

Supporting Information for:

Exploring Acidity-Dependent PCET Pathways in Imino-Bipyridyl Cobalt Complexes

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Experimental Details

CV of Proton Sources with Intermediate Acidity

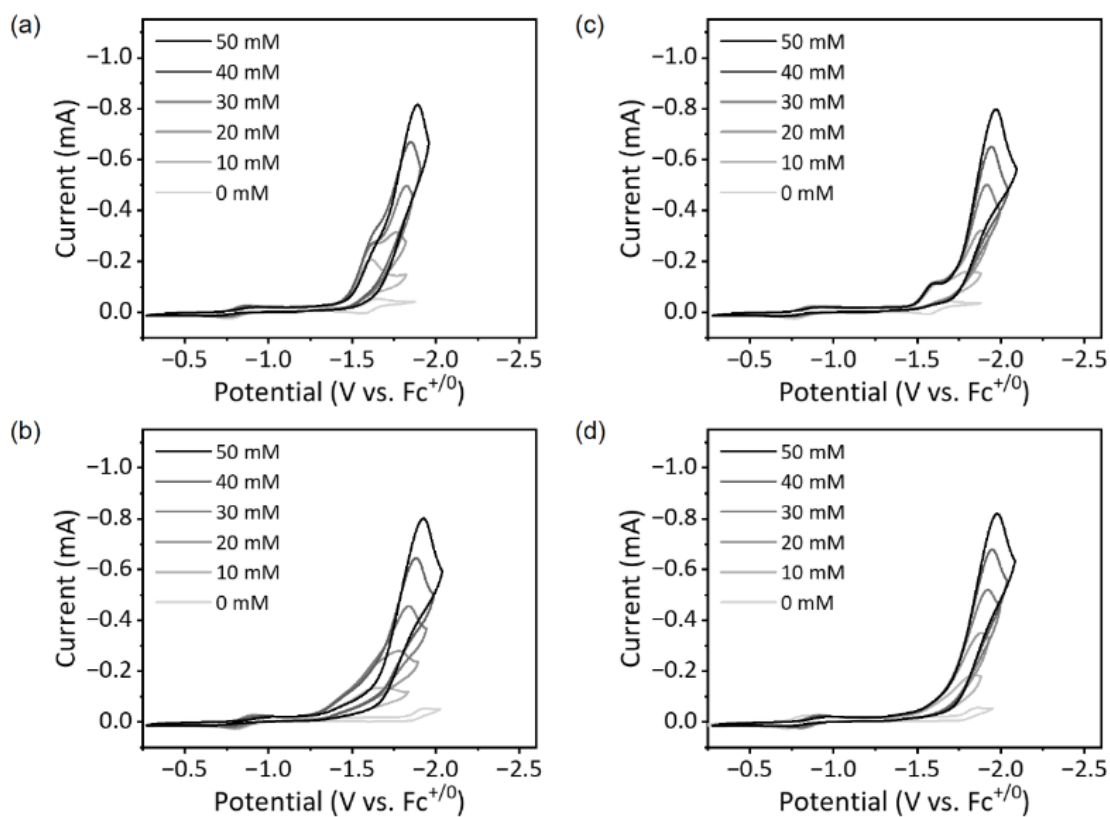
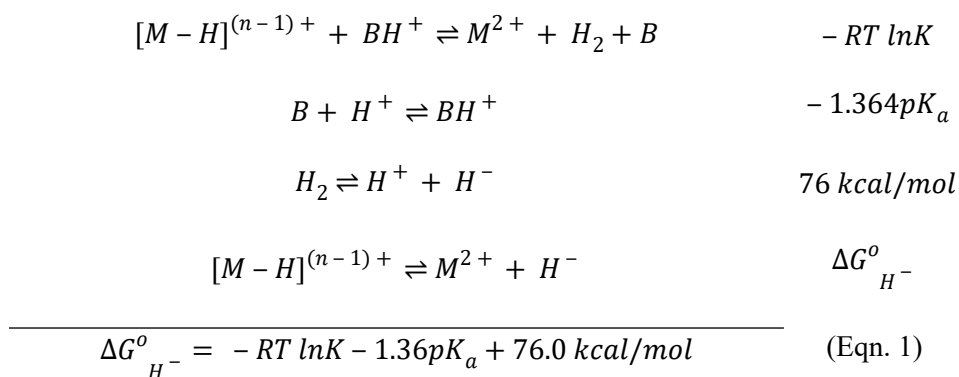


Figure S1. CVs of (a) ${}^4[1]^{2+}$ and (b) ${}^4[2]^{2+}$ in the presence of 2-picoline·HBF₄, and (c) ${}^4[1]^{2+}$ and (d) ${}^4[2]^{2+}$ in the presence of 2,6-lutidine·HBF₄. Experimental conditions: 2 mM of complex, 0-50 mM of proton source in CH₃CN.

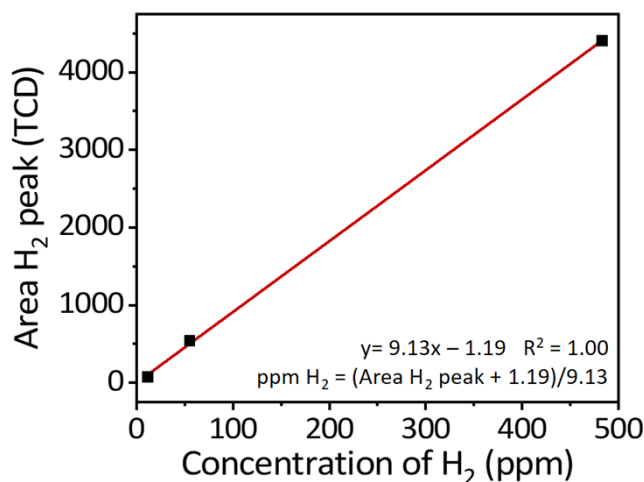
Correlation between hydricity and pK_a of a proton source

The hydricity of a metal hydride can be calculated from the redox potential of the complex, as reported by the Kubiak group,¹ which demonstrated the correlation between these two parameters. Furthermore, the process in which the metal hydride reacts with an external proton to form H_2 can be depicted by Scheme S1.² Based on this, the appropriate proton source for HER can be considered using Eqn. 1, selecting one with a suitable pK_a for efficient hydrogen evolution.



Scheme S1. Evolution of hydrogen considering metal hydride hydricity

Calibration curve



Calibration plots for measuring H_2 produced during chronopotentiometry experiments, the gas was quantified by TCD detectors. Calibration is for 1 ml of reference gases.

Calculation of Faradaic Efficiency (FE)

Chronoamperometry experiments were conducted three times in 4-neck pear shaped cells at constant currents for 1 h (Figure S2, S3). After chronoamperometry experiments, samples captured with a gas-tight syringe were injected into a gas chromatograph for analysis. Calibration curves were constructed using known amounts of H₂ with N₂ reference gas to quantify the concentration of gaseous products from respective chromatograms. The amount of gas produced was calculated from the concentration of gas using the ideal gas law, and Faradaic efficiency was determined using eqn.2

$$FE(\%) = \frac{z * F * n}{Q} \times 100 \text{ (Eqn.2)}$$

, where z is the number of electrons, n is the moles of analyte produced, F is the Faraday constant and Q is the specific charge passed during the chronopotentiometry experiments.



Figure S2. Photographic depiction of the controlled potential electrochemistry setup

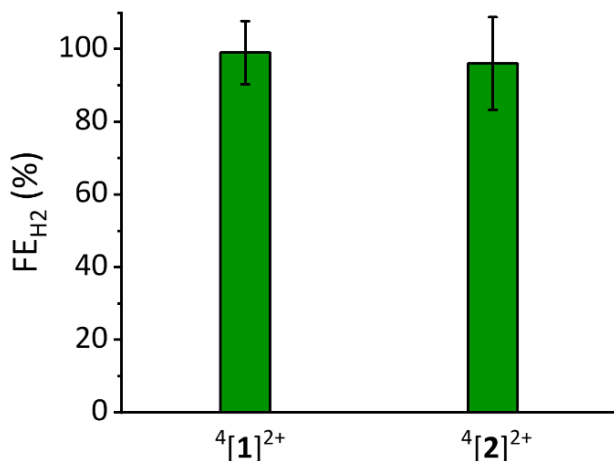


Figure S3. Faradaic efficiency values of ⁴[1]²⁺ and ⁴[2]²⁺.

Turnover Frequency and Tafel plot

Foot of the Wave Analysis (FOWA), developed by Savéant and Costentin, is a useful analytical method when an ideal S-shaped electrocatalytic wave cannot be achieved due to side phenomena such as substrate limitations, catalyst decomposition, product inhibition, or surface passivation.³ ⁴[1]²⁺ followed an ET-CPET-PT process, while ⁴[2]²⁺ followed an ET-PT-ET-PT (ECEC) process. Therefore, the TOF values for both complexes were determined using the same method, eqn. 3.⁴

The benchmarking of complex ⁴[1]²⁺ and ⁴[2]²⁺ proceeded by comparing catalytic Tafel plots of other reported proton reduction catalysts in Figure S5. Each catalytic Tafel plot was constructed using equation from previously reported literature (Eqn. 4).⁵ The TOF_{max} values were obtained from the reported values,⁶⁻⁹ and the thermodynamic potentials for H₂ evolution (E^o_{HA/H₂}) were calculated using the acid dissociation constant (pK_a) of the proton source at the solvent media (Eqn. 5).¹⁰ The pK_a values at the solvent media were taken from the reported literature.^{11, 12} The E_{cat/2} value of each catalyst were also obtained from the reported literature.

$$\frac{i}{i_p} = \frac{2.24 \sqrt{\frac{RT}{Fv}} \sqrt{k_{obs}}}{1 + \exp\left[\frac{F}{RT}(E - E_{redox})\right]} \quad (\text{Eqn.3})$$

$$TOF = \frac{TOF_{max}}{1 + \exp\left[\frac{F}{RT}\left(E_{HA^o/H_2} - E_{cat/2}\right)\right] \exp\left[-\frac{F}{RT}\eta\right]} \quad (Eqn.4)$$

$$E_{HA^o/H_2} = E_{H^+/H_2} - \frac{2.31RT}{F} \times pK_a \quad (Eqn.5)$$

Computational details

The geometries were calculated in Orca 5.01 software¹³ using the unrestricted B3LYP functional.¹⁴⁻¹⁷ Optimization and Frequency calculation were proceeded using def2-SVP basis set¹⁸ with the auxiliary def2/J basis set¹⁹ was used for all atoms. Single point energy of optimized geometries was calculated using def2-TZVPP basis set¹⁸ with the auxiliary def2/J basis set¹⁹ for all atoms. Each structure was confirmed by a frequency calculation at the same level of theory to be a real local minimum on the potential energy surface. Solvation free energies in acetonitrile were calculated by using the polarizable continuum model (C-PCM) using Bondi atomic radii.²⁰⁻²² In the proposed mechanism, for ΔG , values were calculated considering the dissociation of acetonitrile or variations depending on ET-PT and CPET. The calculations included the complexation energy correction to account for the differences in the number of molecules in the model before and after the reaction.²³ This involved taking into account relevant proton sources such as $Et_3N/[Et_3NH]^+$, and additionally generated H_2 . The activation energy barrier was determined through the TS structure in the system, including the proton source. The reduction potentials of cobalt complexes were calculated by eqn.6 and 7.²⁴

$$E^o = -\frac{\Delta G_{solv}^{redox}}{F} \left(F = 23.1 \frac{kcal}{mol * V} \right) \quad (Eqn. 6)$$

$$\Delta G_{solv}^{redox} = \Delta G_{solv}^{red} - \Delta G_{solv}^{ox} \quad (Eqn. 7)$$

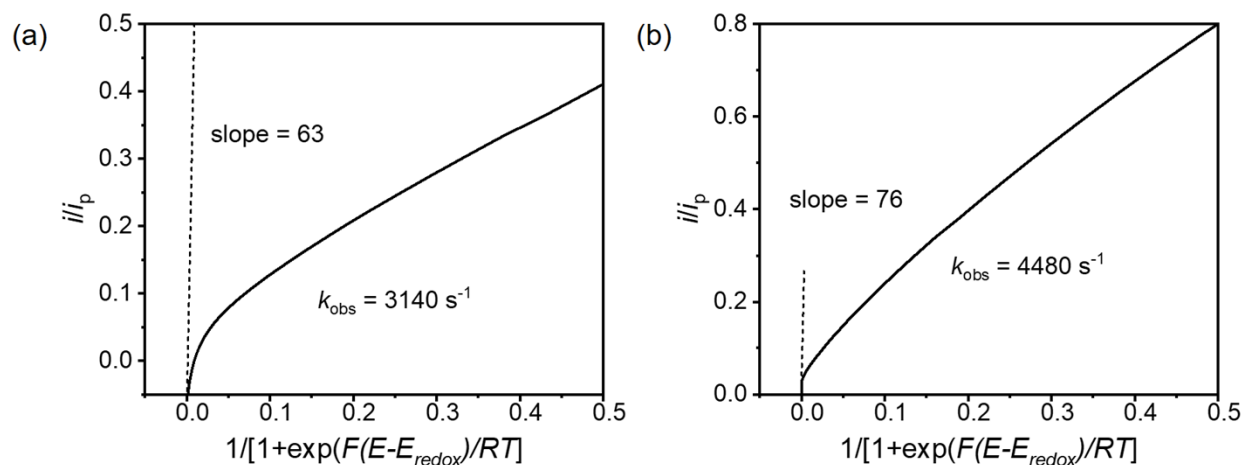


Figure S4. FOWA plots of (a) $4[1]^{2+}$ and (b) $4[2]^{2+}$.

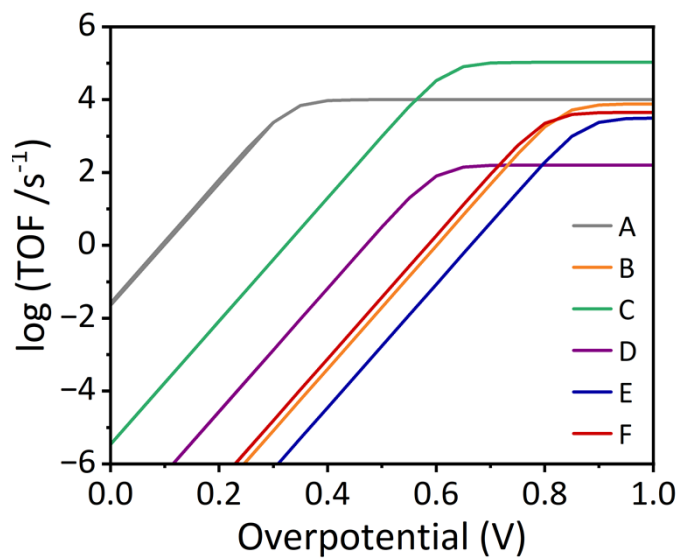


Figure S5. Compared Tafel plots of Co complexes of this work and previously reported in literatures. (a) $[\text{Co}(\text{dmgH})_2(\text{Py})](\text{Cl})^6$ (b) $[\text{Co}(\text{bapbpy})\text{Cl}]^+$,⁷ (c) $[\text{Ni}(\text{P}^{\text{Ph}}_2\text{N}^{\text{Ph}})_2](\text{OTf})_2$,⁸ (d) $4[1]^{2+}$, (e) $4[2]^{2+}$.

Table S1. Compared catalytic parameters of known HER catalysts, $^4[1]^{2+}$, and $^4[2]^{2+}$.

	Catalyst	$E_{\text{cat}/2}$	Solvent	Proton source	$E_{\text{HA}/\text{H}_2}^{\circ}$	TOF_{max} (s^{-1})	Ref.
A	$[\text{Co}(\text{dmgH})_2(\text{Py})](\text{Cl})$	-1.53 V	CH_3CN	$[\text{Et}_3\text{NH}]^+$	-1.20 V	10,000	6
B	$[\text{Co}(\text{bapbpy})\text{Cl}]^+$	-1.65 V	CH_3CN	1M HBF_4	-0.82 V	7,600	7
C	$[\text{Ni}(\text{P}^{\text{Ph}}_2\text{N}^{\text{Ph}})_2](\text{OTf})_2$	-1.13 V	CH_3CN	$[\text{DMFH}]^+/\text{H}_2\text{O}$	-0.51 V	106,000	8
D	Ni(PNP)	-1.83 V	CH_3CN	Acetic acid	-1.23 V	160	9
E	$^4[1]^{2+}$	-2.01 V	CH_3CN	50mM $\text{Et}_3\text{N}\cdot\text{HBF}_4$	-1.14 V	3,140	This work
F	$^4[2]^{2+}$	-1.93 V	CH_3CN	50mM $\text{Et}_3\text{N}\cdot\text{HBF}_4$	-1.14 V	4,480	This work

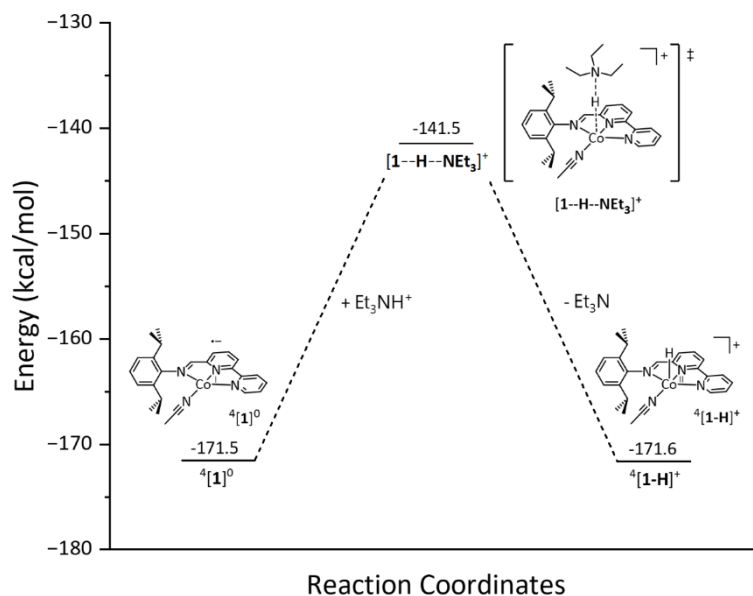


Figure S6. Activation barrier for the formation of ${}^4[1-H]^+$. B3LYP/Def2-SVP//Def2-TZVPPD solution phase calculations in CH_3CN .

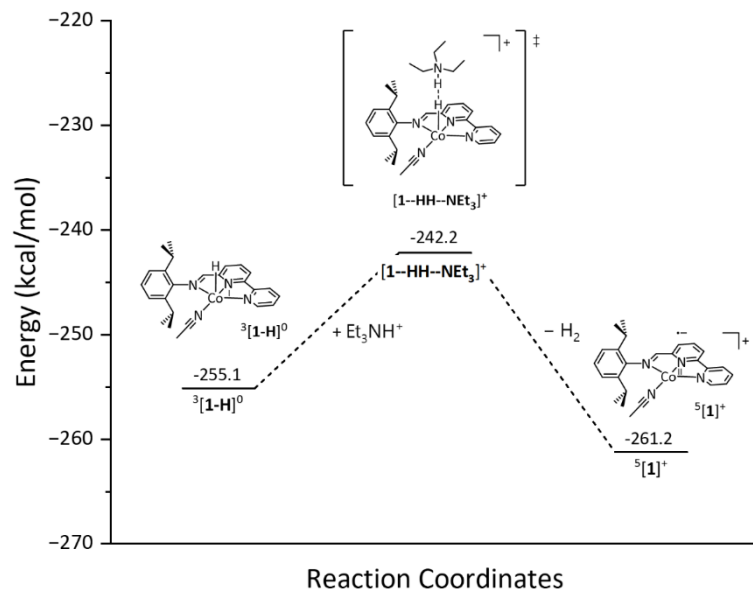


Figure S7. Activation barrier for the formation of H_2 from ${}^3[1-H]^0$. B3LYP/Def2-SVP//Def2-TZVPPD solution phase calculations in CH_3CN .

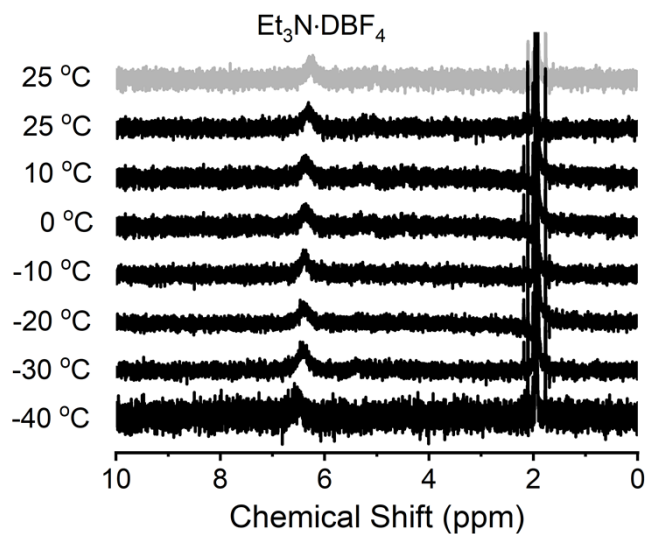


Figure S8. Temperature-dependent ^2H NMR spectra of $^3[2]^+$ with $\text{Et}_3\text{N}\cdot\text{DBF}_4$ in CH_3CN , a free $\text{Et}_3\text{N}\cdot\text{DBF}_4$ peak (gray) is given for comparison.

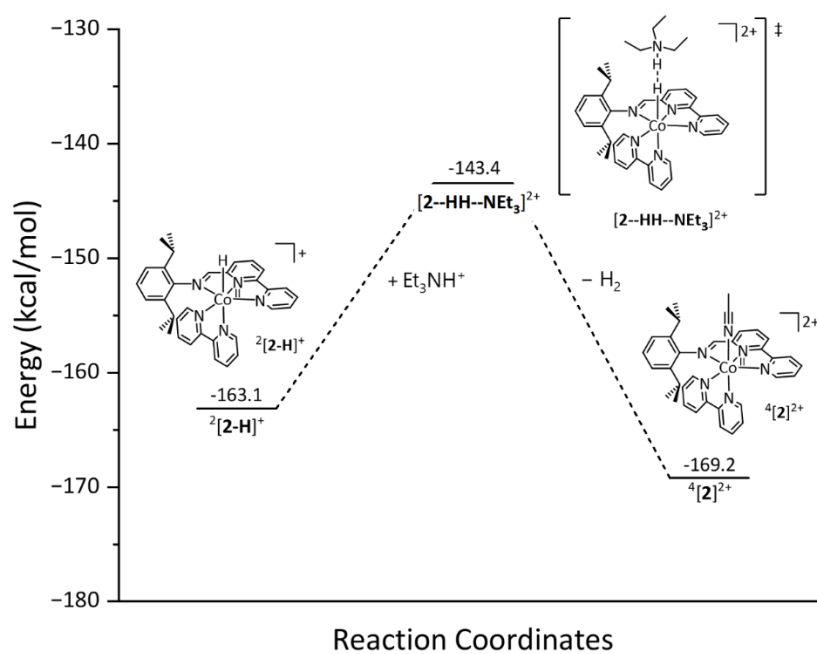


Figure S9. Activation barrier for the formation of H_2 from $^2[2-\text{H}]^+$. B3LYP/Def2-SVP//Def2-TZVPPD solution phase calculations in CH_3CN .

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Cartesian coordinates of DFT-optimized structures

(Format)

Structure name

Spin multiplicity / Charge

Atom number XYZ

$4[1]^{2+}$

Spin multiplicity : Quartet / Charge : 2+

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Spin multiplicity : Triplet / Charge : 1+

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$^5[1-2\text{CH}_3\text{CN}]^+$

Spin multiplicity : Quintet / Charge : 1+

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7	9.113204000	11.674396000	3.796291000
6	7.922835000	12.013265000	0.655108000
1	8.902467000	12.423589000	0.918292000
6	7.144177000	12.604533000	-0.340634000
1	7.507949000	13.488238000	-0.868689000
6	5.901349000	12.035087000	-0.635573000
1	5.260203000	12.465385000	-1.408951000
6	5.486633000	10.905896000	0.070407000
1	4.522262000	10.444421000	-0.145420000
6	6.327052000	10.371893000	1.058478000
6	5.991474000	9.175549000	1.873559000
6	4.813178000	8.441960000	1.776806000
1	4.032169000	8.714213000	1.067238000
6	4.648853000	7.318623000	2.632558000
1	3.732894000	6.725868000	2.572655000
6	5.638266000	6.977856000	3.536881000
1	5.524515000	6.118443000	4.202348000
6	6.821210000	7.762525000	3.602574000
6	7.914973000	7.553997000	4.485471000

1	7.884632000	6.724403000	5.201725000
6	10.034824000	8.211972000	5.363986000
6	9.963011000	8.829666000	6.642620000
6	11.032110000	8.652646000	7.534744000
1	10.987232000	9.113204000	8.525116000
6	8.742138000	9.645426000	7.064014000
1	8.187297000	9.888696000	6.145483000
6	7.802000000	8.819788000	7.964155000
1	7.474224000	7.894326000	7.465119000
1	6.902741000	9.402145000	8.227027000
1	8.306395000	8.535607000	8.903349000
6	9.110677000	10.975600000	7.743067000
1	9.584073000	10.820673000	8.726554000
1	8.204031000	11.580408000	7.909785000
1	9.805892000	11.566834000	7.125624000
6	11.077168000	9.612406000	0.764479000
6	12.123110000	9.526672000	-0.237189000
1	12.355109000	10.534321000	-0.615107000
1	11.782144000	8.893188000	-1.070697000
1	13.026354000	9.085201000	0.211231000
6	9.328569000	12.708365000	4.265997000
6	9.592849000	14.008328000	4.853238000
1	9.089506000	14.788705000	4.261754000
1	10.677704000	14.196275000	4.858810000
1	9.214187000	14.028585000	5.886745000
6	12.152249000	7.897466000	7.183820000

1	12.974095000	7.770364000	7.894261000
6	12.219214000	7.307359000	5.920980000
1	13.099330000	6.716970000	5.652562000
6	11.176026000	7.451614000	4.993050000
6	11.259524000	6.760998000	3.634095000
1	10.488414000	7.216764000	2.995723000
6	10.926254000	5.261060000	3.752811000
1	11.657523000	4.743363000	4.396915000
1	10.947255000	4.777255000	2.761696000
1	9.925754000	5.103680000	4.186667000
6	12.614200000	6.967914000	2.936486000
1	13.435763000	6.461850000	3.469703000
1	12.584176000	6.553251000	1.915345000
1	12.870048000	8.037269000	2.862149000

$^5[1]^+$

Spin multiplicity : Quintet / Charge : 1+

27	8.239440000	9.956643000	3.249858000
7	7.362885000	10.811931000	1.467860000
7	6.673309000	8.783240000	2.917323000
7	8.613661000	8.462015000	4.605941000
7	9.655800000	11.363231000	3.628729000
6	7.823900000	11.859759000	0.767449000
1	8.770376000	12.292559000	1.102569000
6	7.144040000	12.384079000	-0.330054000
1	7.557592000	13.237182000	-0.871121000
6	5.933758000	11.792730000	-0.708134000
1	5.369388000	12.176616000	-1.561426000
6	5.452678000	10.701124000	0.015073000
1	4.513527000	10.222382000	-0.265016000
6	6.191407000	10.222242000	1.104088000
6	5.797490000	9.049800000	1.924669000
6	4.683321000	8.244506000	1.729848000
1	3.969062000	8.446003000	0.931279000
6	4.500189000	7.128494000	2.593123000
1	3.627805000	6.484868000	2.457700000
6	5.424130000	6.843363000	3.584521000
1	5.303555000	5.975626000	4.237491000
6	6.550945000	7.691912000	3.740015000
6	7.630152000	7.547642000	4.652992000
1	7.663908000	6.713578000	5.362209000

6	9.720626000	8.365199000	5.496721000
6	9.592185000	8.802122000	6.842511000
6	10.710108000	8.703019000	7.685890000
1	10.625521000	9.027415000	8.726770000
6	8.286259000	9.377574000	7.388177000
1	7.588151000	9.470501000	6.543736000
6	7.638293000	8.435165000	8.419695000
1	7.450416000	7.437876000	7.990384000
1	6.674468000	8.843541000	8.767004000
1	8.285395000	8.305172000	9.303537000
6	8.474818000	10.790406000	7.970442000
1	9.135093000	10.786197000	8.853493000
1	7.503615000	11.206747000	8.285755000
1	8.911039000	11.474873000	7.224792000
6	10.471935000	12.143468000	3.878729000
6	11.495931000	13.118606000	4.192476000
1	11.160955000	14.118013000	3.874230000
1	12.424940000	12.856237000	3.662767000
1	11.679930000	13.120027000	5.277978000
6	11.927934000	8.203504000	7.222610000
1	12.785798000	8.133973000	7.897440000
6	12.046799000	7.797539000	5.892661000
1	13.003918000	7.408441000	5.534244000
6	10.959249000	7.870894000	5.009021000
6	11.122249000	7.396974000	3.566392000
1	10.186053000	7.632316000	3.037398000

6	11.311890000	5.870071000	3.494746000
1	12.236624000	5.558092000	4.008743000
1	11.381514000	5.536530000	2.445868000
1	10.469172000	5.338785000	3.966057000
6	12.257486000	8.133689000	2.833773000
1	13.240620000	7.923893000	3.286677000
1	12.304043000	7.814480000	1.779353000
1	12.102274000	9.224683000	2.851357000

$^4[1]^0$

Spin multiplicity : Quartet / Charge : 0

27	8.338709000	10.161559000	3.273351000
7	7.232125000	11.228441000	1.674411000
7	7.044814000	8.833148000	2.671023000
7	8.838246000	8.505918000	4.572857000
7	9.578533000	11.502817000	3.890397000
6	7.414174000	12.479930000	1.230613000
1	8.215077000	13.051028000	1.711603000
6	6.642722000	13.044942000	0.217297000
1	6.828767000	14.069540000	-0.111613000
6	5.630615000	12.261968000	-0.356797000
1	4.999794000	12.664275000	-1.153702000
6	5.436325000	10.960747000	0.100442000
1	4.654212000	10.336946000	-0.334546000
6	6.256737000	10.458783000	1.126575000
6	6.143000000	9.093243000	1.689507000
6	5.213432000	8.144186000	1.272189000
1	4.496312000	8.368929000	0.481800000
6	5.214350000	6.866599000	1.896488000
1	4.493909000	6.106799000	1.583563000
6	6.130952000	6.596188000	2.899045000
1	6.150994000	5.621396000	3.395420000
6	7.059536000	7.593401000	3.294378000
6	8.047148000	7.457667000	4.300105000
1	8.151680000	6.506763000	4.840185000

6	9.875162000	8.381679000	5.516973000
6	9.754587000	9.045317000	6.774368000
6	10.798010000	8.939487000	7.704216000
1	10.706557000	9.434963000	8.674306000
6	8.479190000	9.812658000	7.113958000
1	8.044754000	10.126119000	6.150955000
6	7.448599000	8.894491000	7.799617000
1	7.218682000	8.014473000	7.178254000
1	6.504324000	9.433592000	7.987946000
1	7.830078000	8.531769000	8.769740000
6	8.719125000	11.080259000	7.947830000
1	9.073936000	10.848774000	8.966020000
1	7.780076000	11.648316000	8.054422000
1	9.462928000	11.741918000	7.474418000
6	10.317529000	12.312345000	4.279460000
6	11.239619000	13.325150000	4.767552000
1	11.192401000	14.220642000	4.128309000
1	12.268974000	12.933199000	4.759793000
1	10.974838000	13.606901000	5.799094000
6	11.952224000	8.203660000	7.420902000
1	12.753033000	8.126454000	8.162070000
6	12.077441000	7.577321000	6.180439000
1	12.989101000	7.015899000	5.954467000
6	11.064192000	7.658577000	5.211448000
6	11.275855000	7.000379000	3.848706000
1	10.416544000	7.273148000	3.219679000

6	11.306097000	5.464303000	3.946299000
1	12.146819000	5.117876000	4.571253000
1	11.424667000	5.011663000	2.947135000
1	10.375673000	5.072417000	4.387942000
6	12.536090000	7.532788000	3.141293000
1	13.456694000	7.271082000	3.689140000
1	12.620746000	7.103096000	2.128837000
1	12.503817000	8.630220000	3.041684000

$^4[1-H]^+$

Spin multiplicity : Quartet / Charge : 1+

27	8.194039000	10.370662000	3.472685000
7	7.505689000	11.001048000	1.502502000
7	6.822646000	8.902949000	2.851844000
7	8.685886000	8.566055000	4.655945000
7	9.962696000	11.383299000	3.564965000
6	7.945802000	12.089722000	0.859654000
1	8.838447000	12.571525000	1.268089000
6	7.312287000	12.600561000	-0.275045000
1	7.710630000	13.489092000	-0.768661000
6	6.171656000	11.950854000	-0.750462000
1	5.644437000	12.322072000	-1.632532000
6	5.711203000	10.812311000	-0.085226000
1	4.824782000	10.286375000	-0.441511000
6	6.404947000	10.357547000	1.041711000
6	6.037308000	9.132369000	1.797476000
6	5.014243000	8.224595000	1.470380000
1	4.358253000	8.397071000	0.616363000
6	4.860700000	7.077573000	2.253489000
1	4.071232000	6.360773000	2.016463000
6	5.733322000	6.832560000	3.321239000
1	5.656602000	5.925728000	3.924629000
6	6.725508000	7.783552000	3.581700000
6	7.778008000	7.657301000	4.600777000
1	7.774222000	6.783535000	5.267801000

6	9.729351000	8.495162000	5.630391000
6	9.459272000	8.767297000	6.994231000
6	10.537719000	8.709827000	7.893537000
1	10.358469000	8.910394000	8.952944000
6	8.068442000	9.130544000	7.513831000
1	7.397925000	9.239370000	6.649460000
6	7.492361000	8.018674000	8.410845000
1	7.447315000	7.054383000	7.879527000
1	6.471219000	8.276840000	8.736812000
1	8.107982000	7.876455000	9.314693000
6	8.063392000	10.487958000	8.240786000
1	8.677916000	10.466731000	9.155749000
1	7.035903000	10.755085000	8.538091000
1	8.447876000	11.290177000	7.590687000
6	10.931359000	12.003614000	3.688478000
6	12.141612000	12.783292000	3.863396000
1	12.328061000	13.387039000	2.961920000
1	12.993500000	12.106987000	4.033647000
1	12.024470000	13.449724000	4.732110000
6	11.828237000	8.404705000	7.465000000
1	12.648922000	8.361740000	8.186322000
6	12.073873000	8.159637000	6.111606000
1	13.089278000	7.923072000	5.786451000
6	11.039484000	8.207735000	5.168105000
6	11.294563000	7.889399000	3.696918000
1	10.504513000	8.393991000	3.116320000

6	11.157490000	6.376713000	3.431130000
1	11.922507000	5.812953000	3.991105000
1	11.290268000	6.157520000	2.358678000
1	10.169977000	5.995076000	3.735707000
6	12.643333000	8.411385000	3.179492000
1	13.493815000	7.873171000	3.628799000
1	12.707652000	8.268027000	2.088780000
1	12.772352000	9.485017000	3.389965000
1	7.090814000	11.077117000	4.473490000

$^4[1-NH]^+$

Spin multiplicity : Quartet / Charge : 1+

27	8.383416000	9.832176000	3.450822000
7	7.742425000	10.902223000	1.720671000
7	7.115343000	8.582490000	2.735805000
7	8.235735000	8.363514000	5.183469000
7	9.742511000	11.094473000	4.215710000
6	8.138655000	12.111856000	1.296371000
1	8.834780000	12.652674000	1.944225000
6	7.694746000	12.664494000	0.097884000
1	8.038846000	13.653668000	-0.210095000
6	6.807284000	11.918921000	-0.687486000
1	6.437271000	12.315728000	-1.635808000
6	6.395632000	10.661470000	-0.249248000
1	5.705688000	10.067636000	-0.849649000
6	6.878820000	10.169009000	0.972044000
6	6.503319000	8.853115000	1.545310000
6	5.621154000	7.963402000	0.964191000
1	5.134047000	8.184954000	0.014787000
6	5.353682000	6.729781000	1.638675000
1	4.665939000	6.011900000	1.184957000
6	5.942864000	6.452904000	2.843164000
1	5.737826000	5.521621000	3.376583000
6	6.841983000	7.414734000	3.440221000
6	7.451503000	7.260493000	4.665233000
1	7.337199000	6.366262000	5.280859000

6	9.399934000	8.005566000	5.963434000
6	9.398946000	8.237754000	7.364756000
6	10.552417000	7.904983000	8.091089000
1	10.579179000	8.081342000	9.167972000
6	8.196980000	8.859305000	8.081608000
1	7.287237000	8.585281000	7.519611000
6	7.981850000	8.317743000	9.504403000
1	7.949085000	7.216665000	9.519295000
1	7.026484000	8.692863000	9.905103000
1	8.775365000	8.644926000	10.195600000
6	8.291066000	10.398945000	8.096437000
1	9.179761000	10.725258000	8.661997000
1	7.400848000	10.838706000	8.575686000
1	8.371384000	10.816651000	7.079968000
6	10.533530000	11.819851000	4.647852000
6	11.523602000	12.729813000	5.187835000
1	11.980746000	13.305215000	4.367976000
1	12.301680000	12.157031000	5.715763000
1	11.036326000	13.420669000	5.893580000
6	11.664021000	7.337325000	7.467815000
1	12.548250000	7.075852000	8.055191000
6	11.640769000	7.102985000	6.093821000
1	12.515186000	6.658406000	5.612052000
6	10.522340000	7.435313000	5.313670000
6	10.568629000	7.176641000	3.808023000
1	9.661400000	7.608810000	3.356710000

6	10.545280000	5.669485000	3.490998000		
1	11.442344000	5.168152000	3.891118000		
1	10.525855000	5.504880000	2.400909000		
1	9.659460000	5.181819000	3.926677000		
6	11.773748000	7.860003000	3.134609000		
1	12.729739000	7.434157000	3.480175000		
1	11.726068000	7.722568000	2.041690000		
1	11.791519000	8.942019000	3.341137000		
1		7.629105000		8.955403000	5.757672000

$^3[1-H]^0$

Spin multiplicity : Triplet / Charge : 0

27	8.208602000	10.362311000	3.753997000
7	7.202408000	11.430609000	1.896476000
7	7.079862000	8.980800000	2.797001000
7	8.764509000	8.637368000	4.790446000
7	9.991584000	11.079406000	2.983828000
6	7.333422000	12.706261000	1.519841000
1	8.048896000	13.309077000	2.089319000
6	6.611059000	13.264322000	0.464252000
1	6.755295000	14.311430000	0.189305000
6	5.704321000	12.446172000	-0.220227000
1	5.114345000	12.840882000	-1.051451000
6	5.560727000	11.116722000	0.172137000
1	4.858135000	10.463953000	-0.347437000
6	6.333747000	10.631673000	1.242489000
6	6.267723000	9.233526000	1.740379000
6	5.452537000	8.246099000	1.195926000
1	4.803010000	8.460193000	0.346838000
6	5.474483000	6.946528000	1.763381000
1	4.838457000	6.160851000	1.348586000
6	6.306514000	6.684462000	2.837677000
1	6.349464000	5.692038000	3.294135000
6	7.124401000	7.721405000	3.350914000
6	8.042905000	7.578773000	4.430684000
1	8.146290000	6.612212000	4.939452000

6	9.725086000	8.493225000	5.829064000
6	9.375526000	8.827176000	7.165068000
6	10.347090000	8.686974000	8.168280000
1	10.087931000	8.928937000	9.202497000
6	7.964514000	9.291119000	7.518411000
1	7.489264000	9.591765000	6.573401000
6	7.131910000	8.141988000	8.118301000
1	7.081398000	7.280807000	7.432715000
1	6.099640000	8.473437000	8.322870000
1	7.567150000	7.789692000	9.069375000
6	7.949742000	10.521679000	8.440008000
1	8.359128000	10.298680000	9.439308000
1	6.915603000	10.877167000	8.582238000
1	8.535602000	11.350783000	8.010854000
6	10.958612000	11.574384000	2.585287000
6	12.167435000	12.206398000	2.085316000
1	12.028651000	12.490253000	1.030779000
1	13.013657000	11.507168000	2.165780000
1	12.385293000	13.108500000	2.677907000
6	11.636336000	8.240818000	7.873046000
1	12.378110000	8.135212000	8.669928000
6	11.974483000	7.934094000	6.554028000
1	12.987028000	7.589767000	6.327547000
6	11.040463000	8.056815000	5.513340000
6	11.436044000	7.701688000	4.081024000
1	10.668995000	8.136634000	3.422692000

6	11.427848000	6.176805000	3.857090000
1	12.171982000	5.679424000	4.502422000
1	11.674709000	5.934414000	2.809527000
1	10.442101000	5.740847000	4.083572000
6	12.789948000	8.301904000	3.665262000
1	13.630588000	7.847889000	4.215676000
1	12.970108000	8.125733000	2.591820000
1	12.821535000	9.389103000	3.841599000
1	7.579563000	11.537583000	4.749302000

TS-[1--H--NEt₃]⁺

Spin multiplicity : Quartet / Charge : 1+

27	8.120556000	9.814173000	3.641155000
7	7.329707000	10.446656000	1.695849000
7	7.084190000	8.233428000	3.003932000
7	8.920704000	8.257898000	4.827468000
7	9.431543000	11.305797000	3.979206000
6	7.540253000	11.623539000	1.086432000
1	8.304262000	12.269944000	1.528328000
6	6.834787000	12.021307000	-0.047552000
1	7.043956000	12.987050000	-0.511863000
6	5.862355000	11.155642000	-0.563906000
1	5.283898000	11.432130000	-1.448858000
6	5.639898000	9.931702000	0.064395000
1	4.887044000	9.242448000	-0.320440000
6	6.395769000	9.594881000	1.197190000
6	6.268568000	8.314446000	1.929353000
6	5.450077000	7.244836000	1.574436000
1	4.798706000	7.300580000	0.701115000
6	5.496351000	6.064127000	2.352906000
1	4.854783000	5.219009000	2.093502000
6	6.382188000	5.971427000	3.420126000
1	6.464103000	5.055718000	4.011000000
6	7.204549000	7.078102000	3.721465000
6	8.235657000	7.131876000	4.714144000
1	8.450760000	6.256003000	5.338592000

6	10.011413000	8.333846000	5.740398000
6	9.791350000	8.477454000	7.134683000
6	10.909888000	8.557259000	7.981297000
1	10.757905000	8.659867000	9.059187000
6	8.389278000	8.552194000	7.733796000
1	7.679241000	8.632401000	6.898222000
6	8.037507000	7.276099000	8.521332000
1	8.119107000	6.376754000	7.890093000
1	7.005388000	7.329352000	8.906397000
1	8.711813000	7.143375000	9.384207000
6	8.196089000	9.807143000	8.603861000
1	8.835129000	9.789123000	9.502081000
1	7.150174000	9.877012000	8.945477000
1	8.430910000	10.724320000	8.039863000
6	10.190554000	12.150080000	4.205003000
6	11.141183000	13.207578000	4.492457000
1	12.092542000	12.767185000	4.828645000
1	10.741040000	13.858758000	5.285188000
1	11.316028000	13.805222000	3.584526000
6	12.208616000	8.510921000	7.476761000
1	13.064562000	8.572894000	8.154701000
6	12.411620000	8.390126000	6.100012000
1	13.432242000	8.355979000	5.711541000
6	11.331124000	8.304021000	5.210983000
6	11.569135000	8.120198000	3.713638000
1	10.660602000	8.474245000	3.200703000

6	11.732711000	6.627953000	3.362095000
1	12.627031000	6.206129000	3.851570000
1	11.847351000	6.494411000	2.273259000
1	10.861570000	6.037212000	3.687151000
6	12.749130000	8.940716000	3.170790000
1	13.716855000	8.582159000	3.558303000
1	12.789791000	8.860544000	2.072129000
1	12.654939000	10.007722000	3.430160000
7	5.195107000	10.716558000	5.039796000
6	4.469095000	11.203973000	3.853509000
6	3.186818000	12.012985000	4.087220000
1	4.242436000	10.320949000	3.237060000
1	5.170050000	11.816522000	3.264384000
1	2.779632000	12.321713000	3.110484000
1	2.409259000	11.434565000	4.606136000
1	3.374289000	12.929473000	4.668112000
6	4.733829000	9.435824000	5.603328000
6	3.398428000	9.420918000	6.356626000
1	5.528757000	9.091011000	6.284333000
1	4.697175000	8.712629000	4.773566000
1	3.254172000	8.424280000	6.805145000
1	3.374506000	10.157780000	7.175036000
1	2.540611000	9.611704000	5.694718000
6	5.535452000	11.727387000	6.051979000
6	6.307353000	12.924387000	5.504410000
1	6.147742000	11.217280000	6.812597000

1	4.625743000	12.082315000	6.574184000
1	6.629577000	13.564004000	6.341134000
1	7.203441000	12.595502000	4.957820000
1	5.700588000	13.546469000	4.828671000
1	6.723352000	10.188949000	4.366243000

IRC backward-[1--H--NEt₃]⁺

Spin multiplicity : Quartet / Charge : 1+

27	8.438410000	9.846549000	3.396928000
7	7.333149000	10.634153000	1.626587000
7	7.150263000	8.432842000	2.997624000
7	9.033822000	8.363243000	4.840826000
7	9.717265000	11.280365000	3.667495000
6	7.500890000	11.807780000	0.998554000
1	8.263801000	12.473640000	1.414751000
6	6.760485000	12.180582000	-0.120728000
1	6.933851000	13.146278000	-0.600094000
6	5.797231000	11.283308000	-0.605300000
1	5.192982000	11.534485000	-1.480793000
6	5.616204000	10.064698000	0.043234000
1	4.868996000	9.356679000	-0.317575000
6	6.404842000	9.755651000	1.166041000
6	6.306231000	8.490857000	1.927614000
6	5.454172000	7.439401000	1.609729000
1	4.786370000	7.498309000	0.749172000
6	5.475679000	6.267681000	2.415812000
1	4.808167000	5.434561000	2.183372000
6	6.366092000	6.184049000	3.474102000
1	6.425062000	5.282083000	4.090172000
6	7.231542000	7.270357000	3.753734000
6	8.246426000	7.285740000	4.741889000
1	8.391954000	6.408805000	5.386595000

6	10.080145000	8.388571000	5.788142000
6	9.818128000	8.534914000	7.179987000
6	10.901625000	8.572947000	8.073127000
1	10.707203000	8.677455000	9.144441000
6	8.396673000	8.664819000	7.724580000
1	7.727171000	8.774754000	6.858850000
6	7.957664000	7.402279000	8.490254000
1	8.025334000	6.502972000	7.857499000
1	6.914047000	7.497631000	8.835176000
1	8.590206000	7.236075000	9.378829000
6	8.217885000	9.921400000	8.596046000
1	8.824243000	9.875655000	9.515731000
1	7.164634000	10.027887000	8.905539000
1	8.505195000	10.833285000	8.047758000
6	10.500220000	12.127279000	3.809155000
6	11.489555000	13.178363000	3.979065000
1	12.499322000	12.738875000	4.003032000
1	11.311412000	13.714643000	4.924428000
1	11.427608000	13.893080000	3.143569000
6	12.219491000	8.487019000	7.625026000
1	13.048378000	8.518292000	8.338057000
6	12.472236000	8.366443000	6.255921000
1	13.506752000	8.301064000	5.909563000
6	11.427204000	8.316090000	5.323255000
6	11.718478000	8.126815000	3.836345000
1	10.860245000	8.557538000	3.295297000

6	11.778077000	6.630242000	3.470785000
1	12.615735000	6.132549000	3.989192000
1	11.926386000	6.497851000	2.385449000
1	10.850145000	6.108112000	3.752798000
6	12.981262000	8.853946000	3.350933000
1	13.901856000	8.417443000	3.772713000
1	13.061794000	8.779806000	2.253783000
1	12.962515000	9.923377000	3.617600000
7	5.089613000	10.471570000	4.946413000
6	4.260115000	11.114374000	3.844800000
6	3.090703000	11.979770000	4.288765000
1	3.922935000	10.283146000	3.210768000
1	4.969543000	11.708919000	3.253714000
1	2.592254000	12.344666000	3.377209000
1	2.344831000	11.429933000	4.877011000
1	3.411509000	12.862597000	4.860440000
6	4.551313000	9.147315000	5.461051000
6	3.283651000	9.202318000	6.297589000
1	5.378575000	8.714704000	6.041046000
1	4.411026000	8.521970000	4.568597000
1	3.091285000	8.183338000	6.667750000
1	3.383683000	9.857441000	7.175481000
1	2.403892000	9.511902000	5.716980000
6	5.494176000	11.409764000	6.058861000
6	6.353487000	12.568899000	5.578144000
1	6.049644000	10.792336000	6.777691000

1	4.578349000	11.757853000	6.552450000
1	6.707320000	13.127754000	6.457554000
1	7.236872000	12.205127000	5.029253000
1	5.803187000	13.269845000	4.933498000
1	5.975251000	10.196125000	4.475508000

IRC forward-[1--H--NEt₃]⁺

Spin multiplicity : Quartet / Charge : 1+

27	8.594886000	9.970000000	3.511594000
7	7.819834000	10.599522000	1.563836000
7	7.432120000	8.368320000	2.823118000
7	9.304555000	8.200487000	4.643457000
7	10.275980000	11.143156000	3.573639000
6	8.095588000	11.770568000	0.977462000
1	8.918088000	12.350607000	1.405048000
6	7.381280000	12.246234000	-0.124504000
1	7.645741000	13.206092000	-0.572354000
6	6.335035000	11.469691000	-0.625790000
1	5.748305000	11.809456000	-1.482604000
6	6.045804000	10.245715000	-0.018415000
1	5.233481000	9.622079000	-0.393745000
6	6.812683000	9.833602000	1.076968000
6	6.621134000	8.536473000	1.776005000
6	5.725528000	7.518421000	1.403910000
1	5.054592000	7.642986000	0.553163000
6	5.719861000	6.328859000	2.136871000
1	5.030842000	5.526139000	1.864818000
6	6.613247000	6.157980000	3.201993000
1	6.652780000	5.226771000	3.770922000
6	7.472694000	7.217654000	3.508478000
6	8.522723000	7.185477000	4.538253000
1	8.623235000	6.292861000	5.171933000

6	10.344072000	8.215558000	5.626911000
6	10.037183000	8.477201000	6.984022000
6	11.104229000	8.505557000	7.897804000
1	10.896239000	8.698771000	8.953295000
6	8.612790000	8.729354000	7.476800000
1	7.958698000	8.811402000	6.596746000
6	8.096753000	7.557100000	8.332496000
1	8.126361000	6.606660000	7.775672000
1	7.054694000	7.737232000	8.644469000
1	8.704479000	7.432219000	9.244296000
6	8.490444000	10.064343000	8.233511000
1	9.074112000	10.063857000	9.168660000
1	7.437484000	10.252281000	8.500962000
1	8.838812000	10.907062000	7.615083000
6	11.203051000	11.832902000	3.628884000
6	12.363251000	12.700461000	3.698885000
1	13.271189000	12.090468000	3.824219000
1	12.260183000	13.383846000	4.556020000
1	12.441765000	13.286780000	2.770382000
6	12.419421000	8.293698000	7.487181000
1	13.231966000	8.317038000	8.218545000
6	12.699338000	8.056419000	6.139197000
1	13.733562000	7.893396000	5.828209000
6	11.676323000	8.020311000	5.182160000
6	11.975023000	7.714274000	3.716150000
1	11.150121000	8.141810000	3.122605000

6	11.978407000	6.193438000	3.460946000
1	12.781367000	5.703521000	4.036903000
1	12.146552000	5.979595000	2.392398000
1	11.024388000	5.727357000	3.754310000
6	13.276702000	8.353049000	3.209182000
1	14.167288000	7.901567000	3.675818000
1	13.368637000	8.204480000	2.121109000
1	13.301891000	9.436318000	3.408266000
7	4.067700000	10.978749000	5.500604000
6	3.203460000	11.209226000	4.345833000
6	1.753866000	11.658991000	4.602185000
1	3.192021000	10.276598000	3.756153000
1	3.681579000	11.964991000	3.696552000
1	1.241878000	11.829718000	3.640087000
1	1.175250000	10.908010000	5.161501000
1	1.713522000	12.605035000	5.166785000
6	4.000003000	9.665344000	6.130874000
6	2.801426000	9.349782000	7.043842000
1	4.923861000	9.538681000	6.725761000
1	4.047169000	8.906595000	5.329540000
1	2.936863000	8.358567000	7.509163000
1	2.704669000	10.086659000	7.858498000
1	1.850056000	9.329399000	6.489658000
6	4.253487000	12.096977000	6.417690000
6	4.864694000	13.335907000	5.760465000
1	4.934293000	11.749982000	7.214319000

1	3.314633000	12.395445000	6.936111000
1	5.078754000	14.102035000	6.523278000
1	5.808247000	13.079901000	5.250203000
1	4.189437000	13.791969000	5.018839000
1	7.407445000	10.502916000	4.497229000

TS-[1--HH--NEt₃]⁺

Spin multiplicity : Triplet / Charge : 1+

27	8.682076000	10.656643000	3.958735000
7	7.697194000	11.911822000	2.320435000
7	7.117054000	9.587699000	3.329860000
7	9.002722000	8.903859000	5.006512000
7	10.527539000	11.124780000	3.187977000
6	8.097416000	13.099401000	1.853110000
1	9.020089000	13.505043000	2.279916000
6	7.393499000	13.803822000	0.875477000
1	7.760613000	14.769713000	0.522546000
6	6.217239000	13.238938000	0.371306000
1	5.633401000	13.756622000	-0.393924000
6	5.795298000	12.001521000	0.856137000
1	4.882227000	11.544020000	0.473553000
6	6.563183000	11.354257000	1.837554000
6	6.220794000	10.029404000	2.414348000
6	5.108455000	9.266189000	2.072957000
1	4.386561000	9.621899000	1.337049000
6	4.925311000	8.007097000	2.693609000
1	4.056058000	7.397248000	2.437022000
6	5.855354000	7.550677000	3.615385000
1	5.745535000	6.577363000	4.099929000
6	6.969139000	8.363625000	3.925602000
6	8.030964000	8.020123000	4.821013000
1	8.043426000	7.040175000	5.312428000

6	10.137348000	8.521370000	5.783412000
6	10.246231000	8.961898000	7.128370000
6	11.377863000	8.584263000	7.866638000
1	11.472309000	8.904347000	8.907076000
6	9.133055000	9.780200000	7.776165000
1	8.577364000	10.258153000	6.955680000
6	8.142893000	8.869766000	8.528889000
1	7.712929000	8.103893000	7.864084000
1	7.311377000	9.461412000	8.947534000
1	8.642728000	8.348991000	9.363399000
6	9.651696000	10.898968000	8.692808000
1	10.154383000	10.501740000	9.589827000
1	8.811768000	11.521544000	9.041758000
1	10.364754000	11.554703000	8.167233000
6	11.569381000	11.458487000	2.811944000
6	12.874598000	11.882106000	2.339513000
1	12.754045000	12.592158000	1.506887000
1	13.446068000	11.006456000	1.995195000
1	13.420618000	12.372382000	3.160405000
6	12.384231000	7.800228000	7.299822000
1	13.256806000	7.512935000	7.893276000
6	12.273564000	7.388629000	5.971560000
1	13.068157000	6.779181000	5.533154000
6	11.163446000	7.740228000	5.186909000
6	11.078285000	7.266358000	3.736050000
1	10.284859000	7.852301000	3.248621000

6	10.678546000	5.780208000	3.652334000
1	11.439836000	5.140720000	4.130629000
1	10.583700000	5.461675000	2.600608000
1	9.716732000	5.588192000	4.153293000
6	12.374862000	7.520099000	2.947099000
1	13.211100000	6.905077000	3.317978000
1	12.227705000	7.264661000	1.884733000
1	12.683421000	8.576237000	3.002734000
1	8.373456000	12.015837000	5.067674000
7	6.319371000	12.923202000	5.934449000
6	5.766310000	13.770765000	4.854087000
6	4.665911000	14.770717000	5.220501000
1	5.402783000	13.085309000	4.073637000
1	6.611591000	14.321018000	4.409320000
1	4.394075000	15.341685000	4.317881000
1	3.753952000	14.282215000	5.592372000
1	4.998943000	15.496235000	5.978787000
6	5.557822000	11.694803000	6.250339000
6	4.245868000	11.834715000	7.026796000
1	6.244604000	11.048184000	6.822587000
1	5.371302000	11.181319000	5.293719000
1	3.862920000	10.828055000	7.260229000
1	4.383648000	12.364751000	7.982159000
1	3.469846000	12.357933000	6.449114000
6	6.792731000	13.645638000	7.133905000
6	7.836643000	14.720604000	6.838944000

1	7.231164000	12.885387000	7.800545000
1	5.943492000	14.089666000	7.683907000
1	8.216724000	15.124217000	7.790487000
1	8.691818000	14.312144000	6.278483000
1	7.422108000	15.564112000	6.265946000
1	7.570915000	12.321820000	5.340078000

IRC backward-[1--HH--NEt₃]⁺

Spin multiplicity : Triplet / Charge : 1+

27	8.739296000	10.739903000	4.033860000
7	7.778772000	12.010694000	2.294028000
7	7.200135000	9.668489000	3.286801000
7	9.059686000	8.920966000	4.993962000
7	10.545151000	11.082769000	3.095626000
6	8.169849000	13.208261000	1.846816000
1	9.081671000	13.619381000	2.292817000
6	7.473131000	13.916414000	0.866648000
1	7.834082000	14.890030000	0.528314000
6	6.310491000	13.342563000	0.339010000
1	5.731573000	13.861471000	-0.429256000
6	5.896573000	12.095988000	0.805296000
1	4.993539000	11.633552000	0.405162000
6	6.660501000	11.446117000	1.790825000
6	6.324735000	10.111191000	2.349779000
6	5.226390000	9.347837000	1.966581000
1	4.526409000	9.708855000	1.212454000
6	5.026960000	8.080091000	2.568962000
1	4.167994000	7.470010000	2.279731000
6	5.930438000	7.619786000	3.511624000
1	5.810209000	6.641015000	3.983184000
6	7.037835000	8.430048000	3.861696000
6	8.068667000	8.060631000	4.775016000
1	8.043722000	7.078109000	5.261902000

6	10.161212000	8.503924000	5.794497000
6	10.253824000	8.935012000	7.145137000
6	11.353641000	8.519108000	7.910582000
1	11.430240000	8.832712000	8.954765000
6	9.152249000	9.783491000	7.773282000
1	8.613004000	10.258087000	6.940489000
6	8.145243000	8.902033000	8.537476000
1	7.704390000	8.134213000	7.881858000
1	7.322396000	9.512921000	8.946198000
1	8.632800000	8.384353000	9.381313000
6	9.686434000	10.910975000	8.670206000
1	10.179287000	10.524684000	9.577624000
1	8.855968000	11.555924000	9.002040000
1	10.412578000	11.543130000	8.133571000
6	11.572393000	11.328773000	2.623271000
6	12.859440000	11.643364000	2.027642000
1	12.721694000	12.362698000	1.205758000
1	13.321682000	10.724590000	1.635138000
1	13.521121000	12.084337000	2.789157000
6	12.348474000	7.704080000	7.367808000
1	13.195826000	7.386409000	7.982094000
6	12.257143000	7.300675000	6.035412000
1	13.042519000	6.667261000	5.614344000
6	11.179123000	7.690593000	5.224516000
6	11.119214000	7.225973000	3.769539000
1	10.355097000	7.836936000	3.266357000

6	10.682037000	5.751841000	3.664597000
1	11.411222000	5.088919000	4.160875000
1	10.609982000	5.441320000	2.608556000
1	9.700828000	5.583541000	4.135449000
6	12.443748000	7.447717000	3.018041000
1	13.250061000	6.802124000	3.403313000
1	12.318307000	7.209873000	1.948757000
1	12.784037000	8.492567000	3.096456000
1	8.444080000	12.015969000	5.075509000
7	6.266110000	12.926297000	6.040977000
6	5.573408000	13.664609000	4.917295000
6	4.499574000	14.668384000	5.315648000
1	5.159152000	12.885875000	4.261813000
1	6.370959000	14.168606000	4.353206000
1	4.074275000	15.084120000	4.388802000
1	3.676742000	14.216236000	5.885133000
1	4.903601000	15.510661000	5.895874000
6	5.580190000	11.654838000	6.479444000
6	4.218302000	11.797965000	7.141351000
1	6.290986000	11.165858000	7.161093000
1	5.514365000	11.031177000	5.575973000
1	3.910080000	10.801155000	7.493240000
1	4.241887000	12.464231000	8.016946000
1	3.446721000	12.153084000	6.443587000
6	6.698625000	13.787543000	7.195094000
6	7.677305000	14.882454000	6.793057000

1	7.169853000	13.103183000	7.915134000
1	5.800553000	14.202826000	7.671549000
1	8.020066000	15.395537000	7.704533000
1	8.560028000	14.462950000	6.286311000
1	7.222863000	15.638776000	6.136368000
1	7.172667000	12.557225000	5.600046000

IRC forward-[1--HH--NEt₃]⁺

Spin multiplicity : Triplet / Charge : 1+

27	9.051616000	10.672114000	3.639530000
7	8.077795000	11.995577000	2.157415000
7	7.258370000	9.783153000	3.281847000
7	9.144303000	8.862334000	4.861362000
7	10.948187000	11.061252000	3.252248000
6	8.570773000	13.130424000	1.651294000
1	9.575100000	13.414143000	1.980932000
6	7.861429000	13.928092000	0.749585000
1	8.305990000	14.848042000	0.364319000
6	6.584703000	13.515650000	0.362182000
1	5.995248000	14.108702000	-0.341298000
6	6.065212000	12.330821000	0.888152000
1	5.069149000	11.993350000	0.599348000
6	6.840601000	11.589213000	1.789525000
6	6.383648000	10.316132000	2.411995000
6	5.159976000	9.679835000	2.149976000
1	4.445730000	10.107665000	1.445546000
6	4.864970000	8.479163000	2.804355000
1	3.916477000	7.972160000	2.613459000
6	5.792102000	7.930443000	3.695038000
1	5.597591000	6.989554000	4.214669000
6	6.992979000	8.617902000	3.905560000
6	8.071878000	8.152287000	4.784259000
1	7.938286000	7.213581000	5.340680000

6	10.229639000	8.431011000	5.682670000
6	10.296944000	8.860580000	7.029428000
6	11.389434000	8.434777000	7.801415000
1	11.456545000	8.741531000	8.848468000
6	9.216158000	9.750210000	7.639170000
1	8.600004000	10.126087000	6.809818000
6	8.293222000	8.952676000	8.579028000
1	7.818979000	8.106178000	8.056464000
1	7.492864000	9.598712000	8.976858000
1	8.856831000	8.546526000	9.435810000
6	9.801930000	10.982126000	8.350539000
1	10.388192000	10.705518000	9.242219000
1	8.989927000	11.648991000	8.684524000
1	10.458487000	11.557490000	7.677773000
6	12.046500000	11.284851000	2.953276000
6	13.422152000	11.573183000	2.584666000
1	13.448182000	12.136425000	1.638918000
1	13.981631000	10.632868000	2.461675000
1	13.899217000	12.173677000	3.374984000
6	12.390826000	7.629243000	7.258072000
1	13.231595000	7.306035000	7.878066000
6	12.322575000	7.245805000	5.916785000
1	13.117833000	6.625415000	5.496711000
6	11.252969000	7.641485000	5.100326000
6	11.174512000	7.210352000	3.636957000
1	10.515005000	7.932788000	3.129360000

6	10.532446000	5.815754000	3.498126000
1	11.150414000	5.051685000	3.999301000
1	10.439010000	5.534210000	2.436002000
1	9.528341000	5.780069000	3.948702000
6	12.530856000	7.253312000	2.915511000
1	13.224337000	6.483668000	3.292156000
1	12.390136000	7.064661000	1.838718000
1	13.020541000	8.233807000	3.027893000
1	9.093719000	11.859044000	5.004952000
7	5.777589000	12.900196000	6.042795000
6	4.921486000	13.471037000	5.003237000
6	3.741926000	14.359382000	5.436793000
1	4.537923000	12.629707000	4.401531000
1	5.556185000	14.060640000	4.318133000
1	3.224349000	14.749265000	4.544115000
1	3.002051000	13.810321000	6.038929000
1	4.079280000	15.228261000	6.025433000
6	5.311163000	11.670594000	6.680598000
6	4.236281000	11.774384000	7.777290000
1	6.195607000	11.170718000	7.117875000
1	4.945050000	11.001234000	5.882895000
1	4.047512000	10.775999000	8.207166000
1	4.557440000	12.432389000	8.601318000
1	3.279040000	12.156517000	7.390277000
6	6.426061000	13.844213000	6.948234000
6	7.330111000	14.858991000	6.246700000

1	7.040328000	13.248713000	7.646100000
1	5.701206000	14.396662000	7.586463000
1	7.868139000	15.462927000	6.995403000
1	8.075332000	14.350961000	5.613003000
1	6.761994000	15.556644000	5.610834000
1	8.313610000	11.745262000	4.909102000

$4[2]^{2+}$

Spin multiplicity : Quartet / Charge : 2+

27	10.998632000	3.565362000	3.183807000
7	11.271078000	3.535452000	0.862584000
7	9.720715000	5.072524000	2.451071000
7	10.125495000	4.500802000	4.981854000
7	12.782604000	4.685571000	3.667769000
7	12.372449000	2.061074000	3.797571000
7	9.298170000	2.239782000	3.167646000
6	10.477978000	4.372589000	0.303302000
1	10.398013000	4.465097000	-0.790005000
6	9.619906000	5.247817000	1.124745000
6	8.746428000	6.190639000	0.576966000
1	8.679143000	6.318520000	-0.505263000
6	7.968501000	6.954351000	1.455562000
1	7.272904000	7.701561000	1.067137000
6	8.082111000	6.758130000	2.831290000
1	7.477014000	7.347699000	3.520341000
6	8.985562000	5.790229000	3.308157000
6	9.214389000	5.471792000	4.743723000
6	8.550701000	6.119319000	5.792394000
1	7.819436000	6.902489000	5.590811000
6	8.838373000	5.748157000	7.107863000
1	8.330119000	6.241193000	7.939905000
6	9.779818000	4.745002000	7.340950000
1	10.035379000	4.424369000	8.352698000

6	10.401925000	4.148322000	6.241467000
1	11.147236000	3.359577000	6.379366000
6	12.056901000	2.656899000	0.038568000
6	11.477651000	1.465721000	-0.465222000
6	12.291237000	0.617683000	-1.234681000
1	11.866437000	-0.303974000	-1.640054000
6	13.623845000	0.929100000	-1.498336000
1	14.236391000	0.252996000	-2.100960000
6	14.171878000	2.110661000	-0.996600000
1	15.213008000	2.354121000	-1.219136000
6	13.408564000	2.995259000	-0.221442000
6	10.012431000	1.097554000	-0.237601000
1	9.610411000	1.770851000	0.531417000
6	9.836449000	-0.336797000	0.291121000
1	10.136434000	-1.090251000	-0.455112000
1	8.777809000	-0.521363000	0.537266000
1	10.431998000	-0.506565000	1.202049000
6	9.181527000	1.315846000	-1.517664000
1	9.244546000	2.358143000	-1.869505000
1	8.119884000	1.081791000	-1.333399000
1	9.534508000	0.664327000	-2.334437000
6	13.997950000	4.319559000	0.255538000
1	13.407250000	4.640131000	1.125584000
6	13.846394000	5.409389000	-0.825296000
1	14.414459000	5.142494000	-1.732254000
1	14.228489000	6.375435000	-0.455774000

1	12.794518000	5.551798000	-1.120424000
6	15.460927000	4.209998000	0.712629000
1	15.593663000	3.413221000	1.461786000
1	15.783995000	5.160583000	1.166599000
1	16.141448000	4.002917000	-0.129178000
6	12.886365000	6.018798000	3.598157000
1	12.036596000	6.557273000	3.170406000
6	14.014967000	6.707630000	4.042595000
1	14.056232000	7.795620000	3.964955000
6	15.070041000	5.970867000	4.585127000
1	15.970270000	6.470187000	4.951248000
6	14.962874000	4.581755000	4.656864000
1	15.777193000	3.993982000	5.080082000
6	13.798097000	3.961194000	4.183437000
6	13.588269000	2.490397000	4.209305000
6	14.571383000	1.583012000	4.625586000
1	15.549463000	1.933344000	4.954157000
6	14.289945000	0.216443000	4.609822000
1	15.048165000	-0.502629000	4.928897000
6	13.033592000	-0.213682000	4.180395000
1	12.769259000	-1.272299000	4.150207000
6	12.104331000	0.747235000	3.783150000
1	11.108410000	0.455067000	3.443927000
6	8.310557000	1.647670000	3.275563000
6	7.071777000	0.902883000	3.406025000
1	6.954940000	0.229799000	2.542716000

1	6.222530000	1.602250000	3.442873000
1	7.095314000	0.308069000	4.332054000



Spin multiplicity : Triplet / Charge : 1+

27	10.982837000	3.619018000	3.010927000
7	11.234596000	3.505935000	0.873670000
7	9.754837000	5.111439000	2.374942000
7	10.018418000	4.506347000	4.914163000
7	12.731037000	4.719481000	3.716950000
7	12.456352000	2.083137000	3.592673000
7	9.414699000	2.132123000	3.318941000
6	10.513070000	4.427399000	0.249776000
1	10.524678000	4.523169000	-0.843424000
6	9.693577000	5.308998000	1.020550000
6	8.855975000	6.315043000	0.480651000
1	8.820066000	6.462644000	-0.601752000
6	8.092471000	7.089722000	1.337697000
1	7.436401000	7.870004000	0.944783000
6	8.161554000	6.864430000	2.735126000
1	7.559371000	7.466681000	3.415749000
6	9.005135000	5.865626000	3.213944000
6	9.171998000	5.526112000	4.653350000
6	8.509840000	6.201669000	5.692301000
1	7.830455000	7.026468000	5.474645000
6	8.730944000	5.805695000	7.010829000
1	8.224215000	6.320601000	7.830999000
6	9.606355000	4.745406000	7.266463000
1	9.807354000	4.402088000	8.283389000

6	10.227191000	4.128148000	6.179222000
1	10.921171000	3.294865000	6.330970000
6	12.015643000	2.619147000	0.075013000
6	11.434938000	1.421066000	-0.422884000
6	12.235973000	0.549214000	-1.177431000
1	11.800790000	-0.373232000	-1.570805000
6	13.575022000	0.837835000	-1.441984000
1	14.181537000	0.144671000	-2.031808000
6	14.134099000	2.019289000	-0.952545000
1	15.180856000	2.245074000	-1.170781000
6	13.377438000	2.925330000	-0.193522000
6	9.959935000	1.095857000	-0.194840000
1	9.614617000	1.736066000	0.629161000
6	9.716403000	-0.363089000	0.226516000
1	9.954546000	-1.072711000	-0.582849000
1	8.654992000	-0.510402000	0.486782000
1	10.321455000	-0.639757000	1.104779000
6	9.117177000	1.444906000	-1.437998000
1	9.223509000	2.505438000	-1.715366000
1	8.047861000	1.247708000	-1.251892000
1	9.426116000	0.837938000	-2.306095000
6	13.997060000	4.238240000	0.279985000
1	13.382475000	4.590971000	1.120514000
6	13.929408000	5.313910000	-0.822898000
1	14.513931000	5.007514000	-1.707215000
1	14.342303000	6.270253000	-0.459661000

1	12.893903000	5.495188000	-1.151044000
6	15.437912000	4.086222000	0.794243000
1	15.513878000	3.299909000	1.562215000
1	15.780424000	5.032623000	1.243887000
1	16.143514000	3.837036000	-0.015491000
6	12.776708000	6.057075000	3.753823000
1	11.914736000	6.585626000	3.338346000
6	13.856030000	6.759470000	4.290109000
1	13.849503000	7.851190000	4.297599000
6	14.926384000	6.030071000	4.813808000
1	15.789323000	6.538481000	5.250757000
6	14.881634000	4.636604000	4.772319000
1	15.708579000	4.053804000	5.177863000
6	13.763547000	4.004275000	4.207048000
6	13.627527000	2.527586000	4.097812000
6	14.642814000	1.637594000	4.480176000
1	15.585583000	2.006804000	4.883678000
6	14.438411000	0.265846000	4.332231000
1	15.219241000	-0.440817000	4.623689000
6	13.225920000	-0.183243000	3.805837000
1	13.019885000	-1.246677000	3.669194000
6	12.265930000	0.765491000	3.450541000
1	11.302835000	0.456549000	3.039047000
6	8.462940000	1.506795000	3.525109000
6	7.263762000	0.727548000	3.785749000
1	7.029628000	0.100472000	2.911932000

1	6.418249000	1.403880000	3.984469000
1	7.424166000	0.080928000	4.662082000

$^3[2]^+$

Spin multiplicity : Triplet / Charge :1+

27	11.184949000	3.951348000	2.941439000
7	11.304111000	3.665375000	0.843965000
7	9.739989000	5.165478000	2.307598000
7	10.059436000	4.495173000	4.806281000
7	12.999277000	4.739183000	3.639357000
7	12.180014000	2.217326000	3.670979000
6	10.509265000	4.506926000	0.192028000
1	10.504630000	4.562045000	-0.903104000
6	9.627397000	5.333610000	0.952466000
6	8.671102000	6.232730000	0.426094000
1	8.596630000	6.370665000	-0.655477000
6	7.836125000	6.914582000	1.297730000
1	7.087353000	7.611715000	0.914849000
6	7.940252000	6.691971000	2.694083000
1	7.266766000	7.206014000	3.380667000
6	8.902520000	5.804397000	3.162037000
6	9.110508000	5.438062000	4.585357000
6	8.385849000	5.997557000	5.649315000
1	7.629232000	6.760384000	5.462168000
6	8.644392000	5.567436000	6.949866000
1	8.087253000	5.991429000	7.789020000
6	9.623207000	4.590782000	7.164301000
1	9.856047000	4.224953000	8.166270000
6	10.307240000	4.088354000	6.057826000

1	11.084010000	3.327398000	6.178804000
6	12.129232000	2.784652000	0.081899000
6	11.635396000	1.495271000	-0.258370000
6	12.471655000	0.628251000	-0.978251000
1	12.107694000	-0.364832000	-1.252012000
6	13.759577000	1.010204000	-1.357815000
1	14.394423000	0.318711000	-1.919001000
6	14.231083000	2.278689000	-1.020105000
1	15.237615000	2.574494000	-1.327020000
6	13.436416000	3.184817000	-0.299564000
6	10.211196000	1.073526000	0.100577000
1	9.909975000	1.677569000	0.971862000
6	10.088095000	-0.407547000	0.494541000
1	10.246263000	-1.076685000	-0.367071000
1	9.076835000	-0.612157000	0.882554000
1	10.814878000	-0.687269000	1.273257000
6	9.228833000	1.399805000	-1.043012000
1	9.238924000	2.470292000	-1.298354000
1	8.198109000	1.128498000	-0.758897000
1	9.489022000	0.833707000	-1.953546000
6	13.964858000	4.583002000	0.011582000
1	13.319345000	5.002225000	0.796733000
6	13.849308000	5.504025000	-1.219198000
1	14.467930000	5.127598000	-2.051576000
1	14.192986000	6.523796000	-0.976967000
1	12.809943000	5.571597000	-1.577780000

6	15.403344000	4.580431000	0.554434000
1	15.508488000	3.907070000	1.420005000
1	15.688019000	5.595247000	0.877187000
1	16.132862000	4.264708000	-0.209474000
6	13.297426000	6.045717000	3.633997000
1	12.549154000	6.715706000	3.201439000
6	14.495029000	6.540807000	4.149353000
1	14.698009000	7.613125000	4.125808000
6	15.410614000	5.633821000	4.688694000
1	16.360538000	5.980094000	5.102913000
6	15.097797000	4.274065000	4.698153000
1	15.798465000	3.555743000	5.123385000
6	13.872927000	3.850969000	4.163370000
6	13.427472000	2.433381000	4.149644000
6	14.217705000	1.374238000	4.616773000
1	15.225937000	1.554102000	4.989800000
6	13.699019000	0.079028000	4.601265000
1	14.302104000	-0.757442000	4.962335000
6	12.403136000	-0.128385000	4.124474000
1	11.953940000	-1.122973000	4.100908000
6	11.681617000	0.973820000	3.664653000
1	10.665752000	0.855572000	3.279419000

$^2[2-H]^+$

Spin multiplicity : Doublet / Charge : 1+

27	10.918869000	3.590016000	3.140548000
7	11.399393000	3.606453000	0.784874000
7	9.847380000	5.099013000	2.452425000
7	9.987388000	4.385956000	4.989121000
7	12.640010000	4.557517000	3.581494000
7	11.958174000	2.055105000	3.807551000
6	10.702741000	4.549598000	0.276320000
1	10.693846000	4.769376000	-0.803266000
6	9.849313000	5.387990000	1.133313000
6	9.071464000	6.421290000	0.600672000
1	9.098338000	6.622538000	-0.472373000
6	8.272496000	7.172156000	1.465524000
1	7.651266000	7.985647000	1.084572000
6	8.278155000	6.869738000	2.826229000
1	7.660100000	7.444991000	3.515609000
6	9.083603000	5.819730000	3.299026000
6	9.159719000	5.417696000	4.728097000
6	8.432188000	6.049340000	5.748338000
1	7.763967000	6.882438000	5.528732000
6	8.574315000	5.594383000	7.060027000
1	8.017262000	6.071961000	7.869751000
6	9.435247000	4.524981000	7.318604000
1	9.577123000	4.138343000	8.329998000
6	10.121814000	3.952115000	6.244974000

1	10.806128000	3.112096000	6.401106000
6	12.217453000	2.787945000	-0.045451000
6	11.761620000	1.477194000	-0.347316000
6	12.578146000	0.657755000	-1.137956000
1	12.241157000	-0.349506000	-1.393057000
6	13.814295000	1.105922000	-1.610003000
1	14.436756000	0.451301000	-2.226236000
6	14.252176000	2.389854000	-1.289455000
1	15.221713000	2.732416000	-1.660185000
6	13.475043000	3.256459000	-0.502530000
6	10.390215000	1.008434000	0.130833000
1	10.170955000	1.575345000	1.049867000
6	10.337782000	-0.485912000	0.482014000
1	10.439774000	-1.125890000	-0.409927000
1	9.368195000	-0.729209000	0.946780000
1	11.133031000	-0.765286000	1.191301000
6	9.296949000	1.358371000	-0.899280000
1	9.276162000	2.436115000	-1.125929000
1	8.301102000	1.072925000	-0.520705000
1	9.466662000	0.821061000	-1.847771000
6	13.996587000	4.656480000	-0.181467000
1	13.347666000	5.086071000	0.595321000
6	13.916678000	5.580695000	-1.412280000
1	14.553993000	5.204183000	-2.229953000
1	14.260328000	6.597166000	-1.157661000
1	12.887190000	5.655017000	-1.797700000

6	15.423873000	4.636318000	0.393699000
1	15.494630000	3.974664000	1.271719000
1	15.719500000	5.650530000	0.708451000
1	16.162338000	4.294965000	-0.349926000
6	12.877994000	5.871193000	3.453784000
1	12.078289000	6.474750000	3.018923000
6	14.077383000	6.461550000	3.851390000
1	14.220677000	7.536532000	3.726182000
6	15.070848000	5.650675000	4.405869000
1	16.023261000	6.075230000	4.731919000
6	14.828456000	4.283935000	4.540733000
1	15.586744000	3.631735000	4.974386000
6	13.598325000	3.762294000	4.118099000
6	13.221121000	2.337650000	4.225889000
6	14.068534000	1.340505000	4.725061000
1	15.079970000	1.587111000	5.049485000
6	13.606110000	0.027176000	4.803292000
1	14.253828000	-0.763478000	5.189009000
6	12.303827000	-0.253305000	4.383051000
1	11.894424000	-1.264355000	4.428764000
6	11.516042000	0.787522000	3.893161000
1	10.495175000	0.612196000	3.553847000
1	9.700092000	2.712617000	2.895252000

$^2[2\text{-NH}]^+$

Spin multiplicity : Doublet / Charge : 1+

27	11.138865000	4.315722000	3.452565000
7	11.228660000	3.819955000	0.331929000
7	9.679948000	5.267205000	2.385423000
7	9.885422000	4.716416000	5.025985000
7	13.078554000	4.735494000	3.654372000
7	11.818596000	2.447090000	3.534534000
6	10.447738000	4.894864000	0.093480000
1	10.428922000	5.252503000	-0.937356000
6	9.645937000	5.572833000	1.039623000
6	8.755038000	6.576201000	0.549398000
1	8.773673000	6.819138000	-0.515265000
6	7.877943000	7.197904000	1.406644000
1	7.187852000	7.962993000	1.044387000
6	7.871813000	6.824074000	2.769427000
1	7.176331000	7.301238000	3.458451000
6	8.777925000	5.870386000	3.220348000
6	8.823731000	5.467438000	4.654735000
6	7.837434000	5.818467000	5.589718000
1	6.971472000	6.409169000	5.292718000
6	7.964408000	5.387515000	6.909710000
1	7.200947000	5.650771000	7.645794000
6	9.070744000	4.614330000	7.275849000
1	9.206085000	4.257317000	8.298535000
6	10.009464000	4.301039000	6.295803000

1	10.892447000	3.698974000	6.527052000
6	12.033364000	3.182615000	-0.664036000
6	11.716147000	1.848165000	-1.031168000
6	12.495337000	1.235927000	-2.021527000
1	12.272188000	0.212171000	-2.327941000
6	13.543638000	1.920394000	-2.641546000
1	14.131798000	1.428242000	-3.421029000
6	13.843755000	3.226674000	-2.261260000
1	14.675815000	3.746920000	-2.742535000
6	13.112205000	3.883206000	-1.257104000
6	10.514532000	1.124601000	-0.424377000
1	10.364722000	1.514909000	0.594543000
6	10.710824000	-0.392298000	-0.288669000
1	10.745334000	-0.894063000	-1.269298000
1	9.867723000	-0.828991000	0.270260000
1	11.639258000	-0.634942000	0.252346000
6	9.232990000	1.442333000	-1.221666000
1	9.043909000	2.526031000	-1.274641000
1	8.356975000	0.966615000	-0.750496000
1	9.314058000	1.062405000	-2.253938000
6	13.527895000	5.291040000	-0.833192000
1	12.921783000	5.576409000	0.038500000
6	13.262360000	6.324713000	-1.943936000
1	13.863655000	6.107087000	-2.842359000
1	13.529496000	7.337218000	-1.599077000
1	12.202557000	6.336497000	-2.244848000

6	14.999429000	5.336976000	-0.380967000
1	15.194657000	4.608701000	0.422021000
1	15.246676000	6.340242000	0.003121000
1	15.689958000	5.120672000	-1.212363000
6	13.644239000	5.960499000	3.773715000
1	12.952240000	6.805600000	3.839378000
6	15.013571000	6.158705000	3.809326000
1	15.415884000	7.168299000	3.913129000
6	15.862055000	5.034750000	3.699556000
1	16.948035000	5.154082000	3.709516000
6	15.297131000	3.774367000	3.580461000
1	15.935294000	2.893341000	3.499608000
6	13.892589000	3.629929000	3.574596000
6	13.193577000	2.353899000	3.531602000
6	13.827080000	1.092905000	3.538103000
1	14.916230000	1.030942000	3.515748000
6	13.066564000	-0.065101000	3.594144000
1	13.550137000	-1.044558000	3.606849000
6	11.657600000	0.045199000	3.645542000
1	11.019668000	-0.838875000	3.704729000
6	11.087894000	1.304228000	3.606282000
1	10.001207000	1.430931000	3.620767000
1	11.113857000	3.332793000	1.222545000

$^2[2\text{-H-NH}]^{2+}$

Spin multiplicity : Doublet / Charge : 2+

27	11.170782000	3.791543000	3.027648000
7	11.006437000	3.724839000	0.068266000
7	9.962937000	5.194357000	2.341915000
7	10.022401000	4.109257000	4.755882000
7	12.682040000	4.992626000	3.648453000
7	12.426479000	2.397507000	3.566955000
6	10.624488000	4.958014000	-0.005790000
1	10.758554000	5.486251000	-0.955691000
6	9.939134000	5.669162000	1.068503000
6	9.199355000	6.801402000	0.705184000
1	9.233063000	7.164329000	-0.323764000
6	8.406032000	7.426123000	1.669748000
1	7.812188000	8.307001000	1.418458000
6	8.375975000	6.895092000	2.952345000
1	7.749695000	7.356394000	3.715423000
6	9.170516000	5.774703000	3.270494000
6	9.189801000	5.162870000	4.622071000
6	8.396793000	5.608515000	5.688623000
1	7.725714000	6.459827000	5.576399000
6	8.473460000	4.938304000	6.910804000
1	7.862770000	5.267213000	7.754752000
6	9.335943000	3.847479000	7.035088000
1	9.424991000	3.294645000	7.972373000
6	10.096687000	3.468864000	5.926420000

1	10.788006000	2.623188000	5.981473000
6	11.695594000	2.997753000	-0.962353000
6	11.072481000	1.815659000	-1.434772000
6	11.733224000	1.101863000	-2.441064000
1	11.280571000	0.194872000	-2.845961000
6	12.960973000	1.538584000	-2.945202000
1	13.457777000	0.968296000	-3.734534000
6	13.559889000	2.691558000	-2.442058000
1	14.529818000	3.005968000	-2.834279000
6	12.951004000	3.453465000	-1.430983000
6	9.695665000	1.384030000	-0.935030000
1	9.559605000	1.786980000	0.081674000
6	9.538375000	-0.139606000	-0.825195000
1	9.543189000	-0.626974000	-1.813351000
1	8.575133000	-0.379958000	-0.347741000
1	10.341630000	-0.587152000	-0.218595000
6	8.586820000	1.994727000	-1.816375000
1	8.654955000	3.093692000	-1.855265000
1	7.593279000	1.728487000	-1.420562000
1	8.658058000	1.614833000	-2.848999000
6	13.690823000	4.666476000	-0.868654000
1	13.097608000	5.097231000	-0.048996000
6	13.869559000	5.767676000	-1.930376000
1	14.487559000	5.414228000	-2.771713000
1	14.372035000	6.643211000	-1.488446000
1	12.900513000	6.097876000	-2.338156000

6	15.042730000	4.258443000	-0.252752000
1	14.913576000	3.484965000	0.521091000
1	15.521934000	5.133544000	0.215306000
1	15.734422000	3.866421000	-1.015735000
6	12.720915000	6.333142000	3.632867000
1	11.841592000	6.851483000	3.245566000
6	13.823322000	7.058474000	4.085035000
1	13.805387000	8.149250000	4.048835000
6	14.927685000	6.360061000	4.575800000
1	15.809580000	6.891842000	4.940409000
6	14.891948000	4.965193000	4.595098000
1	15.743624000	4.399577000	4.973566000
6	13.752820000	4.305012000	4.120663000
6	13.605528000	2.834720000	4.082192000
6	14.579229000	1.936110000	4.531572000
1	15.519866000	2.301635000	4.943340000
6	14.332723000	0.565310000	4.449603000
1	15.083240000	-0.149492000	4.794810000
6	13.117431000	0.126890000	3.920711000
1	12.880732000	-0.935355000	3.836282000
6	12.191858000	1.075345000	3.488303000
1	11.232631000	0.777998000	3.063983000
1	10.767779000	3.212627000	0.970890000
1	10.267720000	2.751291000	2.364004000

CH₃CN

Spin multiplicity : Singlet / Charge : 0

6	-2.066454000	-0.000019000	-1.057054000
7	-2.066335000	0.000020000	-2.216701000
6	-2.066530000	-0.000004000	0.400235000
1	-1.032148000	0.000001000	0.776779000
1	-2.583584000	-0.895735000	0.777031000
1	-2.583584000	0.895738000	0.777008000

Et₃N

Spin multiplicity : Singlet / Charge : 0

6	-2.465749000	0.355331000	0.152781000
1	-2.889803000	-0.662619000	0.147654000
1	-2.175628000	0.615803000	-0.878104000
1	-3.262297000	1.053462000	0.456037000
6	-1.248459000	0.428042000	1.076937000
1	-0.844097000	1.465244000	1.051613000
1	-0.450086000	-0.209299000	0.658525000
7	-1.511064000	-0.050662000	2.428027000
6	-2.544815000	0.646768000	3.187227000
1	-2.630231000	0.139522000	4.163601000
1	-3.516445000	0.487766000	2.684907000
6	-2.379343000	2.159393000	3.420595000
1	-2.318691000	2.715156000	2.470378000
1	-3.251911000	2.548364000	3.972208000
1	-1.478526000	2.396411000	4.007200000
6	-0.339777000	-0.511703000	3.163493000
1	-0.695922000	-0.998278000	4.088858000
1	0.134996000	-1.310165000	2.562431000
6	0.747080000	0.515515000	3.528835000
1	0.380106000	1.275652000	4.236065000
1	1.602105000	0.004815000	4.003731000
1	1.128401000	1.038141000	2.635996000

[Et₃NH]⁺

Spin multiplicity : Singlet / Charge : 1+

6	-2.434586000	0.407370000	0.120586000
1	-2.911663000	-0.583884000	0.051143000
1	-2.060939000	0.671799000	-0.880263000
1	-3.196221000	1.150543000	0.398498000
6	-1.254415000	0.393216000	1.078605000
1	-0.828152000	1.395581000	1.209528000
1	-0.459306000	-0.267839000	0.705587000
7	-1.606564000	-0.135302000	2.450767000
6	-2.680791000	0.650651000	3.182784000
1	-2.887155000	0.074918000	4.096046000
1	-3.574756000	0.588086000	2.548151000
6	-2.351463000	2.097484000	3.507861000
1	-2.083545000	2.682724000	2.615462000
1	-3.256000000	2.552542000	3.939984000
1	-1.547864000	2.191227000	4.251183000
6	-0.378123000	-0.471586000	3.288661000
1	-0.759074000	-0.691258000	4.295689000
1	0.005983000	-1.410171000	2.863247000
6	0.728194000	0.570727000	3.327807000
1	0.403000000	1.532906000	3.744968000
1	1.519416000	0.174808000	3.983534000
1	1.178179000	0.743229000	2.339691000
1	-2.045257000	-1.049982000	2.284960000

H₂

Spin multiplicity : Singlet / Charge : 0

1	-1.182459000	0.897436000	0.000000000
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1	-1.944036000	0.897436000	0.000000000
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