10.11012400	1.49351000
H	-4.90034000	10.30302500	0.31120500
H	-2.05139700	3.34934100	0.17808500
C	-6.65804100	2.81470600	-2.24001700
C	-5.66690100	3.75428800	-1.98333500
C	-4.40029200	3.36385300	-1.45157100
C	-4.16613500	1.97106200	-1.28819300
C	-5.15514400	1.04070400	-1.55941100
C	-6.42438500	1.44351700	-2.02235800
H	-7.61662300	3.13842100	-2.63029800
H	-5.83342700	4.79992200	-2.22109700
H	-3.19166100	1.62635700	-0.95938600
H	-4.95676100	-0.01843300	-1.43004300
C	-3.33960000	4.40454700	-1.24023600
C	-1.98090600	3.91882200	-0.75338400
H	-3.22867900	4.96182900	-2.17234100
H	-1.33081400	4.77459500	-0.56260800
H	-1.49969600	3.27981700	-1.50498500
C	-7.44126500	0.41208000	-2.29206100
O	-7.28550400	-0.79012200	-2.12956300
O	-8.60830100	0.92480100	-2.75190800
C	-9.65789800	-0.01511900	-3.03978200
H	-10.50064800	0.58636600	-3.37821800
H	-9.34761300	-0.70977000	-3.82398800
H	-9.92738400	-0.57764200	-2.14278400
C	-0.40729000	8.36433400	-1.36870600
O	-1.81224000	8.36479300	-1.72605900
C	-1.98977600	8.67148300	-3.13318600
C	-0.61422400	9.12634200	-3.62266000
C	0.33964400	8.34681100	-2.70168000
H	-0.19516800	9.27232000	-0.79130000
H	-0.22170600	7.48915800	-0.74190500
H	-2.33077200	7.76144700	-3.63842000
H	-2.76447200	9.43824800	-3.21887800
H	-0.46265600	8.90871400	-4.68252000
H	-0.49244000	10.20443800	-3.47426900
H	0.46069200	7.31820900	-3.05754000
H	1.33044400	8.80092900	-2.62519400
C	-4.61373100	1.88138300	2.08351500
C	-4.73201100	1.15576200	3.26668400
C	-5.52179300	1.67803700	4.28958400
C	-6.16068100	2.89907300	4.08921300
C	-5.99093500	3.56951200	2.87303300
N	-5.21698700	3.06224100	1.88223300
H	-5.63814400	1.14776500	5.22920100
H	-4.02498200	1.50438400	1.25481500
H	-4.21698100	0.20766200	3.37526100
H	-6.76937000	3.32779000	4.87605100
C	-6.62422200	4.87348500	2.57034700
C	-7.63195500	5.44531000	3.35448100
N	-6.17380200	5.48596400	1.44734400
C	-8.18427900	6.66582500	2.97498100
H	-7.99267400	4.93862500	4.24131100
C	-6.71466000	6.66166400	1.08089700
C	-7.71959200	7.28513900	1.81462300
H	-8.96827700	7.11970000	3.57231600
H	-6.30547600	7.09308100	0.17231100
H	-8.12396100	8.23336800	1.47818700

TS₂₀₋₁_pyridine

scf done: -3235.34354405

Ni	-5.03985300	4.74426800	-0.39569000
Zn	-3.14195500	8.40378400	-0.20552900
C	-3.80631500	6.11128600	-0.84293000
O	-2.88263100	6.30360700	0.03398100

O	-4.29005800	7.15124800	-1.44553300
C	-2.46707200	11.13238100	0.78304800
H	-1.43493700	10.82869500	0.99710000
H	-2.68910300	11.98282100	1.44490600
H	-2.47245700	11.52130800	-0.24271000
C	-3.45480000	9.96753200	0.95989500
H	-3.43707500	9.63242400	2.00621600
H	-4.47793700	10.33146500	0.79081000
H	-1.63779400	4.24658500	-1.04390300
C	-6.37554000	2.10636800	-2.08180700
C	-5.62938500	3.25992800	-2.30694900
C	-4.32634400	3.42712900	-1.74102100
C	-3.84737300	2.37253800	-0.90409900
C	-4.59836200	1.22620900	-0.69225900
C	-5.86710100	1.06591500	-1.28441300
H	-7.35216600	2.00287300	-2.54115100
H	-6.01170000	4.01923800	-2.98315000
H	-2.86474500	2.45326700	-0.45246100
H	-4.20835300	0.42971200	-0.06692300
C	-3.55100400	4.67264700	-2.00097200
C	-2.03371500	4.51993000	-2.02391700
H	-3.92747300	5.16255400	-2.89762300
H	-1.55916500	5.46071000	-2.31420800
H	-1.74347200	3.74648100	-2.74541300
C	-6.61280100	-0.18299800	-1.03894800
O	-6.21810100	-1.11084800	-0.34865500
O	-7.81180400	-0.21517600	-1.66609700
C	-8.60719700	-1.39970700	-1.47910400
H	-9.51372600	-1.23420300	-2.05966900
H	-8.07519000	-2.28070000	-1.84536400
H	-8.85046900	-1.53528000	-0.42270700
C	-0.12643800	8.47176200	-1.20392400
O	-1.52004900	8.68065000	-1.55284900
C	-1.64012500	9.34101500	-2.84077200
C	-0.22610900	9.81092800	-3.18072500
C	0.64978000	8.75197800	-2.49001300
H	0.13661000	9.17316700	-0.40353200
H	-0.02433100	7.44893800	-0.83460000
H	-2.02021200	8.61113100	-3.56371700
H	-2.36416700	10.15380800	-2.73874400
H	-0.06080700	9.86885300	-4.25908000
H	-0.03902700	10.80092200	-2.75176700
H	0.71288800	7.84698700	-3.10343000
H	1.66583000	9.09961600	-2.28902100
C	-6.57268800	4.69998700	2.01764200
C	-7.44123300	5.15812800	3.00273900
C	-7.92654200	6.46372700	2.92319100
C	-7.51662500	7.26336700	1.85627900
C	-6.64110900	6.73620100	0.91209400
N	-6.17243300	5.47045500	0.98108600
H	-8.60616600	6.84899600	3.67655700
H	-6.17801900	3.69033100	2.04430600
H	-7.72604100	4.49715100	3.81385500
H	-7.86355800	8.28542900	1.75116700
H	-6.28132000	7.32358900	0.07410900

TS₂₀₋₁_Cs₂CO₃

scf done: -3062.93283808

Ni	-5.04077400	4.49027400	-0.18941800
Zn	-2.97667600	8.10597100	-0.15890000
C	-3.84265400	5.84025100	-0.62290200
O	-2.80160600	6.04717000	0.14883500
O	-4.40083600	6.94491900	-1.09422300
C	-2.70056600	11.05381200	0.12527700
H	-1.86918300	11.04176900	-0.59040900
H	-2.55928400	11.94062900	0.76114100
H	-3.61286000	11.22823900	-0.45953300

C	-2.77785100	9.74503600	0.93094600	H	-2.60245800	5.18719000	-2.05358400
H	-1.87158300	9.65327600	1.54838000	H	-1.26934000	4.99809500	0.01137000
H	-3.60667500	9.80972800	1.64982900	H	-1.27218900	3.43235700	-0.83231300
H	-2.00158200	3.53516500	-0.82375300	C	-0.28237100	8.84448400	-1.41983500
C	-6.83598700	2.77594700	-2.88190300	O	-1.61311200	8.58072500	-1.93519800
C	-5.87123000	3.76525800	-2.70068700	C	-1.60976900	8.54885200	-3.38687100
C	-4.66644200	3.50182500	-1.99207600	C	-0.24810100	9.11143700	-3.79355200
C	-4.48997400	2.18952800	-1.47908600	C	0.64961100	8.68315200	-2.62042200
C	-5.46448600	1.20572300	-1.66802600	H	-0.26403200	9.86456900	-1.01861600
C	-6.63899200	1.48799800	-2.36942200	H	-0.08949000	8.13613300	-0.61038500
H	-7.74117100	3.00709900	-3.43763500	H	-1.74045200	7.50962000	-3.70736500
H	-6.01830000	4.74960800	-3.13757100	H	-2.45778900	9.14112300	-3.73993300
H	-3.57256300	1.93412900	-0.96010800	H	0.08738400	8.71964600	-4.75666500
H	-5.29668500	0.20891300	-1.26869600	H	-0.29087100	10.20349100	-3.86377500
C	-3.61229200	4.58233100	-1.86080300	H	0.95127700	7.63632400	-2.73130000
C	-2.17963100	4.06761000	-1.76160200	H	1.55257100	9.29076100	-2.52510000
H	-3.72917000	5.24899900	-2.71552800	N	-6.32785300	4.86788300	1.20360000
H	-1.47506300	4.90141300	-1.79603400	Si	-6.02797900	3.78237600	2.52622100
H	-1.95685700	3.38344400	-2.59019400	Si	-7.91706800	5.22559100	0.59512700
C	-0.22268100	8.17480000	-1.77009000	K	-5.01066700	7.21691500	2.19801200
O	-1.66367200	8.28297500	-1.87011900	C	-4.36681900	4.16914600	3.39025600
C	-2.05262600	8.82912000	-3.15732100	H	-4.41450900	5.07419100	4.01193700
C	-0.74970800	9.29700700	-3.80816000	H	-4.10389600	3.34913400	4.06996500
C	0.28759700	8.33776300	-3.20078000	H	-3.54221000	4.28749900	2.67958600
H	0.14296000	8.97244400	-1.11163200	C	-5.97644800	1.93993400	2.05365500
H	0.00900400	7.20515800	-1.32254400	H	-6.93153700	1.62450200	1.61813800
H	-2.53928200	8.03320200	-3.73110000	H	-5.19692100	1.74006300	1.31162000
H	-2.77093900	9.63448700	-2.98191100	H	-5.78349100	1.30950900	2.93077600
H	-0.79444700	9.24788000	-4.89864400	C	-7.32605300	3.91499100	3.92212400
H	-0.52741700	10.33031500	-3.52153200	H	-8.33060100	3.62381800	3.59611900
H	0.27223900	7.37511100	-3.72263100	H	-7.04669500	3.25142900	4.75020200
H	1.30722400	8.72889900	-3.23372700	H	-7.39216000	4.93277300	4.32504800
H	-7.38686800	0.71559100	-2.52238500	C	-7.89024200	6.12670400	-1.07597700
Cs	-7.15198100	7.61302200	0.55655600	H	-8.91675500	6.33288300	-1.40585800
Cs	-2.26586700	5.64302500	3.25660800	H	-7.36107000	7.08414500	-1.01467500
C	-5.51862100	5.05420600	2.55116800	H	-7.39640600	5.53099900	-1.85018000
O	-5.52632700	6.27160000	2.95340900	C	-9.00618200	3.68118200	0.34792800
O	-6.07471900	4.78979900	1.36073200	H	-8.54494800	2.99883500	-0.37584800
O	-5.00859600	4.10383900	3.22773000	H	-9.15386200	3.12203800	1.27882700
				H	-9.99824000	3.95218700	-0.03405500
				C	-8.88123300	6.39372400	1.76270500
				H	-9.87658500	6.61030100	1.35441300
				H	-9.01879700	5.96773500	2.76172800
				H	-8.36710800	7.35719500	1.88037300
				H	-6.20104500	0.85485500	-3.44008200

TS_{20-1_KHMDS}

scf done: -4232.42750417

Ni	-4.93663900	4.73377200	-0.12695800
Zn	-3.38540300	8.56874400	-0.71665900
C	-3.76653500	6.11429400	-0.56084900
O	-3.08797200	6.73280500	0.38448200
O	-4.20678700	6.90688800	-1.52387000
C	-3.14280400	10.95439100	1.09352800
H	-3.28649300	10.33267100	1.98726800
H	-3.46467800	11.97150600	1.36276000
H	-2.06030500	11.00180300	0.92124600
C	-3.89285800	10.39361700	-0.12793800
H	-4.97415400	10.41762400	0.07085900
H	-3.74462800	11.07285900	-0.97971800
H	-2.26892500	3.67796300	0.61071400
C	-5.59790800	2.93323000	-3.44546100
C	-4.79469800	3.90604600	-2.85678800
C	-3.95247600	3.59819600	-1.75667400
C	-3.94245000	2.25929000	-1.30149100
C	-4.74930200	1.28794500	-1.90072800
C	-5.58302500	1.61506800	-2.97131800
H	-6.23256900	3.20069500	-4.28648400
H	-4.79800600	4.92219600	-3.23819900
H	-3.28790100	1.97192300	-0.48610100
H	-4.71577600	0.26669700	-1.53009700
C	-3.02392800	4.66367300	-1.19360100
C	-1.89657800	4.15971000	-0.29796900