

Supporting Information

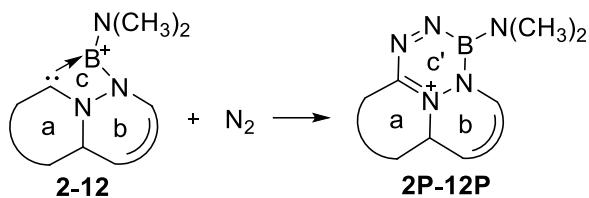
Predicting Dinitrogen Activation by Boremium and Borinium Cations

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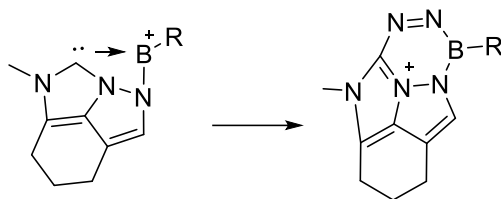
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Table S1. The NICS(1)_{zz} values of ring a, b, c, a', b' and c' in reactants (**2-12**) and products (**2P-12P**).



Compound	a	b	c(c')
2/2P	0.6/0.2	-5.1/-2.4	2.5/-2.5
3/3P	-20.8/-29.3	-10.8/-24.5	6.1/-3.3
4/4P	-3.6/-1.2	-6.2/-3.8	-2.4/-6.3
5/5P	-19.2/-29.5	-10.5/-23.2	4.8/-1.1
6/6P	1.5/2.3	-3.1/2.3	-0.3/-2.1
7/7P	2.3/4.9	-3.5/-3.8	2.4/-5.5
8/8P	-24.3/-28.4	-14.7/-22.7	10.6/-2.0
9/9P	-5.2/-0.1	-5.7/-3.5	-1.2/-2.9
10/10P	4.5/-1.2	-9.8/-2.7	4.3/0.3
11/11P	-16.2/-25.1	-8.4/-21.0	-7.3/-2.2
12/12P	-13.1/-22.4	-5.7/-19.7	4.4/-0.5

Table S2. The thermodynamic result (ΔG) of the dinitrogen activation by borenium (or borinium) cation with different substituent. Note that the value in the parenthesis for **12d** was calculated based on the thermodynamically more stable open form.



Entry	Reagent	R	ΔG (kcal/mol)
1	12	N(CH ₃) ₂	-5.5
2	12a	OCH ₃	-11.0

3	12b	CH ₃	-11.8
4	12c	<i>t</i> Bu	-10.1
5	12d	Si(CH ₃) ₃	-9.2 (-7.8)
6	12e	Ph	-9.8

Table S3. The gibbs free isomerization energy from closed to open form. $\Delta G_s = G_{\text{open}} - G_{\text{closed}}$, and were given in kcal/mol.

Reagent	3	3a	3b	3c	3d	3e
ΔG	3.9	5.8	4.0	2.5	-1.0	3.3
Reagent	12	12b	12b	12c	12d	12e
ΔG	2.3	6.1	3.5	0.7	-1.4	2.0

Table S4. LBO of B-C in compounds **12** and **12a-12e**.

Compound	12	12a	12b	12c	12d	12e
LBO	0.509	0.583	0.558	0.515	0.501	0.526

Table S5. Activation strain model of **TS-2** with the open form as reference. $\Delta E(\text{barrier}) = \Delta E_{\text{deform}}(\text{N}_2) + \Delta E_{\text{deform}}(\text{LP}) + \Delta E_{\text{b}}$. LP means Lewis pairs.

Compound	ΔE_{b}	$\Delta E_{\text{deform}}(\text{N}_2)$	$\Delta E_{\text{deform}}(\text{LP})$	$\Delta E(\text{barrier})$
3	-7.6	0.0	6.7	-0.9
3a	-8.4	0.0	4.4	-4.0
3b	-6.4	0.0	2.6	-3.8
3c	-6.8	0.0	3.0	-3.8
3d	-5.8	0.0	2.6	-3.2
3e	-6.5	0.0	3.7	-2.8

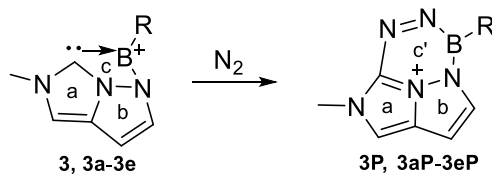
Table S6. Activation strain model of **TS-3** with the closed form as reference. $\Delta E(\text{barrier}) = \Delta E_{\text{deform}}(\text{N}_2) + \Delta E_{\text{deform}}(\text{LP}) + \Delta E_{\text{b}}$. LP means Lewis pairs.

Compound	ΔE_b	$\Delta E_{\text{deform}}(\text{N}_2)$	$\Delta E_{\text{deform}}(\text{LP})$	$\Delta E(\text{barrier})$
3	-28.8	0.0	30.8	2.0
3a	-36.0	0.0	34.4	-1.6
3b	-39.6	1.8	28.6	-9.2
3c	-38.1	3.7	28.4	-6.0
3d	-33.5	6.2	19.8	-7.4
3e	-35.9	1.4	28.6	-6.0

Table S7. Activation strain model of **TS-3** with the open form as reference. $\Delta E(\text{barrier}) = \Delta E_{\text{deform}}(\text{N}_2) + \Delta E_{\text{deform}}(\text{LP}) + \Delta E_b$. LP means Lewis pairs.

Compound	ΔE_b	$\Delta E_{\text{deform}}(\text{N}_2)$	$\Delta E_{\text{deform}}(\text{LP})$	$\Delta E(\text{barrier})$
3	-28.8	0.0	24.9	-3.9
3a	-36.0	0.0	26.1	-9.9
3b	-39.6	1.8	22.6	-15.2
3c	-38.1	3.7	23.7	-10.7
3d	-33.5	6.2	19.1	-8.2
3e	-35.9	1.4	23.8	-10.7

Table S8. The NICS(1)_{zz} values of ring a, b, c, a', b' and c' in reactants (**3**, **3a-3e**) and products (**3P**, **3aP-3eP**).



Compound	a	b	c	a'	b'	c'
3/3P	-20.8	-10.8	6.1	-29.3	-24.5	-3.3
3a/3aP	-18.9	-8.9	8.7	-31.1	-27.3	-11.3
3b/3bP	-21.2	-8.9	6.0	-32.4	-26.6	-16.8

3c/3cP	-21.9	-10.5	4.5	-32.1	-26.7	-17.0
3d/3dP	-24.6	-13.4	-2.9	-32.8	-26.4	-18.3
3e/3eP	-20.6	-9.5	6.5	-31.4	-27.4	-13.1

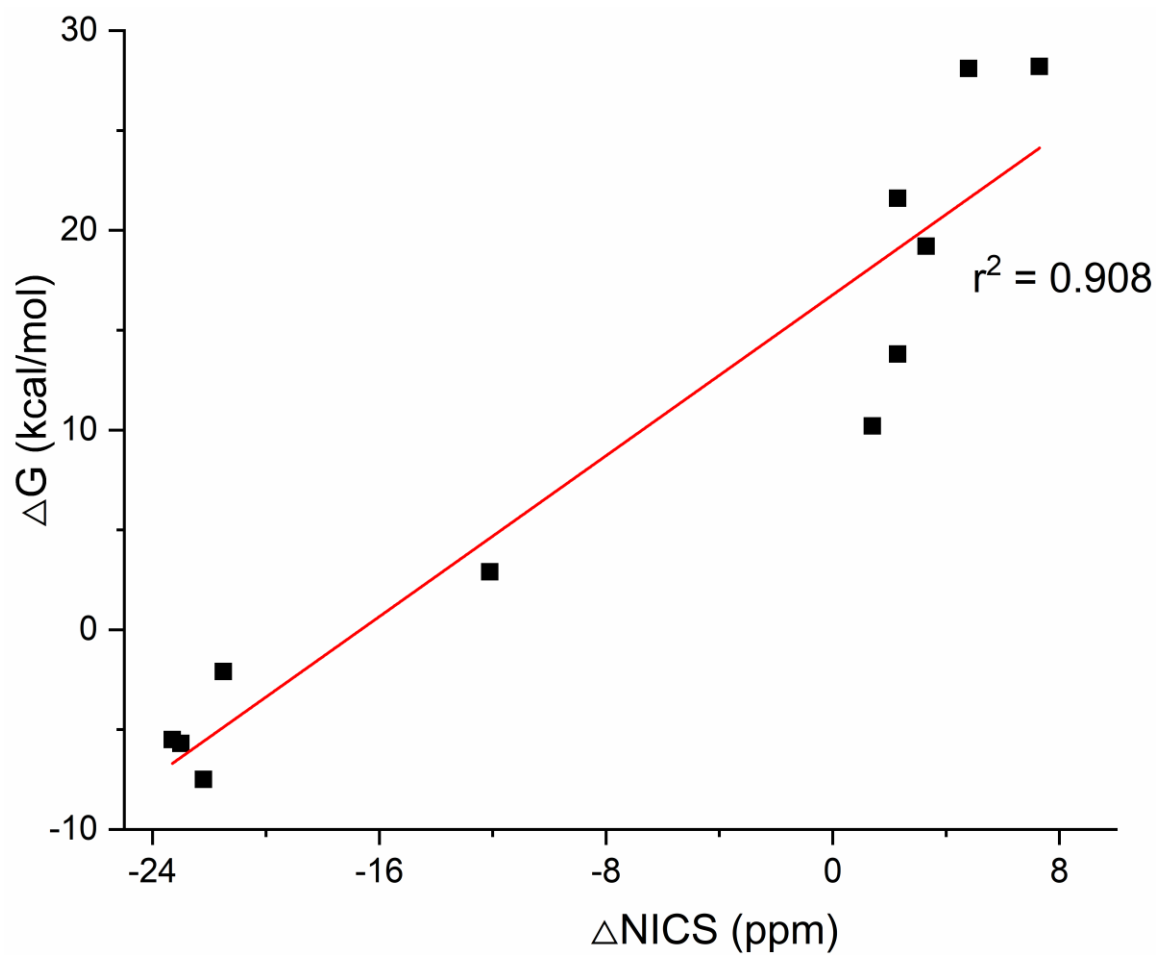


Figure S1. The result of linear fitting between ΔNICS and ΔG for **2-12**.

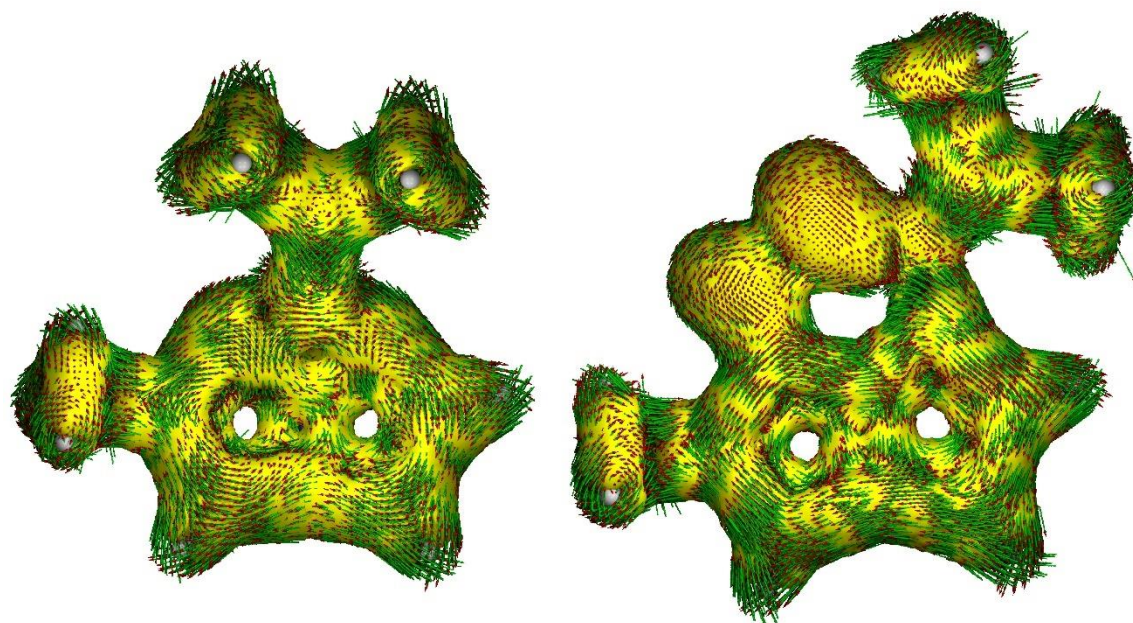


Figure S2. The ACID plots of the reactant (left) and product (right) for **3**. The isovalue is 0.03.

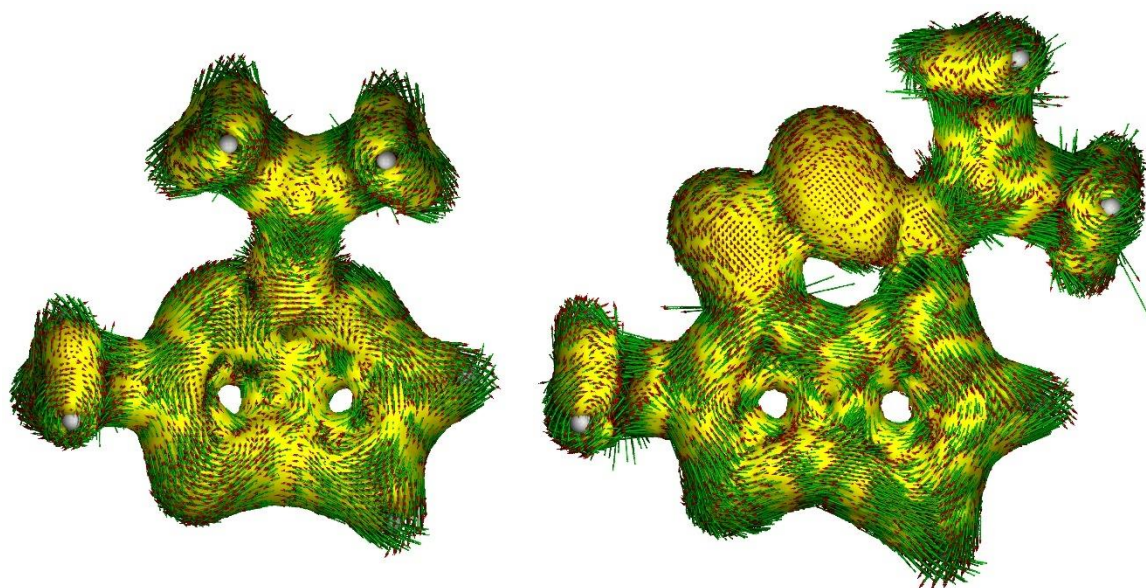


Figure S3. The ACID plots of the reactant (left) and product (right) for **5**. The isovalue is 0.03.

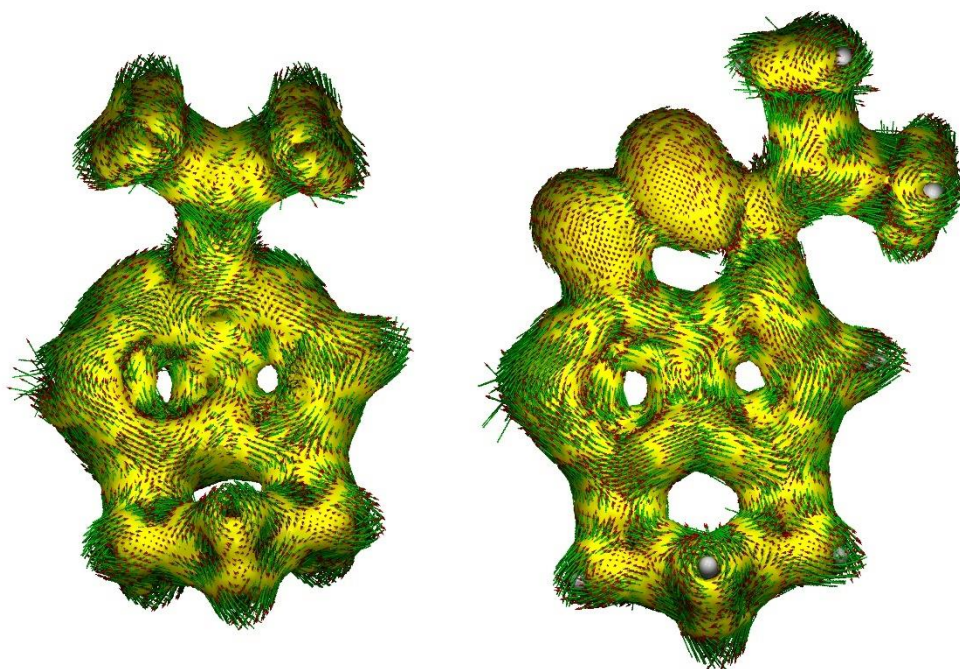


Figure S4. The ACID plots of the reactant (left) and product (right) for **11**. The isovalue is 0.03.

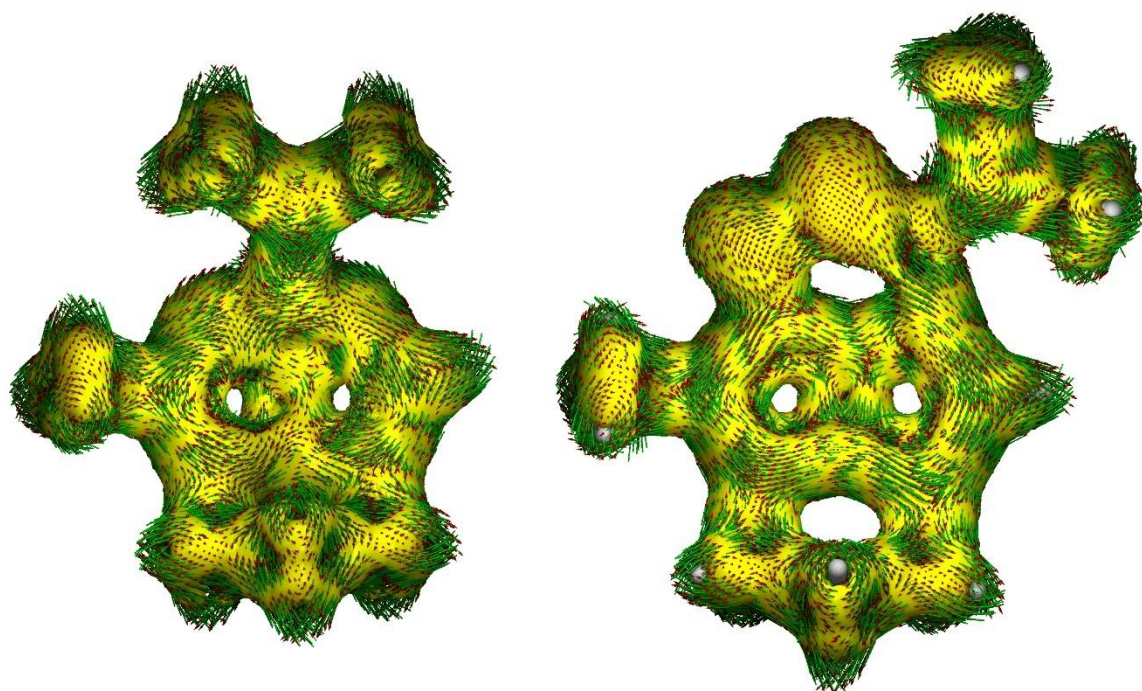


Figure S5. The ACID plots of the reactant (left) and product (right) for **12**. The isovalue is 0.03.

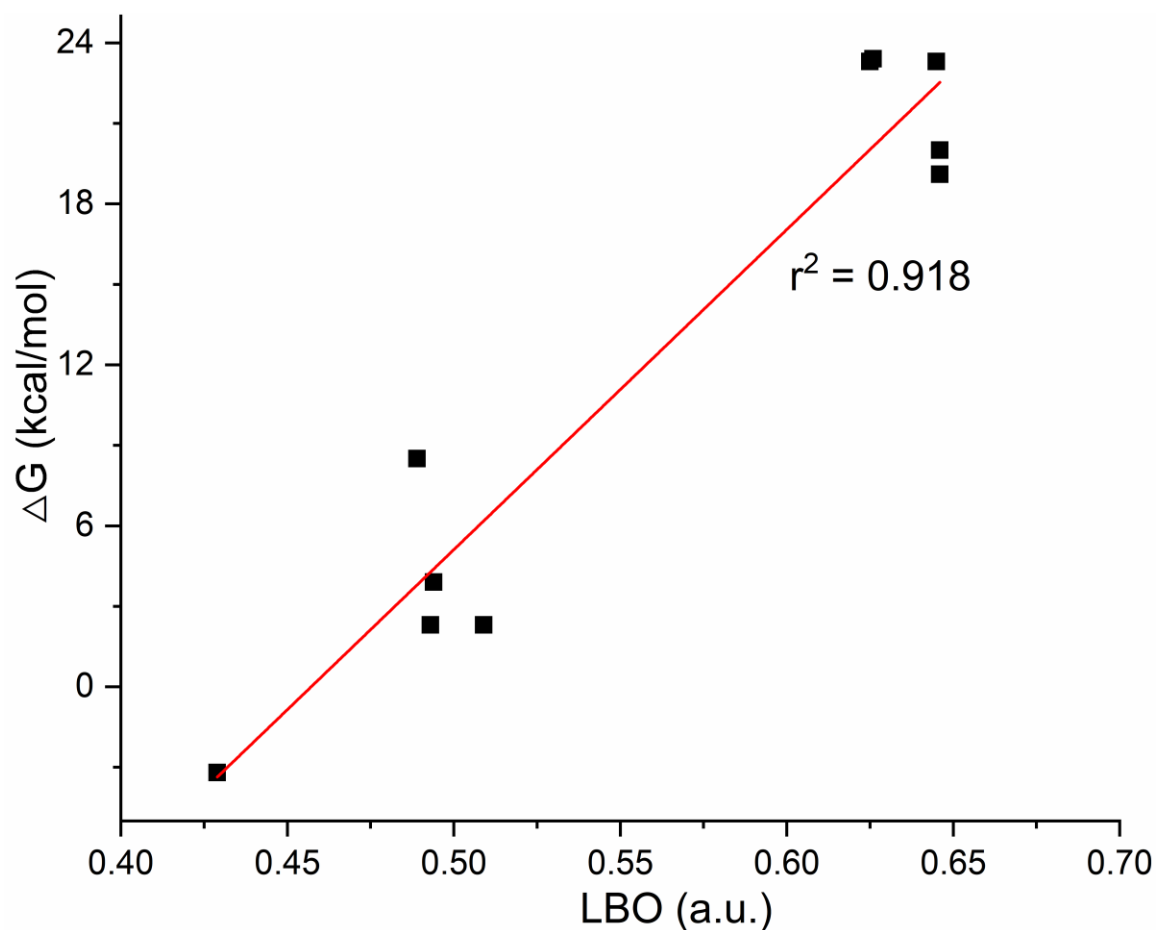


Figure S6. The result of linear fitting between LBO and Gibbs free isomerization energy for 2-12, except 6.

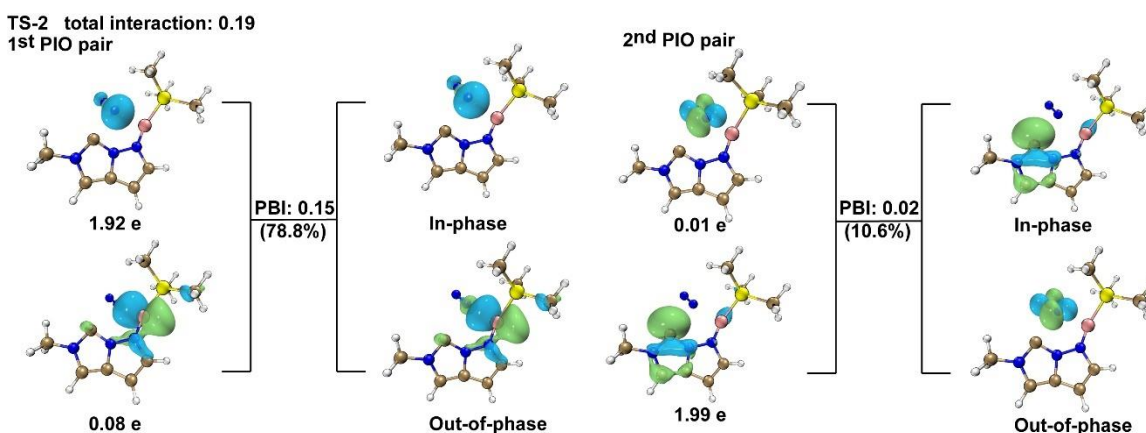


Figure S7. PIO analysis for TS-2 of **3d** via separating to two fragments including N₂ and the remaining part. The primary interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

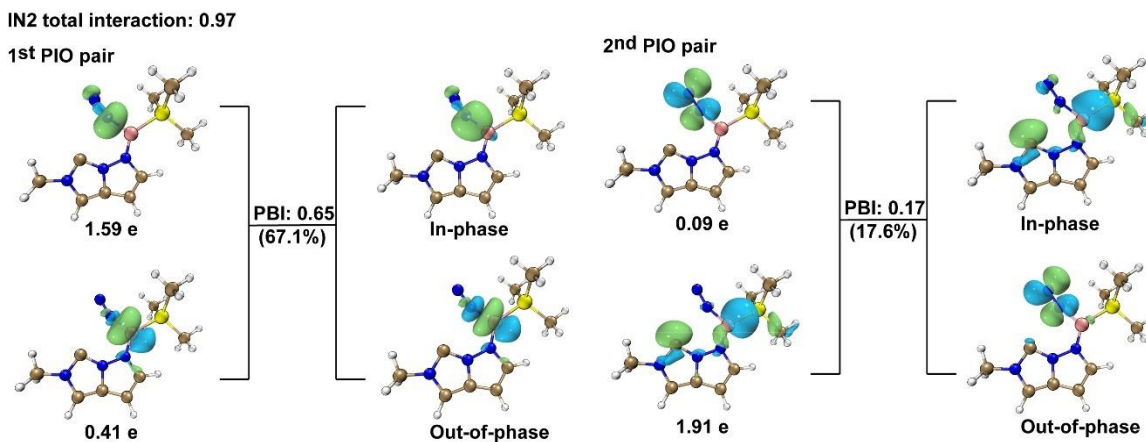


Figure S8. PIO analysis for **IN2** of **3d** via separating to two fragments including N_2 and the remaining part. The primary interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

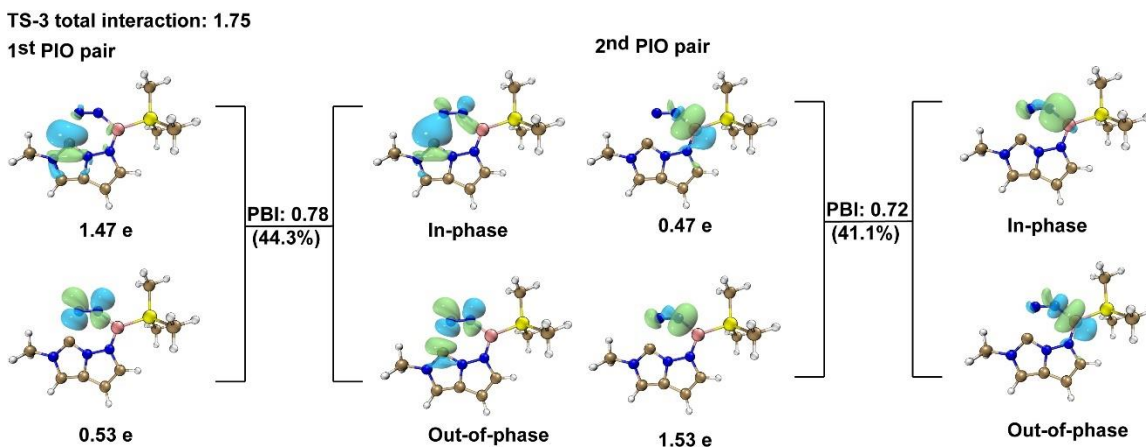


Figure S9. PIO analysis for **TS-3** of **3d** via separating to two fragments including N_2 and the remaining part. The primary interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

P total interaction: 2.64

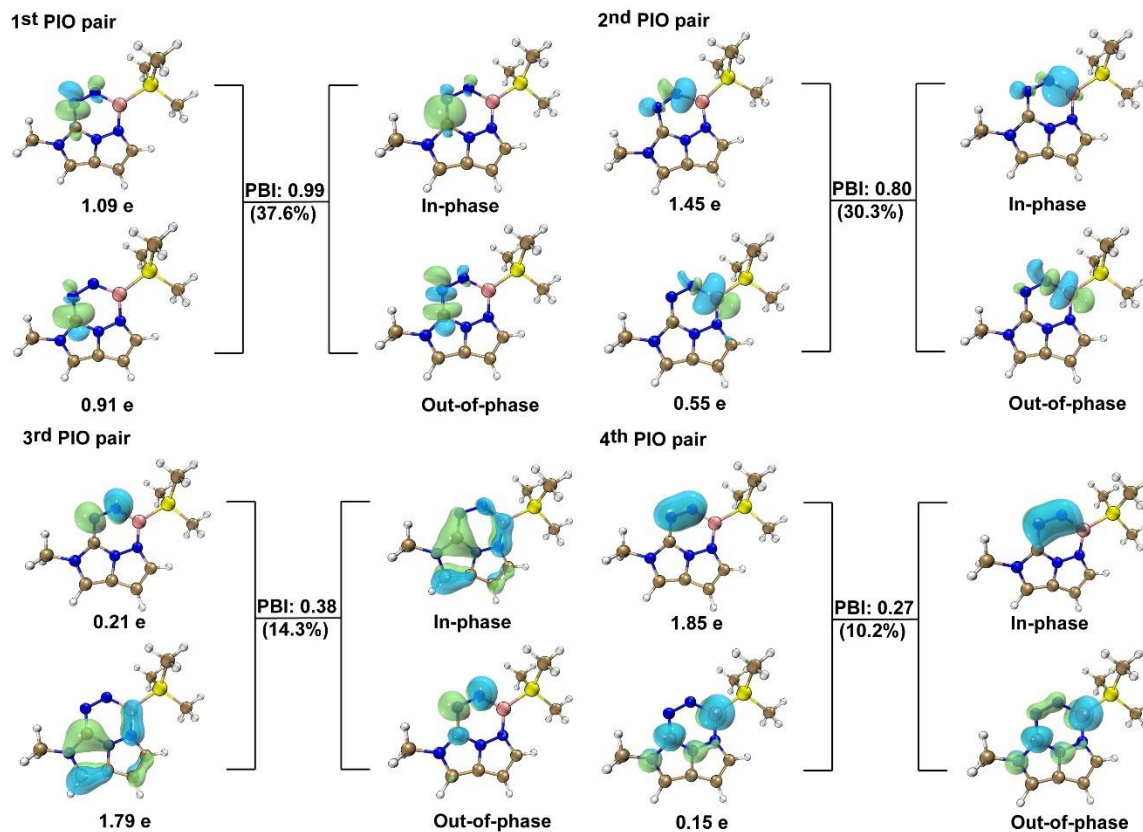


Figure S10. PIO analysis for **P** of **3d** via separating to two fragments including N_2 and the remaining part. The third and fourth interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

TS-2 total interaction: 0.23

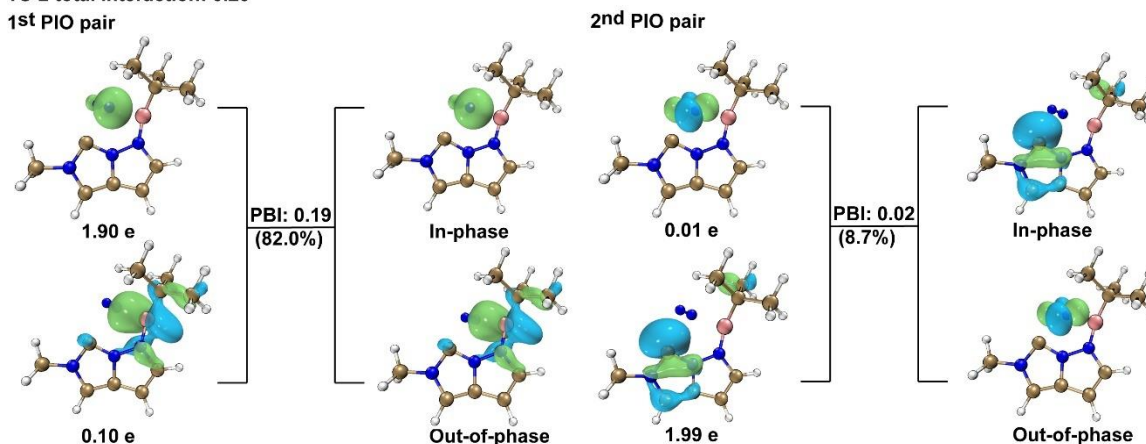


Figure S11. PIO analysis for **TS-2** of **3c** via separating to two fragments including N_2 and the remaining part. The primary interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

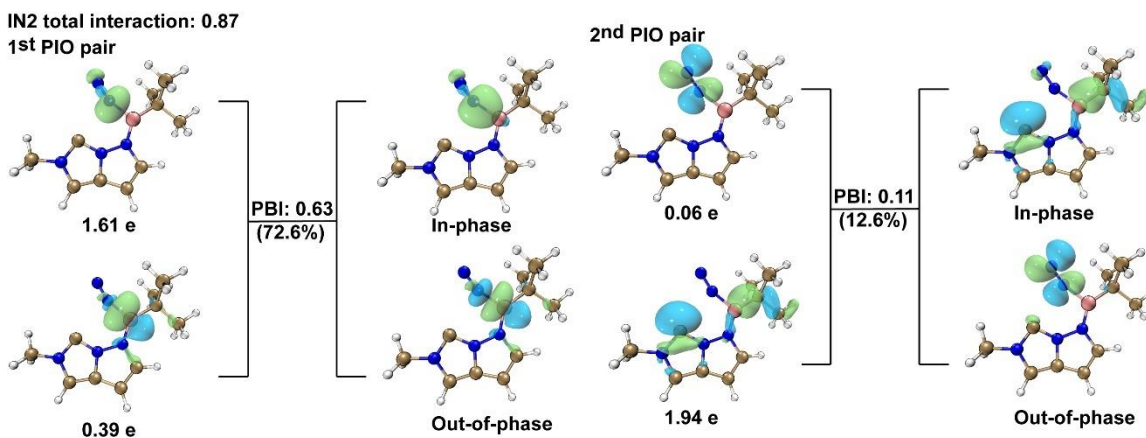


Figure S12. PIO analysis for **IN2** of **3c** via separating to two fragments including N_2 and the remaining part. The primary interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

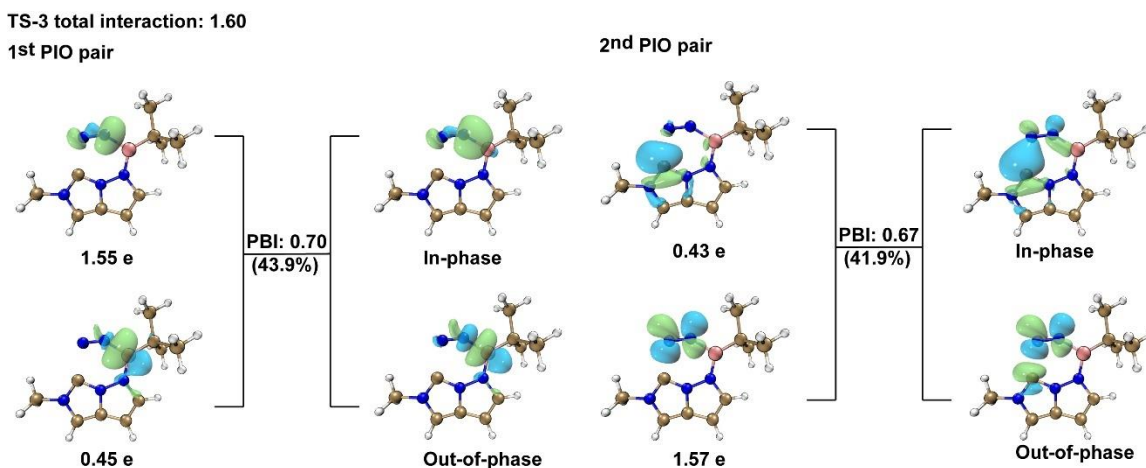
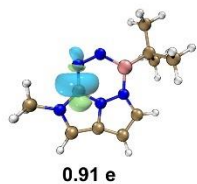
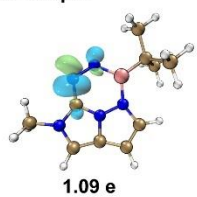
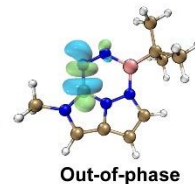
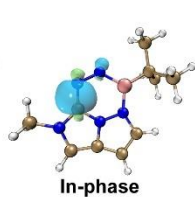


Figure S13. PIO analysis for **TS-3** of **3c** via separating to two fragments including N_2 and the remaining part. The primary interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

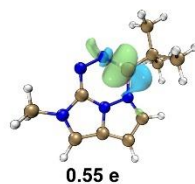
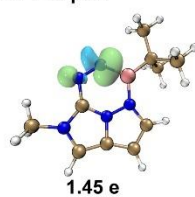
P total interaction: 2.64
1st PIO pair



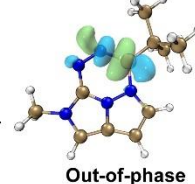
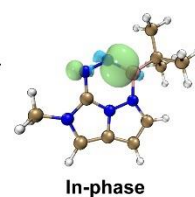
PBI: 0.99
(37.5%)



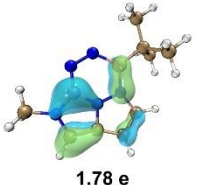
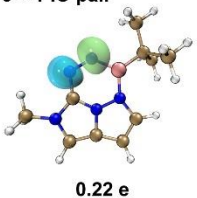
2nd PIO pair



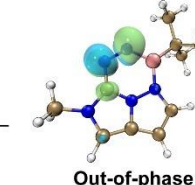
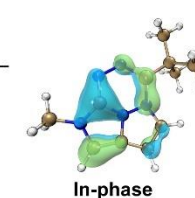
PBI: 0.79
(30.1%)



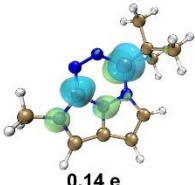
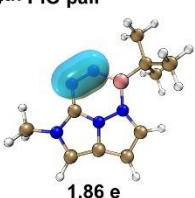
3rd PIO pair



PBI: 0.39
(14.6%)



4th PIO pair



PBI: 0.27
(10.1%)

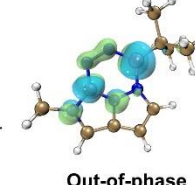
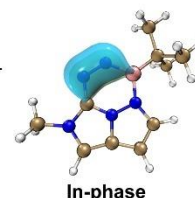


Figure S14. PIO analysis for **P** of **3c** via separating to two fragments including N_2 and the remaining part. The primary interaction between two fragments and their corresponding PBIs and contribution to total interaction are given. In-phase and out-of-phase means in-phase and out-of-phase combination, respectively. The isovalue is 0.05 a.u.

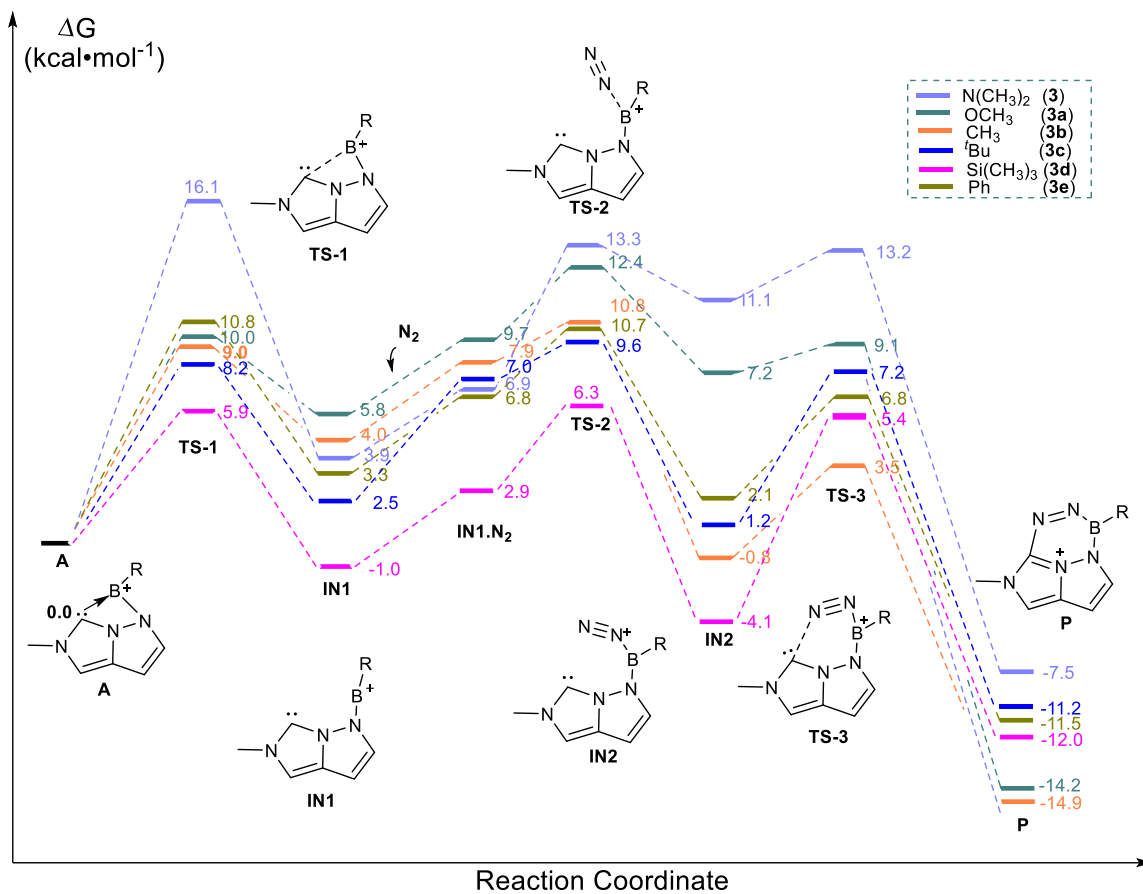


Figure S15. Gibbs energy profiles for the activation of N₂ activation by boronium (or borinium) cation with different substituents.

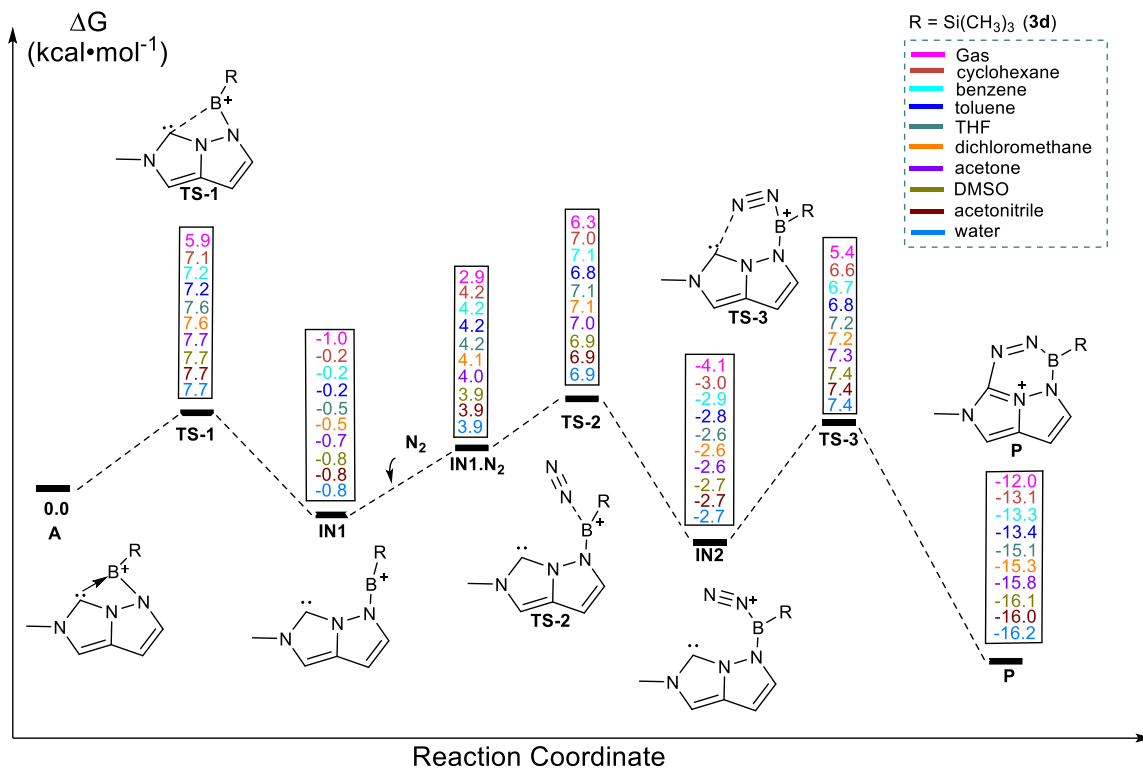


Figure S16. Gibbs energy profiles for the activation of N_2 activation by **3d** considering different solvents.

Cartesian coordinates

N_2

E = -109.519139 a.u.

N	0.00000000	0.00000000	0.54500700
N	0.00000000	0.00000000	-0.54500700

1.closed

E = -618.119950 a.u.

C	-1.67391000	0.79578900	0.07487000
C	0.07260000	-0.88900700	-0.34069200
C	-2.64331400	0.14985900	-0.94137000
C	-1.90018300	0.09525700	1.45440500
C	-1.11214800	-1.78868300	-0.10208900
H	-3.66261600	0.24135900	-0.56608300
H	-2.58475700	0.67333000	-1.89512000
C	-2.22751800	-1.35235800	-1.10972400
C	-1.65627800	-1.42979600	1.32152000
H	-2.91660200	0.31584200	1.78230900
H	-1.21178800	0.54063400	2.17407300
H	-0.88981900	-2.84859200	-0.18880500
H	-3.08812500	-1.99951900	-0.93935700
H	-1.88401000	-1.53053000	-2.12855500
H	-2.58727900	-1.98332200	1.45122800
H	-0.96450300	-1.77491900	2.08935300

N	-0.37952800	0.30672100	-0.33076600
C	-1.29596000	2.27000400	0.13881900
H	-1.99032200	3.07117500	0.33477100
C	0.03285500	2.42211900	-0.02157600
H	0.61267300	3.33087100	0.01142400
N	0.66589400	1.20232700	-0.35071300
B	1.52261400	-0.04875800	-0.24122500
N	2.83822100	-0.29304300	-0.04690600
C	3.81670000	0.78409000	0.11044300
H	4.29103100	0.71176400	1.09105300
H	4.58292900	0.69652700	-0.66206500
H	3.32729600	1.75225100	0.01865200
C	3.39649700	-1.64355700	0.01954100
H	4.14608000	-1.76793700	-0.76429100
H	3.87080500	-1.79892600	0.99047000
H	2.60779000	-2.38054900	-0.11912400

1.open

E = -618.091399 a.u.

C	-1.59873500	0.82288800	-0.00002100
C	-0.29824500	-1.29136400	0.00004200
C	-2.37793000	0.38893400	-1.25599200
C	-2.37790900	0.38901900	1.25599300

C	-1.75130500	-1.73674300	0.00006700
H	-3.36931000	0.84438700	-1.22564900
H	-1.86731200	0.76140600	-2.14542200
C	-2.45222500	-1.15937500	-1.25792500
C	-2.45221100	-1.15929000	1.25802700
H	-3.36928600	0.84447500	1.22564100
H	-1.86727000	0.76154600	2.14538900
H	-1.81355600	-2.82304200	0.00010400
H	-3.48908000	-1.49863300	-1.25763000
H	-1.98210300	-1.56079800	-2.15611800
H	-3.48906800	-1.49854200	1.25776200
H	-1.98208500	-1.56065700	2.15624200
N	-0.36551500	-0.00282200	-0.00002000
C	-1.02629400	2.20848700	-0.00007200
H	-1.62328800	3.10880900	-0.00009600
C	0.30222000	2.18389400	-0.00008700
H	1.01766700	2.99095700	-0.00012200
N	0.78428500	0.83946000	-0.00004200
B	2.00235000	0.26361500	-0.00002800
N	3.24339600	-0.20101700	-0.00000500
C	3.96170800	-0.52870100	1.24559600
H	4.16636900	-1.59963100	1.26036300
H	4.89878200	0.02830100	1.27019000
H	3.35599100	-0.26483200	2.11046600
C	3.96179000	-0.52862900	-1.24557700
H	4.89889800	0.02832200	-1.27004300
H	4.16639100	-1.59956900	-1.26042400
H	3.35616000	-0.26464400	-2.11047200

1P

E = -727.659278 a.u.

C	1.58204600	1.07265700	-0.05688700
C	0.77331000	-1.18387900	0.05562900
C	2.36566000	0.88049100	1.26393900
C	2.48507300	0.65940000	-1.24798200
C	2.23522700	-1.42259100	0.18431700
H	3.24992500	1.51743000	1.21906600
H	1.75157200	1.22259800	2.09745000
C	2.73822600	-0.61813700	1.41358200
C	2.91450600	-0.81794900	-1.07711200
H	3.34168300	1.33442200	-1.25994300
H	1.93164300	0.80858500	-2.17583000
H	2.42879700	-2.48936500	0.27962800
H	3.81905100	-0.74491400	1.47646200
H	2.30808200	-1.02836800	2.32689200
H	3.99347500	-0.89848500	-0.94248700
H	2.64929600	-1.39989700	-1.95905900
N	0.49126300	0.07607500	-0.02367400
C	0.77287600	2.32080300	-0.23392900
H	1.19781000	3.30793600	-0.32336800
C	-0.52377600	2.01546800	-0.29046100
H	-1.37699700	2.65530400	-0.44203600
N	-0.74003100	0.62202300	-0.13767500
N	-3.18445800	-0.02993300	0.07561300
C	-3.68762300	1.30691500	0.36738900

H	-3.99307300	1.83035500	-0.54423100
H	-4.55902900	1.22616500	1.01900200
H	-2.93945000	1.89633300	0.89769700
C	-4.23962500	-1.03549400	-0.08097800
H	-4.80007200	-1.12984600	0.85182500
H	-4.92597400	-0.72428400	-0.87219000
H	-3.80506100	-1.99735100	-0.33800600
B	-1.84883800	-0.33875200	-0.07791400
N	-1.41341800	-1.76139000	-0.19547500
N	-0.22805300	-2.15805600	-0.10541000

2.closed

E = -580.016254 a.u.

C	-0.37164000	-0.43031100	-0.45972000
B	1.20769400	-0.03039000	-0.39055300
C	0.52650000	2.32532900	0.36080100
C	-0.76177100	2.43391500	0.70999700
H	1.36313700	2.89444600	0.73920000
H	-1.15690300	3.15122400	1.41366200
N	2.39565700	-0.59074500	-0.06924600
C	3.63290800	0.19220500	-0.03334700
H	4.02707500	0.21798400	0.98459200
H	4.37300600	-0.27180800	-0.68783000
H	3.44292100	1.20691900	-0.37994100
C	2.55206300	-2.00410400	0.27083800
H	2.95237200	-2.09776900	1.28222700
H	1.58946100	-2.50955900	0.21561800
H	3.24604700	-2.47394300	-0.42870200
N	0.76564400	1.39971500	-0.70648600
N	-0.54400100	0.80340900	-0.77776900
C	-2.39122800	0.32080000	0.53317300
H	-2.31972300	0.40532500	1.61889800
H	-3.44610200	0.30407000	0.26129100
C	-1.64757300	1.52085900	-0.12862700
H	-2.26179100	2.07792300	-0.83967900
C	-1.67016500	-1.00381700	0.04886300
C	-2.44057000	-1.66839200	-1.10478100
H	-1.88327100	-2.51316100	-1.51316000
H	-3.39441000	-2.04061300	-0.72653900
H	-2.64001000	-0.95981900	-1.91139700
C	-1.43956400	-1.98820200	1.19434200
H	-2.39985400	-2.25476600	1.64066800
H	-0.97290300	-2.90661800	0.83255700
H	-0.81238000	-1.55422200	1.97658100

2.open

E = -579.975970 a.u.

C	0.68560600	-0.88575100	-0.15017600
B	-1.94685100	0.26477300	-0.02774000
C	-0.46577900	2.33520600	-0.42187100
C	0.83231000	2.55409400	-0.23012000
H	-1.23820500	2.98553300	-0.80110600
H	1.33104500	3.48811400	-0.44118300
N	-3.06503000	-0.44353800	-0.00136300
C	-3.96469000	-0.49930100	1.16521300
H	-4.95983700	-0.17626600	0.85830100

H	-4.00632400	-1.52704400	1.52691300
H	-3.59778700	0.15131600	1.95667300
C	-3.45345700	-1.29546100	-1.14414400
H	-4.42260700	-0.96605500	-1.51955000
H	-2.70471900	-1.22867300	-1.93141200
H	-3.51752900	-2.32753100	-0.79867100
N	-0.81939000	0.99622600	-0.04221600
N	0.41913400	0.33399800	0.17841400
C	2.65676600	0.57737600	-0.18987900
H	2.75540800	0.80406300	-1.25438900
H	3.60078400	0.79654100	0.30847800
C	1.48037800	1.35211600	0.40308500
H	1.60727400	1.52023100	1.47868100
C	2.21526600	-0.91719900	-0.00713200
C	2.55024300	-1.43263300	1.40119500
H	2.12263800	-2.42474500	1.55463400
H	3.63365500	-1.50647800	1.51637700
H	2.16651700	-0.77278600	2.18402300
C	2.83605000	-1.82147700	-1.06759000
H	3.92649600	-1.77602600	-1.00674100
H	2.52340800	-2.85554900	-0.91564900
H	2.53487500	-1.51714100	-2.07199800

2P

E = -689.536504 a.u.

C	1.04501400	-0.68855900	0.09685300
B	-1.69635800	-0.40664200	0.00173400
C	-0.79719400	2.12723800	-0.39333800
C	0.43613600	2.63982200	-0.37525000
H	-1.72916700	2.57906800	-0.69352600
H	0.70137600	3.65342300	-0.62896200
N	-3.06895100	-0.37601000	0.08827000
C	-3.82874100	0.83257900	0.38333000
H	-4.28678100	1.24252600	-0.52192000
H	-4.62608900	0.59378600	1.08960400
H	-3.19058900	1.58712200	0.84415100
C	-3.90188600	-1.56000800	-0.13581900
H	-4.60524100	-1.36322700	-0.94829600
H	-3.27861100	-2.41129700	-0.39527000
H	-4.46811100	-1.78731200	0.77013000
N	-0.81686900	0.77429600	0.06066900
N	-0.96497800	-1.69501900	-0.20445200
N	0.28054600	-1.83914100	-0.16729100
N	0.48255200	0.46188500	0.22820900
C	2.62680100	0.99825300	-0.40425500
H	2.56045600	1.06991300	-1.49247500
H	3.54998900	1.46872900	-0.06905900
C	1.37753200	1.63060600	0.23482900
H	1.57388800	1.90089800	1.28142800
C	2.54483500	-0.51102300	0.03307100
C	3.16261900	-0.73608300	1.42271200
H	2.98878200	-1.76116500	1.75408600
H	4.24038400	-0.57422800	1.36901900
H	2.75104900	-0.05813100	2.17478900
C	3.15977100	-1.45394700	-0.99880900

H	4.22244900	-1.22573600	-1.10328700
H	3.05779700	-2.49230800	-0.68127200
H	2.68478800	-1.34418500	-1.97558100

4.closed

E = -556.773527 a.u.

C	0.38832300	0.55389600	-0.55376100
B	-1.03713000	-0.15472700	-0.28814200
N	1.32327900	1.28710900	-0.04161700
C	1.17910500	2.57805300	0.61815000
H	1.73275700	3.33563300	0.06279700
H	0.12499800	2.84436600	0.65034300
H	1.57582100	2.50549000	1.63107400
C	0.37092600	-1.93817500	0.73685200
C	1.67530100	-1.67547800	0.82614500
H	-0.23325100	-2.51658300	1.42215300
H	2.32919400	-2.02830400	1.60969400
N	-2.33601000	0.14758200	-0.05199100
C	-3.32757000	-0.90907200	0.16901000
H	-3.72400200	-0.84331200	1.18438100
H	-4.14842500	-0.78951100	-0.54049100
H	-2.86846100	-1.88487700	0.01689000
C	-2.87102400	1.50552500	-0.01028100
H	-3.27273700	1.72084800	0.98210900
H	-2.08987800	2.22510100	-0.25100900
H	-3.67402200	1.60467500	-0.74335500
N	-0.26138800	-1.42969100	-0.43471400
N	0.85679400	-0.63181900	-1.06181500
C	2.62260400	0.56793100	-0.12470200
H	3.16602900	0.70013900	0.81074700
H	3.21194200	0.95888200	-0.95615100
C	2.15053800	-0.88907000	-0.37705600
H	2.84773900	-1.43283100	-1.01365500

4.open

E = -556.732906 a.u.

C	0.87094100	1.00608100	-0.10930100
B	-1.71172100	-0.29703200	0.04723800
N	2.17880900	1.04059900	-0.09707500
C	2.95982000	2.21167000	0.27264100
H	3.55542100	2.54806900	-0.57775200
H	2.27054100	2.99663600	0.57163000
H	3.62551900	1.96140600	1.10062000
C	0.07818400	-1.87513300	0.94390000
C	1.35403700	-2.05355400	0.62594700
H	-0.53505900	-2.36151200	1.68662000
H	2.01796600	-2.76097300	1.10022200
N	-2.89469700	0.29798000	-0.01412900
C	-4.00617900	-0.17387200	-0.85766400
H	-4.87072000	-0.37511500	-0.22423500
H	-4.25439400	0.60394700	-1.58042900
H	-3.72065900	-1.08223300	-1.38453000
C	-3.15434500	1.53488600	0.75071800
H	-3.95862900	1.35264800	1.46402500
H	-2.24939800	1.84380500	1.27132100

H	-3.44913000	2.31734600	0.05082700
N	-0.50674500	-0.88036800	0.10079300
N	0.54778600	-0.26688200	-0.64307400
C	2.87173200	-0.20596400	-0.47543200
H	3.61449900	-0.46615500	0.28068000
H	3.37052600	-0.08439700	-1.43873000
C	1.70723900	-1.19992100	-0.56945400
H	1.77746900	-1.81277200	-1.47019400

4P

E = -666.270006 a.u.

C	-1.20532300	-0.70736600	-0.26109100
B	1.46904900	-0.32728700	-0.15282600
N	-2.46372700	-0.66370800	0.06121000
C	-3.30553000	-1.78995100	0.45522200
H	-4.12529100	-1.89151200	-0.25644400
H	-2.69885700	-2.69219800	0.46330100
H	-3.70470800	-1.59743800	1.45146100
C	0.34226100	1.91150300	0.55560500
C	-0.92352000	2.33521700	0.54621600
H	1.18307400	2.31841800	1.09807200
H	-1.30443800	3.20177800	1.06247800
N	2.83392200	-0.23718500	-0.00766400
C	3.54806000	1.03209100	-0.09554300
H	3.86602000	1.36943200	0.89545500
H	4.43973800	0.90095100	-0.71174900
H	2.91826700	1.79138000	-0.55777900
C	3.70123400	-1.38063800	0.28055600
H	4.22441900	-1.21432100	1.22523000
H	3.11426400	-2.29197200	0.34604600
H	4.44292700	-1.48202500	-0.51467100
N	0.56949900	0.81196400	-0.29503700
N	0.82784400	-1.70274200	-0.10754500
N	-0.40254100	-1.87789100	-0.10694900
N	-0.73025400	0.44449000	-0.74116800
C	-2.96777700	0.72190400	-0.03732900
H	-3.38309100	1.02451200	0.92595200
H	-3.74578800	0.76749900	-0.80023900
C	-1.70648700	1.52817000	-0.46264000
H	-1.91248300	2.10186300	-1.36889000

5.closed

E = -571.550803 a.u.

C	0.46524100	0.73781200	-0.63869500
C	1.88748500	-0.85593300	0.01793600
B	-1.00733800	-0.02316000	-0.38452700
N	1.54541500	1.24482500	-0.02742100
C	1.84705600	2.64523100	0.25039500
H	2.57548800	3.00401200	-0.47537900
H	0.92321100	3.21305200	0.16511300
H	2.25702100	2.70775700	1.25545700
C	0.24497500	-2.38776800	0.19343100
C	1.56277900	-2.18801500	0.50477000
H	-0.36300500	-3.24711200	0.43317600
H	2.19431700	-2.85785000	1.06321100

N	-2.24599000	0.33292900	0.01027400
C	-3.28004500	-0.66241200	0.31039400
H	-3.56516200	-0.59259800	1.36161600
H	-4.15591400	-0.46952200	-0.31114300
H	-2.91047600	-1.66445000	0.09892100
C	-2.66723200	1.72478200	0.17831800
H	-2.94297500	1.90303500	1.21918700
H	-1.85880400	2.39577700	-0.10547400
H	-3.53234200	1.91967400	-0.45763100
N	-0.29370700	-1.36373800	-0.61162900
N	0.82344500	-0.55192300	-0.75361400
N	2.46423300	0.29817000	0.35043200

5.open

E = -571.553282 a.u.

C	1.03942200	-1.16641700	-0.00011000
C	1.77272100	1.00486900	-0.00011500
B	-1.68773500	0.22348600	-0.00022300
N	2.37833600	-0.99405100	0.00014400
C	3.36333600	-2.06873900	-0.00012400
H	3.98568700	-1.98421000	0.88900100
H	2.81933500	-3.00881800	0.00326800
H	3.98124300	-1.98817300	-0.89273400
C	-0.10626700	2.23651200	0.00012700
C	1.23126300	2.35109700	0.00012600
H	-0.87973400	2.98704900	0.00024300
H	1.78784600	3.27385600	0.00026100
N	-2.86764700	-0.36794000	-0.00008500
C	-3.55888700	-0.75205500	1.24959200
H	-4.53568200	-0.26868100	1.27040400
H	-3.67769100	-1.83556500	1.25878700
H	-2.97547900	-0.44245800	2.11459400
C	-3.55991100	-0.75181500	-1.24920600
H	-4.53680500	-0.26859500	-1.26901000
H	-2.97733300	-0.44188500	-2.11464200
H	-3.67857800	-1.83533900	-1.25858800
N	-0.49144100	0.85028900	-0.00011400
N	0.69963900	0.14979200	-0.00032200
N	2.85765600	0.30114900	0.00006100

5P

E = -681.101795 a.u.

C	1.28300000	-0.79532200	0.03587100
C	1.68855500	1.37317200	0.00466600
B	-1.43826400	-0.35677300	-0.01896700
N	2.59863000	-0.54477600	0.02995200
C	3.67398800	-1.53829900	0.04097500
H	4.24929400	-1.41380500	0.95590500
H	3.21304400	-2.52338800	0.00379300
H	4.30209200	-1.36973800	-0.83082700
C	-0.38134000	2.22193800	-0.08740000
C	0.93631400	2.59530100	-0.06972200
H	-1.25280900	2.85135000	-0.15445500
H	1.31746500	3.60066100	-0.11386600
N	-2.80711800	-0.31108900	0.02964400

C	-3.56802000	0.92763800	0.15593500
H	-3.95587400	1.24803300	-0.81481600
H	-4.41239700	0.76275200	0.82694500
H	-2.95566400	1.71822900	0.58674000
C	-3.65037000	-1.50630900	-0.08471000
H	-4.32087200	-1.39248700	-0.93934600
H	-3.03290400	-2.38897500	-0.22012700
H	-4.25029400	-1.61455100	0.82107400
N	-0.52849400	0.83400900	-0.01647500
N	-0.74265100	-1.70198700	-0.06346100
N	0.48872400	-1.94024300	-0.02837100
N	0.73995900	0.41166900	0.03651600
N	2.87916000	0.77199900	0.01221300

6.closed

E = -596.091758 a.u.

C	0.23124900	0.51742600	-0.45836500
B	-1.20535600	-0.18948000	-0.25551400
N	0.98435900	1.46009600	0.01150700
C	2.42782500	1.23085300	0.26163500
H	2.52617000	1.17387100	1.34939100
H	2.96929200	2.11396600	-0.08058200
C	2.96636600	-0.03011000	-0.40974100
H	3.88361900	-0.33030900	0.09810900
H	3.22888200	0.19148800	-1.44586000
N	-0.43331600	-1.46972600	-0.37293800
C	0.16692900	-2.00852300	0.80564100
H	-0.47091300	-2.52792200	1.50715900
C	1.49039600	-1.84381100	0.85961600
H	2.13996000	-2.23600200	1.62796800
C	0.44192900	2.71184000	0.53793800
H	-0.64348500	2.66886600	0.53567800
H	0.79964200	2.84982300	1.55893800
H	0.78267600	3.54330000	-0.08027100
C	1.97531300	-1.19435200	-0.42431700
H	2.34202100	-1.95347500	-1.12120200
N	0.69911100	-0.67040200	-0.93654500
N	-2.52808500	0.06956700	-0.08977800
C	-3.14498300	1.39149900	-0.13314100
H	-3.51643300	1.67530900	0.85423500
H	-2.43175200	2.13320000	-0.48753600
H	-3.98599400	1.37295100	-0.82902000
C	-3.47311400	-1.03078300	0.12452100
H	-4.26029000	-0.98617700	-0.63042400
H	-2.95600300	-1.98524300	0.03800000
H	-3.92656000	-0.94723100	1.11453600

6P

E = -705.602337 a.u.

C	1.08465300	-0.76990100	0.09194200
N	2.38989800	-0.98014000	0.08668700
C	3.33687700	0.14680700	0.02882000
H	4.13672000	-0.14832400	-0.65249700
H	3.77590900	0.28414400	1.02160200
C	2.66523400	1.42194800	-0.46707600
H	2.39272800	1.32969500	-1.52087900

H	3.35340600	2.26038800	-0.36178100
N	-0.75479100	0.72775300	0.02355600
C	-0.79028000	2.10547000	-0.25008700
H	-1.73010600	2.54419000	-0.54455300
C	0.39919900	2.68490100	-0.10854000
H	0.62179300	3.73025600	-0.24674700
C	2.98083700	-2.32337700	0.12847700
H	2.20725700	-3.06605000	0.28879000
H	3.48976300	-2.52276500	-0.81555600
H	3.70385400	-2.35322400	0.94509300
C	1.40348800	1.66613500	0.35804900
H	1.67408800	1.82342000	1.41013900
N	0.58988800	0.43535400	0.26555900
N	-3.04963100	-0.32517100	0.03911200
C	-3.90741300	-1.47505900	-0.25276600
H	-4.56693300	-1.23851100	-1.09164300
H	-3.30262500	-2.34175000	-0.50378400
H	-4.52308100	-1.70604200	0.61966600
C	-3.78942400	0.89045800	0.35228900
H	-3.16607000	1.58708000	0.91298200
H	-4.16325900	1.37855600	-0.55373600
H	-4.64777900	0.63668300	0.97709100
B	-1.66949700	-0.38516300	-0.01970400
N	-1.00102600	-1.72145900	-0.15897000
N	0.22463200	-1.90151300	-0.12341700

7.closed

E = -670.109252 a.u.

C	-0.17090500	-0.43452200	-0.45630900
B	1.41188700	-0.04837400	-0.30295700
N	-1.19243700	-1.22846600	-0.17537500
C	-2.43059900	0.87240300	0.47159800
N	0.98673300	1.35128600	-0.63312200
C	0.76399800	2.40235700	0.29332000
H	1.61661500	2.93025100	0.69490200
C	-0.52937900	2.66348400	0.49758900
H	-0.92275400	3.46988000	1.09776700
C	-1.08899500	-2.69055500	-0.07304700
H	-0.21058100	-3.01735400	-0.62339500
H	-1.03086900	-2.99345100	0.97247800
H	-1.98131200	-3.12163100	-0.52169500
C	-1.41520800	1.72533000	-0.31309300
H	-1.88912300	2.22815400	-1.15965700
N	-0.36275700	0.82389900	-0.79840200
N	2.59152900	-0.61079700	0.05450500
C	2.77212300	-2.02034200	0.39153800
H	3.18399100	-2.10754300	1.39887700
H	1.81839300	-2.54273500	0.35452800
H	3.46492100	-2.48400200	-0.31357600
C	3.81448700	0.19305500	0.13445800
H	4.59018600	-0.26809800	-0.47967300
H	3.62578000	1.19898100	-0.23770700
H	4.16291600	0.24178600	1.16816300
C	-2.47040000	-0.61292400	0.12368400
O	-3.43615700	-1.29765600	0.21480900

H -3.44566300 1.24667700 0.35504500
H -2.18488200 0.90102400 1.53857900

7.open

E = -670.069350 a.u.

C -0.41810800 -0.86521900 -0.04830700
B 2.08575200 0.20695300 0.00502400
N -1.71352800 -1.25437400 -0.09955200
C -2.50751500 1.07023800 0.35415700
C -2.02944200 -2.69024800 -0.11232000
H -1.08716400 -3.22928900 -0.09351300
H -2.63791700 -2.94342500 0.75498400
H -2.58910900 -2.93414400 -1.01410100
C -1.26794300 1.50813400 -0.40904000
H -1.49837500 1.59348900 -1.47916000
N -0.27472700 0.44072100 -0.21592400
N 3.22676800 -0.46767200 0.03454800
C 3.66145400 -1.19670400 1.24147700
H 4.64170000 -0.82819000 1.54531100
H 2.94516700 -1.04898000 2.04763700
H 3.72165500 -2.25936300 1.00442100
C 4.09768300 -0.62548400 -1.14441100
H 4.14929600 -1.68305200 -1.40521400
H 3.69871200 -0.06279000 -1.98615500
H 5.09443600 -0.25789600 -0.89860800
C -2.83103000 -0.38472400 0.03981900
O -3.94482400 -0.81549800 0.00445100
H -3.38194500 1.66726700 0.10219200
H -2.33127200 1.13830100 1.43246800
C 0.78708700 2.39712700 0.23509700
H 1.62758800 3.01144100 0.51723200
C -0.49122600 2.71075600 0.05907600
H -0.91118500 3.69762000 0.18378800
N 1.00184100 1.00774900 -0.01411400

7P

E = -779.616452 a.u.

C -0.84796700 -0.77206100 -0.20100500
N -2.17770300 -0.94030500 -0.05511900
C -3.01541300 0.14580700 0.36833500
C -2.32841900 1.49449800 0.52968600
N 0.97997400 0.73097300 -0.27773500
C 1.03904000 2.14054000 -0.30967800
H 2.00682400 2.61347700 -0.29423800
C -0.16664800 2.70070100 -0.38084500
H -0.37829400 3.75574100 -0.44093300
C -2.80494700 -2.27732300 -0.11861500
H -2.12822100 -2.96000300 -0.62063700
H -3.01721600 -2.62776800 0.89054700
H -3.73777300 -2.17796900 -0.66755300
C -1.21041200 1.62620800 -0.49403900
H -1.63928700 1.59514500 -1.50626800
N -0.36569000 0.42669100 -0.34830000
N 3.22923800 -0.33835500 0.22186300
C 4.10019500 -1.51615800 0.14780500
H 4.51829000 -1.72759000 1.13437000

H 3.53901100 -2.38002100 -0.19635700
H 4.92087700 -1.31845800 -0.54581500
C 3.92736600 0.88024200 0.61682600
H 4.37911000 1.38339800 -0.24407600
H 3.25325400 1.56393100 1.13297200
H 4.72491200 0.62328000 1.31496100
B 1.88823200 -0.38935700 -0.10209900
N 1.23097300 -1.72422300 -0.28212600
N 0.00098800 -1.90934500 -0.28464700
O -4.16328700 -0.05938600 0.60416800
H -3.08685700 2.26542600 0.40418800
H -1.93071700 1.56050000 1.54760600

8.closed

E = -859.069385 a.u.

C -0.30317500 -0.92467600 -0.45633900
C -2.01310900 0.65423600 0.03467900
B 1.07733000 -0.02316100 -0.28720800
C -0.47328200 2.33081400 0.06078700
C -1.79431700 2.07080800 0.30691300
H 0.05309100 3.26505000 0.17821700
H -2.52014800 2.78078600 0.66440000
N 2.37583400 -0.20276400 0.02438300
C 3.29764100 0.91865800 0.22265600
H 3.67490400 0.90809800 1.24673400
H 4.13703500 0.82224800 -0.46792300
H 2.78923000 1.86255900 0.03372500
C 2.97535900 -1.52828600 0.19524700
H 3.35708100 -1.62918300 1.21267500
H 2.23325900 -2.30176500 0.00796400
H 3.80095100 -1.64497800 -0.50875300
N 0.17962800 1.22305000 -0.49154400
N -0.81984800 0.29203700 -0.49686300
S -1.59684600 -1.89471800 0.07140200
C -2.66260300 -0.53897700 0.30728100
H -3.67089600 -0.71323800 0.64740500

8.open

E = -859.053114 a.u.

C -0.78973400 -1.29927700 -0.00002100
C -1.93696600 0.81853800 -0.00000700
B 1.58815200 0.30664100 -0.00012600
C -0.14092200 2.19749500 -0.00005100
C -1.48091500 2.19571700 -0.00003600
H 0.56408000 3.01277700 -0.00006800
H -2.10689100 3.07317500 -0.00003300
N 2.81365300 -0.18470000 0.00000800
C 3.52910700 -0.52067100 -1.24880700
H 4.47051400 0.02846300 -1.27105200
H 3.72180300 -1.59357100 -1.25841100
H 2.92538900 -0.25249500 -2.11374000
C 3.52921800 -0.51986500 1.24897200
H 4.47063900 0.02926300 1.27077700
H 2.92558600 -0.25111800 2.11378700
H 3.72189500 -1.59276300 1.25925600
N 0.35310900 0.85524200 -0.00008800

N	-0.78117400	0.02493300	-0.00003400
S	-2.46472400	-1.65064900	0.00003000
C	-3.01590600	0.00829000	0.00001500
H	-4.06059300	0.27375600	0.00003500

8P

E = -968.606893 a.u.

C	1.22905800	-1.02775400	0.03833400
C	1.82730000	1.21880000	-0.00716200
B	-1.43480900	-0.33237300	-0.04418200
C	-0.22012500	2.11632300	-0.14514000
C	1.09789100	2.45116900	-0.10729900
H	-1.08017800	2.75748700	-0.24001600
H	1.51007200	3.44412500	-0.15520900
N	-2.78810400	-0.11531800	0.04835800
C	-3.39228500	1.19767600	0.25129600
H	-3.64234600	1.67385500	-0.70147300
H	-4.31217400	1.08158600	0.82516500
H	-2.73127000	1.84434900	0.82827500
C	-3.76519900	-1.20141300	-0.09235800
H	-4.43904800	-0.97584800	-0.92185700
H	-3.25488000	-2.14071600	-0.28351400
H	-4.35132000	-1.28564200	0.82498100
N	-0.39650200	0.73677900	-0.06020200
N	-0.90106300	-1.72720400	-0.11501600
N	0.30634300	-2.06502300	-0.05857100
N	0.85730300	0.24483500	0.00780600
S	2.92813100	-1.09561900	0.08329700
C	3.06389000	0.61121700	0.04512800
H	4.03607100	1.07798100	0.05838600

9.closed

E = -537.308974 a.u.

C	0.42913600	0.89761700	-0.34518700
B	-0.92547000	0.01379800	-0.27155400
C	0.63107000	-1.75304200	0.49043900
C	1.87879000	-1.34865600	0.73799300
H	0.07493500	-2.52361500	1.00632900
H	2.52596700	-1.76278400	1.49672000
N	-2.23878000	0.15457300	-0.00073000
C	-3.15421600	-0.99038100	-0.03304700
H	-3.55289100	-1.17329500	0.96665100
H	-3.98102400	-0.77006400	-0.71035900
H	-2.63007800	-1.87641500	-0.38859300
C	-2.86045300	1.43417400	0.34535100
H	-3.32312700	1.36046300	1.33102600
H	-2.11254700	2.22525400	0.35769100
H	-3.62911600	1.67584800	-0.39077900
N	-0.00229600	-1.12699600	-0.63118000
N	1.04638000	-0.09973700	-0.98387200
O	1.18602900	1.68957900	0.30448200
C	2.56525600	1.14233000	0.21175600
H	3.09865400	1.74291700	-0.52258900
H	3.00025600	1.24331300	1.20161000
C	2.32774300	-0.31149700	-0.27109400
H	3.12699300	-0.64539300	-0.93257700

9.open

E = -537.274825 a.u.

C	0.94659700	-1.40088400	-0.12541700
B	-1.39401800	0.32602300	-0.00930000
C	0.62916700	1.69564100	-0.76437200
C	1.92489300	1.60765300	-0.48967900
H	0.08854300	2.38252100	-1.39691900
H	2.68815500	2.25887400	-0.88896700
N	-2.65894200	-0.06096800	0.02435200
C	-3.65090100	0.45833700	0.98394000
H	-4.47950500	0.89920200	0.42912400
H	-4.01499700	-0.36943200	1.59298100
H	-3.19796600	1.21184600	1.62525400
C	-3.15214900	-1.10359600	-0.90212900
H	-3.93441600	-0.67834200	-1.53117400
H	-2.33239500	-1.47297200	-1.51618800
H	-3.55522000	-1.92545000	-0.30991000
N	-0.10341800	0.69709800	-0.04001500
N	0.85755700	-0.17591000	0.53169200
O	2.20224800	-1.70507400	-0.15788700
C	3.09498500	-0.63991400	0.30670400
H	3.57002500	-0.98600300	1.22158400
H	3.83647200	-0.48103700	-0.47233200
C	2.15357500	0.54215700	0.55901900
H	2.34002900	0.99336900	1.53553600

9P

E = -646.805371 a.u.

C	-1.32071900	-1.16553500	-0.15693200
B	1.25905600	-0.27504000	-0.06285900
C	-0.23497000	1.90634700	0.38542300
C	-1.56071800	2.08399800	0.38552700
H	0.53745100	2.55859800	0.76337100
H	-2.07789800	2.96449600	0.73096800
N	2.59246100	0.05033900	-0.03762000
C	3.07809500	1.40537200	-0.27593700
H	3.37405600	1.88466800	0.66178600
H	3.95201100	1.36477700	-0.92851300
H	2.31371500	2.00537000	-0.77004900
C	3.65405200	-0.91552000	0.25910200
H	4.22044300	-0.57688200	1.12944400
H	3.22669300	-1.89331500	0.46142900
H	4.33117700	-0.98357500	-0.59484800
N	0.15790800	0.68646600	-0.22518400
N	0.83911600	-1.71383300	0.11503700
N	-0.33139000	-2.14762000	0.09422000
N	-1.04382300	0.05990800	-0.46747000
C	-3.22716000	-0.05371600	0.22380200
H	-4.17278800	-0.08044400	-0.30676500
H	-3.37738400	0.06178800	1.29718500
C	-2.20837900	0.94930800	-0.37753600
H	-2.51577100	1.26628500	-1.38005500
O	-2.58601300	-1.37561200	0.02959500

10.closed

E = -566.195473 a.u.

C	-0.00704900	-0.75255200	-0.48313200
B	1.49951900	-0.13455400	-0.31850600
C	0.43084500	2.20682800	0.19729700
C	-0.89445200	2.17937400	0.54989900
H	1.17519700	2.92318000	0.52419700
H	-1.30428200	2.92691200	1.21286800
N	2.74526700	-0.51278100	0.04225200
C	3.85112600	0.44430900	0.12780500
H	4.20263300	0.51193100	1.15917300
H	4.67219100	0.10373200	-0.50546200
H	3.52455800	1.42504800	-0.21441200
C	3.10084500	-1.89392700	0.36997700
H	3.48905800	-1.93992600	1.38906800
H	2.22615700	-2.53649700	0.28674000
H	3.87143200	-2.24470400	-0.31890400
N	0.85795600	1.20633900	-0.68361000
N	-0.33680700	0.45009600	-0.84936500
C	-2.37166700	-0.41770300	0.09721700
B	-1.49806600	0.91129500	-0.03511000
C	-1.23182400	-1.51601300	-0.06629700
H	-1.47614200	-2.30459300	-0.78630600
H	-1.01540300	-2.01747700	0.88229700
C	-3.39408400	-0.53914400	-1.04798000
H	-3.90749400	-1.50238300	-0.98867000
H	-4.15078000	0.24414700	-0.97627100
H	-2.92196400	-0.46492500	-2.03083600
C	-3.06713400	-0.57381900	1.45285300
H	-3.84383000	0.18464400	1.56929100
H	-3.54570800	-1.55390900	1.52902200
H	-2.36744500	-0.46858200	2.28551100

10.open

E = -566.160965 a.u.

C	0.29474900	-1.36718500	-0.00025000
B	-2.06001300	0.26237600	0.00006300
C	-0.30788900	2.12782900	0.00004500
C	1.03886300	2.18526400	-0.00007100
H	-1.03470000	2.92928200	0.00016900
H	1.54968100	3.13681800	-0.00005000
N	-3.29577700	-0.20749800	0.00008100
C	-4.01515800	-0.53189500	1.24821600
H	-4.94977400	0.02886700	1.27056900
H	-4.22178100	-1.60224500	1.26169100
H	-3.40855500	-0.26912400	2.11286400
C	-4.01512800	-0.53225700	-1.24797100
H	-4.94977500	0.02844800	-1.27046800
H	-3.40854000	-0.26966500	-2.11268300
H	-4.22169500	-1.60262100	-1.26118000
N	-0.81950900	0.79625900	0.00000700
N	0.31251900	-0.04702800	-0.00015200
C	2.66577000	-0.37204200	-0.00012700
B	1.54742400	0.72573700	-0.00020900
C	3.54745800	-0.30709100	1.26027000
H	4.24312700	-1.15054100	1.26901800
H	4.13565100	0.61257100	1.28066000

H	2.95462200	-0.35311900	2.17752200
C	3.54871800	-0.30679400	-1.25958000
H	4.13703100	0.61281100	-1.27907600
H	4.24431500	-1.15030900	-1.26791500
H	2.95680000	-0.35244600	-2.17743900
C	1.77695400	-1.67835900	-0.00060100
H	1.97516400	-2.31864100	0.86728100
H	1.97471900	-2.31759300	-0.86937200

10P

E = -675.720164 a.u.

C	0.70973800	-1.22754800	0.00608400
B	-1.87819800	-0.26671500	-0.05224500
C	-0.39873400	2.01881200	-0.24783400
C	0.93852100	2.28158300	-0.23998200
H	-1.21440400	2.71623400	-0.37699900
H	1.30713100	3.28820800	-0.35832100
N	-3.20674200	0.05990400	0.07578500
C	-3.67185400	1.42419800	0.30485000
H	-3.93776100	1.91469400	-0.63632900
H	-4.55851300	1.39839300	0.93935700
H	-2.91156000	2.00869900	0.82313700
C	-4.29003900	-0.92128600	-0.04739800
H	-4.96143300	-0.61737400	-0.85357600
H	-3.88396500	-1.90482400	-0.26368300
H	-4.85587100	-0.95804600	0.88572600
N	-0.74009200	0.65970900	-0.08851800
N	-1.49385100	-1.72654900	-0.14438700
N	-0.33464800	-2.19142800	-0.10032900
N	0.45612000	0.03538900	0.00049600
C	2.86987000	-0.04293800	0.05496000
C	3.57585400	0.17290500	1.41228500
H	4.37764800	-0.55986700	1.53245800
H	4.01909200	1.16876800	1.45900700
H	2.88949700	0.06692300	2.25663800
C	3.88807200	0.08991400	-1.08972700
H	4.35122200	1.07780500	-1.07395700
H	4.68019600	-0.65453300	-0.97673300
H	3.42519100	-0.05110800	-2.06917700
C	2.18046700	-1.46149900	0.02989300
H	2.43931400	-2.09194800	0.88754800
H	2.44206600	-2.04225500	-0.86270600
B	1.64125400	0.94195600	-0.07025800

11.closed

E = -975.772625 a.u.

C	-0.71503800	1.14839200	-0.76479300
C	1.23761600	-0.10524600	-0.73281300
B	-1.80377500	-0.03076000	-0.39450900
C	0.09807300	-1.99214200	-0.42163300
C	1.35980200	-1.48058300	-0.33346300
H	-0.25737400	-2.97881400	-0.16584100
N	-2.95775000	-0.14083500	0.29991000
C	-3.57934000	-1.43661300	0.57842900
H	-3.59979700	-1.61618200	1.65518000
H	-4.60282100	-1.43574700	0.19926800

H	-3.02348500	-2.23337600	0.08663500
C	-3.67886400	1.01492500	0.83330000
H	-3.73573500	0.94527200	1.92134700
H	-3.16829600	1.93483700	0.55457000
H	-4.69123000	1.03157300	0.42561000
N	-0.82773600	-1.06264000	-1.00310100
N	-0.02712800	0.07021500	-1.13919100
S	0.45988400	2.20541500	-0.08300800
C	1.75227300	1.02859200	-0.17892400
C	3.07109000	0.86868700	0.52782900
H	3.88975400	0.95477200	-0.19071800
H	3.22058600	1.63137500	1.29175700
C	3.07344700	-0.54332000	1.20630100
H	4.07258600	-0.71371900	1.60881300
H	2.38687100	-0.50217700	2.05584800
C	2.67832300	-1.77162200	0.32606900
H	3.43852400	-1.94316000	-0.44093300
H	2.63516400	-2.66108600	0.95398500

11.open

E = -975.765788 a.u.

C	-0.28395100	1.76607700	0.00120400
C	1.18723900	-0.07623500	-0.06907600
B	-2.30597800	-0.41995000	-0.00005400
C	-0.15590900	-1.84158800	-0.07900300
C	1.14521600	-1.50045900	-0.10346000
H	-0.66419700	-2.79200300	-0.09003400
N	-3.61283700	-0.22128300	0.03526300
C	-4.41824800	-0.04396300	-1.18994600
H	-5.20430600	-0.79926700	-1.20584700
H	-4.85982600	0.95270200	-1.17344600
H	-3.79005100	-0.14784300	-2.07254500
C	-4.35683300	-0.08550500	1.30385200
H	-5.14214900	-0.84118800	1.33300000
H	-3.68610200	-0.21880400	2.15047300
H	-4.79733800	0.91101600	1.34248600
N	-0.97733100	-0.63585500	-0.03731100
N	-0.07551100	0.45576200	-0.03793500
C	2.16180500	0.83447600	-0.05584100
C	3.57146800	0.30395100	-0.07728300
H	3.96752400	0.35802600	-1.09576300
H	4.23235700	0.89694900	0.55635800
C	3.56249500	-1.16482800	0.43783000
H	4.55268100	-1.59341200	0.27901200
H	3.39339000	-1.13937700	1.51748500
C	2.51159100	-2.12313400	-0.19288900
H	2.73659000	-2.27843200	-1.25342400
H	2.55255600	-3.09684700	0.29507900
S	1.33433000	2.39281900	-0.00968800

11P

E = -1085.317476 a.u.

C	0.11145700	1.67495100	-0.06623200
C	1.34484700	-0.23315300	-0.13411300
B	-2.17647000	0.11609000	0.03892500
C	-0.17389300	-1.81207500	0.01183900

C	1.17949500	-1.63312700	-0.05887600
H	-0.75940100	-2.71108500	0.10660600
N	-3.39522100	-0.52087400	-0.00721200
C	-3.55565200	-1.95224100	-0.23097800
H	-3.67512300	-2.49244400	0.71298100
H	-4.44722700	-2.12276200	-0.83644600
H	-2.70727800	-2.35653100	-0.78242500
C	-4.66007300	0.18747800	0.20955300
H	-5.18581600	-0.25842600	1.05719300
H	-4.46912600	1.23722800	0.41188200
H	-5.28776900	0.09676300	-0.67962700
N	-0.85062700	-0.56386500	-0.03275900
N	-2.11404800	1.60856300	0.15679500
N	-1.09156700	2.34274200	0.10190400
N	0.13609100	0.34984300	-0.11260000
S	1.74715100	2.24418000	-0.07854600
C	2.38715300	0.63816600	-0.12226900
C	3.74675500	-0.00960300	-0.11130900
H	4.12486300	-0.06100500	-1.13710600
H	4.46638200	0.56449600	0.47293600
C	3.60732600	-1.43930400	0.50386400
H	4.56780800	-1.94268800	0.39165600
H	3.43151000	-1.32050700	1.57604100
C	2.49418700	-2.37028500	-0.06776000
H	2.45602700	-3.28645600	0.52091500
H	2.73105400	-2.65361600	-1.09770200

12.closed

E = -672.235161 a.u.

C	-0.57764800	0.97647800	-1.00407800
C	1.26515900	-0.30669900	-0.90559200
B	-1.66738500	-0.12723200	-0.46488200
C	0.08211100	-2.09462100	-0.32488700
C	1.34948200	-1.59503200	-0.27229400
H	-0.29726600	-3.02367500	0.07436300
N	-2.76529900	-0.13802900	0.33075700
C	-3.40941200	-1.38541000	0.74334900
H	-3.33494800	-1.50735000	1.82616100
H	-4.46397600	-1.36015400	0.46237300
H	-2.93731800	-2.23259400	0.24809800
C	-3.39870900	1.07577300	0.83883400
H	-3.32526900	1.11284700	1.92799600
H	-2.91727400	1.95249300	0.40901000
H	-4.45345100	1.08246800	0.55721500
N	-0.82286200	-1.25769200	-1.07001200
N	0.02758800	-0.17397800	-1.39198100
C	1.60743800	0.90878200	-0.35882900
C	2.81451800	0.92935700	0.53214900
H	3.72367000	1.00859600	-0.06752000
H	2.80858000	1.76997600	1.22641400
C	2.80603500	-0.40837100	1.35151800
H	3.75178300	-0.47591900	1.89044000
H	2.01375200	-0.33050000	2.10107300
C	2.58614200	-1.74408300	0.56732500
H	3.44637600	-1.94928000	-0.07481300

H	2.50180300	-2.56193300	1.28247600
N	0.45171900	1.66940000	-0.40972400
C	0.32633100	3.03539800	0.09624800
H	-0.71260800	3.20828400	0.36758400
H	0.96115200	3.15096600	0.97231000
H	0.62521500	3.74460200	-0.67451400

12.open

E = -672.227172 a.u.

C	0.00793500	1.72224100	-0.01175600
C	-1.11328100	-0.26559600	-0.06719600
B	2.37851300	-0.34643300	-0.00612200
C	0.33243200	-1.90930400	0.10711300
C	-0.99446600	-1.66469900	0.06734500
H	0.92037600	-2.80656600	0.20570300
N	3.67497200	-0.07640300	-0.01483100
C	4.42664600	0.22365700	1.21992700
H	5.24539100	-0.48994800	1.31591700
H	4.82377700	1.23651000	1.14864900
H	3.77204700	0.15121300	2.08620700
C	4.45968800	0.00569600	-1.26236900
H	5.28012900	-0.71049000	-1.20980200
H	3.82905900	-0.22087500	-2.11977500
H	4.85622800	1.01666500	-1.35926300
N	1.06558600	-0.63289500	0.00882200
N	0.08465100	0.36208500	-0.06953800
C	-2.07777000	0.65410100	-0.01979500
C	-3.48296200	0.13627600	0.09315000
H	-3.84134500	0.23773800	1.12249300
H	-4.18488200	0.67374500	-0.54786200
C	-3.46253000	-1.36637500	-0.34668600
H	-4.43015100	-1.80706900	-0.10422600
H	-3.36871900	-1.38408700	-1.43533100
C	-2.35385500	-2.30226900	0.23774900
H	-2.51246200	-2.44965000	1.31090200
H	-2.42022700	-3.28154600	-0.23636600
N	-1.36771400	1.86355600	0.00184000
C	-2.00732700	3.17464200	0.02680700
H	-1.22448500	3.92147100	0.12476500
H	-2.55996900	3.34112600	-0.89824800
H	-2.68686500	3.23929700	0.87707000

12P

E = -781.786123 a.u.

C	0.27236800	1.48792000	-0.26574700
C	1.27409200	-0.45966400	-0.46413400
B	-2.14741700	0.18566200	0.00301800
C	-0.31253600	-1.90842300	-0.03782600
C	1.05411500	-1.81321100	-0.16503900
H	-0.93996200	-2.75193900	0.19973000
N	-3.42632100	-0.32213200	0.06286600
C	-3.75427000	-1.71461600	-0.20938000
H	-3.94620300	-2.26402500	0.71723800
H	-4.65472400	-1.76108800	-0.82532700
H	-2.95020800	-2.20044200	-0.76190800
C	-4.58190000	0.49513600	0.43505700

H	-5.07282000	0.05898600	1.30859700
H	-4.26090000	1.50681300	0.66635400
H	-5.29663400	0.51958000	-0.39093900
N	-0.92586900	-0.64658700	-0.24242900
N	-1.89109000	1.64397900	0.22612600
N	-0.78661600	2.25733300	0.13524200
N	0.10638000	0.18042400	-0.49887000
C	2.26960600	0.45737900	-0.25019800
C	3.61824200	-0.13197600	0.04508900
H	4.18766700	-0.24327900	-0.88183200
H	4.20692700	0.49310300	0.71802100
C	3.37952800	-1.53020300	0.72520800
H	4.34559900	-2.03062500	0.79715000
H	3.04296500	-1.33739100	1.74703600
C	2.36088700	-2.53118600	0.07574300
H	2.24767800	-3.39000900	0.73628100
H	2.74847500	-2.89891700	-0.87832500
N	1.63214700	1.66864500	-0.14851600
C	2.24574500	2.98316600	0.06531900
H	3.04604400	2.87808100	0.79519800
H	2.63981400	3.36291200	-0.87589000
H	1.47768800	3.65236100	0.44804200

12a.closed

E = -652.799745 a.u.

C	-0.71188500	1.26339800	-0.81207900
C	0.87437800	-0.31892300	-0.95478400
B	-1.90831800	0.32909300	-0.23582500
C	-0.57092100	-1.90980600	-0.38002900
C	0.76581900	-1.64407600	-0.40134100
H	-1.08366400	-2.78496700	-0.00870300
N	-1.36118800	-0.87440100	-1.00576800
N	-0.34637400	0.06366200	-1.33334800
C	1.45969800	0.77355200	-0.34572400
C	2.70530100	0.51517400	0.44839700
H	3.57091000	0.47753100	-0.21623000
H	2.89745800	1.29049200	1.19011400
C	2.50896300	-0.85759500	1.18102500
H	3.45973800	-1.12927900	1.64082400
H	1.79331300	-0.69993000	1.99255900
C	2.00517200	-2.07049800	0.33174900
H	2.77194900	-2.37289000	-0.38584700
H	1.81925400	-2.91355500	0.99657100
N	0.45582800	1.71631100	-0.24547600
C	0.57910300	3.02441400	0.40060800
H	-0.40316200	3.31526900	0.76690100
H	1.27944600	2.94723400	1.22940300
H	0.93520100	3.75753600	-0.32180800
O	-2.82621200	0.46645200	0.67558700
C	-3.68605400	-0.61197200	1.09453800
H	-3.35753300	-0.94593100	2.07662100
H	-4.69299300	-0.20891000	1.15738000
H	-3.65395100	-1.43070000	0.37463100

12a.open

E = -652.785106 a.u.

C	-0.39523200	1.67257300	-0.12508000
C	0.80107200	-0.26816700	-0.27233500
B	-2.67729200	-0.40895600	-0.21923200
C	-0.59532800	-1.96233500	-0.10417300
C	0.72163800	-1.67223800	-0.14578100
H	-1.15321800	-2.87977000	-0.01892100
N	-1.36662700	-0.70556800	-0.20888800
N	-0.41704600	0.32159000	-0.28911100
C	1.72616100	0.68177700	-0.12309100
C	3.13997200	0.20805500	0.06706800
H	3.68843000	0.24447000	-0.87839000
H	3.68848100	0.82393000	0.78231600
C	3.07555900	-1.25613900	0.62225000
H	4.07877000	-1.68241100	0.58453200
H	2.79636200	-1.19030700	1.67688100
C	2.10101000	-2.27664500	-0.05709400
H	2.43414200	-2.49152200	-1.07737400
H	2.11309600	-3.21433700	0.49746800
N	0.97253300	1.86379200	-0.06800600
C	1.56063000	3.19404800	0.05396500
H	0.75120700	3.89874400	0.22253400
H	2.24993300	3.21616500	0.89841200
H	2.09190300	3.45631700	-0.86096900
O	-3.90377400	-0.16558000	-0.29894000
C	-4.94975000	0.28886800	0.61814900
H	-5.78268600	-0.39273500	0.48064500
H	-4.56942700	0.26778900	1.63567700
H	-5.20675100	1.29560200	0.30362400

12ap

E = -762.359076 a.u.

C	-0.16831400	1.38116800	-0.24759200
C	1.08048100	-0.42083000	-0.46202800
B	-2.38456700	-0.23939900	-0.04904100
C	-0.32274300	-2.07609200	-0.14316000
C	1.02636600	-1.80170000	-0.22287200
H	-0.85985500	-2.99535600	0.02772600
N	-1.07383000	-0.88700400	-0.30151700
N	-2.35541800	1.23562500	0.12342100
N	-1.33038900	1.99527100	0.08891300
N	-0.15358300	0.06735000	-0.50764300
C	1.94501000	0.61386100	-0.20360500
C	3.35396800	0.18819900	0.09000300
H	3.93826800	0.18697200	-0.83464600
H	3.85353300	0.85600400	0.79312300
C	3.28785400	-1.25665000	0.71201600
H	4.30964600	-1.63123700	0.77744000
H	2.92204000	-1.14823100	1.73616600
C	2.41177700	-2.35626100	0.01373100
H	2.40180800	-3.24462700	0.64392400
H	2.85170300	-2.63910300	-0.94650500
N	1.16037900	1.73171200	-0.09609400
C	1.59904700	3.11014400	0.14918500
H	2.39654200	3.09406200	0.88938100
H	1.95312800	3.55354900	-0.78001100

H	0.74724300	3.66945800	0.53097300
O	-3.46284100	-0.99222000	0.08172400
C	-4.77025100	-0.46612500	0.36525800
H	-5.41501800	-0.71245000	-0.47576900
H	-5.13507600	-0.96088100	1.26263400
H	-4.72768800	0.61162900	0.51180300

12b.closed

E = -577.541463 a.u.

C	-1.43624163	0.74336876	-0.71243562
C	0.56304050	-0.27315204	-0.93240885
B	-2.11548348	-0.46673690	0.13848215
C	-0.22613514	-2.17690816	-0.09655980
C	0.94257269	-1.50154691	-0.28660206
H	-0.39824648	-3.12814849	0.38484163
N	-1.36424880	-1.49691482	-0.67758282
N	-0.74191036	-0.33103830	-1.18902704
C	0.81719966	1.00507564	-0.46616971
C	2.15243558	1.23105921	0.17676441
H	2.91077585	1.39693530	-0.59146840
H	2.15974045	2.09856771	0.83664389
C	2.48412213	-0.05463891	1.01303366
H	3.51223776	0.03453921	1.36533307
H	1.84076096	-0.04953811	1.89716160
C	2.31889719	-1.44292318	0.31194292
H	3.06782774	-1.56002520	-0.47522658
H	2.48097303	-2.23069171	1.04693412
N	-0.41630445	1.59180774	-0.31670542
C	-0.65771364	2.93995541	0.20050013
H	-1.63692426	2.95212682	0.67463205
H	0.11360970	3.18775300	0.92645973
H	-0.64055931	3.65493676	-0.62102741
C	-2.91088299	-0.57147190	1.44123232
H	-3.97231877	-0.48444309	1.16884116
H	-2.78015245	-1.52679794	1.95003071
H	-2.70682772	0.24858042	2.13185622

12b.open

E = -577.531526 a.u.

C	0.73946200	1.71158900	-0.00110300
C	-0.39053200	-0.27274700	-0.14461400
B	3.08118700	-0.29354700	-0.01854200
C	1.05384000	-1.91929200	0.09537400
C	-0.27140500	-1.66717000	0.02903100
H	1.63766100	-2.81448700	0.22717900
N	1.79126300	-0.63941400	-0.01958900
N	0.80902800	0.35507300	-0.13145000
C	-1.34767900	0.65161900	-0.04532600
C	-2.74973900	0.13843500	0.11468300
H	-3.06850700	0.24481400	1.15661600
H	-3.47149100	0.67841100	-0.50155500
C	-2.74947500	-1.36434600	-0.32193000
H	-3.71074600	-1.79988300	-0.04784000
H	-2.69022400	-1.38623500	-1.41281300
C	-1.62794200	-2.30210100	0.23232900
H	-1.75619500	-2.45250600	1.30909300

H	-1.70605600	-3.28063200	-0.24163200
N	-0.63369000	1.85749800	0.01769100
C	-1.27033500	3.16973500	0.09334200
H	-0.49064200	3.90610200	0.26646900
H	-1.78493100	3.39168400	-0.84159600
H	-1.98230100	3.18493000	0.91876900
C	4.50143800	0.15806700	-0.01345900
H	5.01460700	-0.09302500	0.91799600
H	5.06400500	-0.20361900	-0.87685400
H	4.44688300	1.25735000	-0.07765700

12bP

E = -687.102420 a.u.

C	-0.56038200	1.34346500	-0.20561800
C	0.75747100	-0.40219000	-0.45999500
B	-2.69983500	-0.38680900	0.06616600
C	-0.56729300	-2.11376800	-0.09373600
C	0.76406800	-1.78514600	-0.21504100
H	-1.05723700	-3.05497700	0.09732800
N	-1.37604300	-0.94952600	-0.22149300
N	-2.73301400	1.09562600	0.20351300
N	-1.74198000	1.90568100	0.14180000
N	-0.49585100	0.03451100	-0.46654300
C	1.58354100	0.66600700	-0.22634600
C	3.01697600	0.30030400	0.02734300
H	3.57434500	0.32508100	-0.91343500
H	3.50683200	0.98851900	0.71743400
C	3.02931700	-1.14632000	0.64918400
H	4.06687600	-1.47939700	0.68182800
H	2.69220800	-1.05278500	1.68456300
C	2.17750600	-2.28205000	-0.02171600
H	2.22413800	-3.17046700	0.60662900
H	2.59629200	-2.54566300	-0.99687100
N	0.75502200	1.75349100	-0.09910900
C	1.14133800	3.15058100	0.13135900
H	1.94047100	3.17345300	0.86969500
H	1.47483800	3.59790900	-0.80349500
H	0.26899200	3.67953300	0.51020300
C	-3.96259000	-1.24643400	0.29473500
H	-3.78033100	-2.32047500	0.34086500
H	-4.47424700	-0.93063700	1.20702100
H	-4.67065700	-1.06122200	-0.52079300

12c.closed

E = -695.453715 a.u.

C	-0.40101657	1.02863336	-1.25866863
C	1.42739653	-0.26412471	-0.97692517
B	-1.42625691	-0.12529957	-0.72058264
C	0.21294605	-2.08810118	-0.60365808
C	1.45444344	-1.57164899	-0.38126600
H	-0.19959991	-3.03937781	-0.30257981
N	-0.62163005	-1.21045525	-1.39806217
N	0.25849434	-0.11763999	-1.60144402
C	1.69052108	0.93542495	-0.34498665
C	2.79379359	0.93064277	0.67015975
H	3.75948851	1.03596465	0.17090300

H	2.70612953	1.74606490	1.38831772
C	2.71130097	-0.43751096	1.43412434
H	3.59424508	-0.51754329	2.06907795
H	1.84279265	-0.39228481	2.09703895
C	2.59407478	-1.74471496	0.58236049
H	3.52062677	-1.91926513	0.02983551
H	2.44102669	-2.58976517	1.25292196
N	0.55727958	1.69593450	-0.51477624
C	0.35512889	3.04215281	0.02208936
H	-0.71303886	3.19567588	0.16090763
H	0.87249903	3.12815086	0.97567962
H	0.74206100	3.77981709	-0.67981352
C	-2.44690793	-0.16205186	0.43585137
C	-3.46653334	0.97936220	0.27533368
H	-4.14368155	0.98384778	1.13349005
H	-2.97789173	1.95554901	0.22590728
H	-4.07031125	0.85778283	-0.62626707
C	-3.16279946	-1.52033594	0.49689920
H	-3.72342532	-1.72275019	-0.41796754
H	-2.46050978	-2.34237521	0.65804080
H	-3.86965796	-1.52550636	1.33064945
C	-1.63228808	0.05461312	1.73520830
H	-0.88686740	-0.73221304	1.88527940
H	-1.12516806	1.02429978	1.74468968
H	-2.31679973	0.03150767	2.58764744

12c.open

E = -695.447996 a.u.

C	0.35694800	1.75013300	-0.00836600
C	1.34730800	-0.29550000	-0.05524500
B	-2.16842700	-0.20498900	-0.00065200
C	-0.20041900	-1.84808400	-0.07176100
C	1.14031100	-1.69091300	-0.09018000
H	-0.84527300	-2.71113900	-0.08762900
N	-0.85193900	-0.53060100	-0.03204100
N	0.19119400	0.40004800	-0.03334500
C	2.36823700	0.56192400	-0.04714500
C	3.74206500	-0.04567400	-0.07422800
H	4.15985900	-0.00033900	-1.08453500
H	4.44169400	0.46767800	0.58851900
C	3.60361600	-1.53064300	0.40874700
H	4.55001200	-2.03968700	0.22279400
H	3.46295800	-1.50576200	1.49224600
C	2.46114500	-2.41618900	-0.19316700
H	2.65125500	-2.60338600	-1.25491100
H	2.45035600	-3.38265200	0.31035900
N	1.73514500	1.81422400	-0.02350900
C	2.45397400	3.08410400	-0.00445600
H	1.71699700	3.88188700	0.01909900
H	3.08538300	3.14128300	0.88253900
H	3.06881800	3.17762100	-0.89984500
C	-4.38502400	-0.42501200	1.31648900
H	-5.29720500	0.17453900	1.36204500
H	-4.66730600	-1.47842000	1.32211900
H	-3.78939000	-0.22448300	2.20782400

C	-4.43302500	-0.38076300	-1.24153900
H	-3.87080000	-0.15010200	-2.14715900
H	-4.71702200	-1.43327300	-1.27247500
H	-5.34532100	0.22026800	-1.23258700
C	-3.02047900	1.40173700	0.04253400
H	-3.31285700	1.89678200	0.96515100
H	-1.89703700	1.56010300	0.02774400
H	-3.34194800	1.92692600	-0.85332000
C	-3.63163000	-0.11155300	0.02790700

12cP

E = -805.012301 a.u.

C	0.55150400	1.51902600	-0.21457100
C	1.50909400	-0.44699500	-0.44960300
B	-1.89733400	0.24075500	-0.03670400
C	-0.12753100	-1.87869900	-0.15614000
C	1.24394700	-1.80903900	-0.23765700
H	-0.79270700	-2.71193900	-0.00223500
N	-0.69940200	-0.57592300	-0.27738700
N	-1.63777700	1.70518800	0.10681300
N	-0.50902300	2.30747300	0.08707600
N	0.36419300	0.22301300	-0.47597100
C	2.52249200	0.43812200	-0.19721900
C	3.85423100	-0.20113500	0.07035700
H	4.42303500	-0.27070000	-0.86130500
H	4.45532300	0.36911300	0.77990200
C	3.57662700	-1.63180800	0.66677900
H	4.52958800	-2.15980900	0.70756100
H	3.24687300	-1.48974800	1.69901400
C	2.53233600	-2.57189200	-0.03434500
H	2.39727100	-3.46172100	0.57907800
H	2.90791700	-2.89732400	-1.00847400
N	1.91788900	1.66650300	-0.08035900
C	2.56352600	2.96176500	0.16282900
H	3.31664900	2.83608700	0.93837300
H	3.02152900	3.32185700	-0.75683900
H	1.79746100	3.65829300	0.49782200
C	-3.34979600	-0.30040500	0.10685400
C	-3.44200900	-1.82977600	0.04522800
H	-2.93466600	-2.30054900	0.89348400
H	-4.48871000	-2.14145800	0.08868000
H	-3.02667400	-2.22838200	-0.88612500
C	-4.14840700	0.31388900	-1.06680900
H	-5.19783400	0.01780100	-0.98015900
H	-4.10116200	1.40485300	-1.04886800
H	-3.78328500	-0.03564200	-2.03675400
C	-3.95197600	0.20655200	1.43262500
H	-3.90800900	1.29493500	1.49520600
H	-4.99997300	-0.09977200	1.49514100
H	-3.43135400	-0.21108200	2.29884100

12d.closed

E = -946.848990 a.u.

C	-0.00263006	1.10954473	-1.47716541
C	1.72956032	-0.23516547	-0.92539241
B	-1.08092933	-0.05526824	-1.12265625

C	0.46317194	-2.05837304	-0.87373856
C	1.64152457	-1.56597765	-0.39697261
H	-0.00353292	-3.01716697	-0.70407226
N	-0.21202114	-1.12952030	-1.75897552
N	0.69199237	-0.04316737	-1.74250700
C	1.89177540	0.93383192	-0.20842480
C	2.81469373	0.86956226	0.97117632
H	3.84806326	0.99241332	0.63900296
H	2.61134073	1.64931213	1.70551955
C	2.61210403	-0.53302508	1.64685066
H	3.39490780	-0.65465386	2.39628325
H	1.65984464	-0.50233362	2.18146184
C	2.60619522	-1.80226451	0.73087087
H	3.60556483	-1.97953336	0.32562497
H	2.33284337	-2.66836018	1.33294078
N	0.82901140	1.73019611	-0.55152685
C	0.55916649	3.06573198	-0.02002940
H	-0.51987908	3.19910180	0.03292275
H	0.99539184	3.14986914	0.97316366
H	0.98843528	3.81866928	-0.67974682
Si	-2.42247125	-0.14155294	0.38919902
C	-3.32541312	-1.77942610	0.35127942
H	-2.63929405	-2.62699019	0.41733936
H	-4.00863344	-1.84493254	1.20219437
H	-3.91923982	-1.89185284	-0.55799120
C	-3.58092109	1.32249074	0.26374083
H	-4.26159109	1.32904312	1.11903917
H	-3.04532824	2.27441627	0.26101250
H	-4.18938547	1.27653346	-0.64169759
C	-1.31266462	-0.01901362	1.90985607
H	-0.68014645	-0.90627043	2.00019950
H	-0.66965725	0.86629246	1.88519773
H	-1.92271525	0.04446934	2.81486011

12d.open

E = -946.846733 a.u.

C	-0.43294400	1.55675400	0.02706800
C	-1.74902000	-0.30648500	-0.13153100
B	1.70778100	-0.66322900	0.03280300
C	-0.47739400	-2.08365700	0.13192200
C	-1.77193000	-1.70554900	0.04560300
H	0.01003900	-3.03341200	0.27329500
N	0.38209600	-0.89151500	0.02404500
N	-0.49270100	0.19701200	-0.10058300
C	-2.61281000	0.70708000	-0.04901000
C	-4.06063700	0.33474300	0.09233700
H	-4.38228100	0.47391100	1.12956300
H	-4.71743300	0.94142800	-0.53454300
C	-4.20224700	-1.16179700	-0.34255400
H	-5.20608900	-1.49944900	-0.08317000
H	-4.12824200	-1.19207200	-1.43236700
C	-3.18666900	-2.20340700	0.23010800
H	-3.34615500	-2.33688700	1.30493000
H	-3.35440500	-3.17099200	-0.24322100
N	-1.78501600	1.83707600	0.02406600

C	-2.29092700	3.20489300	0.08879000
H	-1.44584800	3.86192000	0.27414300
H	-2.76669300	3.47474500	-0.85419500
H	-3.01124700	3.29208500	0.90252300
Si	3.63677300	-0.02494200	-0.00881200
C	4.61456700	-1.25125000	-1.02048200
H	5.63955100	-0.88127000	-1.11411300
H	4.66305800	-2.23289300	-0.54612700
H	4.21207700	-1.36641500	-2.02823100
C	4.19952000	0.10651300	1.76431800
H	3.55992800	0.77502700	2.34336600
H	4.23200700	-0.86500300	2.26039800
H	5.21196800	0.51989600	1.78064300
C	3.39574800	1.63193300	-0.84558100
H	3.12050600	1.51571000	-1.89547900
H	2.62988300	2.23519200	-0.35365500
H	4.34345300	2.17716500	-0.80302900

12dP

E = -1056.405946 a.u.

C	0.96220600	1.55472600	-0.25443400
C	1.81267200	-0.46254100	-0.50358300
B	-1.56054500	0.40863600	-0.13440600
C	0.07803400	-1.78450600	-0.24222200
C	1.45430700	-1.80410800	-0.29015100
H	-0.64920300	-2.56789900	-0.09723000
N	-0.40051600	-0.45165700	-0.37843900
N	-1.22548800	1.85640400	0.02379800
N	-0.05587800	2.39147000	0.04217100
N	0.71223200	0.27810200	-0.56175900
C	2.86415000	0.35691900	-0.18578300
C	4.13922500	-0.36319100	0.14245900
H	4.74443100	-0.46902800	-0.76247200
H	4.74107900	0.17044200	0.87922200
C	3.74659000	-1.77321000	0.72279700
H	4.66229000	-2.35883800	0.80731900
H	3.37787600	-1.61016200	1.73861900
C	2.68042700	-2.64642600	-0.02932700
H	2.46046500	-3.52544200	0.57502500
H	3.08076400	-2.99547900	-0.98522500
N	2.33025000	1.61652200	-0.06468800
C	3.04044400	2.86445800	0.23759300
H	3.76480500	2.67133000	1.02652100
H	3.54186500	3.22778100	-0.65787200
H	2.30539900	3.59164300	0.57706400
Si	-3.46900300	-0.21545600	0.11242900
C	-4.07181800	0.43814500	1.76371100
H	-5.13122600	0.20478500	1.89699500
H	-3.52676600	-0.00033300	2.60254300
H	-3.95730900	1.52322500	1.81305200
C	-3.53470300	-2.09831100	0.07235500
H	-4.57121200	-2.43421600	0.15960700
H	-3.14702200	-2.50521400	-0.86599000
H	-2.98630400	-2.54607100	0.90614900
C	-4.47124700	0.51260700	-1.29793900

H	-5.52796200	0.26355800	-1.17021100
H	-4.38499600	1.60138100	-1.31568300
H	-4.15413600	0.12849400	-2.26983400

12e.closed

E = -769.254232 a.u.

C	0.36623880	1.05494936	-1.33630884
C	2.08961504	-0.28070831	-0.76625296
B	-0.80030936	-0.06351752	-1.08120828
C	0.77931687	-2.06979065	-0.63896187
C	1.97754279	-1.59615110	-0.19628614
H	0.29298919	-3.00804656	-0.41799427
N	0.12729013	-1.16917404	-1.56248986
N	1.05173601	-0.09716546	-1.58192112
C	2.26528521	0.90347420	-0.07881164
C	3.16808721	0.85541713	1.11787668
H	4.21065141	0.93635328	0.80277908
H	2.97534402	1.66497342	1.82187114
C	2.91067790	-0.51674603	1.83357933
H	3.65885984	-0.62776141	2.61918624
H	1.93545281	-0.45519072	2.32412010
C	2.91901320	-1.81029352	0.95443398
H	3.92619403	-2.00337526	0.57666276
H	2.62596350	-2.65823087	1.57273081
N	1.19020408	1.69101353	-0.42624664
C	0.92945920	3.03351595	0.09183611
H	-0.14722680	3.18124356	0.13434876
H	1.35399844	3.11878937	1.08958137
H	1.37702728	3.77554971	-0.56795515
C	-2.10836610	-0.08437717	-0.33981617
C	-2.74721255	1.12073576	0.00307996
C	-2.72792465	-1.30406827	-0.00906556
C	-3.96428620	1.10859815	0.66450691
H	-2.29656822	2.06603153	-0.27980257
C	-3.94276202	-1.31578349	0.65485820
H	-2.25918227	-2.24224353	-0.28626232
C	-4.55611489	-0.10968605	0.99202595
H	-4.45872271	2.03732737	0.91920531
H	-4.41996677	-2.25475227	0.90486924
H	-5.50929752	-0.12031406	1.50714056

12e.open

E = -769.246843 a.u.

C	-0.78240900	1.71032500	-0.04258600
C	-1.94782200	-0.25519700	-0.09371000
B	1.54115000	-0.42462900	0.00274900
C	-0.54073200	-1.92588600	0.14911700
C	-1.86078400	-1.65096400	0.08844300
H	0.02641600	-2.83174500	0.28350300
N	0.22287400	-0.66678300	0.01639200
N	-0.73520900	0.34626900	-0.09947100
C	-2.89048500	0.68690700	-0.04904300
C	-4.30564100	0.20421100	0.09048600
H	-4.64859600	0.33785900	1.12149000
H	-5.00244100	0.74352500	-0.55456500
C	-4.32484200	-1.30767400	-0.31434700

H	-5.30002200	-1.71971100	-0.05266100
H	-4.24195700	-1.35321200	-1.40303500
C	-3.23266900	-2.25423900	0.28266200
H	-3.38539200	-2.37495000	1.35995300
H	-3.32339000	-3.24208000	-0.16921900
N	-2.15394400	1.88060400	-0.03469500
C	-2.76458200	3.20586700	-0.02034700
H	-1.96717000	3.93477200	0.09390500
H	-3.29538900	3.38554400	-0.95559400
H	-3.45859700	3.28382900	0.81699300
C	2.98862800	-0.21439200	-0.00172200
C	3.70925000	-0.26682200	-1.21934600
C	3.66544400	0.06213000	1.21075500
C	5.07349700	-0.05190900	-1.21458500
H	3.19250500	-0.47094800	-2.14943200
C	5.02990000	0.27554400	1.19719100
H	3.11463200	0.11163700	2.14236800
C	5.72675500	0.21722100	-0.01077200
H	5.63327600	-0.08920600	-2.13998700
H	5.55611000	0.48978800	2.11822400
H	6.79716600	0.38668400	-0.01444600

12eP

E = -878.812761 a.u.

C	1.18968800	1.52589900	-0.32545100
C	1.93160700	-0.54297500	-0.46639400
B	-1.38465100	0.54171600	-0.13210800
C	0.14219900	-1.75047100	-0.07004300
C	1.51410400	-1.84383900	-0.14199700
H	-0.61084500	-2.48457700	0.16711800
N	-0.27668700	-0.41738000	-0.31581800
N	-0.96099300	1.95559100	0.03653600
N	0.22850300	2.42209500	0.00552500
N	0.86601600	0.24778700	-0.56094700
C	3.02874900	0.23934000	-0.20913500
C	4.26912600	-0.51870600	0.16229100
H	4.85627100	-0.72859500	-0.73622500
H	4.90747500	0.03914300	0.84866200
C	3.81178900	-1.85475200	0.85663300
H	4.69703600	-2.47838500	0.98356300
H	3.45996900	-1.59269900	1.85764300
C	2.69666700	-2.72585900	0.17886800
H	2.43506900	-3.54221800	0.85085100
H	3.07219900	-3.16902700	-0.74758400
N	2.55948500	1.52665200	-0.15260000
C	3.33334300	2.75141400	0.07866400
H	4.08174500	2.55034100	0.84263900
H	3.81186900	3.06415300	-0.84792100
H	2.64496700	3.52025100	0.42416700
C	-2.84857400	0.12839700	-0.02697700
C	-3.30261000	-1.13033700	-0.45723000
C	-3.78002500	1.03518500	0.50596000
C	-4.63950700	-1.47809900	-0.34658200
H	-2.61472000	-1.83121800	-0.92047700
C	-5.11698400	0.68396000	0.62445500

H	-3.44047600	2.01377300	0.82446300
C	-5.54474000	-0.57110200	0.20138400
H	-4.98277700	-2.44524300	-0.69193500
H	-5.82781300	1.38659300	1.04091500
H	-6.58997800	-0.84242200	0.28911400

3

E = -555.537679 a.u.

C	-0.48231400	0.72457000	0.66715600
C	-2.43941800	0.30017500	-0.38679800
C	-1.88318400	-0.94083300	-0.06229500
B	0.97910500	-0.00071400	0.40836400
N	-1.54197400	1.27460400	0.02115300
H	-3.36288000	0.56560900	-0.87269900
C	-1.75944900	2.70969900	-0.16687800
H	-2.35408200	3.10429400	0.65586400
H	-0.79043100	3.20338700	-0.18705200
H	-2.27369900	2.86653100	-1.11274700
C	-0.17817600	-2.43236700	-0.13745400
C	-1.48590800	-2.27615500	-0.49891700
H	0.45793200	-3.28648200	-0.31192500
H	-2.08210400	-2.99400600	-1.03635000
N	0.29658000	-1.36177000	0.64467600
N	-0.83649000	-0.56982200	0.70812400
N	2.21353200	0.35033700	-0.01656000
C	3.24789300	-0.64236000	-0.31502300
H	2.88768400	-1.64269100	-0.08079500
H	3.51788200	-0.59169300	-1.37163100
H	4.13344400	-0.43575100	0.28856700
C	2.62314700	1.73943400	-0.21872000
H	2.86389600	1.90768900	-1.27025000
H	1.82187700	2.41107100	0.08391100
H	3.50787000	1.94917800	0.38511300

3.TS-1.

E = -555.509292 a.u.

C	-0.67918200	-0.93902200	-0.33139500
C	-2.68179500	-0.00841200	0.32768400
C	-1.83656700	1.04246000	0.06761400
B	1.38766600	0.18060800	-0.27172400
N	-1.95016700	-1.18121100	0.09776200
H	-3.72034100	-0.04159100	0.60795500
C	-2.53400000	-2.51535400	0.22414900
H	-1.72679000	-3.24062300	0.16890300
H	-3.03957600	-2.60033200	1.18488100
H	-3.24090300	-2.69291600	-0.58565200
C	-0.08007300	2.47716300	-0.20404300
C	-1.40205900	2.43824600	0.09008500
H	0.58890500	3.31756800	-0.28214500
H	-2.00606400	3.30325200	0.30902000
N	0.40822900	1.15984700	-0.44411900
N	-0.71626700	0.38601100	-0.34849500
N	2.55613400	-0.39474900	0.01190500
C	2.91691500	-1.73853600	-0.47276600
H	3.78158500	-1.66269400	-1.13319500
H	3.16325400	-2.36370400	0.38650500

H	2.07497000	-2.17380400	-1.00657100
C	3.56934300	0.27135100	0.85089700
H	3.21021300	1.24533200	1.18049600
H	3.77094500	-0.35061200	1.72385000
H	4.48448100	0.40041900	0.27184000

3.IN1.

E = -555.528269 a.u.

C	1.00171300	-1.11823300	-0.00007400
C	2.86728100	0.26561700	0.00001300
C	1.78361200	1.08592700	-0.00006200
B	-1.66897600	0.23047700	-0.00005200
N	2.36254700	-1.03303900	0.00003500
H	3.92252400	0.47774300	0.00007300
C	3.22376800	-2.21299100	0.00003500
H	3.85030600	-2.21605400	0.89167500
H	2.57970700	-3.08764500	0.00075500
H	3.84932100	-2.21680100	-0.89229400
C	-0.13467600	2.27729600	0.00001300
C	1.20169400	2.41088100	0.00001900
H	-0.92082000	3.01376700	0.00004400
H	1.72945100	3.35072500	0.00006900
N	-0.48954400	0.88412700	-0.00001800
N	0.71711000	0.20046100	-0.00010300
N	-2.84446500	-0.37456300	-0.00001100
C	-3.52925900	-0.77017400	1.24755600
H	-4.51433500	-0.30360200	1.27017000
H	-3.63111000	-1.85554300	1.25822500
H	-2.95099400	-0.45138400	2.11261400
C	-3.52940900	-0.77027000	-1.24745900
H	-2.95196500	-0.45029300	-2.11262500
H	-3.63006400	-1.85574400	-1.25870300
H	-4.51501500	-0.30478000	-1.26930300

3.IN1. N2.

E = -665.054328 a.u.

C	0.93003700	1.13703000	-0.47285600
C	2.80115800	-0.23913600	-0.42836000
C	1.72130800	-1.06389500	-0.46967800
B	-1.72564600	-0.21905000	-0.35960700
N	2.29075600	1.05708600	-0.43364300
H	3.85678400	-0.44678300	-0.39663000
C	3.14672900	2.24061900	-0.40711900
H	2.49895300	3.11179200	-0.37082800
H	3.78401500	2.21686900	0.47653400
H	3.76134400	2.27648600	-1.30631000
C	-0.19238600	-2.26180800	-0.46583100
C	1.14469600	-2.39138000	-0.45669000
H	-0.97582400	-3.00121900	-0.46401300
H	1.67617800	-3.32893500	-0.44047200
N	-0.55118600	-0.87149700	-0.48447000
N	-0.12449900	-0.09005900	2.41372100
N	0.93236500	-0.14015100	2.67684600
N	0.65163000	-0.18359000	-0.50742500
N	-2.89613300	0.38565600	-0.25530700
C	-3.67042100	0.81803600	-1.43623700

H	-4.65685500	0.35550500	-1.39719500
H	-3.76713400	1.90356600	-1.40918100
H	-3.16069800	0.52153600	-2.35094400
C	-3.48431700	0.74168700	1.05246300
H	-2.83603200	0.40459000	1.85861300
H	-3.59162200	1.82560900	1.09918300
H	-4.46222500	0.26720800	1.13708100

3.TS-2.

E = -665.048801 a.u.

C	-1.28781200	0.85168600	0.55196200
C	-3.04067800	-0.56242700	-0.01329600
C	-1.89644800	-1.22089000	-0.34181200
B	1.50727000	-0.14919000	-0.05610200
N	-2.63777100	0.66435200	0.50613700
H	-4.07540600	-0.84828300	-0.08905500
C	-3.58589800	1.66855100	0.97978800
H	-4.20322900	1.25094000	1.77489400
H	-3.01123700	2.50620000	1.36459500
H	-4.21909300	2.00176300	0.15763800
C	0.10491100	-2.16447200	-0.76635700
C	-1.21761900	-2.39792700	-0.83803400
H	0.94478800	-2.78075500	-1.04252500
H	-1.67164300	-3.30536600	-1.20015900
N	0.35022300	-0.86189000	-0.23540400
N	1.10980900	1.66072000	-1.00713000
N	0.84604600	2.58094800	-1.52675700
N	-0.89860200	-0.32370500	0.00867700
N	2.74683800	-0.05487100	0.43761600
C	3.10574000	-0.89150400	1.60303500
H	3.43076500	-0.23908600	2.41443300
H	2.24353900	-1.47009500	1.92929800
H	3.91811700	-1.56406600	1.32579700
C	3.83950400	0.80185200	-0.03858000
H	4.11077200	1.50596100	0.74942400
H	4.70106100	0.17527100	-0.27274500
H	3.54921400	1.34537400	-0.93329800

3.IN2.

E = -665.055837 a.u.

C	-1.49210400	-0.92792500	0.29472400
C	-3.04920100	0.75739600	-0.02434100
C	-1.82516400	1.31768500	-0.23111000
B	1.45987000	-0.19133300	-0.07687300
N	-2.80844200	-0.57923300	0.27572300
H	-4.03965300	1.17717400	-0.04559400
C	-3.87980200	-1.52687200	0.56605700
H	-3.41973300	-2.48004000	0.81049500
H	-4.46702000	-1.17545300	1.41421600
H	-4.52376600	-1.64094100	-0.30583700
C	0.28281600	2.05791100	-0.47998100
C	-1.00031100	2.46897900	-0.51587600
H	1.19075700	2.60731300	-0.66780900
H	-1.33244300	3.47113300	-0.72857300
N	0.36067600	0.67321400	-0.19287700
N	1.08851900	-1.71424600	-0.45691400

N	0.98359100	-2.75304700	-0.76863000
N	-0.94869300	0.26115000	-0.03958500
N	2.77170600	-0.01391400	0.27089900
C	3.88680700	-0.92025100	-0.01270900
H	4.62665400	-0.40384000	-0.62747700
H	4.35678700	-1.22470600	0.92409700
H	3.55937100	-1.80728900	-0.55056200
C	3.19328700	1.22649400	0.93698000
H	3.84938500	0.96924800	1.77003300
H	3.74211600	1.86586500	0.24139200
H	2.32873100	1.76023000	1.32720800

3.TS-3.

E = -665.053510 a.u.

C	-1.56336400	-0.92244200	0.24666300
C	-2.99334600	0.87504200	-0.01474100
C	-1.73172700	1.35776000	-0.17868500
B	1.52764300	-0.26400600	-0.08327100
N	-2.84833000	-0.48293900	0.23021500
H	-3.95232000	1.36212200	-0.04338700
C	-3.98422900	-1.37169800	0.45759800
H	-3.59219800	-2.36845200	0.63815900
H	-4.54895300	-1.03621900	1.32711600
H	-4.62963700	-1.38205100	-0.42047200
C	0.40376300	1.99696500	-0.40842500
C	-0.85477000	2.47238100	-0.43305400
H	1.33736700	2.50531200	-0.58501700
H	-1.13933300	3.49375000	-0.62140800
N	0.41956000	0.60502400	-0.14561500
N	1.07135700	-1.74766900	-0.42195700
N	0.37850000	-2.58989300	-0.51981300
N	-0.91803700	0.24292700	-0.01692800
N	2.85260900	-0.09922800	0.21054900
C	3.90834300	-1.05810900	-0.12342500
H	4.60319000	-0.60775400	-0.83526400
H	4.45369300	-1.32866200	0.78213200
H	3.49424800	-1.95982200	-0.57240800
C	3.34876500	1.12628100	0.84539600
H	4.04942000	0.85180200	1.63541600
H	3.87026300	1.75293100	0.11755300
H	2.52583200	1.68243700	1.29080200

3.P.

E = -665.091422 a.u.

C	-1.29164200	-0.76498800	-0.03805300
C	-2.88412000	0.79396500	-0.01804100
C	-1.65588000	1.45972700	-0.00275900
B	1.42711200	-0.38158900	0.02414700
N	-2.62590600	-0.55079100	-0.03615200
H	-3.89211400	1.17176700	-0.01342900
C	-3.62466400	-1.62840000	-0.06047900
H	-3.09572700	-2.57255100	0.04978600
H	-4.31538300	-1.48775900	0.76817000
H	-4.15432800	-1.60506700	-1.01095600
C	0.45850300	2.21037500	0.10405900
C	-0.83982500	2.63924800	0.08273500

H	1.35918300	2.79534300	0.18047400
H	-1.17047000	3.66212000	0.13145900
N	0.53568600	0.82078100	0.02524300
N	0.72178400	-1.70520100	0.08268700
N	-0.52351900	-1.90230600	0.04394900
N	-0.75072700	0.44680600	-0.03367200
N	2.80028100	-0.33729700	-0.03822200
C	3.63300000	-1.53585300	0.09864000
H	4.22934100	-1.67214400	-0.80609700
H	4.30816200	-1.41371100	0.94888800
H	3.00633500	-2.40894900	0.25447900
C	3.56502000	0.89405900	-0.19612000
H	3.90419600	1.27846300	0.77036600
H	4.44346700	0.69397900	-0.81138900
H	2.97623100	1.65371500	-0.70919800

3a.

E = -536.100189 a.u.

C	-0.55838600	-0.74703300	-0.64065100
C	-2.18126400	0.46031800	0.36447300
C	-1.16763100	1.36249800	0.01669400
B	1.05507500	-0.67254600	-0.34832800
N	-1.75110000	-0.80465800	0.00165800
H	-3.13401900	0.60607300	0.84485900
C	-2.51587300	-2.03242600	0.23835100
H	-3.21266000	-2.19308100	-0.58301500
H	-1.81522800	-2.86252300	0.29497200
H	-3.05460300	-1.93366700	1.17821600
C	0.99976400	2.02992300	0.11045400
C	-0.26180000	2.43048600	0.44034300
H	1.92757800	2.55349800	0.28275200
H	-0.51961300	3.34196100	0.95298400
N	1.00603700	0.83279200	-0.64155200
N	-0.35728400	0.57796600	-0.72221500
O	1.95225100	-1.47787000	0.12199400
C	3.30708800	-1.09177300	0.43568100
H	3.42068500	-1.12879900	1.51637400
H	3.96104100	-1.82066200	-0.03478800
H	3.51848300	-0.09176700	0.05602600

3a. TS-1.

E = -536.080364 a.u.

C	0.20444300	-0.93359500	0.22140500
C	2.36537700	-0.22088100	-0.13296100
C	1.60299700	0.91276400	-0.00296200
B	-1.73626100	0.41415200	0.03428800
N	1.49441300	-1.31011900	0.00279500
H	3.42037400	-0.36178600	-0.29103100
C	1.95039000	-2.69854600	-0.04267200
H	2.50468200	-2.93904400	0.86380800
H	1.07431600	-3.33718300	-0.11527600
H	2.58411300	-2.84351000	-0.91623000
C	-0.01538500	2.52756900	-0.03487700
C	1.32052400	2.34159800	-0.13630800
H	-0.60100500	3.43019500	-0.08076700
H	2.03502200	3.13082100	-0.30344100

N	-0.66596700	1.27673800	0.19656100
N	0.37444700	0.38028100	0.26050100
O	-2.90067700	-0.02554800	-0.14127300
C	-3.52182000	-1.34436500	-0.07598400
H	-4.21630200	-1.31945000	0.75806100
H	-4.04114000	-1.48339600	-1.01855600
H	-2.73274900	-2.07858700	0.06934300

3a.IN1.

E = -536.086523 a.u.

C	0.67951500	-1.10998800	-0.08283200
C	2.51138000	0.30479600	0.08669000
C	1.41244100	1.10709600	0.05988300
B	-1.96717800	0.09558000	-0.20418400
N	2.03641600	-1.00220400	-0.00211700
H	3.56017800	0.53471400	0.16199500
C	2.92244000	-2.16456200	-0.00703900
H	3.50669100	-2.18932500	0.91237300
H	2.29887400	-3.05168500	-0.07044900
H	3.58771600	-2.12002900	-0.86883000
C	-0.54235200	2.24879200	0.02177600
C	0.78896400	2.41375100	0.10164800
H	-1.34682500	2.96490900	0.01476000
H	1.28580800	3.36706300	0.18173300
N	-0.85169900	0.84720800	-0.08020500
N	0.37310000	0.19909400	-0.04688000
O	-3.02884200	-0.53261300	-0.39355600
C	-3.97119100	-1.36418800	0.35656000
H	-3.87445000	-1.13994300	1.41499400
H	-4.95454500	-1.11187900	-0.02528000
H	-3.70872300	-2.39368900	0.13237600

3a.IN1.N2.

E = -645.614407 a.u.

C	-0.85315000	-0.83592200	-0.65238300
C	-2.75825100	0.24496000	0.11723800
C	-1.73340400	1.12741400	0.26722100
B	1.68399500	0.64068100	-0.53683000
N	-2.19647600	-0.90703700	-0.42820300
H	-3.80806300	0.32716000	0.33977700
C	-2.98607500	-2.09545500	-0.74390400
H	-2.31099200	-2.83552300	-1.16393200
H	-3.44655100	-2.48768800	0.16248900
H	-3.75647400	-1.84539000	-1.47275800
C	0.09812100	2.44628500	0.40911800
C	-1.22281700	2.42534200	0.65534200
H	0.83309100	3.22070100	0.55165600
H	-1.78569400	3.24732600	1.06669000
N	0.50922900	1.18602000	-0.14502100
N	1.63856100	-1.37261100	1.26864600
N	1.28821400	-2.15819600	1.93763100
N	-0.64172600	0.41748900	-0.20501700
O	2.78432700	0.30592300	-1.02484600
C	3.93033100	-0.52936000	-0.67849100
H	4.73714600	-0.19876600	-1.32326800
H	4.16406500	-0.38167200	0.37188600

H	3.64573900	-1.55617800	-0.89070700
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3a.TS-2.

E = -645.611975 a.u.

C	-1.04295700	-0.91555600	-0.44441700
C	-2.83406400	0.44215400	0.13591100
C	-1.71985800	1.21181300	0.25100800
B	1.72371500	0.41815800	-0.32413000
N	-2.39014600	-0.81289200	-0.26880800
H	-3.87531800	0.66899300	0.28649200
C	-3.29934000	-1.93160100	-0.50552400
H	-2.70678400	-2.76293300	-0.87646800
H	-3.79251200	-2.21481600	0.42413100
H	-4.04472700	-1.65111700	-1.24922800
C	0.21764700	2.36346800	0.27593700
C	-1.10204900	2.49801900	0.48250600
H	1.02175600	3.07779100	0.34144100
H	-1.59575000	3.41473500	0.76031100
N	0.52260800	1.00508300	-0.07877800
N	1.56231300	-1.54550400	0.66678300
N	1.54024500	-2.50475700	1.18264900
N	-0.69194300	0.34125300	-0.08655300
O	2.90461800	0.37473900	-0.77292300
C	4.13025800	-0.28599700	-0.35627100
H	4.93605600	0.23819600	-0.85868000
H	4.22841200	-0.21609900	0.72453500
H	4.07399500	-1.31952400	-0.69044500

3a.IN2.

E = -645.623479 a.u.

C	-0.85315000	-0.83592200	-0.65238300
C	-2.75825100	0.24496000	0.11723800
C	-1.73340400	1.12741400	0.26722100
B	1.68399500	0.64068100	-0.53683000
N	-2.19647600	-0.90703700	-0.42820300
H	-3.80806300	0.32716000	0.33977700
C	-2.98607500	-2.09545500	-0.74390400
H	-2.31099200	-2.83552300	-1.16393200
H	-3.44655100	-2.48768800	0.16248900
H	-3.75647400	-1.84539000	-1.47275800
C	0.09812100	2.44628500	0.40911800
C	-1.22281700	2.42534200	0.65534200
H	0.83309100	3.22070100	0.55165600
H	-1.78569400	3.24732600	1.06669000
N	0.50922900	1.18602000	-0.14502100
N	1.63856100	-1.37261100	1.26864600
N	1.28821400	-2.15819600	1.93763100
N	-0.64172600	0.41748900	-0.20501700
O	2.78432700	0.30592300	-1.02484600
C	3.93033100	-0.52936000	-0.67849100
H	4.73714600	-0.19876600	-1.32326800
H	4.16406500	-0.38167200	0.37188600
H	3.64573900	-1.55617800	-0.89070700

3a.TS-3.

E = -645.621578 a.u.

C	1.26226200	-0.97369900	-0.00038100
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C	2.79130000	0.76209600	-0.00000700
C	1.55948400	1.33656200	0.00028700
B	-1.81026200	-0.01647200	0.00026600
N	2.57009200	-0.60897400	-0.00037600
H	3.77781700	1.19210600	-0.00001300
C	3.65737100	-1.58455200	0.00003800
H	4.26745000	-1.45919700	0.89419100
H	3.21157900	-2.57496500	-0.00442000
H	4.27291700	-1.45362100	-0.88954400
C	-0.53882800	2.13384600	-0.00020000
C	0.74623700	2.52788000	0.00009600
H	-1.45406400	2.70330800	-0.00035000
H	1.09163200	3.54819100	0.00019800
N	-0.62761900	0.71455400	-0.00023400
N	-1.51178000	-1.58022500	0.00032700
N	-1.01049300	-2.55098300	0.00021000
N	0.68420100	0.25700900	0.00011600
O	-3.05132000	0.39588500	0.00070900
C	-4.26620600	-0.37132600	-0.00060900
H	-4.82697100	-0.10103600	0.89039600
H	-4.82478700	-0.10168700	-0.89319300
H	-4.05422400	-1.44231900	0.00008500

3a.P.

E = -645.664351 a.u.

C	-0.92779900	-0.79346600	-0.00089400
C	-2.64206600	0.63148800	-0.00002500
C	-1.47113300	1.40062400	-0.00014500
B	1.73834100	-0.16782200	-0.00051600
N	-2.27973700	-0.68618800	-0.00017100
H	-3.67786800	0.92673300	0.00008700
C	-3.19058800	-1.84089300	0.00131700
H	-2.58124600	-2.74199300	-0.00796500
H	-3.80073900	-1.81140500	0.90178700
H	-3.81463800	-1.80232000	-0.88918400
C	0.58630600	2.31641800	0.00032700
C	-0.74314700	2.64246900	0.00064400
H	1.45690800	2.95233300	0.00064500
H	-1.15201300	3.63818700	0.00130800
N	0.75364300	0.93419700	-0.00082400
N	1.16949800	-1.54630000	-0.00056500
N	-0.06224100	-1.85047400	-0.00069700
N	-0.49424400	0.46159200	-0.00093800
O	3.02522700	0.11539500	0.00013600
C	4.06809900	-0.87731100	0.00097900
H	3.64410100	-1.87975000	0.00068900
H	4.67367200	-0.71572600	-0.88787500
H	4.67183800	-0.71588300	0.89114500

3b.

E = -460.841173 a.u.

C	0.67264900	0.54424600	-0.68387200
C	1.21417700	-1.40367200	0.33939600
C	-0.14585000	-1.48845900	0.01413600
B	-0.66010200	1.43913500	-0.24793100
N	1.65315900	-0.15099800	-0.04384600

H	1.88044500	-2.10726700	0.81027300
C	3.02499300	0.32927600	0.14669700
H	3.64327900	0.00991500	-0.69108600
H	3.00108700	1.41581500	0.19111600
H	3.41287400	-0.07482600	1.07927200
C	-2.26452400	-0.68012000	0.14069500
C	-1.51168000	-1.76867100	0.46209700
H	-3.31429200	-0.51370800	0.32665400
H	-1.86143100	-2.64427000	0.98323200
N	-1.53216500	0.27129000	-0.61558000
N	-0.30782200	-0.37831000	-0.73181600
C	-0.88766100	2.70831000	0.56594800
H	-0.31908300	3.54268100	0.14721000
H	-1.94120500	2.97956000	0.63732300
H	-0.50599600	2.55709600	1.58376000

3b.TS-1.

E = -460.825687 a.u.

C	-0.51190700	-0.95490900	-0.24263800
C	-1.86288900	0.86736600	0.14314600
C	-0.59255500	1.35907400	-0.00904800
B	1.82485800	-0.98838700	-0.02861200
N	-1.77840700	-0.52815400	0.00241400
H	-2.80719100	1.35594700	0.31043200
C	-2.94830400	-1.40468200	0.06564400
H	-3.55164200	-1.28516500	-0.83339200
H	-2.59442200	-2.42971000	0.13538400
H	-3.53758200	-1.15695400	0.94705000
C	1.66687000	1.73008300	0.03128900
C	0.47250200	2.35554900	0.13011200
H	2.66859500	2.12180900	0.08471000
H	0.35147400	3.41254600	0.30424800
N	1.46666000	0.32620700	-0.18649100
N	0.10005500	0.21972100	-0.30034100
C	2.65277800	-2.21991000	0.19002800
H	2.52472200	-2.91037600	-0.64879700
H	3.71215100	-1.95694100	0.27936100
H	2.33248100	-2.72906900	1.10379000

3b.IN1.

E = -460.831716 a.u.

C	0.62694600	-1.10350200	0.00009300
C	1.96418900	0.79301000	0.00011800
C	0.67927100	1.23819600	-0.00008200
B	-2.25649000	-0.72649500	0.00022200
N	1.89249500	-0.59949500	0.00011500
H	2.90151500	1.32251400	0.00018700
C	3.08199100	-1.45071700	-0.00011500
H	3.67695000	-1.25475000	0.89126800
H	2.74556900	-2.48347100	0.00209500
H	3.67455800	-1.25778200	-0.89375600
C	-1.52587100	1.75728500	-0.00000600
C	-0.29899600	2.30528500	-0.00007900
H	-2.50537400	2.20485700	-0.00000900
H	-0.10207400	3.36549200	-0.00010400
N	-1.41390000	0.31742100	0.00003100

N	-0.05132200	0.06177500	-0.00007800
C	-3.18643500	-1.88851000	-0.00007100
H	-3.80710100	-1.92584600	0.89879000
H	-3.80560400	-1.92649500	-0.89991400
H	-2.53347200	-2.77623300	0.00071700

3b.IN1.N2.

E = -570.358098 a.u.

C	-0.66442400	-0.74333300	-0.71755000
C	-2.34162700	0.53688200	0.25040100
C	-1.19815800	1.26304300	0.36730300
B	2.05056800	0.36515500	-0.70704300
N	-1.98427300	-0.64657400	-0.39345500
H	-3.35326000	0.74765300	0.55215400
C	-2.95207300	-1.69762500	-0.70538400
H	-2.42027700	-2.48824100	-1.22688200
H	-3.38478900	-2.08827600	0.21510200
H	-3.73791400	-1.29799400	-1.34550900
C	0.80040300	2.32341900	0.41559700
C	-0.48992400	2.46110100	0.76355200
H	1.64319400	2.98324400	0.53509900
H	-0.90491000	3.32844100	1.25143700
N	0.99942800	1.04122200	-0.21463500
N	1.72786300	-1.75906900	1.07925000
N	1.38350800	-2.57739300	1.71114100
N	-0.24869400	0.44017500	-0.21719900
C	3.22674000	-0.30562700	-1.32642600
H	3.97726900	-0.59074700	-0.58558800
H	2.82714400	-1.22885200	-1.77546600
H	3.67026700	0.29330700	-2.12580700

3b.TS-2.

E = -570.356983 a.u.

C	0.74536900	-0.85197000	0.51323000
C	2.42859300	0.58094500	-0.19727900
C	1.26790900	1.27644000	-0.31054500
B	-2.09602200	0.32588800	0.43336000
N	2.07597700	-0.67745000	0.28300400
H	3.44902900	0.86208000	-0.39373000
C	3.06025200	-1.72785800	0.53890900
H	2.53384200	-2.56924700	0.98019700
H	3.52892200	-2.03414500	-0.39591200
H	3.81752900	-1.36256100	1.23185700
C	-0.73237600	2.32007000	-0.29173200
C	0.56790500	2.51549300	-0.55951800
H	-1.57906000	2.98319300	-0.35700000
H	0.99527500	3.44712600	-0.89377600
N	-0.94595100	0.95142500	0.12059300
N	-1.76688100	-1.80100400	-0.67339500
N	-1.67788200	-2.76328900	-1.17654500
N	0.30538900	0.36148900	0.09852900
C	-3.46920400	0.01414800	0.94104800
H	-4.14116100	-0.33265500	0.15391500
H	-3.37855700	-0.77740300	1.69690100
H	-3.89096000	0.89237000	1.44076300

3b.IN2.

E = -570.380515 a.u.

C	-0.93556000	-0.95417600	-0.00003500
C	-2.43893500	0.80628300	0.00008800
C	-1.19878800	1.36110400	0.00005400
B	2.08769200	-0.14342200	0.00003700
N	-2.23979800	-0.57205300	-0.00010600
H	-3.41951100	1.25031100	0.00000400
C	-3.34458400	-1.52860700	-0.00019800
H	-2.91581400	-2.52651000	-0.00051300
H	-3.95468300	-1.39031300	0.89196700
H	-3.95492800	-1.38985500	-0.89212400
C	0.92748100	2.09252000	0.00009300
C	-0.34503900	2.52615100	0.00010200
H	1.85272500	2.64350900	0.00012200
H	-0.65488600	3.55827000	0.00013900
N	0.97342400	0.66506000	0.00005100
N	1.74159300	-1.69094000	-0.00000400
N	1.73703500	-2.78159200	-0.00002900
N	-0.34965600	0.26482000	0.00002800
C	3.60120300	0.14978900	0.00005500
H	4.08716600	-0.28249400	0.88011600
H	4.08717800	-0.28245100	-0.88002100
H	3.80143600	1.22120000	0.00008200

3b.TS-3.

E = -570.374997 a.u.

C	0.97607000	-0.85860500	-0.00003100
C	2.24231700	1.04437600	0.00000900
C	0.93853800	1.44069300	0.00003000
B	-2.14273400	-0.46741600	-0.00002300
N	2.22340300	-0.34372400	-0.00002800
H	3.15926100	1.60830600	0.00001500
C	3.43372100	-1.16731300	0.00005900
H	4.02041400	-0.95446900	-0.89245000
H	4.01977400	-0.95526200	0.89317800
H	3.12822100	-2.20986400	-0.00051900
C	-1.25432100	1.92116200	-0.00004700
C	-0.04142800	2.50114200	-0.00001000
H	-2.23761100	2.36131700	-0.00008000
H	0.15259000	3.56065400	-0.00001000
N	-1.14408300	0.50470100	-0.00003600
N	-1.49377600	-1.87605100	-0.00004000
N	-0.52878000	-2.44763000	-0.00004900
N	0.22137900	0.25650300	0.00001200
C	-3.67237600	-0.33777800	0.00008600
H	-4.09370100	-0.84254100	0.87561900
H	-4.02351700	0.69297900	0.00004200
H	-4.09388400	-0.84269600	-0.87526600

3b.P.

E = -570.407174 a.u.

C	-0.79125000	-0.71375300	0.00009900
C	-2.09751000	1.09264600	-0.00023900
C	-0.77469000	1.54549300	0.00013500
B	1.96039300	-0.75380300	0.00004400
N	-2.07505000	-0.27578300	-0.00032100

H	-3.02765900	1.63618100	-0.00055100
C	-3.24387600	-1.16932100	0.00051400
H	-2.87536200	-2.19290000	-0.00849700
H	-3.82809600	-0.99019900	0.90084300
H	-3.83822700	-0.97802600	-0.89058700
C	1.44823800	1.91916200	-0.00009600
C	0.24528600	2.56564000	-0.00019800
H	2.44828700	2.32162300	-0.00025600
H	0.09979700	3.63251600	-0.00042900
N	1.26619500	0.53034400	0.00018700
N	1.06389900	-1.95133600	-0.00047800
N	-0.20896100	-1.94697600	-0.00055500
N	-0.06293900	0.39351700	0.00045900
C	3.49437100	-0.90124200	0.00027000
H	4.04842600	0.03729800	0.00006100
H	3.80250000	-1.48840100	0.87126300
H	3.80295000	-1.48919400	-0.87002400

3c.

E = -578.753685 a.u.

C	0.68559300	0.70816600	-0.80299700
C	2.55719800	0.37209300	0.43135400
C	2.07835500	-0.89660600	0.08155600
B	-0.71847000	-0.09733200	-0.46960000
N	1.66770500	1.30144000	-0.06727100
H	3.42353700	0.67633100	0.99481500
C	1.81148200	2.74883200	0.10982400
H	2.43271100	3.15547900	-0.68696300
H	0.82041700	3.19503800	0.06808200
H	2.26584100	2.94078200	1.07944100
C	0.42693900	-2.45059600	0.07273600
C	1.69271100	-2.23328400	0.52897800
H	-0.19508400	-3.32035500	0.21787200
H	2.26969600	-2.91136600	1.13538200
N	-0.02688600	-1.40780000	-0.77224300
N	1.09217200	-0.58004100	-0.78363000
C	-2.06875600	0.25835600	0.15241600
C	-2.64861800	-0.89029300	0.98757000
H	-2.05716400	-1.06820300	1.88904100
H	-3.66597000	-0.64204500	1.30000200
H	-2.69855000	-1.82009500	0.41462500
C	-2.92609500	0.45337100	-1.13903200
H	-2.54765200	1.26054100	-1.77059000
H	-2.99335800	-0.46011700	-1.73432500
H	-3.93774400	0.72249800	-0.82175300
C	-2.03296100	1.57118400	0.94291200
H	-1.41547900	1.48321900	1.84028800
H	-1.65095200	2.39348100	0.33206500
H	-3.04391800	1.83894200	1.26011500

3c.TS-1.

E = -578.739040 a.u.

C	-0.86576000	-0.89002200	-0.34674600
C	-2.94733600	-0.07969400	0.20391700
C	-2.14833800	1.01745900	0.00917600
B	1.10930300	0.27827600	-0.15551500

N	-2.14219100	-1.21108200	-0.01072400
H	-3.99222200	-0.17483200	0.44358000
C	-2.65682800	-2.57761900	0.07190700
H	-3.28772500	-2.79108200	-0.79013900
H	-1.80730900	-3.25526400	0.07961300
H	-3.22925600	-2.69264300	0.99100200
C	-0.42543600	2.52356900	0.00543100
C	-1.76310900	2.42137600	0.17655000
H	0.22035400	3.38418700	0.05455000
H	-2.41259800	3.24642600	0.42001100
N	0.13060900	1.24046000	-0.29770700
N	-0.98092000	0.43185700	-0.38745100
C	2.46990600	-0.34034000	0.05235400
C	3.47778300	0.82901700	0.20070300
H	3.25812500	1.45249500	1.06993500
H	4.47192500	0.39767000	0.34273400
H	3.51267800	1.45715400	-0.69185500
C	2.82590700	-1.21184900	-1.17263200
H	2.10698200	-2.02193300	-1.30201100
H	2.86824100	-0.62673300	-2.09319800
H	3.81374600	-1.64720200	-1.00212100
C	2.44852400	-1.20450400	1.33185400
H	2.20947100	-0.61750400	2.22082800
H	1.73199000	-2.02241300	1.24299000
H	3.44471100	-1.63271300	1.46775000

3c.IN1.

E = -578.746210 a.u.

C	-1.12425400	-1.03416800	-0.00005300
C	-3.09080300	0.19665700	-0.00009000
C	-2.07680400	1.10398100	-0.00007900
B	1.37225700	0.38020700	-0.00009300
N	-2.48660300	-1.06003000	-0.00008100
H	-4.15985600	0.32215100	-0.00014900
C	-3.25485200	-2.30393200	0.00013500
H	-3.87915700	-2.35360800	-0.89142500
H	-2.54629600	-3.12721600	-0.00131700
H	-3.87686200	-2.35478600	0.89323700
C	-0.23955800	2.42911900	0.00006800
C	-1.58352000	2.46609900	0.00000900
H	0.49176600	3.21967400	0.00016300
H	-2.17305700	3.36872800	0.00001800
N	0.20970400	1.06242400	0.00001000
N	-0.94955100	0.30184300	-0.00004100
C	2.65605800	-0.38687100	-0.00003200
C	3.83706800	0.62304700	0.00041400
H	3.84108600	1.25318400	0.89132800
H	4.75838300	0.03518100	0.00054600
H	3.84151100	1.25345900	-0.89030200
C	2.69552700	-1.26987200	-1.27318400
H	1.85489900	-1.96500900	-1.30086500
H	2.69554400	-0.67081100	-2.18506900
H	3.62229600	-1.84839300	-1.24345500
C	2.69496400	-1.27030200	1.27286300
H	2.69462400	-0.67153600	2.18494300

H 1.85429800 -1.96541400 1.29996900
H 3.62173200 -1.84883400 1.24332000

3c.IN1.N2.

E = -688.272089 a.u.

C -1.27923200 -0.73794500 -0.65805700
C -3.17452300 0.48647100 -0.10911100
C -2.11115500 1.25604500 0.24376300
B 1.35641100 0.52262200 -0.02620400
N -2.64082700 -0.68780500 -0.63546300
H -4.23446100 0.66176300 -0.04235100
C -3.47653500 -1.77859300 -1.13339400
H -2.81446800 -2.55267200 -1.51063400
H -4.08782500 -2.17764200 -0.32436500
H -4.11620400 -1.41703200 -1.93799200
C -0.22092800 2.40097700 0.71098000
C -1.56030500 2.48886400 0.76231100
H 0.54647200 3.09888100 1.00150100
H -2.10906200 3.34193700 1.12717600
N 0.16482500 1.12454400 0.16925500
N 0.56677000 -1.56059900 1.67557000
N 0.13289300 -2.37945600 2.24932800
N -1.02366400 0.46702000 -0.10008100
C 2.68526600 -0.02382100 -0.43856800
C 2.26830100 -1.25779800 -1.31441100
H 1.61922900 -0.98242400 -2.14712100
H 3.19973700 -1.66454200 -1.71776000
H 1.76829100 -2.02751400 -0.72714500
C 3.39287900 1.02289600 -1.33777000
H 3.71008300 1.89614400 -0.76581900
H 4.28546900 0.55038800 -1.75483600
H 2.76403400 1.34795200 -2.16842300
C 3.60147700 -0.46990400 0.71309700
H 3.13286400 -1.23144800 1.33541400
H 4.50758600 -0.89694200 0.27694900
H 3.89474600 0.37095900 1.34311500

3c.TS-2.

E = -688.271369 a.u.

C 1.50597900 -0.82576400 0.47704500
C 3.26710900 0.61060900 -0.00041100
C 2.13076200 1.29160500 -0.30026200
B -1.30098900 0.31241500 -0.05667000
N 2.85529700 -0.64227100 0.44593200
H 4.30327700 0.89856100 -0.04630400
C 3.79708200 -1.67761800 0.86628100
H 3.21647700 -2.51592900 1.24043300
H 4.40278600 -1.99693500 0.01853400
H 4.44016700 -1.29271100 1.65722400
C 0.14231900 2.31365900 -0.59446800
C 1.46662300 2.52040500 -0.67086100
H -0.69057500 2.96751400 -0.79440400
H 1.93240100 3.45086800 -0.95216400
N -0.11948200 0.95390700 -0.19761900
N -0.75125400 -1.81115400 -1.11454100
N -0.54751700 -2.76087300 -1.60849000

N 1.12445900 0.37480300 -0.02310500
C -2.71376500 0.01953100 0.36164800
C -2.59955800 -0.97926400 1.54958800
H -1.96389100 -0.60146600 2.35283800
H -3.60718000 -1.12095000 1.94909100
H -2.21678900 -1.94792400 1.22602500
C -3.25499500 1.38269100 0.88532500
H -3.37907200 2.10809500 0.07862700
H -4.24026900 1.19812700 1.32023800
H -2.62046100 1.81185900 1.66355900
C -3.63451800 -0.53737900 -0.73389600
H -3.30708500 -1.51799100 -1.07892200
H -4.63716600 -0.64830700 -0.31453300
H -3.70041800 0.13337300 -1.59206800

3c.IN2.

E = -688.290612 a.u.

C -1.80653800 -0.94917500 -0.00011000
C -3.32421500 0.79652400 -0.00014200
C -2.08833700 1.35977000 -0.00002800
B 1.20443100 -0.14228700 0.00007100
N -3.11376600 -0.57957500 -0.00018100
H -4.30782100 1.23350900 -0.00019500
C -4.20926500 -1.54576400 -0.00015000
H -3.77184000 -2.53991300 -0.00097400
H -4.82067000 -1.41357700 0.89214000
H -4.82161600 -1.41251300 -0.89163000
C 0.02838400 2.11428900 0.00007200
C -1.24830500 2.53267500 0.00003600
H 0.94048000 2.68220300 0.00013000
H -1.56843400 3.56151900 0.00005000
N 0.09758700 0.68504400 0.00005100
N 0.79475700 -1.69139200 0.00001300
N 0.81057500 -2.78230000 -0.00000800
N -1.22832100 0.27217900 -0.00000900
C 2.75866500 0.01237700 0.00008700
C 3.33204000 -0.67354400 -1.26188100
H 2.95146100 -0.22148800 -2.18054800
H 4.41847600 -0.55686000 -1.25819700
H 3.12712900 -1.74665600 -1.29133800
C 3.19481200 1.48721900 0.00008700
H 2.85281300 2.01589900 0.89282000
H 4.28651400 1.52568400 0.00011500
H 2.85286000 2.01588200 -0.89267300
C 3.33203000 -0.67353400 1.26206600
H 3.12715700 -1.74665300 1.29151400
H 4.41846200 -0.55681500 1.25841200
H 2.95141600 -0.22149500 2.18072700

3c.TS-3.

E = -688.282391 a.u.

C -1.79031300 -0.86943900 0.00001200
C -3.18240800 0.92978300 0.00000700
C -1.90552900 1.41471700 0.00000400
B 1.25998000 -0.35007800 0.00000200
N -3.07260200 -0.45294500 0.00000200

H	-4.13565800	1.42994000	0.00000900
C	-4.22090700	-1.36190200	-0.00001000
H	-4.82021700	-1.19152600	0.89305400
H	-4.82018900	-1.19152200	-0.89309100
H	-3.84244200	-2.38047300	0.00000000
C	0.25436900	2.02570500	-0.00000600
C	-0.99283400	2.53311300	-0.00000800
H	1.20583300	2.52955900	-0.00001000
H	-1.25066200	3.57871500	-0.00001400
N	0.23440700	0.60866200	0.00000300
N	0.64436100	-1.76857500	-0.00000200
N	-0.34916700	-2.32040800	-0.00000300
N	-1.11195300	0.28417100	0.00001100
C	2.80580300	-0.16166800	0.00000000
C	3.23633300	0.61742600	-1.26337600
H	2.80452700	1.61954000	-1.31113700
H	4.32361100	0.72875000	-1.25692000
H	2.96362300	0.08738700	-2.17908200
C	3.50547800	-1.53262400	0.00000600
H	3.24936800	-2.12048200	0.88494300
H	3.24937000	-2.12048800	-0.88492600
H	4.58789700	-1.38637200	0.00000600
C	3.23633500	0.61743800	1.26336800
H	2.96362800	0.08740800	2.17907900
H	4.32361400	0.72876300	1.25690800
H	2.80452900	1.61955200	1.31112000

3c.P.

E = -688.314865 a.u.

C	-1.55162100	-0.77104300	-0.00049600
C	-3.11709000	0.81530200	0.00012700
C	-1.87774300	1.46381400	-0.00032200
B	1.18010300	-0.39986200	-0.00022200
N	-2.88796900	-0.53244600	0.00008000
H	-4.11863000	1.21236300	0.00044500
C	-3.90690300	-1.59342200	0.00025000
H	-3.38658200	-2.54884300	0.00162400
H	-4.51828600	-1.49933000	0.89541700
H	-4.51682400	-1.50110300	-0.89610400
C	0.25969800	2.17156300	0.00018500
C	-1.02846500	2.62710100	0.00034000
H	1.18363700	2.72599300	0.00046900
H	-1.33497000	3.65927900	0.00077500
N	0.29472300	0.77146100	-0.00044000
N	0.46674200	-1.71451000	0.00004900
N	-0.79414500	-1.90061300	0.00006300
N	-0.99798200	0.43398600	-0.00083500
C	2.73459300	-0.27933700	-0.00003600
C	3.18797700	0.49372500	-1.25823600
H	2.78528900	1.51011000	-1.29771900
H	4.27817300	0.57537300	-1.25709200
H	2.89735900	-0.02221600	-2.17678600
C	3.38511900	-1.67056300	-0.00118200
H	3.09630300	-2.24908800	0.87834200
H	3.09662400	-2.24747200	-0.88188400

H	4.47312500	-1.56530400	-0.00091500
C	3.18722100	0.49126600	1.26001300
H	2.89597500	-0.02643300	2.17737800
H	4.27742700	0.57281200	1.25972200
H	2.78456400	1.50760100	1.30116200

3d.

E = -830.148668 a.u.

C	1.04145800	0.67520600	-1.07505100
C	2.44320100	0.51085300	0.70578000
C	2.15631500	-0.79899200	0.31131600
B	-0.33191800	-0.22623000	-0.97762600
N	1.72900200	1.35844300	-0.10992700
H	3.07045900	0.89269000	1.49458500
C	1.75401500	2.81903000	-0.00355100
H	2.55955600	3.22040700	-0.61687200
H	0.79882800	3.19996000	-0.35989200
H	1.90009900	3.09392200	1.03909400
C	0.71131900	-2.48622900	-0.13078800
C	1.74350000	-2.14502400	0.69066800
H	0.14376900	-3.40378100	-0.14950100
H	2.14804500	-2.75415900	1.48203800
N	0.46736000	-1.50600100	-1.12756100
N	1.47322400	-0.59087200	-0.84091900
Si	-2.00361000	0.17578700	0.09171500
C	-3.05938600	-1.36394500	0.18538400
H	-2.52129800	-2.19818700	0.64178700
H	-3.94081800	-1.16958800	0.80216500
H	-3.41060800	-1.67764100	-0.79970500
C	-1.25370000	0.60619600	1.76608600
H	-0.63734300	1.50779700	1.71593200
H	-2.05309500	0.79783500	2.48717400
H	-0.64393500	-0.20946200	2.16465700
C	-2.89152700	1.63516900	-0.66648400
H	-3.29383700	1.39699800	-1.65298700
H	-3.73069000	1.92477400	-0.02855700
H	-2.23728000	2.50400300	-0.76711700

3d.TS-1.

E = -830.138327 a.u.

C	-1.04129100	-0.82285200	-0.50618200
C	-3.15069600	-0.40767900	0.30741600
C	-2.59082200	0.81738900	0.05364000
B	0.67630400	0.59029100	-0.27200600
N	-2.18351400	-1.37275200	-0.02529200
H	-4.13070500	-0.69466700	0.64790700
C	-2.42952200	-2.81067700	0.07878400
H	-3.09620800	-3.13379200	-0.71987800
H	-1.47458500	-3.32118900	-0.01468000
H	-2.87398400	-3.03045000	1.04818700
C	-1.14756700	2.58864500	-0.00543500
C	-2.43058000	2.25926000	0.26614600
H	-0.64856500	3.54196800	0.04541800
H	-3.18195500	2.95052000	0.61152200
N	-0.41737700	1.43223500	-0.42287200
N	-1.39764400	0.46218300	-0.50879300

Si	2.52944300	-0.16016300	0.06791900
C	3.67533800	1.27453600	0.41985600
H	3.37614400	1.83338200	1.30851200
H	4.68068900	0.88382300	0.60091800
H	3.74041100	1.96510900	-0.42305500
C	2.29603500	-1.29374300	1.53676300
H	1.55126600	-2.06463900	1.32923500
H	3.24333700	-1.79598200	1.75143200
H	1.99917600	-0.75130500	2.43628300
C	2.95790300	-1.08604100	-1.49629400
H	3.06484600	-0.41812900	-2.35293500
H	3.91187200	-1.60177700	-1.35616200
H	2.20150000	-1.83675400	-1.73298900

3d.IN1.

E = -830.147508 a.u.

C	-1.33066500	-1.00470800	0.00000300
C	-3.42941000	-0.01519600	0.00000300
C	-2.53099400	1.00557500	0.00000000
B	0.98870200	0.71434500	0.00000200
N	-2.67977000	-1.19136200	0.00000500
H	-4.50584600	-0.01770300	0.00000400
C	-3.29494600	-2.51743200	-0.00000600
H	-2.49360600	-3.25072600	0.00008100
H	-3.90784400	-2.64136000	0.89228000
H	-3.90770100	-2.64141500	-0.89238200
C	-0.86840000	2.54163500	0.00000100
C	-2.20723700	2.41691000	0.00000000
H	-0.23852400	3.41509700	0.00000200
H	-2.90200700	3.24131400	0.00000000
N	-0.25651900	1.24093200	0.00000100
N	-1.31431300	0.34556800	0.00000000
Si	2.76390400	-0.28370800	0.00000000
C	2.67335900	-1.30448100	-1.55968500
H	2.68339100	-0.68656800	-2.45911500
H	3.54453000	-1.96486100	-1.59737700
H	1.77845300	-1.93009800	-1.57044500
C	4.11616600	1.00409000	-0.00006600
H	4.08584300	1.63733000	0.88818300
H	5.07911100	0.48516400	-0.00006800
H	4.08580900	1.63727100	-0.88835600
C	2.67342900	-1.30439500	1.55974600
H	1.77851700	-1.93000100	1.57059100
H	3.54459400	-1.96478300	1.59742800
H	2.68351800	-0.68643000	2.45914100

3d.IN1.N2.

E = -939.673434 a.u.

C	-1.47425500	-0.73917400	-0.63228300
C	-3.51432200	0.27997200	-0.19505800
C	-2.55917700	1.18031200	0.15762900
B	0.96388800	0.79710400	-0.00438900
N	-2.83215900	-0.84575000	-0.65438600
H	-4.58909100	0.33382200	-0.16938500
C	-3.52075800	-2.04336500	-1.13170600
H	-2.76202100	-2.75182700	-1.45153400

H	-4.11417000	-2.47623000	-0.32679000
H	-4.16520500	-1.78954700	-1.97283200
C	-0.82307700	2.54320100	0.64401400
C	-2.16577800	2.48382200	0.64698900
H	-0.14860900	3.33151900	0.93298800
H	-2.81781800	3.28264700	0.96138400
N	-0.27957800	1.30113400	0.16513500
N	0.38274400	-1.40043800	1.80870800
N	0.06413100	-2.31311300	2.31253700
N	-1.37846900	0.50911900	-0.11843600
Si	2.78641700	-0.01619700	-0.39333900
C	2.28580700	-1.62742000	-1.20060000
H	1.71669700	-1.46293400	-2.11692000
H	3.19831900	-2.17391900	-1.45775000
H	1.68563200	-2.25266600	-0.53859900
C	3.64966300	1.15941100	-1.55913700
H	3.85889000	2.12526900	-1.09596300
H	4.60924100	0.71891700	-1.84475300
H	3.07807400	1.32459800	-2.47405800
C	3.67152300	-0.22118300	1.23582500
H	3.12063200	-0.85970500	1.92750000
H	4.63864300	-0.69502100	1.04439000
H	3.86706100	0.73618100	1.72208400

3d.TS-2.

E = -939.671704 a.u.

C	1.91064500	-0.85090400	0.39773000
C	3.67692000	0.60715700	0.01042500
C	2.54374400	1.31190800	-0.23549800
B	-0.93127500	0.41648200	-0.04939900
N	3.25964400	-0.67079700	0.37355900
H	4.71448000	0.89187700	-0.02436900
C	4.19769400	-1.73642700	0.71996100
H	3.61360900	-2.60041200	1.02347500
H	4.80945700	-1.98965200	-0.14558700
H	4.83492200	-1.41474000	1.54326700
C	0.56667400	2.36265900	-0.48361300
C	1.89209200	2.56382600	-0.54034600
H	-0.26062900	3.03300500	-0.64978900
H	2.36635000	3.50459800	-0.76837800
N	0.29194700	0.98253500	-0.16239500
N	-0.51053800	-1.91713800	-0.89118800
N	-0.42916500	-2.94823400	-1.23504400
N	1.52992000	0.38636600	-0.01247400
Si	-2.90572600	0.05549700	0.26287000
C	-2.93485300	-1.22560300	1.62184800
H	-2.46187300	-0.86562400	2.53712700
H	-3.97828700	-1.45685800	1.85483200
H	-2.44910300	-2.15602700	1.32265300
C	-3.58310700	1.71585200	0.79788300
H	-3.51476300	2.46760900	0.00889900
H	-4.64356300	1.59418400	1.03713400
H	-3.08768000	2.09634900	1.69314300
C	-3.63290900	-0.54486500	-1.34658300
H	-3.20143500	-1.49374300	-1.66880600

H -4.70565400 -0.70395600 -1.20394700
H -3.51335700 0.18328500 -2.15087400

3d.IN2.

E = -939.693596 a.u.

C 2.19364200 -0.95294200 0.00004100
C 3.65014800 0.84683000 0.00001700
C 2.39563300 1.36793900 -0.00001200
B -0.85641100 -0.22335500 0.00004800
N 3.48734500 -0.53715300 0.00002100
H 4.61872600 1.31650700 0.00001200
C 4.61640700 -1.46415400 -0.00006700
H 4.21349100 -2.47281400 0.00048300
H 5.22278800 -1.31045300 -0.89235000
H 5.22346900 -1.30975200 0.89163100
C 0.25105500 2.04040200 0.00003900
C 1.51120400 2.50986000 0.00001600
H -0.69216400 2.56019800 0.00006400
H 1.79372400 3.54970800 0.00001700
N 0.24125900 0.61383700 0.00003100
N -0.45730500 -1.74298500 0.00004800
N -0.48517400 -2.83603000 0.00005000
N 1.57558200 0.25023300 -0.00000200
Si -2.88518400 0.03176300 -0.00000900
C -3.50696700 -0.82155500 1.54773300
H -3.11406700 -0.36240800 2.45715900
H -4.59717200 -0.74409900 1.58450200
H -3.26253900 -1.88663400 1.56667700
C -3.28594700 1.85974000 -0.00053100
H -2.91275400 2.36952700 -0.89171000
H -4.37404900 1.97098500 -0.00080300
H -2.91316400 2.36992600 0.89059100
C -3.50686700 -0.82240400 -1.54732900
H -3.26321800 -1.88768000 -1.56521700
H -4.59699900 -0.74418100 -1.58464400
H -3.11325200 -0.36434100 -2.45699300

3d.TS-3.

E = -939.679652 a.u.

C -2.11569200 -0.85652600 -0.00021500
C -3.50899700 0.93315900 0.00018800
C -2.23060400 1.42208700 0.00007700
B 0.90319300 -0.38867100 -0.00004500
N -3.40061000 -0.45048200 0.00002400
H -4.46382500 1.43050700 0.00035800
C -4.54627600 -1.36404800 -0.00008400
H -5.14471300 -1.19590800 -0.89398600
H -4.16469700 -2.38169500 0.00095500
H -5.14589500 -1.19455300 0.89276500
C -0.06099700 2.01028300 -0.00009200
C -1.30402400 2.53287000 0.00008000
H 0.90162400 2.49600900 -0.00013900
H -1.55179600 3.58083500 0.00019500
N -0.09820600 0.59637900 -0.00018700
N 0.25015800 -1.78924000 0.00012500
N -0.79133800 -2.27954100 0.00012900

N -1.44186800 0.29261100 -0.00013600
Si 2.92093200 -0.13636000 0.00000500
C 3.37631100 0.82853000 1.54523200
H 4.45998100 0.97076800 1.57466700
H 2.91931700 1.82067900 1.57412500
H 3.09114600 0.29809300 2.45622300
C 3.37636100 0.82879200 -1.54504500
H 4.46006100 0.97078600 -1.57456100
H 3.09097600 0.29865000 -2.45613800
H 2.91960300 1.82105900 -1.57364200
C 3.68481300 -1.84388500 -0.00012500
H 3.39611000 -2.41702900 0.88390600
H 3.39598200 -2.41696200 -0.88415700
H 4.77480200 -1.76449700 -0.00020000

3d.TS-3.

E = -939.679652 a.u.

C -2.11569200 -0.85652600 -0.00021500
C -3.50899700 0.93315900 0.00018800
C -2.23060400 1.42208700 0.00007700
B 0.90319300 -0.38867100 -0.00004500
N -3.40061000 -0.45048200 0.00002400
H -4.46382500 1.43050700 0.00035800
C -4.54627600 -1.36404800 -0.00008400
H -5.14471300 -1.19590800 -0.89398600
H -4.16469700 -2.38169500 0.00095500
H -5.14589500 -1.19455300 0.89276500
C -0.06099700 2.01028300 -0.00009200
C -1.30402400 2.53287000 0.00008000
H 0.90162400 2.49600900 -0.00013900
H -1.55179600 3.58083500 0.00019500
N -0.09820600 0.59637900 -0.00018700
N 0.25015800 -1.78924000 0.00012500
N -0.79133800 -2.27954100 0.00012900
N -1.44186800 0.29261100 -0.00013600
Si 2.92093200 -0.13636000 0.00000500
C 3.37631100 0.82853000 1.54523200
H 4.45998100 0.97076800 1.57466700
H 2.91931700 1.82067900 1.57412500
H 3.09114600 0.29809300 2.45622300
C 3.37636100 0.82879200 -1.54504500
H 4.46006100 0.97078600 -1.57456100
H 3.09097600 0.29865000 -2.45613800
H 2.91960300 1.82105900 -1.57364200
C 3.68481300 -1.84388500 -0.00012500
H 3.39611000 -2.41702900 0.88390600
H 3.39598200 -2.41696200 -0.88415700
H 4.77480200 -1.76449700 -0.00020000

3d.P.

E = -939.710932 a.u.

C -1.87693700 -0.78199300 -0.00008300
C -3.49151400 0.75600000 -0.00011300
C -2.27429200 1.44301000 0.00010500
B 0.84655300 -0.30988600 0.00001100
N -3.21993800 -0.58610800 -0.00025400

H	-4.50548500	1.12003800	-0.00019700
C	-4.20540100	-1.67798100	-0.00018200
H	-3.65544200	-2.61669500	-0.00262400
H	-4.81723300	-1.60562500	0.89670800
H	-4.82036700	-1.60279500	-0.89468100
C	-0.15477500	2.21327800	0.00018500
C	-1.45519400	2.63126800	0.00012500
H	0.76005500	2.78443600	0.00024000
H	-1.79199300	3.65396000	0.00012300
N	-0.08199500	0.81369400	0.00015200
N	0.17620700	-1.65548100	-0.00027300
N	-1.07935700	-1.88581200	-0.00034900
N	-1.36481400	0.44013900	0.00015100
Si	2.86750500	-0.19378600	0.00008400
C	3.46112300	-1.07499400	1.54572700
H	4.55335800	-1.11876600	1.55101900
H	3.14536600	-0.56548800	2.45863100
H	3.08575100	-2.10025300	1.57790000
C	3.40884200	1.60939100	0.00026300
H	4.50063400	1.66389700	0.00028200
H	3.06673200	2.14447200	-0.89019200
H	3.06670600	2.14430600	0.89080800
C	3.46123300	-1.07473200	-1.54566300
H	3.08579600	-2.09996100	-1.57806700
H	3.14559400	-0.56503300	-2.45850000
H	4.55346500	-1.11857200	-1.55085800

3e.

E = -652.555346 a.u.

C	1.22182400	0.74416700	-0.79817000
C	2.94790700	0.68280800	0.66893000
C	2.69974900	-0.64110000	0.29034200
B	-0.10573600	-0.24761000	-0.70021400
N	2.00785900	1.47604300	0.03758800
H	3.68556200	1.11110500	1.32652900
C	1.92641200	2.92875500	0.20054000
H	2.58600000	3.41721600	-0.51536500
H	0.89842100	3.23438800	0.01973600
H	2.21561000	3.18521800	1.21743400
C	1.30610400	-2.41848300	0.08618000
C	2.45833800	-2.02415000	0.69845700
H	0.80574100	-3.37147100	0.16104200
H	3.04490100	-2.61673200	1.38024100
N	0.81840200	-1.44695900	-0.81863800
N	1.79616200	-0.46938000	-0.69688600
C	-1.53534200	-0.07894800	-0.29374700
C	-2.10294700	1.20733900	-0.22162200
C	-2.33550400	-1.20089500	-0.00024300
C	-3.43051700	1.36822300	0.13606200
H	-1.49983800	2.07487400	-0.46677900
C	-3.66169400	-1.03758200	0.35868200
H	-1.91427900	-2.19853800	-0.06275900
C	-4.20423900	0.24574200	0.42700900
H	-3.86899800	2.35663300	0.18516600
H	-4.27810200	-1.89905600	0.58130200

H	-5.24385300	0.37122100	0.70555100
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3e.TS-1.

E = -652.535943 a.u.

C	1.30153700	0.93162900	-0.26191000
C	3.49165300	0.42343800	0.23960300
C	2.85281300	-0.77599700	0.05812800
B	-0.51280000	-0.59341100	-0.18888600
N	2.53063000	1.42701400	0.04677600
H	4.51689800	0.66434300	0.46042100
C	2.84909100	2.85191400	0.12139200
H	3.43630800	3.14918800	-0.74674000
H	1.91329000	3.40392900	0.13594200
H	3.40713900	3.05097500	1.03500300
C	1.39374400	-2.53299300	-0.02457300
C	2.69849100	-2.22608900	0.16320400
H	0.89583600	-3.48778900	-0.01915400
H	3.47187900	-2.94717900	0.37124100
N	0.64179800	-1.34686100	-0.27497000
N	1.59826000	-0.36139300	-0.28792100
C	-1.92341400	-0.17457100	-0.06980000
C	-2.27250500	1.18806700	-0.14327300
C	-2.92406600	-1.15598200	0.10811600
C	-3.60240800	1.55788900	-0.03924200
H	-1.49332400	1.92727200	-0.28147600
C	-4.24742700	-0.76859800	0.20844000
H	-2.66575300	-2.20708000	0.16608300
C	-4.58280500	0.58364700	0.13517000
H	-3.87906100	2.60277100	-0.09484000
H	-5.02021400	-1.51414400	0.34422700
H	-5.62204300	0.87933000	0.21499800

3e.IN1.

E = -652.547689 a.u.

C	1.69679400	1.15766700	-0.00030000
C	3.74356100	0.05888600	0.00007200
C	2.79205300	-0.91119500	0.00018000
B	-0.74944500	-0.57271600	0.00006800
N	3.05502000	1.27078000	-0.00024800
H	4.81851600	0.00334400	0.00014800
C	3.73539000	2.56386200	-0.00036400
H	4.35463400	2.65755100	-0.89212300
H	2.97059300	3.33517900	-0.00132000
H	4.35331200	2.65845000	0.89221900
C	1.06596400	-2.36891500	0.00013800
C	2.40748700	-2.30610400	0.00037500
H	0.39372700	-3.21056500	0.00013400
H	3.06513400	-3.16025700	0.00056300
N	0.51299200	-1.03856900	0.00013900
N	1.60785100	-0.19010800	0.00002300
C	-2.14920800	-0.15902400	0.00005600
C	-2.82428600	0.05222900	1.22738500
C	-2.82455900	0.05103900	-1.22733300
C	-4.14404400	0.45792400	1.21752700
H	-2.30695400	-0.09890700	2.16721100
C	-4.14428500	0.45683900	-1.21757300

H	-2.30741200	-0.10096500	-2.16712100
C	-4.79721400	0.65739200	-0.00004600
H	-4.66906500	0.62310300	2.14927200
H	-4.66949200	0.62119000	-2.14935900
H	-5.83272500	0.97712900	-0.00008500

3e.IN1.N2.

E = -762.073457 a.u.

C	1.71188400	0.67704100	-0.85716600
C	3.71871200	-0.33880200	-0.27493600
C	2.73494800	-1.10263400	0.26833500
B	-0.79151400	-0.63383300	0.17031500
N	3.07253500	0.70753400	-0.93064800
H	4.79017800	-0.44050600	-0.26140000
C	3.79622100	1.75424000	-1.64835200
H	3.05831500	2.42445000	-2.07990200
H	4.43586000	2.30440300	-0.95856200
H	4.39974100	1.31184600	-2.44051900
C	0.96279100	-2.25574600	1.06021200
C	2.30512600	-2.26315700	1.01773200
H	0.26289100	-2.93566300	1.51659500
H	2.93378300	-3.01407000	1.46800500
N	0.45584300	-1.10815800	0.35565000
N	0.03759200	1.75780800	1.58606000
N	0.56287700	2.67759100	1.84257000
N	1.57577000	-0.44126500	-0.10895500
C	-2.19384000	-0.30385700	-0.07528400
C	-2.94269800	0.49843100	0.81831000
C	-2.80388900	-0.81992700	-1.24573200
C	-4.26876200	0.76676900	0.54413000
H	-2.47541000	0.89970400	1.70838600
C	-4.13063200	-0.53657800	-1.50680700
H	-2.23119500	-1.42866200	-1.93551600
C	-4.85620200	0.25201900	-0.61367400
H	-4.85088100	1.37766800	1.22170900
H	-4.60347200	-0.92302100	-2.40020800
H	-5.89651800	0.47165200	-0.82351200

3e.TS-2.

E = -762.071250 a.u.

C	-2.06773600	0.79052100	0.62442800
C	-3.81592100	-0.63583400	0.07333300
C	-2.68136200	-1.23575200	-0.37087600
B	0.74777300	-0.19845600	-0.23425100
N	-3.41104000	0.56591000	0.64788600
H	-4.84508800	-0.94995800	0.04807000
C	-4.35177200	1.50873200	1.24765600
H	-3.77243400	2.32428000	1.67087800
H	-5.03033600	1.89358900	0.48662600
H	-4.92061800	1.01429400	2.03472500
C	-0.69435500	-2.12817700	-0.94478800
C	-2.01376600	-2.37574700	-0.95662600
H	0.14196200	-2.71105100	-1.29454900
H	-2.47382900	-3.27330400	-1.33631600
N	-0.44073700	-0.83247200	-0.37464400
N	0.17192000	1.95100700	-0.84359400

N	0.00878100	2.99780100	-1.09792000
N	-1.68266200	-0.33053600	-0.03358200
C	2.19235100	-0.08075400	0.03113700
C	3.06378300	0.76524800	-0.68832100
C	2.70882200	-0.92533500	1.04176100
C	4.41496500	0.75729900	-0.40559600
H	2.67710600	1.41861800	-1.46080000
C	4.06550900	-0.92104700	1.31630900
H	2.04364600	-1.56980500	1.60541600
C	4.91147200	-0.08246000	0.59455900
H	5.08823300	1.40282100	-0.95450900
H	4.46427300	-1.56163200	2.09213200
H	5.97245700	-0.07770700	0.81469600

3e.IN2.

E = -762.089521 a.u.

C	2.39442900	-0.89894400	0.19825700
C	3.77700500	0.93931700	-0.06886900
C	2.50359500	1.39156400	-0.21576300
B	-0.66915300	-0.34068400	-0.06148700
N	3.66955700	-0.42798100	0.17157900
H	4.72429500	1.44900200	-0.10470900
C	4.83297800	-1.28489100	0.38471300
H	4.47052500	-2.29237300	0.56731500
H	5.46805100	-1.27660700	-0.50082300
H	5.39786500	-0.93540500	1.24857100
C	0.33488100	1.95153400	-0.40877800
C	1.57501100	2.47256000	-0.44873600
H	-0.62519600	2.41288600	-0.56965400
H	1.81512600	3.50571000	-0.63785800
N	0.38548400	0.55020500	-0.15933700
N	-0.20975600	-1.85717800	-0.02045100
N	-0.11986300	-2.94390500	0.00044700
N	1.73021000	0.25228600	-0.05266300
C	-2.17662100	-0.15133000	0.01553000
C	-2.69880400	0.96850000	0.68932700
C	-3.06718400	-1.07119400	-0.56513600
C	-4.06868300	1.16538500	0.76455600
H	-2.03292400	1.66684800	1.18448900
C	-4.43540800	-0.86307000	-0.49865800
H	-2.69681800	-1.94606500	-1.09017900
C	-4.93494300	0.25430000	0.16564500
H	-4.46347500	2.02210100	1.29577500
H	-5.11352800	-1.56992300	-0.95936600
H	-6.00512700	0.41087100	0.22431800

3e.TS-3.

E = -762.083985 a.u.

C	-2.36455300	-0.88110900	0.15160000
C	-3.72305900	0.95146200	-0.03713500
C	-2.44197900	1.39828400	-0.16213800
B	0.73624400	-0.35610200	-0.05717700
N	-3.63411200	-0.42117300	0.14819700
H	-4.66541700	1.47083700	-0.06206400
C	-4.80028800	-1.28735900	0.32061400
H	-5.35448800	-0.98306400	1.20756100

H	-5.43868100	-1.22229500	-0.55949500
H	-4.44370000	-2.30631500	0.44214000
C	-0.28077900	1.96750200	-0.35169500
C	-1.52107100	2.48874200	-0.36940400
H	0.67473100	2.43909200	-0.50936800
H	-1.76957500	3.52421300	-0.53010600
N	-0.31570700	0.56713700	-0.13671300
N	0.15748500	-1.79761100	-0.05658600
N	-0.76105900	-2.42906600	0.02372200
N	-1.66650900	0.25640100	-0.04142300
C	2.23893500	-0.18374100	0.02133100
C	3.07196800	-1.22401300	-0.43004500
C	2.83273800	0.97812200	0.54889200
C	4.45105700	-1.09155200	-0.39042500
H	2.63966500	-2.13866800	-0.82254000
C	4.21106000	1.10080200	0.60221900
H	2.21753600	1.77094700	0.95933200
C	5.01885200	0.07071600	0.12344600
H	5.08350800	-1.89297100	-0.75026500
H	4.66047200	1.99119200	1.02312100
H	6.09675400	0.17058900	0.16363500

3e.P.

E = -762.116757 a.u.

C	2.04997400	-0.78702600	-0.07450500
C	3.67794600	0.73336300	0.00220800
C	2.46616000	1.42715600	0.06342200
B	-0.65888700	-0.31788100	0.02322800
N	3.39231200	-0.60278200	-0.07823400
H	4.69460500	1.08871300	0.01319200
C	4.36638200	-1.70069400	-0.16632200
H	3.81640700	-2.63615000	-0.08861200
H	4.88100400	-1.64767100	-1.12383700
H	5.07247500	-1.61279900	0.65658100
C	0.36332000	2.21315300	0.22503600
C	1.66876300	2.61667500	0.21261500
H	-0.53222900	2.80026200	0.34045600
H	2.01942200	3.62991600	0.30890300
N	0.26567200	0.82556600	0.08216500
N	0.00375900	-1.65910500	0.01357900
N	1.25058200	-1.89402700	-0.03667000
N	1.54309400	0.43652200	-0.00546800
C	-2.17645100	-0.21086300	-0.01830300
C	-2.93363200	-1.35977500	0.27321900
C	-2.85541500	0.97765200	-0.34227700
C	-4.32014300	-1.31128000	0.26916800
H	-2.42135800	-2.28658400	0.50237300
C	-4.23917000	1.02221300	-0.35898100
H	-2.30407000	1.86808600	-0.62512300
C	-4.97091900	-0.12235500	-0.04427800
H	-4.89446800	-2.19887500	0.50261400
H	-4.75248800	1.93849900	-0.62194700
H	-6.05369400	-0.08653500	-0.05436400