

Electronic Supplementary Information

Ion-pairs as a Gateway to Transmetalation: Aryl Transfer from Boron to Nickel and Magnesium.

Kimberly C. Fabijanczuk,^a Weam A. O. Altalhi,^{b,c} Asma M. O. Aldajani,^{b,d} Allan J. Canty,^e Scott A. McLuckey^{*,a} and Richard A. J. O'Hair^{*,b}

a. Department of Chemistry, Purdue University, West Lafayette, Indiana 47907-2084, United States of America

b. School of Chemistry and Bio21 Institute of Molecular Science and Biotechnology, The University of Melbourne, Victoria 3010, Australia

c. Department of Chemistry, Prince Sattam Bin Abdulaziz University, Hotat Bani Tamim, 16511 Saudi Arabia

d. Department of Chemistry, College of Science, University of Bisha, Bisha 61922, P.O. Box 551, Saudi Arabia

e. School of Physical Sciences - Chemistry, University of Tasmania, Private Bag 75, Hobart, Tasmania 7001, Australia.

Contents of Supplementary Information

Figure S1: Mass spectra of magnesium hydrolysis reactions.

Cartesian coordinates and energies (in Hartrees) of all Ni and Mg species.

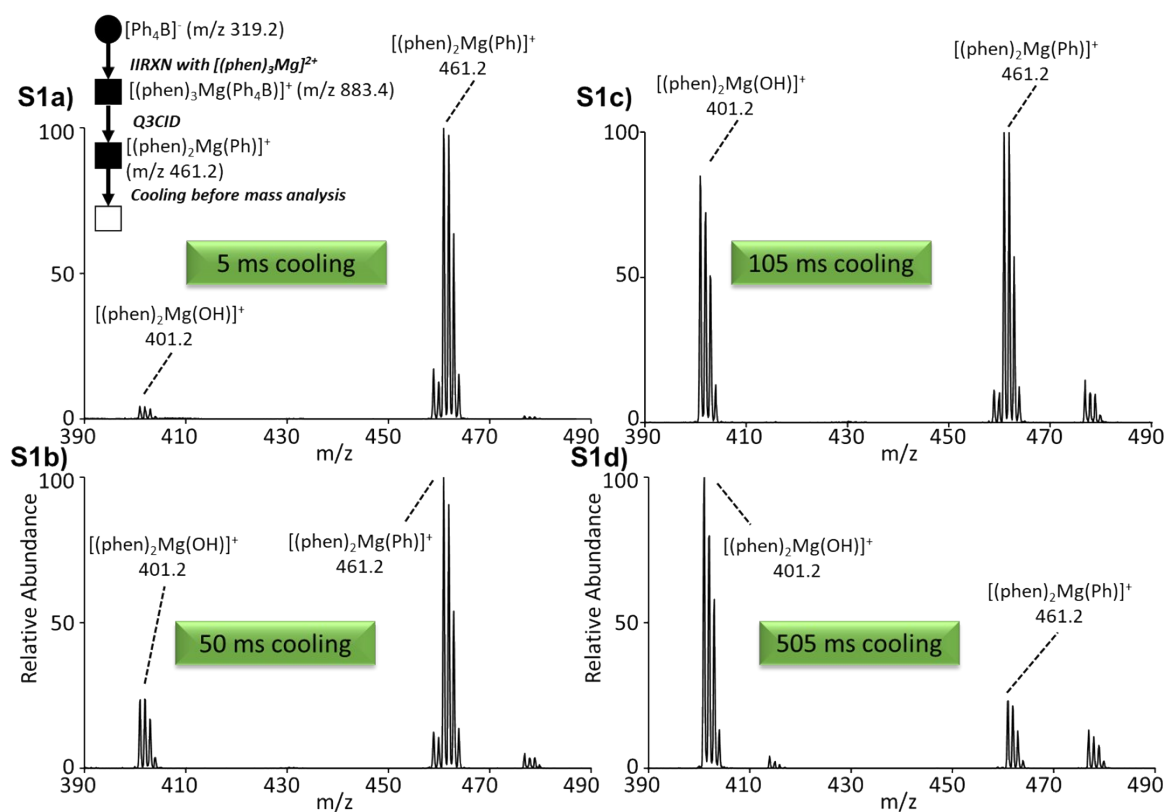


Figure S1: Mass spectra showing the reaction of mass-selected of $[(\text{phen})_2\text{Mg}(\text{Ph})]^+$ (m/z 461) reacting with background water yielding the hydroxide product $[(\text{phen})_2\text{Mg}(\text{OH})]^+$ (m/z 401) as a function of cooling time post isolation: **(a)** the mass spectrum for 5 ms of cooling time allowed after isolation of $[(\text{phen})_2\text{Mg}(\text{Ph})]^+$ (m/z 461) that is then immediately mass analysed; **(b)** the analogous spectrum for 50 ms cooling time; **(c)** the analogous spectrum for 105 ms of cooling time; and **(d)** the analogous spectrum for 505 ms of cooling time.

Cartesian coordinates and energies (in Hartrees) of all Ni and Mg species.

3

Charge = -1 Multiplicity = 1
 E= -950.450045
 H= -950.428688
 G= -950.500796
 SPE= -951.9884227

B	-0.00004800	0.00010900	-0.00007600
C	-0.99210100	1.01350300	0.83381200
C	-0.98297500	1.18311100	2.22560300
C	-1.97067300	1.74968000	0.13888500
C	-1.87292500	2.03554400	2.88434800
H	-0.25930300	0.62421500	2.82278700
C	-2.86047500	2.60920300	0.77570600
H	-2.03713800	1.63244900	-0.94665100
C	-2.81625900	2.75996600	2.16264500
H	-1.82782600	2.12909800	3.97137200
H	-3.59913500	3.15964500	0.18964500
H	-3.51326600	3.42790800	2.67111700
C	0.99175300	-0.83436400	1.01305300
C	0.98198300	-2.22621600	1.18234200
C	1.97066400	-0.14006300	1.74934700
C	1.87173200	-2.88556500	2.03450700
H	0.25796700	-2.82292300	0.62340400
C	2.86026400	-0.77751000	2.60862300
H	2.03758700	0.94547700	1.63240100
C	2.81546700	-2.16446300	2.75900600
H	1.82615800	-3.97259200	2.12780400
H	3.59922200	-0.19191900	3.15916700
H	3.51231700	-2.67341100	3.42675000
C	-0.99265700	-1.01256000	-0.83422300
C	-1.97119200	-1.74886100	-0.13936900
C	-0.98395000	-1.18154400	-2.22609800
C	-2.86140700	-2.60783600	-0.77635400
H	-2.03725500	-1.63220000	0.94625300
C	-1.87432800	-2.03340000	-2.88499900
H	-0.26032600	-0.62255900	-2.82324500
C	-2.81765900	-2.75790900	-2.16338100
H	-3.60002000	-3.15839300	-0.19034000
H	-1.82957400	-2.12643200	-3.97208100
H	-3.51500300	-3.42540600	-2.67197600
C	0.99288700	0.83375100	-1.01285400
C	0.98467700	2.22563400	-1.18198000
C	1.97137400	0.13853200	-1.74885100
C	1.87535900	2.88413300	-2.03383200
H	0.26116900	2.82307200	-0.62317700
C	2.86189100	0.77512100	-2.60781800
H	2.03720900	-0.94707500	-1.63191300
C	2.81854600	2.16212400	-2.75813800
H	1.83094800	3.97121700	-2.12703000
H	3.60042900	0.18881200	-3.15815900
H	3.51611800	2.67040600	-3.42563700

4a

Charge = 2 Multiplicity = 3
 E= -1883.742979
 H= -1883.710381
 G= -1883.806492
 SPE= -3223.73426

Ni	0.00307000	-0.00156500	0.00242200
N	1.47714100	-1.01657600	1.11482700
N	1.72088200	0.48935000	-1.11417200
N	0.15494900	1.78856800	1.10446300
N	-1.29049200	1.23575600	-1.10981500
N	-1.61947300	-0.76048800	1.11683500
N	-0.42816500	-1.74266600	-1.10121400
C	-2.19539800	-0.25778700	2.19987800
H	-1.77449900	0.67134900	2.58773400

C	-2.23226500	4.78873600	-0.56413600
H	-2.86453800	5.55077600	-1.01784400
C	-0.66579700	4.07220200	1.14855400
C	-1.49769100	5.06971900	0.54588100
H	-1.53129700	6.06076000	0.99649100
C	-3.65446200	-3.82018700	0.55983100
H	-4.49843700	-4.33963300	1.01173100
C	-1.99887900	0.94086900	-2.19100000
H	-1.89902000	-0.07539700	-2.57558900
C	1.33422700	-1.75790300	2.20455800
H	0.32004600	-1.85956500	2.59415700
C	-3.19745800	-2.60446100	1.16256000
C	-3.04932100	-4.31856100	-0.55198200
H	-3.39998300	-5.24429200	-1.00624300
C	0.87836100	2.04117500	2.18632200
H	1.47710500	1.21565300	2.57461900
C	-1.46885100	-2.43893900	-0.58035800
C	-2.10610700	-1.91387200	0.59476300
C	1.81870900	1.23740300	-2.20438200
H	0.88867600	1.65672700	-2.59154400
C	0.17539600	-2.21174000	-2.18471900
H	1.00845400	-1.62257700	-2.57125300
C	-2.19179300	3.48851500	-1.16236300
C	4.12164800	0.13811100	-1.16766400
C	2.71780100	-0.85984900	0.58996700
C	-1.94052500	-3.63945700	-1.15147200
C	3.86500400	-1.44857800	1.16212800
C	-1.37998500	2.48581300	-0.59166000
C	-0.60652100	2.78166200	0.58188200
C	5.14431400	-1.23521500	0.55533000
H	6.01940200	-1.69763900	1.01002700
C	2.84809600	-0.05455200	-0.59222800
C	5.26781400	-0.47190100	-0.56396900
H	6.24348100	-0.31239800	-1.02109500
C	0.11274300	4.30835600	2.30002000
H	0.09528100	5.29229700	2.76805200
C	0.88694200	3.29320700	2.81995500
H	1.49817600	3.44615000	3.70582900
C	-2.93038900	3.14456500	-2.31286100
H	-3.57011400	3.89060700	-2.78367000
C	-2.83578200	1.86956000	-2.82829200
H	-3.39425300	1.57520700	-3.71330300
C	3.68044100	-2.22782800	2.32253000
H	4.54125000	-2.69997800	2.79538000
C	2.41433500	-2.38454700	2.84474500
H	2.24137100	-2.98059700	3.73726000
C	4.19201900	0.93536100	-2.32829300
H	5.15719900	1.10850800	-2.80362300
C	3.04047100	1.48710000	-2.84778200
H	3.06409800	2.10690000	-3.74056800
C	-0.22033900	-3.39730400	-2.82244800
H	0.30882100	-3.73620400	-3.70951900
C	-1.28048900	-4.11000500	-2.30466900
H	-1.61483700	-5.03402800	-2.77568100
C	-3.78593100	-2.04575300	2.31555600
H	-4.63138400	-2.54825700	2.78479800
C	-3.28616800	-0.87091800	2.83534300
H	-3.71987700	-0.41616700	3.72241600

4b

Charge = 2 Multiplicity = 1
 E= -1912.927701
 H= -1912.894932
 G= -1912.991788
 SPE= -1915.509983

H	-3.04074400	5.56134900	-1.04520700
C	-2.39460700	4.81800200	-0.58154000
C	-2.29636000	3.52662400	-1.18804200
C	-1.69658800	5.11157900	0.54535400

C	-1.46615900	2.54079500	-0.61331200
C	-3.00014400	3.18160600	-2.35827000
C	-0.85024300	4.13476300	1.15745200
H	-1.77001500	6.09576400	1.00472300
N	-1.32743400	1.30245300	-1.15195900
C	-0.73433000	2.84868200	0.58816000
C	-2.85908900	1.92138900	-2.89342600
H	-3.65062600	3.91862300	-2.82744800
C	-0.11218600	4.39592700	2.32827500
C	-2.00757800	1.01144700	-2.25349900
N	0.04540800	1.88024800	1.13282400
H	-3.39026700	1.62600400	-3.79387800
C	0.68184300	3.41034700	2.86917100
H	-0.17818500	5.37866100	2.79337300
H	-1.87198400	0.00560800	-2.65417400
C	0.72905200	2.16235200	2.23463700
H	1.26378900	3.58302100	3.77012600
H	1.34642100	1.35903800	2.63975200
Mg	0.01363500	-0.00511300	0.00411300
C	3.12065500	1.44321600	-2.92667400
C	4.28055000	0.94023100	-2.38247900
C	4.22525000	0.18417800	-1.19531000
C	2.95618100	-0.02175000	-0.61361800
C	1.90632100	1.18151400	-2.27895100
C	5.39023900	-0.37047600	-0.57852300
C	2.85413300	-0.78207300	0.60526000
C	4.02325900	-1.32012800	1.18404800
C	5.29269400	-1.09684900	0.56441100
C	3.87710700	-2.06374500	2.37139000
H	4.75896400	-2.49415800	2.84418400
C	2.62620800	-2.23833200	2.91851700
C	1.52464600	-1.66086500	2.27381800
H	6.35748800	-0.19864600	-1.04751300
H	3.13242400	2.03122900	-3.84006300
H	5.24430200	1.11932600	-2.85740900
H	0.96855000	1.56297000	-2.68599100
H	6.17992900	-1.52096100	1.03132100
H	2.48239800	-2.80850500	3.83198200
H	0.51997400	-1.77748100	2.68322700
N	1.62535800	-0.95240600	1.15647400
N	1.81643800	0.47161700	-1.16163900
C	-3.26782600	-1.08925300	2.91342400
C	-3.75517700	-2.25500600	2.36772900
C	-3.17744900	-2.77080000	1.19136000
C	-2.10680700	-2.04951900	0.62153900
C	-2.19791100	-0.44580100	2.27752800
C	-3.63275100	-3.97831800	0.57508500
C	-1.49212600	-2.53876500	-0.58545700
C	-1.96157800	-3.73725000	-1.16365500
C	-3.04561700	-4.44523900	-0.55656500
C	-1.32661800	-4.18500700	-2.33823900
H	-1.66416500	-5.10712200	-2.80960700
C	-0.28972000	-3.45603800	-2.87460300
C	0.10303500	-2.27486900	-2.23203200
H	-4.45964000	-4.51609300	1.03560800
H	-3.69387600	-0.66661800	3.81900900
H	-4.58419500	-2.78637200	2.83335600
H	-1.78707800	0.47884600	2.68608600
H	-3.39043300	-5.36625800	-1.02328700
H	0.22093500	-3.77771600	-3.77790100
H	0.91909800	-1.67202600	-2.63330900
N	-0.47477800	-1.82139600	-1.12665200
N	-1.62764000	-0.90373600	1.17036700

5a

Charge = 1 Multiplicity = 3

E= -2834.269579

H= -2834.215245

G= -2834.358549

SPE= -2835.1564857

Ni	-2.40087900	-0.09258000	-0.22300700
N	-1.61208300	0.35143500	-2.12155400

N	-0.73174100	-1.35754300	-0.21945300
N	-3.63627700	-1.67946800	-0.89090600
N	-3.13590300	-0.81994700	1.61626300
N	-3.91514000	1.39048500	-0.42974500
N	-1.44488500	1.56563900	0.61301900
C	-5.13601300	1.27688500	-0.92976500
H	-5.47539300	0.26508400	-1.15591500
C	-5.37527800	-3.69315300	2.32795600
H	-5.81113500	-4.20217600	3.18624800
C	-5.05124900	-3.46758100	-0.06748600
C	-5.62836700	-4.12583600	1.06450200
H	-6.27147700	-4.98734200	0.89138700
C	-3.62957700	5.06848400	-0.00698000
H	-4.22075500	5.96632800	-0.18057900
C	-2.84754500	-0.39896300	2.83798800
H	-2.17060500	0.45321500	2.91030200
C	-2.05551500	1.20322200	-3.03725000
H	-2.99005700	1.71952700	-2.81182700
C	-4.19983600	3.80070200	-0.34314600
C	-2.37912700	5.15231400	0.52200900
H	-1.95177800	6.12015300	0.78029500
C	-3.84605800	-2.09643900	-2.12946100
H	-3.34933400	-1.53150200	-2.91952700
C	-2.12681700	2.72166600	0.42117000
C	-3.44599100	2.62709700	-0.12987300
C	-0.33576300	-2.23334000	0.69752100
H	-0.95078500	-2.30701300	1.59625900
C	-0.24676000	1.61777600	1.17077000
H	0.26578300	0.67021600	1.34070000
C	-4.52498100	-2.56636500	2.56367000
C	1.19954400	-1.94905300	-1.56405900
C	-0.45396100	-0.31426200	-2.35338800
C	-1.59508500	3.97895300	0.75912100
C	0.29839500	-0.13590300	-3.53323900
C	-3.95481500	-1.88791900	1.46786800
C	-4.21923600	-2.34733000	0.13258600
C	1.52250200	-0.85195000	-3.70519000
H	2.11066800	-0.66464100	-4.60188700
C	0.00985500	-1.22699100	-1.34763700
C	1.95595500	-1.72223200	-2.75784500
H	2.89773700	-2.25642500	-2.86794500
C	2.64136200	2.30427000	-2.97370500
H	2.21321500	2.87792000	-3.79731500
C	1.89115500	2.02109900	-1.83625800
H	0.85669000	2.37696100	-1.75249300
C	2.46455700	1.30328800	-0.78884600
H	1.86373300	1.09386100	0.09429500
C	3.79637000	0.86650400	-0.78745000
C	4.52135200	1.17297700	-1.95415900
H	5.57579500	0.89386700	-2.00437300
C	3.96291300	1.86344700	-3.02730300
H	4.57457200	2.08762400	-3.90181600
C	6.00278900	0.63288000	0.72927100
C	7.03643000	-0.18879600	1.19994500
H	6.84112200	-1.25079500	1.36071300
C	8.31374400	0.29823100	1.46792300
H	9.08680600	-0.37999600	1.83026200
C	8.60639100	1.64335200	1.27099800
H	9.60482800	2.02850300	1.47586800
C	6.33436200	1.98556200	0.54022700
H	5.56712700	2.67055400	0.16914600
C	1.97813000	1.00565700	4.14778100
H	1.38906300	1.22284200	5.03884200
C	4.54883600	-1.53494000	0.19445800
C	3.86481900	1.47920000	2.70508400
H	4.74479500	2.09013600	2.49917200
C	3.09087100	1.78107100	3.82503800
H	3.37286200	2.61725600	4.46581300
C	3.57652300	0.40338000	1.84720900
C	2.43915000	-0.34434800	2.19900000
H	2.16422800	-1.19283500	1.57020900
C	5.02097700	-3.38788200	-1.35318400
H	5.27332400	-3.71592100	-2.36323300
C	4.85275200	-2.03045600	-1.08523700
H	4.97541800	-1.32159400	-1.90721200

C	4.45345600	-2.50956700	1.20418800
H	4.26560400	-2.18800800	2.23033700
C	1.65874100	-0.06992700	3.32306100
H	0.80128400	-0.70953700	3.55884800
C	7.60478300	2.48959200	0.80451100
H	7.81543500	3.54717000	0.64161800
C	4.60953200	-3.87334000	0.95696800
H	4.53491400	-4.58537500	1.77999900
C	4.88454000	-4.32625900	-0.33122500
H	5.02074300	-5.38871600	-0.53026800
B	4.47562700	0.08325800	0.49743000
C	-5.26242700	-3.88294600	-1.39700900
H	-5.89844300	-4.74528100	-1.59379800
C	-4.65888600	-3.20012200	-2.42958700
H	-4.79872400	-3.50175700	-3.46410300
C	-4.20517800	-2.09212100	3.85141000
H	-4.62252800	-2.59155000	4.72500500
C	-3.36370900	-1.01106600	3.99066000
H	-3.09124500	-0.62899500	4.97066900
C	-0.20262300	0.76916100	-4.48575300
H	0.35958800	0.93920000	-5.40346500
C	-1.38027400	1.44110100	-4.24074900
H	-1.78730100	2.15010500	-4.95672800
C	1.59638900	-2.86779000	-0.57261700
H	2.51568300	-3.44304100	-0.69916500
C	0.81057900	-3.02143500	0.55130000
H	1.10341000	-3.70847100	1.34183200
C	0.36884200	2.82542700	1.55031300
H	1.36291900	2.78829500	1.99598700
C	-0.30311200	4.00434200	1.32996000
H	0.14526900	4.96084400	1.59594300
C	-5.48983600	3.64471300	-0.88544700
H	-6.10348900	4.52619400	-1.06862200
C	-5.96272100	2.38300400	-1.17486000
H	-6.95621800	2.23368100	-1.58905000

5b

Charge = 1 Multiplicity = 1
E= -2863.518041
H= -2863.463660
G= -2863.605973
SPE= -2867.6831552

N	1.80262900	0.93216400	2.00629900
N	0.86694000	-1.31907000	0.78430300
N	3.96653400	-1.30761300	0.76719200
N	2.82548400	-1.20323700	-1.70123200
N	3.84498100	1.72082000	-0.20557300
N	1.29441200	1.58721300	-1.15234000
C	5.09746500	1.76959300	0.22499400
H	5.52806300	0.82778300	0.56631400
C	4.98460500	-4.20561400	-2.06794600
H	5.22649400	-4.95055800	-2.82429300
C	5.23185100	-3.28399300	0.15990000
C	5.55739100	-4.25504700	-0.83782000
H	6.26868800	-5.03983400	-0.58571600
C	3.28112100	5.27978200	-1.11406700
H	3.82096800	6.22508600	-1.09614800
C	2.23770000	-1.16653300	-2.88881800
H	1.51320600	-0.36823900	-3.05363700
C	2.25578600	2.03100000	2.60058300
H	3.11184900	2.51977200	2.13205000
C	3.94441000	4.10590000	-0.64394400
C	2.00703400	5.21229500	-1.57948200
H	1.50060500	6.10484700	-1.94370800
C	4.49004600	-1.36675800	1.98257400
H	4.16951500	-0.59310000	2.68309200
C	1.91572600	2.79842200	-1.13981600
C	3.26569200	2.86580800	-0.64915300
C	0.47550700	-2.47114400	0.25327400
H	0.99062400	-2.78579300	-0.65628600
C	0.07525700	1.51540000	-1.67208600
H	-0.39475100	0.53045900	-1.71056900
C	4.04345200	-3.18092800	-2.39956100

C	-0.83764200	-1.58845900	2.48868400
C	0.73809100	0.29481800	2.55747300
C	1.29841600	3.97157500	-1.61397800
C	0.09825300	0.76118100	3.72722500
C	3.71534100	-2.19559200	-1.44669200
C	4.31872300	-2.25024500	-0.13955400
C	-1.03421300	0.06471400	4.24896200
H	-1.52920800	0.46845900	5.13031700
C	0.25004200	-0.89841400	1.91922400
C	-1.48577500	-1.06621600	3.65142600
H	-2.35641200	-1.59880600	4.02932500
C	-2.29120800	3.12150800	2.14135600
H	-1.86810000	3.94713800	2.71478900
C	-1.47763300	2.30565200	1.36406800
H	-0.39959100	2.49518700	1.31567200
C	-2.03553000	1.25447200	0.63726400
H	-1.37272700	0.59185600	0.07744600
C	-3.41254000	1.00496500	0.58306000
C	-4.20051900	1.84148000	1.39363300
H	-5.28152100	1.69165400	1.40218600
C	-3.66040300	2.86509300	2.16731900
H	-4.31790700	3.48542900	2.77657800
C	-5.55305100	0.23701200	-0.86459300
C	-6.61222100	-0.67154700	-0.99275100
H	-6.47060600	-1.70399500	-0.66913400
C	-7.85168300	-0.30627000	-1.51266600
H	-8.64577800	-1.04924300	-1.58957500
C	-8.08103600	1.00024100	-1.92774700
H	-9.04984900	1.29121500	-2.33201200
C	-5.82375400	1.55006600	-1.28812900
H	-5.04060200	2.30765200	-1.19330800
C	-1.36937900	-0.84249300	-3.91405500
H	-0.74124500	-1.01119400	-4.79208500
C	-4.19371000	-1.56001400	0.58349400
C	-3.21939900	0.29471000	-2.84334100
H	-4.02766200	1.02423100	-2.91996900
C	-2.38230800	0.11461800	-3.94343700
H	-2.53944300	0.70937000	-4.84404200
C	-3.09182600	-0.44855700	-1.65578100
C	-2.05469700	-1.39627500	-1.66580800
H	-1.92702900	-2.01863100	-0.78282800
C	-4.63647000	-2.62914500	2.75153300
H	-4.82581200	-2.52146800	3.82155700
C	-4.40411700	-1.49749600	1.97065200
H	-4.40256500	-0.51944800	2.45756100
C	-4.23597700	-2.85239200	0.02890900
H	-4.11751000	-2.96549500	-1.05101000
C	-1.21719600	-1.60925400	-2.76148600
H	-0.46028500	-2.39944900	-2.72307100
C	-7.05493500	1.93259500	-1.81154700
H	-7.21660900	2.96464500	-2.12433800
C	-4.44965600	-3.99749200	0.79376400
H	-4.48520500	-4.97430200	0.31011400
C	-4.64943900	-3.89436500	2.16874100
H	-4.84000800	-4.78231400	2.77058300
B	-4.06316000	-0.20054800	-0.33527100
C	5.77777700	-3.30939500	1.45756600
H	6.48604300	-4.09338000	1.72297700
C	5.40614700	-2.35282800	2.37464300
H	5.80432100	-2.35209600	3.38548500
C	3.40063800	-3.11161800	-3.65180800
H	3.62584400	-3.86120500	-4.40946800
C	2.49453900	-2.10751500	-3.89761600
H	1.97319800	-2.03196700	-4.84811500
C	0.60740500	1.92650800	4.32406800
H	0.12827900	2.31705100	5.22104500
C	1.69152200	2.56456300	3.76404100
H	2.10670000	3.46828400	4.20157900
C	-1.25227100	-2.78514000	1.87348600
H	-2.12029800	-3.32103000	2.26247500
C	-0.55983000	-3.25077800	0.77883300
H	-0.85590900	-4.16984000	0.27886700
C	-0.62302700	2.63431300	-2.16083300
H	-1.63218500	2.48857200	-2.53875500
C	-0.01491100	3.86178500	-2.12014300

H	-0.52577000	4.75502300	-2.47721500
C	5.26826300	4.11857900	-0.16675700
H	5.81835700	5.05882200	-0.14833300
C	5.85286500	2.94879800	0.26262500
H	6.87592300	2.92650500	0.62766400
Mg	2.37638300	0.07229600	0.03651600

8a

Charge = 1 Multiplicity = 1
 E= -2263.233458
 H= -2263.190153
 G= -2263.307857
 SPE= -3603.9523627

Ni	0.97373800	0.16907100	-0.33524200
N	0.47869600	1.94142500	-0.97440100
N	1.68227700	1.18325500	1.24268600
N	3.03316400	0.03915200	-1.41079700
N	1.62393900	-1.44269600	0.40775000
C	3.69549700	0.75860300	-2.29749500
H	3.20892100	1.67436500	-2.64062100
C	5.40132500	-2.76615300	-0.84223700
H	6.37895500	-3.10078500	-1.18739800
C	-0.02827500	2.32269500	-2.14278900
H	-0.15816700	1.56091300	-2.90853200
C	4.86095400	-1.55626800	-1.38009800
C	4.71236200	-3.47837500	0.08891000
H	5.12722100	-4.39497900	0.50670900
C	2.85793200	-1.87224700	0.01286300
C	3.59390500	-1.10211500	-0.95146200
C	2.33912700	0.76936300	2.31726200
H	2.59408800	-0.28783300	2.36954500
C	0.95670000	-2.11438300	1.34141600
H	-0.00817400	-1.70807800	1.64475600
C	1.64676500	3.43450700	2.16431000
C	0.69956600	2.90523000	-0.03733700
C	3.42635500	-3.04704200	0.54637800
C	0.35244500	4.25548000	-0.21938300
C	0.62619700	5.18857600	0.83153000
H	0.33273500	6.22778100	0.68904500
C	1.35134900	2.49604500	1.15777200
C	1.24893700	4.79641100	1.97677000
H	1.46251300	5.51511000	2.76678000
C	0.61376900	-2.90739800	-2.20785600
H	1.35124000	-3.47605400	-2.77321400
C	-0.24782300	-3.55245700	-1.30578600
H	-0.16713100	-4.63268900	-1.17435000
C	-1.22106800	-2.85318200	-0.59956000
H	-1.89310300	-3.40833600	0.05738200
C	-1.42097400	-1.47012800	-0.76448200
C	-0.49327700	-0.82363500	-1.63301800
H	-0.82323300	0.13890500	-2.00742300
C	0.47237100	-1.54620000	-2.38818400
H	1.08726500	-1.01599800	-3.11811700
C	-4.06108300	-1.49908800	-0.19237800
C	-5.14079000	-1.19652700	0.65434500
H	-4.99401800	-0.47588700	1.46367800
C	-6.39539600	-1.77730300	0.49701200
H	-7.20504500	-1.51474700	1.17821700
C	-6.61908400	-2.68957300	-0.53369100
H	-7.59902600	-3.14759700	-0.66283100
C	-4.32230000	-2.40992600	-1.22553400
H	-3.52992200	-2.67155900	-1.93244100
C	-1.16305800	-0.80268200	4.23318000
H	-0.79222900	0.84696800	5.25678800
C	-2.94347300	0.79198000	-0.67186600
C	-2.46961900	-1.74205700	2.42656100
H	-3.12453400	-2.53908900	2.06881300
C	-1.97107400	-1.82135200	3.72615700
H	-2.23264900	-2.67279500	4.35518300
C	-2.18039600	-0.66435100	1.56715500
C	-1.35924400	0.33686800	2.11046000
H	-1.10086200	1.19940100	1.49236100
C	-3.52213100	2.08380700	-2.68794300

H	-3.68776300	2.10063500	-3.76637700
C	-3.13888600	0.89849300	-2.06408100
H	-3.03950000	0.00119800	-2.68210000
C	-3.18973900	1.96550400	0.05919100
H	-3.12153900	1.94338400	1.14843700
C	-0.86821300	0.28639300	3.41676600
H	-0.26189700	1.10878200	3.80355500
C	-5.57521200	-3.00059400	-1.39891500
H	-5.73487300	-3.70432200	-2.21639200
C	-3.57555800	3.16361200	-0.54785300
H	-3.77860000	4.03971400	0.07023900
C	-3.73584000	3.23432400	-1.92891700
H	-4.05967000	4.16073100	-2.40399800
B	-2.65587900	-0.68307600	-0.00929000
C	-0.23484000	4.61066500	-1.44890500
H	-0.54193900	5.64084900	-1.62614200
C	-0.40026700	3.64654400	-2.41607300
H	-0.83925900	3.87920400	-3.38250000
C	2.33932900	2.96209900	3.29644000
H	2.59128500	3.65120700	4.10200300
C	2.69391700	1.63271900	3.36514300
H	3.23274100	1.23459300	4.22117500
C	1.46896700	-3.27883900	1.93311300
H	0.87578000	-3.78173300	2.69343600
C	2.69452500	-3.75104700	1.52671100
H	3.11682900	-4.65934400	1.95649000
C	5.53952600	-0.76721200	-2.33158600
H	6.51849100	-1.08510400	-2.68986500
C	4.95974700	0.39323900	-2.79360000
H	5.45960100	1.02240300	-3.52620500

8b

Charge = 1 Multiplicity = 1
 E= -2292.442117
 H= -2292.398368
 G= -2292.518403
 SPE= -2295.7555332

N	-0.98759400	1.36769700	1.53120400
N	-0.81117800	2.21530400	-1.04587300
N	-1.91771800	-1.63218200	0.68021700
N	-3.19649200	0.15791800	-0.92367600
C	-0.86298500	1.78684000	3.88887700
H	-0.89281300	1.37650400	4.89424200
C	-0.66085400	3.12979300	3.66439400
H	-0.52667400	3.82146000	4.49512600
C	-0.62925700	3.62088400	2.34659300
C	-0.44467800	5.00625100	2.04176100
H	-0.33368400	5.70708800	2.86751500
C	-0.41096600	5.43736000	0.75547600
H	-0.27343300	6.49243000	0.52453900
C	-0.53798100	4.51438200	-0.32935800
C	-0.71133000	3.13994600	-0.06286400
C	-0.77850900	2.68732200	1.30168800
C	-0.48434100	4.91258000	-1.67616600
H	-0.35603000	5.96709400	-1.91717900
C	-0.57402700	3.96485400	-2.67109400
H	-0.51822100	4.23664600	-3.72138900
C	-1.85820100	-3.73089700	1.84697600
H	-1.28300600	-4.40565100	2.47503300
C	-3.13081800	-4.03496800	1.43016100
H	-3.61024500	-4.96974000	1.71874500
C	-3.83288200	-3.12143800	0.61853200
C	-5.16504000	-3.36663100	0.16136800
H	-5.64725900	-4.29881000	0.45132600
C	-5.81671000	-2.45873000	-0.60880700
H	-6.83385700	-2.64292600	-0.95032200
C	-5.17919900	-1.23863400	-0.99226100
C	-3.85935400	-0.97203900	-0.56921500
C	-3.17694400	-1.92472100	0.26524900
C	-5.81363600	-0.26869700	-1.79082400
H	-6.83330600	-0.44275400	-2.13232100
C	-5.14151400	0.88333400	-2.12758900
H	-5.60506800	1.65292900	-2.73824400

B	2.52746300	-0.82929000	-0.19677500
C	1.17753100	-1.43367100	-0.94257600
C	0.84139000	-2.79692800	-0.79481100
H	1.43465400	-3.39982500	-0.10373400
C	-0.93781300	-2.67456100	-2.43476000
H	-1.72504600	-3.15668500	-3.01190700
C	0.39109200	-0.72726300	-1.87852000
H	0.69105400	0.29410100	-2.12893400
C	3.80975100	-1.26573200	-1.11748400
C	3.74828200	-2.02931600	-2.28828400
H	2.78408400	-2.39317500	-2.65217600
C	6.13689800	-1.91255100	-2.60631700
H	7.03036800	-2.16166300	-3.17701100
C	5.08770100	-0.83114900	-0.72560000
H	5.18047400	-0.22408700	0.17868600
C	2.60758400	-1.52160400	1.28958000
C	1.70488000	-1.18375700	2.30766900
H	0.98697700	-0.38012200	2.12118500
C	2.59046600	-2.82841500	3.82588300
H	2.59419700	-3.32340100	4.79575300
C	3.50285400	-2.55491000	1.60181300
H	4.22949100	-2.86595300	0.85027900
C	2.51852200	0.81822700	-0.15235500
C	2.64808600	1.53409800	-1.35998700
H	2.76487900	0.97119000	-2.28961700
C	2.66557800	3.66874500	-0.23877400
H	2.73951400	4.75642700	-0.26875100
C	2.50084700	1.60622500	1.01035500
H	2.47147000	1.12146400	1.98694000
C	-1.03704900	0.94206000	2.78747100
H	-1.21541100	-0.12406700	2.93191800
C	-0.72633400	2.62294600	-2.30640800
H	-0.76437300	1.84782800	-3.07341900
C	-3.82766100	1.05153400	-1.67343500
H	-3.26666200	1.94985900	-1.93077300
C	-1.28461000	-2.51635000	1.44296100
H	-0.26917200	-2.26354700	1.75586000
C	-0.17215300	-3.40597200	-1.52296000
H	-0.37002300	-4.46956900	-1.38650800
C	-0.64373400	-1.33170600	-2.62057600
H	-1.19144500	-0.75142300	-3.36711300
C	1.68575400	-1.80720700	3.55409200
H	0.97003500	-1.48939900	4.31667900
C	3.49831600	-3.19752400	2.83830600
H	4.21520200	-3.99456800	3.03310700
C	6.23218300	-1.14771400	-1.44511000
H	7.20469400	-0.79399100	-1.10348800
C	4.88848800	-2.35011900	-3.02617300
H	4.79610900	-2.94686700	-3.93362600
C	2.70796600	2.92211900	-1.41488000
H	2.82610200	3.42370300	-2.37633900
C	2.57835100	2.99918900	0.97616700
H	2.59571700	3.56201200	1.91104900
Mg	-1.09753100	0.16748900	-0.26723700

TS8a-11a

Charge = 1 Multiplicity = 1

E= -2263.216110

H= -2263.172980

G= -2263.289940

SPE= -3603.931177

Imaginary frequency = -153.63

Ni	0.61718600	0.32882400	0.39866400
N	-0.09968800	2.11981500	-0.04095500
N	1.21643900	1.26971600	2.07677400
N	2.80330300	0.53942900	-0.66746600
N	1.53301000	-1.22998700	1.02053000
C	3.36436600	1.35267400	-1.54153900
H	2.86655400	2.31249000	-1.69979400
C	5.17595100	-2.31829900	-0.73510500
H	6.10302900	-2.60391400	-1.23148100
C	-0.64725700	2.59545600	-1.15208700

H	-0.72043600	1.92918000	-2.00001800
C	4.58236800	-1.05968900	-1.06544800
C	4.60672600	-3.13225400	0.19221800
H	5.06868600	-4.08205800	0.45938800
C	2.74390300	-1.55560700	0.49303800
C	3.38098500	-0.65737600	-0.43727400
C	1.93950200	0.82834100	3.09737400
H	2.38382900	-0.16033400	3.00170700
C	0.97496400	-2.01795600	1.93480500
H	0.01021300	-1.69880700	2.32648100
C	0.83037600	3.34021800	3.29692900
C	-0.01430000	2.97789700	1.01745600
C	3.37889800	-2.77155000	0.83319800
C	-0.53565700	4.28440500	1.00623200
C	-0.40829400	5.09742900	2.17773800
H	-0.83812600	6.09823700	2.15942500
C	0.68431000	2.51319700	2.16540200
C	0.24371500	4.64443000	3.28271500
H	0.34518800	5.27248300	4.16676500
C	1.25691600	-2.56032400	-2.87096900
H	1.85112900	-3.17861000	-3.54336600
C	0.66532900	-3.11869200	-1.73643300
H	0.76918500	-4.18359400	-1.52843000
C	-0.07006400	-2.31379100	-0.88102200
H	-0.52982100	-2.79108500	-0.01453600
C	-0.28847600	-0.92014700	-1.08433200
C	0.30658400	-0.42860800	-2.27385800
H	0.22142600	0.62206200	-2.54228200
C	1.06097100	-1.21034700	-3.14702100
H	1.50405600	-0.75941700	-4.03503700
C	-2.99178900	-1.90570800	-1.43576800
C	-4.29706500	-2.21916800	-1.01307200
H	-4.69333100	-1.74821400	-0.10982100
C	-5.11374000	-3.10441800	-1.71002600
H	-6.11509000	-3.32302300	-1.33939100
C	-4.65516600	-3.70338600	-2.88166000
H	-5.28876100	-4.39680000	-3.43303200
C	-2.57256900	-2.50469300	-2.63003100
H	-1.59006300	-2.26915400	-3.04115400
C	-2.14004800	-1.50680100	3.82610800
H	-2.12768300	-1.69371200	4.89930000
C	-2.87452300	0.63433300	-1.12199300
C	-2.45430200	-2.28252700	1.55676700
H	-2.69815200	-3.10652400	0.88397000
C	-2.42296200	-2.53493100	2.92962200
H	-2.63404100	-3.53871400	3.29889600
C	-2.20989500	-1.00831600	1.01218000
C	-1.93573900	0.00351600	1.95102700
H	-1.76510400	1.02096900	1.59893300
C	-3.58376800	2.00010300	-3.03655400
H	-3.57395000	2.17356900	-4.11298300
C	-2.88769600	0.92169400	-2.50203600
H	-2.35430500	0.25558600	-3.18514100
C	-3.65233900	1.47929400	-0.31406200
H	-3.74564200	1.27313200	0.75258800
C	-1.89726400	-0.22763100	3.32573700
H	-1.69301200	0.59835800	4.01014000
C	-3.38075000	-3.39109900	-3.34284900
H	-3.01039300	-3.83513500	-4.26702700
C	-4.36675300	2.55993700	-0.83655500
H	-4.97426100	3.17588800	-0.17288800
C	-4.32827600	2.83417600	-2.19965700
H	-4.89687900	3.66670700	-2.61319900
B	-2.22597100	-0.74996100	-0.59312800
C	-1.13430300	4.73624000	-0.18689200
H	-1.55313700	5.74085300	-0.23702800
C	-1.16152700	3.89743900	-1.27245900
H	-1.60577300	4.19538200	-2.21844400
C	1.57670000	2.82743600	4.37482700
H	1.71132300	3.42870300	5.27356200
C	2.14198700	1.57616900	4.26666900
H	2.74135000	1.15459700	5.06961000
C	1.56641600	-3.21224800	2.35924700
H	1.05851700	-3.81928800	3.10512600
C	2.75870400	-3.60013400	1.78858500

H	3.23318200	-4.54165100	2.06531100
C	5.15037300	-0.17089600	-1.99996600
H	6.07110200	-0.44973400	-2.51244400
C	4.53825300	1.03743700	-2.24851700
H	4.95269300	1.74541700	-2.96258000

TS8b-11b

Charge = 1 Multiplicity = 1

E= -2292.413115

H= -2292.369247

G= -2292.489735

SPE= -2295.7243764

Imaginary frequency = -159.29

N	2.38753800	0.49896700	1.33869200
N	2.65747300	-0.43189500	-1.21016900
N	-0.34991300	2.08229700	0.92155500
N	0.51905500	1.98255800	-1.66086100
C	3.31071700	0.91754400	3.52331100
H	3.14600800	1.31709900	4.52002600
C	4.51107700	0.35685300	3.15934400
H	5.33986900	0.29166600	3.86324700
C	4.67216100	-0.14593200	1.85638200
C	5.89012400	-0.75769200	1.42744300
H	6.71580800	-0.81745900	2.13457900
C	6.00598500	-1.26480000	0.17527000
H	6.92708600	-1.74605200	-0.14970400
C	4.91887300	-1.18436800	-0.74814800
C	3.71268200	-0.55374300	-0.37080300
C	3.57680200	-0.04441700	0.96849000
C	4.99586100	-1.72660600	-2.04445300
H	5.91166300	-2.22305000	-2.36284800
C	3.90857800	-1.63450600	-2.87760500
H	3.91780500	-2.06011800	-3.87717100
C	-1.37449900	3.28109700	2.74106600
H	-1.73065500	3.24551500	3.76693200
C	-1.46104700	4.42495800	1.98544700
H	-1.88315500	5.34256500	2.39357300
C	-1.03041500	4.39784500	0.64786000
C	-1.17735600	5.52424400	-0.21916900
H	-1.61330600	6.43558200	0.18721500
C	-0.80502000	5.45243200	-1.52109800
H	-0.93464200	6.30272200	-2.18861500
C	-0.23223500	4.25423000	-2.04920500
C	-0.03516000	3.13511400	-1.21105600
C	-0.46616100	3.19753800	0.16118500
C	0.13832900	4.13293500	-3.40020700
H	-0.01029500	4.97731300	-4.07224300
C	0.67591600	2.95142700	-3.85365200
H	0.96634200	2.81886000	-4.89193300
B	-2.24473700	-1.36364100	0.33724400
C	-2.72481300	0.10156400	-0.08617900
C	-3.41554700	0.89480800	0.84431000
H	-3.55555700	0.51840900	1.85967400
C	-3.76230200	2.65917700	-0.76704400
H	-4.16137000	3.63901500	-1.02746900
C	-2.59822600	0.63858900	-1.37816700
H	-2.11332300	0.05142900	-2.15656700
C	-2.85740200	-2.59527000	-0.44402600
C	-3.76905600	-2.43552900	-1.49754000
H	-4.09214200	-1.43287200	-1.77928000
C	-3.90075900	-4.81548800	-1.84448700
H	-4.29974300	-5.67145900	-2.38681700
C	-2.51048700	-3.91208300	-0.09883300
H	-1.81227100	-4.07752800	0.72325400
C	-1.95476100	-1.57574900	1.89207600
C	-0.80966900	-1.18408400	2.59582300
H	0.04650500	-0.78488900	2.04393500
C	-1.74845300	-1.83742800	4.71486400
H	-1.66804400	-1.94486700	5.79505500
C	-2.99405100	-2.11810200	2.66590600
H	-3.90337400	-2.45388400	2.16515600
C	-0.07868800	-1.65117600	-0.60350500

C	-0.28260100	-1.92860600	-1.97390500
H	-0.83895700	-1.22287400	-2.59709800
C	0.85236300	-4.04878000	-1.86627800
H	1.18769800	-4.97003300	-2.34053600
C	0.64278000	-2.65148200	0.08541700
H	0.83392100	-2.53949200	1.15661200
C	2.27978200	0.96205400	2.57822400
H	1.32170900	1.39745900	2.85239200
C	2.76172000	-0.97664300	-2.41250200
H	1.87367000	-0.93715800	-3.04241400
C	0.85539200	1.90595600	-2.94137800
H	1.29775100	0.96866100	-3.27138100
C	-0.83262300	2.12861400	2.15829700
H	-0.81224200	1.19538000	2.72387900
C	-3.93316400	2.14468500	0.51481200
H	-4.47309300	2.72141000	1.26593600
C	-3.09082300	1.89504100	-1.71687500
H	-2.96180800	2.27155900	-2.73287000
C	-0.69283700	-1.31140700	3.97733500
H	0.23067600	-1.01192800	4.47577000
C	-2.90183500	-2.23935900	4.04983600
H	-3.73435900	-2.66124700	4.61077800
C	-3.01299000	-5.00680200	-0.78836100
H	-2.71531300	-6.01464500	-0.50179800
C	-4.28466200	-3.52530800	-2.19180400
H	-4.99427400	-3.36681600	-3.00290500
C	0.14571700	-3.09734600	-2.59684400
H	-0.08136800	-3.27324700	-3.64842600
C	1.11016200	-3.81608600	-0.51869700
H	1.65509000	-4.55564000	0.06776400
Mg	0.69817000	0.35482000	-0.18264300

11a

Charge = 1 Multiplicity = 1

E= -2263.275533

H= -2263.230938

G= -2263.355200

SPE= -3603.987167

Ni	-1.10890300	-0.03510100	0.04977100
N	-0.17470600	1.48415500	0.79684700
N	-1.97336100	1.35484700	-1.12412600
N	-3.24469400	-0.08657600	1.29529700
N	-2.04388200	-1.49004900	-0.76391600
C	-3.80047300	0.56838500	2.29603400
H	-3.25426500	1.44055800	2.66495300
C	-5.75341900	-2.76600800	0.72685700
H	-6.70794000	-3.09370600	1.13784300
C	0.76584300	1.52302400	1.73317000
H	1.08462700	0.56770800	2.14275100
C	-5.11354900	-1.62591800	1.30682800
C	-5.18719800	-3.42026500	-0.31979800
H	-5.67660200	-4.28335200	-0.76969400
C	-3.25482000	-1.89143800	-0.28986400
C	-3.87148100	-1.17327500	0.80257600
C	-2.85807100	1.23740900	-2.10208100
H	-3.16977200	0.22440600	-2.36139200
C	-1.50108600	-2.12904300	-1.79617200
H	-0.52973500	-1.76313100	-2.12951200
C	-2.02982300	3.77075000	-1.39567500
C	-0.58554700	2.66720500	0.26087000
C	-3.92963600	-2.99787300	-0.85753800
C	-0.08407800	3.91642100	0.66612400
C	-0.58547800	5.10084800	0.03442800
H	-0.19642700	6.06476000	0.36153500
C	-1.56122500	2.59623400	-0.77635800
C	-1.51840700	5.03357900	-0.95553400
H	-1.88822400	5.94125500	-1.43142800
C	1.18242400	-3.23288100	2.65287000
H	1.70374900	-3.97645600	3.25409000
C	1.49190700	-3.07547900	1.30400900
H	2.26715300	-3.68764600	0.84053000
C	0.82028500	-2.11991500	0.53766100
H	1.10001400	-2.01201300	-0.51380700

C	-0.17481000	-1.30964500	1.09396200
C	-0.47768900	-1.48339800	2.44978400
H	-1.24778600	-0.86716500	2.92014600
C	0.19813100	-2.42863000	3.22510600
H	-0.05407400	-2.54267000	4.27971700
C	4.23691500	-1.51177500	-1.07178700
C	4.33879200	-1.83551800	-2.43951000
H	3.97629900	-1.12972600	-3.18747400
C	4.93315700	-3.01800400	-2.86778700
H	5.01627200	-3.23213900	-3.93250300
C	5.42982000	-3.92342400	-1.93227800
H	5.89202300	-4.85240000	-2.26370800
C	4.78532600	-2.42992600	-0.15487400
H	4.76258700	-2.19778600	0.91064900
C	0.81600900	2.13854500	-3.08159400
H	0.13732000	2.71313800	-3.71321300
C	4.04841700	0.41571800	0.81674900
C	1.74358700	0.02345100	-2.38839900
H	1.77379700	-1.06360800	-2.48852500
C	0.84996700	0.74823800	-3.17161000
H	0.18970300	0.23202400	-3.87057900
C	2.61124100	0.65050100	-1.47357300
C	2.52069700	2.05035700	-1.37658800
H	3.15330800	2.57807200	-0.66136200
C	3.98697200	0.39637400	3.25788700
H	3.61665000	-0.05471700	4.17922700
C	3.59468100	-0.13099100	2.02855900
H	2.91612500	-0.98776700	2.01420600
C	4.93355300	1.50353500	0.89356300
H	5.33731900	1.93826600	-0.02370000
C	1.65709400	2.78901700	-2.18145100
H	1.63842500	3.87685700	-2.10554800
C	5.35484900	-3.62706400	-0.57181800
H	5.76061100	-4.32282000	0.16149300
C	5.33922900	2.02865300	2.11914900
H	6.03982900	2.86264300	2.14528700
C	4.86094300	1.48091700	3.30809900
H	5.18184900	1.88529000	4.26733300
B	3.61809500	-0.16682800	-0.58250500
C	0.91046300	3.92046700	1.66520800
H	1.33553900	4.86590700	2.00195600
C	1.33884500	2.72207700	2.18814600
H	2.12596600	2.67053000	2.93850600
C	-2.97392500	3.61366800	-2.42913200
H	-3.36722300	4.49250900	-2.93988000
C	-3.38396300	2.34570400	-2.78492600
H	-4.10811300	2.19064500	-3.58103500
C	-2.11759900	-3.21397800	-2.42824300
H	-1.62657500	-3.69740400	-3.26888600
C	-3.32986600	-3.65561500	-1.94742400
H	-3.83441900	-4.50995000	-2.39817500
C	-5.67866500	-0.90651000	2.37871800
H	-6.63177400	-1.23169200	2.79580400
C	-5.02300200	0.19428100	2.88190200
H	-5.43294700	0.76906400	3.70917600

11b

Charge = 1 Multiplicity = 1
E= -2292.431399
H= -2292.386425
G= -2292.511922
SPE= -2295.7393169

N	3.13869700	-0.58210100	1.25036300
N	2.10264400	-1.85788800	-0.93660700
N	0.85865800	1.95628600	0.94355100
N	2.34577400	1.29727200	-1.21772300
C	4.72399200	-0.44849800	3.04373900
H	5.09519600	0.10902500	3.89907200
C	5.28715600	-1.64575800	2.66740300
H	6.12444300	-2.06938900	3.22073700
C	4.77420400	-2.34122800	1.55665500
C	5.30091600	-3.59888500	1.12603700
H	6.13732000	-4.02612100	1.67691900

C	4.76240100	-4.25091300	0.06459100
H	5.15553200	-5.21456400	-0.25548400
C	3.66244600	-3.69146300	-0.65778000
C	3.13275300	-2.44020000	-0.27579100
C	3.69052500	-1.75854400	0.86559800
C	3.06708000	-4.34163200	-1.75503600
H	3.45011500	-5.31073000	-2.07251100
C	2.00803000	-3.75156900	-2.40536500
H	1.52070800	-4.23293600	-3.24864500
C	-0.32219000	3.57283700	2.26188200
H	-1.00824300	3.75608200	3.08423900
C	0.19556900	4.60348100	1.51285700
H	-0.06155400	5.63957900	1.73061900
C	1.06345900	4.31818700	0.44077000
C	1.62995000	5.33164500	-0.39458000
H	1.40367100	6.37344100	-0.17234600
C	2.42877500	5.00411300	-1.44297100
H	2.85969100	5.77699100	-2.07753100
C	2.71002200	3.63575800	-1.75065600
C	2.16608300	2.61171600	-0.94693700
C	1.34900800	2.96230700	0.18430700
C	3.49543200	3.24553400	-2.85172300
H	3.93520400	4.00920900	-3.49231700
C	3.68988400	1.90752800	-3.10855300
H	4.28884300	1.57387900	-3.95142000
B	-3.65018200	0.01939100	-0.57322300
C	-2.42295900	0.66239600	-1.31978100
C	-2.13722800	2.02794900	-1.16191400
H	-2.72593700	2.61025400	-0.45156000
C	-0.39299200	1.92963100	-2.82218000
H	0.36757700	2.42343100	-3.42799000
C	-1.62867300	-0.05509800	-2.23256300
H	-1.83236800	-1.11632800	-2.38760800
C	-4.48588700	-1.10841900	-1.24884400
C	-4.57813900	-1.25200400	-2.64458700
H	-4.06002300	-0.54150500	-3.28971800
C	-6.01828900	-3.16632800	-2.41481000
H	-6.61175700	-3.96025800	-2.86553300
C	-5.19867500	-2.02938200	-0.45890100
H	-5.15325100	-1.93792700	0.62704700
C	-4.08612700	0.58440400	0.81574900
C	-3.14266500	0.80462600	1.83042500
H	-2.10471300	0.52719500	1.64104000
C	-4.85130900	1.59291700	3.33151400
H	-5.15046900	1.97548600	4.30622600
C	-5.42817200	0.87836400	1.10369700
H	-6.18850100	0.70270600	0.34172000
C	-0.20146400	-1.19610000	1.25614700
C	-1.22997000	-2.00467200	0.73789900
H	-1.34113200	-2.11456500	-0.34713500
C	-2.06121200	-2.58450400	2.92735500
H	-2.77587300	-3.10645100	3.56181500
C	-0.14583600	-1.14729800	2.66342000
H	0.64490000	-0.56429600	3.15726800
C	3.64113400	0.04405300	2.30359100
H	3.15889900	0.98225800	2.58247900
C	1.55845400	-2.50181500	-1.95819500
H	0.71964200	-2.00403300	-2.44870300
C	3.08675600	0.96529700	-2.26381700
H	3.20415500	-0.10257700	-2.45061400
C	0.04715500	2.25629100	1.94735200
H	-0.33292100	1.41054700	2.52313200
C	-1.15246100	2.66235400	-1.91638000
H	-0.98672900	3.73509800	-1.80986200
C	-0.61652300	0.56012000	-2.96279000
H	-0.03069900	-0.01262300	-3.68416100
C	-3.51783100	1.27942900	3.08059400
H	-2.77202600	1.38578700	3.87051800
C	-5.80566000	1.39830200	2.33710500
H	-6.85025000	1.63634300	2.53082100
C	-5.94240600	-3.05418900	-1.02900800
H	-6.47394400	-3.76158800	-0.39473300
C	-5.34195300	-2.25764300	-3.22374100
H	-5.41335600	-2.33415400	-4.30751400
C	-2.14108400	-2.68800000	1.54162400

H -2.92137300 -3.29646800 1.08209800
C -1.05166800 -1.81278600 3.49145700
H -0.96720500 -1.73357100 4.57583200
Mg 1.28400600 -0.10442000 0.18697000

9a

Charge = 1 Multiplicity = 3
E= -1544.270792
H= -1544.242592
G= -1544.331869
SPE = -2883.790866

C 0.73296700 2.37084500 -0.37037800
C 0.07945900 3.40465600 -1.06164300
C 1.95160200 2.69591800 0.24315300
C 0.61644900 4.69212500 -1.14698100
H -0.87887300 3.21406100 -1.55641400
C 2.49046600 3.98121800 0.18392800
H 2.50678900 1.93065800 0.79578600
C 1.82344200 4.98444800 -0.51771900
H 0.08808500 5.46802300 -1.70177400
H 3.43411400 4.20202600 0.68368200
H 2.24235600 5.98842500 -0.57181100
C -2.89044400 0.08685300 0.06868700
C -2.29006000 2.11550500 0.99177600
C -4.22845300 0.21709900 0.49237800
C -2.48299400 -1.08047200 -0.66375000
C -3.59743800 2.33430000 1.45752600
H -1.49177200 2.84130800 1.15711400
C -4.56485400 1.38534300 1.20639000
C -5.16626200 -0.82067600 0.18672700
C -3.42955700 -2.08687300 -0.94761000
H -3.82850700 3.24588300 2.00300700
H -5.58913500 1.52667200 1.55114600
C -4.78181500 -1.92806900 -0.50379800
H -6.19730800 -0.70478100 0.51907300
C -2.97844300 -3.21038100 -1.66847600
C -0.79512900 -2.22626000 -1.72874700
H -5.49944900 -2.71473900 -0.73405700
H -3.67824200 -4.01011100 -1.91029900
C -1.65914000 -3.28244700 -2.05898200
H 0.25436700 -2.25318700 -2.02551600
H -1.28055500 -4.13524900 -2.61697200
N -1.94975300 1.02514400 0.32054100
N -1.18846000 -1.15605900 -1.05567600
C 2.45454600 -0.99209500 -0.18299800
C 2.33867700 -0.15863500 -2.32894400
C 3.71924400 -1.57350600 -0.40801200
C 1.85263400 -1.07263900 1.11837500
C 3.59465900 -0.69771600 -2.65044200
H 1.77201600 0.42626700 -3.05515100
C 4.27978500 -1.41322400 -1.69102600
C 4.36751000 -2.27428200 0.65960800
C 2.52060400 -1.75773000 2.15399000
H 4.01046500 -0.54258500 -3.64287100
H 5.25621300 -1.84574200 -1.90835500
C 3.78903500 -2.36745600 1.88758600
H 5.34034700 -2.72654700 0.46986600
C 1.89688900 -1.78366700 3.41664600
C 0.10920600 -0.47410000 2.50386300
H 4.29022100 -2.89671200 2.69724800
H 2.37922900 -2.30407000 4.24376000
C 0.69027000 -1.14113300 3.59306200
H -0.83776600 0.05596000 2.61188000
H 0.18880500 -1.13619100 4.55755400
N 0.66710400 -0.44239300 1.30350400
N 1.77832500 -0.31941700 -1.14094700
Ni -0.01032300 0.53778600 -0.39157100

9b

Charge = 1 Multiplicity = 1
E= -1573.431884

H= -1573.403745
G= -1573.492107
SPE= -1575.5518212

C 0.31147800 2.51415400 -0.35593400
C -0.71717100 3.47456500 -0.38813000
C 1.61673800 3.03727000 -0.42974000
C -0.47514500 4.84293200 -0.49259200
H -1.76312700 3.15059700 -0.33544400
C 1.88449700 4.40166500 -0.52137200
H 2.47819200 2.35742700 -0.41054500
C 0.83302700 5.31151100 -0.55694500
H -1.30715800 5.54687600 -0.52393100
H 2.91398900 4.75786800 -0.56681500
H 1.03183800 6.37955200 -0.63431800
C -2.94253600 -0.25553300 0.35961400
C -2.27789300 1.28615900 1.93813700
C -4.27178900 -0.25074100 0.82923900
C -2.59386200 -1.06094400 -0.78121600
C -3.57179800 1.36450600 2.47370800
H -1.46665900 1.90042500 2.33261500
C -4.56526200 0.58769900 1.92216200
C -5.25088300 -1.07398200 0.18967500
C -3.58416800 -1.86062600 -1.38837500
H -3.77283500 2.03329100 3.30592900
H -5.58181000 0.61945700 2.31253600
C -4.91853500 -1.85189600 -0.87243700
H -6.27026900 -1.06084500 0.57209500
C -3.20013100 -2.63457500 -2.49953000
C -0.99163000 -1.74838800 -2.28569500
H -5.66502000 -2.47789400 -1.35860200
H -3.93897700 -3.26497500 -2.99284600
C -1.90072900 -2.58325300 -2.94866300
H 0.04376600 -1.68366400 -2.62004000
H -1.57308900 -3.16864800 -3.80313500
N -1.96689800 0.48868000 0.92685500
N -1.31737200 -1.00493800 -1.23782200
C 2.74117400 -0.79480200 -0.29346400
C 2.25205200 0.09376700 -2.36065500
C 4.07500800 -1.06589900 -0.66276300
C 2.30458800 -1.08092500 1.04891600
C 3.55823700 -0.12665600 -2.81937800
H 1.51110100 0.57976400 -2.99800900
C 4.46617500 -0.71636800 -1.96941600
C 4.96359300 -1.66649500 0.28328400
C 3.20664200 -1.67518700 1.95591700
H 3.83595800 0.17130500 -3.82648300
H 5.48994100 -0.90708700 -2.28910000
C 4.54360200 -1.96721100 1.53875800
H 5.98641300 -1.87554800 -0.02605200
C 2.73686500 -1.94290900 3.25539100
C 0.62976200 -1.00864500 2.62888300
H 5.22131900 -2.42521600 2.25738900
C 3.40605000 -2.40404100 3.98079900
C 1.44413100 -1.61523200 3.59387900
H -0.39449100 -0.72327100 2.86985600
H 1.05270500 -1.80819300 4.58871600
N 1.03709000 -0.74506100 1.39560800
N 1.84679400 -0.24607400 -1.14646700
Mg -0.02261300 0.43756800 -0.14578000

12a

Charge = 1 Multiplicity = 1
E= -1620.650006
H= -1620.618879
G= -1620.711910
SPE= -2960.273601

H -5.26934600 -2.30535500 1.86181400
C -4.49140100 -1.87577600 1.23123800
C -3.23069100 -1.55217300 1.82426000
C -4.71035700 -1.66123300 -0.09201300
C -2.19872700 -0.98975500 1.03666000
C -2.95364300 -1.78006100 3.18705300

C	-3.69431500	-1.09014000	-0.92296500
H	-5.66627300	-1.91681800	-0.54790200
N	-0.98187100	-0.69788700	1.53860600
C	-2.44757000	-0.72940300	-0.36255800
C	-1.71218200	-1.46511000	3.69223700
H	-3.72793800	-2.20578900	3.82527800
C	-3.89079400	-0.86943200	-2.29938000
C	-0.75192100	-0.92651600	2.81742000
N	-1.47522900	-0.15757300	-1.12228000
H	-1.46862700	-1.62818400	4.73956200
C	-2.87804400	-0.32169000	-3.05442800
H	-4.84510700	-1.13875100	-2.75165800
H	0.24631000	-0.67091100	3.18183700
C	-1.67919600	0.03206600	-2.42346400
H	-2.99471500	-0.14577100	-4.12072300
H	-0.84990300	0.47573800	-2.97590600
C	3.55104800	2.39997200	1.34563500
C	4.49594400	1.39888300	1.29640800
C	4.14413100	0.14739500	0.75347500
C	2.82418100	-0.00469900	0.29109800
C	2.25746200	2.16042700	0.85591200
C	5.04806000	-0.95920300	0.64604200
C	2.40813400	-1.24677900	-0.27409800
C	3.31367200	-2.31868900	-0.37835600
C	4.65134400	-2.14226000	0.10139000
C	2.82987500	-3.50757800	-0.95984800
H	3.49261500	-4.36614700	-1.06512900
C	1.52160900	-3.56606100	-1.38982500
C	0.69580200	-2.44025600	-1.23510600
H	6.06736500	-0.83163900	1.00881500
H	3.78720300	3.37906300	1.75477200
H	5.50744400	1.56249300	1.66741800
H	1.49428700	2.93719100	0.87961800
H	5.34828000	-2.97570200	0.02110300
H	1.11873500	-4.46752900	-1.84483200
H	-0.34398000	-2.46170000	-1.56388200
N	1.12269700	-1.31250100	-0.69157200
N	1.89267700	0.98962200	0.33982600
C	-0.59024800	2.13404300	-0.13011700
C	-0.58312000	3.04628400	-1.19068200
H	-0.22744400	2.74442500	-2.17996100
C	-1.51328600	4.77294100	0.22383500
H	-1.86497100	5.79407700	0.36256200
C	-1.09376300	2.55871300	1.10440600
H	-1.11750100	1.87030300	1.95187100
C	-1.03214200	4.35781400	-1.01560900
H	-1.00898000	5.05494900	-1.85337100
C	-1.54991900	3.86666300	1.28166100
H	-1.93470600	4.17817100	2.25296000
O	1.45407200	0.82307500	-3.11273400
H	1.91718600	0.96927400	-3.94970200
H	1.70981400	1.56411700	-2.54391500
Ni	0.16607600	0.41707000	-0.33651900

12b

Charge = 1 Multiplicity = 1
 E= -1649.818048
 H= -1649.787062
 G= -1649.880431
 SPE= -1652.042514

H	-4.03232800	-2.97571700	3.03201400
C	-3.59458500	-2.50205200	2.15462300
C	-2.36783900	-1.78342800	2.31085100
C	-4.20522900	-2.58301700	0.94511000
C	-1.77253300	-1.15955000	1.19344900
C	-1.71398800	-1.65403200	3.55038000
C	-3.63548300	-1.95607900	-0.20706400
H	-5.14413200	-3.12254200	0.83038100
N	-0.62169900	-0.45172800	1.28188500
C	-2.41675200	-1.25381200	-0.09254300
C	-0.54599700	-0.93217200	3.63101300
H	-2.14580600	-2.12337200	4.43358300
C	-4.24203400	-1.99792400	-1.47662100

C	-0.03810000	-0.34344300	2.46457400
N	-1.82955000	-0.64152400	-1.14686600
H	-0.02088200	-0.80756200	4.57397800
C	-3.64271200	-1.36263400	-2.53972100
H	-5.18487900	-2.52962200	-1.60008100
H	0.88019300	0.24476400	2.49872000
C	-2.43033300	-0.69116800	-2.32670600
H	-4.09070300	-1.37019800	-3.52954300
H	-1.92292700	-0.17216900	-3.14058200
C	3.49536000	2.50823700	1.43997500
C	4.47599700	1.54762300	1.34557500
C	4.21317100	0.34495700	0.65994900
C	2.92841800	0.19092200	0.10032800
C	2.24720900	2.26452200	0.84489500
C	5.17900500	-0.69981300	0.51204400
C	2.60161700	-1.01943300	-0.60795000
C	3.58093300	-2.02622600	-0.74270900
C	4.87555700	-1.83811600	-0.16390000
C	3.22200900	-3.18415500	-1.45868600
H	3.95226600	-3.98269700	-1.58498200
C	1.95795000	-3.28976800	-1.99116300
C	1.05399800	-2.23485500	-1.79607600
H	6.16590100	-0.56023600	0.95067700
H	3.67032700	3.44534500	1.96129900
H	5.45730100	1.70320900	1.79278200
H	1.43683400	2.99551500	0.88911300
H	5.61432700	-2.62977900	-0.27927700
H	1.65208300	-4.16820500	-2.55277400
H	0.04289600	-2.28883400	-2.20202900
N	1.35614700	-1.13459900	-1.12594800
N	1.97205600	1.14263600	0.19534700
C	-0.99101200	2.54851700	-0.39242900
C	-0.41622400	3.74604900	-0.86885800
H	0.58538600	3.72407900	-1.32492700
C	-2.29240300	5.09257400	-0.18971400
H	-2.78989200	6.05801600	-0.11020800
C	-2.26397000	2.71026600	0.18983300
H	-2.79002800	1.83255700	0.58399300
C	-1.03840300	4.99363600	-0.77841300
H	-0.54403800	5.88567400	-1.16423900
C	-2.90607800	3.94102000	0.29822700
H	-3.89048500	4.00802200	0.76241200
Mg	-0.04961200	0.61302600	-0.62563000
O	0.12562000	1.17994600	-2.73955700
H	0.92067100	1.31234300	-3.27375300
H	-0.27568400	2.06214800	-2.60310200

TS12a-13a

Charge = 1 Multiplicity = 1
 E= -1620.598950
 H= -1620.569380
 G= -1620.658633
 SPE= -2960.219635
 Imaginary frequency = -1555.56

H	-4.55744600	-0.93950200	3.19639900
C	-4.02838000	-0.93758900	2.24410600
C	-2.62851300	-0.63862700	2.24645500
C	-4.68471600	-1.19355900	1.08260200
C	-1.91451200	-0.60875000	1.02671700
C	-1.92640800	-0.35142300	3.43211400
C	-3.98089600	-1.22232000	-0.16217600
H	-5.75481400	-1.39915400	1.08184900
N	-0.61066600	-0.22086700	0.98596600
C	-2.59021000	-0.97163700	-0.19610300
C	-0.58488400	-0.04524100	3.37498800
H	-2.45534800	-0.37672600	4.38464900
C	-4.61526300	-1.50622800	-1.38873900
C	0.03187000	0.03012900	2.12148900
N	-1.86320600	-1.05934600	-1.32867600
H	-0.01014400	0.16861000	4.27241400
C	-3.87084200	-1.55406400	-2.54641500
H	-5.68968000	-1.68963100	-1.40455000

H	1.07213200	0.34044400	2.02156200
C	-2.48318200	-1.34021000	-2.46001500
H	-4.33207400	-1.76882000	-3.50765700
H	-1.85513500	-1.39503400	-3.35210900
C	4.34124600	2.77098700	0.65034200
C	5.22415900	1.72369700	0.52745300
C	4.74586000	0.44256100	0.18595700
C	3.35112300	0.29372100	-0.01742200
C	2.97489700	2.51375700	0.44613200
C	5.62417700	-0.67578800	0.04623200
C	2.83416100	-1.00410200	-0.40413000
C	3.73848100	-2.08819200	-0.52656500
C	5.13591300	-1.89623600	-0.29025700
C	3.22853400	-3.34763700	-0.89447100
H	3.91264900	-4.19040000	-0.99164800
C	1.88206400	-3.49519000	-1.12815600
C	1.05551900	-2.37300600	-0.99946100
H	6.69009900	-0.52672100	0.21557600
H	4.67822400	3.77353700	0.90285800
H	6.29295800	1.86758800	0.68555300
H	2.24838500	3.32411200	0.54187900
H	5.79910700	-2.75398600	-0.39622400
H	1.45265500	-4.45147500	-1.41546900
H	-0.01568200	-2.43380000	-1.18958000
N	1.50659800	-1.17258400	-0.65367900
N	2.49036500	1.32467300	0.13370200
C	-0.96518700	2.01857400	-0.73748500
C	-0.83422800	2.79285400	0.42610300
H	0.11458000	2.80310400	0.96625000
C	-3.13330800	3.49529800	0.25919400
H	-3.97635200	4.06182200	0.65262300
C	-2.19661000	2.03589600	-1.41056900
H	-2.29908900	1.47284100	-2.33989800
C	-1.90889900	3.51690200	0.93052200
H	-1.79814700	4.10253900	1.84236100
C	-3.27451000	2.76872100	-0.92227000
H	-4.22218900	2.77714200	-1.45957200
O	0.69324200	0.95435900	-2.37121900
H	1.61836900	1.24412900	-2.33980700
H	-0.01874300	1.78283000	-1.63804200
Ni	0.19360700	0.31017600	-0.68230600

TS12b-13b

Charge = 1 Multiplicity = 1
 E= -1649.813161
 H= -1649.783428
 G= -1649.873894
 SPE= -1652.038371
 Imaginary frequency = -439.54

H	-4.10193700	-2.40027200	3.31283600
C	-3.65321600	-2.06721300	2.37826900
C	-2.43068500	-1.32713900	2.43738400
C	-4.24727400	-2.33868100	1.18788900
C	-1.82125100	-0.88329100	1.24480700
C	-1.79395400	-1.00231900	3.64988900
C	-3.66225500	-1.89684200	-0.03986800
H	-5.18333800	-2.89350300	1.14679900
N	-0.67194800	-0.16481500	1.23351800
C	-2.44645400	-1.18340500	-0.01711600
C	-0.62739800	-0.27424900	3.63058900
H	-2.23671100	-1.32824100	4.59036800
C	-4.24838700	-2.13185400	-1.29907300
C	-0.10320400	0.12516900	2.39312400
N	-1.84249000	-0.74083300	-1.14326400
H	-0.11396700	-0.00229600	4.54864500
C	-3.63367800	-1.66218800	-2.43680600
H	-5.18951700	-2.67788400	-1.35528300
H	0.81715900	0.70878800	2.34853100
C	-2.42241700	-0.96411200	-2.31419700
H	-4.06900600	-1.81849400	-3.41992800
H	-1.89544000	-0.56233600	-3.18057600
C	3.48129000	2.59620400	1.09547300

C	4.45240700	1.62324800	1.14097100
C	4.18285000	0.34384200	0.61767000
C	2.90314400	0.12579900	0.06586600
C	2.24132900	2.28904000	0.51534100
C	5.14313400	-0.71620900	0.62670800
C	2.57708700	-1.17268500	-0.46552200
C	3.55077500	-2.19302900	-0.45080900
C	4.84102500	-1.93449200	0.10906500
C	3.19064600	-3.43798000	-1.00132500
H	3.91851200	-4.24848800	-1.00974400
C	1.93027100	-3.61341300	-1.52358600
C	1.02920700	-2.53937900	-1.48254400
H	6.12531100	-0.52132100	1.05455100
H	3.65759300	3.59198100	1.49269200
H	5.43015600	1.82651500	1.57653300
H	1.44670900	3.03537100	0.45227900
H	5.57607200	-2.73782400	0.11088800
H	1.62542900	-4.56003700	-1.96097000
H	0.02084700	-2.64201400	-1.88521000
N	1.33475800	-1.35979200	-0.96772800
N	1.95730800	1.09548800	0.01104600
C	-0.98546600	2.52227100	-1.12864000
C	-0.26233800	3.72810400	-1.20287800
H	0.70888400	3.73444800	-1.71343900
C	-1.97471800	4.96530900	-0.05323900
H	-2.35573200	5.89898100	0.35784200
C	-2.24443700	2.61390600	-0.50750100
H	-2.88264100	1.72599700	-0.44225500
C	-0.73315800	4.93125800	-0.68133700
H	-0.14457800	5.84389900	-0.77461500
C	-2.73383100	3.80193300	0.03074900
H	-3.71375000	3.82739900	0.50724100
Mg	0.00676400	0.42550700	-0.84621800
O	-0.01278100	0.80912000	-2.86580800
H	0.67495400	1.19143500	-3.42535900
H	-0.53161700	1.65291300	-2.30188000

13a

Charge = 1 Multiplicity = 1
 E= -1620.660949
 H= -1620.630767
 G= -1620.722796
 SPE= -2960.289138

H	-3.89841100	-2.05591000	3.13742700
C	-3.40246800	-1.79837000	2.20215200
C	-2.18575800	-1.04177100	2.26025700
C	-3.93476000	-2.18974600	1.00945500
C	-1.54314200	-0.71642400	1.05390200
C	-1.57553700	-0.58702000	3.44497200
C	-3.29845000	-1.85681300	-0.23125600
H	-4.86051400	-2.76365500	0.98246800
N	-0.38869600	-0.00723200	0.97696600
C	-2.10458400	-1.12162800	-0.18738200
C	-0.40671800	0.14252800	3.36516000
H	-2.02965300	-0.80979400	4.41023400
C	-3.78061200	-2.19720200	-1.51177100
C	0.15878900	0.41261200	2.10927100
N	-1.42308200	-0.73782100	-1.29049400
H	0.08705000	0.51111800	4.26091600
C	-3.07976700	-1.79472700	-2.63083700
H	-4.70320800	-2.76948300	-1.60820500
H	1.08130000	0.98762400	2.02514700
H	-1.89118400	-1.05741800	-2.48674600
C	-3.43298300	-2.04025900	-3.62935500
H	-1.28998200	-0.69859000	-3.32351400
C	2.81542400	3.35202900	-0.19920800
C	4.00113300	2.74863700	0.15655800
C	4.09137200	1.34424800	0.18922800
C	2.93680200	0.59109200	-0.13430200
C	1.72026000	2.54026400	-0.51298400
C	5.31039500	0.67545600	0.52784800
C	3.00773100	-0.85371000	-0.11938100
C	4.23648100	-1.47363300	0.21058200

C	5.38100800	-0.68068400	0.53635100
C	4.27465800	-2.88279900	0.19884200
H	5.20563300	-3.39340600	0.44499100
C	3.14096900	-3.59145100	-0.12639700
C	1.96998200	-2.87470000	-0.43446300
H	6.18158800	1.28221300	0.77182800
H	2.71713700	4.43329200	-0.24902100
H	4.87981400	3.34394000	0.40413600
H	0.76733600	2.96976700	-0.81970600
H	6.31201000	-1.18783300	0.78820400
H	3.13950500	-4.67874900	-0.14925000
H	1.05224300	-3.40531200	-0.69781200
N	1.90191500	-1.55826100	-0.43032700
N	1.77128700	1.21146700	-0.46760500
C	-3.15473500	2.04850400	-1.40508900
C	-2.06800700	2.75564500	-0.89286100
H	-1.30840000	3.13019800	-1.57985300
C	-2.95702200	2.50518600	1.33923100
H	-2.88678200	2.69654500	2.41001100
C	-4.14009200	1.56761000	-0.54585900
H	-4.99565400	1.02422800	-0.94746000
C	-1.97269300	2.98892300	0.47801600
H	-1.13443300	3.55850400	0.88276000
C	-4.04000200	1.79272900	0.82750000
H	-4.81619100	1.42466200	1.49829400
O	0.37214800	0.54019400	-2.65442200
H	1.29608600	0.72074000	-2.87651500
H	-3.22823200	1.87631600	-2.47870200
Ni	0.17145600	0.23860800	-0.88879100

13b

Charge = 1 Multiplicity = 1

E= -1649.857958

H= -1649.827376

G= -1649.919016

SPE= -1652.088447

H	-4.21080500	-0.88927900	3.45232300
C	-3.67711600	-0.96964200	2.50641600
C	-2.46018700	-0.23258000	2.34869200
C	-4.16654800	-1.73826400	1.49881900
C	-1.74572100	-0.31854100	1.13576600
C	-1.93878000	0.61039500	3.34725400
C	-3.46936700	-1.84461600	0.25408500
H	-5.10120800	-2.28388100	1.62016100
N	-0.61215600	0.38414400	0.89768800
C	-2.25192900	-1.15805300	0.08227400
C	-0.78544500	1.31943100	3.10148800
H	-2.45935200	0.69795100	4.30034000
C	-3.94223700	-2.59074400	-0.84424800
C	-0.16052600	1.17961700	1.85440200
N	-1.54848600	-1.20327600	-1.06666400
H	-0.35986200	1.98443200	3.84800800
C	-3.22741400	-2.60665300	-2.02166600
H	-4.88049700	-3.13736500	-0.75322900
H	0.74451300	1.74401900	1.62596500
C	-2.02274300	-1.88851200	-2.09608900
H	-3.58222100	-3.15821100	-2.88805900
H	-1.41942000	-1.82821500	-3.00377400
C	3.51019100	3.08889400	-0.32972400
C	4.53637600	2.29804400	0.13290100
C	4.34657600	0.90831700	0.25254800
C	3.08623800	0.38928800	-0.11447100
C	2.29384600	2.48019200	-0.66854600
C	5.37077200	0.02709600	0.72156200
C	2.85521800	-1.03054500	-0.01909600
C	3.89005900	-1.87152400	0.44092700
C	5.15109000	-1.30926200	0.81297200
C	3.62267900	-3.25257500	0.50396400
H	4.40016000	-3.93083500	0.85355800
C	2.39026300	-3.72716100	0.11951400
C	1.42672500	-2.81116600	-0.32634100
H	6.33322000	0.45364200	0.99967500
H	3.62626500	4.16374600	-0.43730600

H	5.49801700	2.73077500	0.40635200
H	1.45759400	3.07719700	-1.03442800
H	5.93351400	-1.97918100	1.16605800
H	2.15644800	-4.78762000	0.15135200
H	0.44100800	-3.15000300	-0.64728200
N	1.64576600	-1.50824300	-0.39237000
N	2.07970600	1.17694300	-0.56588400
C	-2.16195100	1.88895900	-2.04654000
C	-1.27192800	2.86709900	-1.60384100
H	-0.40799300	3.11146900	-2.22401600
C	-2.64301000	3.25173500	0.34206200
H	-2.83751100	3.78891300	1.26915100
C	-3.29921700	1.60350000	-1.29472700
H	-4.00504500	0.84986500	-1.64519100
C	-1.51320400	3.55214800	-0.41398500
H	-0.82855100	4.33262900	-0.08095400
C	-3.53695100	2.27807800	-0.10022600
H	-4.42804200	2.05158900	0.48486200
Mg	0.25889900	0.01496400	-1.17861800
O	0.20687200	0.01415400	-3.03460000
H	0.91952700	0.21358900	-3.64475300
H	-1.93987900	1.34725500	-2.96488200

10a

Charge = 1 Multiplicity = 1

E= -1388.689301

H= -1388.665556

G= -1388.741810

SPE= -2727.915166

H	-4.79462100	2.85387900	1.28372500
C	-4.24295500	1.99747000	0.89805000
C	-2.86376300	1.85281300	1.26256400
C	-4.85936700	1.08756500	0.09108900
C	-2.15336500	0.74779500	0.76385300
C	-2.15222600	2.73870700	2.09549900
C	-4.15082200	-0.04757000	-0.42348300
H	-5.90887400	1.21028300	-0.17378600
N	-0.84679200	0.49773800	1.03964600
C	-2.79954700	-0.19691500	-0.07822100
C	-0.82526200	2.48394400	2.37513700
H	-2.65262200	3.61210900	2.51260200
C	-4.70091400	-1.04530200	-1.25564600
C	-0.20438200	1.35056000	1.82695900
N	-2.02932600	-1.22699300	-0.50020700
H	-0.25004600	3.14681000	3.01659600
C	-3.90734200	-2.09256000	-1.67649800
H	-5.74640500	-0.98284500	-1.55654900
H	0.84249000	1.13141500	2.03678700
C	-2.56002600	-2.15752400	-1.27861500
H	-4.30874300	-2.87611200	-2.31416200
H	-1.87576900	-2.95485600	-1.57132700
O	0.08292900	-2.69565000	-0.68905100
H	1.02962200	-2.86164500	-0.79616800
C	1.80614300	1.90386600	-3.19993500
C	3.07755800	1.92630600	-2.67453800
C	3.36040500	1.19236400	-1.50481500
C	2.29818100	0.45853500	-0.92540600
C	0.82179300	1.14629800	-2.53880200
C	4.66046300	1.17299600	-0.90928800
C	2.55837700	-0.32205500	0.26354500
C	3.85741100	-0.31942800	0.82590100
C	4.89873100	0.44850700	0.21448300
C	4.08395500	-1.09321800	1.98002500
H	5.07743100	-1.10162400	2.42801900
C	3.05891000	-1.83768700	2.52037600
C	1.80534000	-1.79930100	1.90047600
H	5.45673200	1.75079700	-1.37771000
H	1.55697600	2.45455600	-4.10399700
H	3.87266400	2.50046100	-3.15003500
H	-0.19718700	1.10833900	-2.92934100
H	5.88858800	0.43063600	0.66890000
H	3.20522000	-2.45597700	3.40208600
H	0.97141600	-2.39194800	2.27422700

N	1.55926200	-1.05831000	0.82233400
N	1.05333100	0.45163400	-1.44212300
Ni	-0.22105000	-1.11552000	0.11102600

10b

Charge = 1 Multiplicity = 1

E= -1417.883522

H= -1417.858892

G= -1417.938074

SPE= -1419.711461

H	-5.07512800	1.98577700	-2.12915600
C	-4.46016300	1.36392600	-1.48052200
C	-3.12226700	1.78841300	-1.20191600
C	-4.95900800	0.22383700	-0.93644200
C	-2.29958800	1.00243200	-0.36846400
C	-2.57464700	2.98047800	-1.71219000
C	-4.15465300	-0.59292500	-0.08115300
H	-5.98344000	-0.08557800	-1.13772700
N	-1.03366100	1.36172000	-0.03735300
C	-2.82155400	-0.22101000	0.18121100
C	-1.28637600	3.33340700	-1.38217100
H	-3.18032400	3.61298900	-2.36017500
C	-4.62565200	-1.76705200	0.53900600
C	-0.55278300	2.49105900	-0.53615100
N	-2.00273300	-0.95167200	0.96651400
H	-0.83606400	4.24813800	-1.75737400
C	-3.79501400	-2.47986800	1.37364300

H	-5.65123500	-2.08925000	0.36204500
H	0.46785700	2.74876600	-0.25268000
C	-2.47869700	-2.03139900	1.56627600
H	-4.14103200	-3.37444000	1.88394300
H	-1.78755100	-2.54274900	2.23622900
Mg	-0.00790500	-0.11326100	1.31362400
O	-0.07280300	-0.55469500	3.09215700
O	0.57840100	-0.47296800	3.79044100
C	1.36837400	-3.20497000	-1.65550800
C	2.65875300	-2.80740700	-1.91901700
C	3.17158300	-1.64914600	-1.30458400
C	2.31370700	-0.94056500	-0.43837800
C	0.59501600	-2.43796500	-0.77348700
C	4.50776900	-1.18487700	-1.51761500
C	2.79922700	0.24506500	0.22023500
C	4.12866000	0.66410400	0.00407400
C	4.96933300	-0.07518300	-0.88610200
C	4.56546100	1.80953700	0.69682900
H	5.58670100	2.16147200	0.55557600
C	3.70391700	2.46354500	1.54810200
C	2.39912900	1.97115700	1.69329500
H	5.15013900	-1.74850100	-2.19231300
H	0.94632300	-4.09660400	-2.11050500
H	3.29400200	-3.37922800	-2.59441100
H	-0.42865400	-2.72826900	-0.53543800
H	5.99012200	0.26999300	-1.04226900
H	4.01620700	3.34313700	2.10410900
H	1.68908800	2.45951800	2.36295500
N	1.95436100	0.90511700	1.04524600
N	1.04470500	-1.34131700	-0.18266900