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Coordenadas Cartesianas das Estruturas Otimizadas

^{2}N

Energia *single-point*:

CCSD/6−311++G(d,p) : E = –54.381473 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = –54.412431851 u. a.

^{4}N

Energia *single-point*:

CCSD/6−311++G(d,p) : E = –54.4922323 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = –54.512702846 u. a.

^{2}P

Energia *single-point*:

CCSD/6−311++G(d,p) : E = –340.7110074 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = –340.74999726 u. a.

^{4}P

Energia *single-point*:

CCSD/6−311++G(d,p) : E = –340.7847141 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = –340.81281045 u. a.

^{1}S

Energia *single-point*:

CCSD/6−311++G(d,p) : E = –397.5421169 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = –397.59580065 u. a.

^{3}S

Energia *single-point*:

CCSD/6−311++G(d,p) : E = – 397.5996196 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = –397.64537260 u. a.

^{1}NH

CCSD/6–311++G(d,p)

1	7	0	0.000000	0.000000	-0.908973
2	1	0	0.000000	0.000000	0.129853

Energia *single-point*:

CCSD/6−311++G(d,p) : E = – 55.0319529 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = – 55.070987329 u. a.

^{3}NH

CCSD/6–311++G(d,p)

1	7	0	0.000000	0.000000	0.130277
2	1	0	0.000000	0.000000	-0.911941

Energia *single-point*:

CCSD/6−311++G(d,p) : E = –55.1105292 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = –55.141277691 u. a.

$^{2}NH_{2}$

CCSD/6–311++G(d,p)

1	7	0	0.000000	0.000000	0.143118
2	1	0	0.000000	0.802610	-0.500914
3	1	0	0.000000	-0.802610	-0.500914

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –55,736460 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –55,795972236 u. a.

NH_{3}

CCSD/6–311++G(d,p)

1	7	0	0.000000	-0.000072	0.112598
2	1	0	-0.817120	-0.470004	-0.262795
3	1	0	0.815898	-0.472120	-0.262795
4	1	0	0.001222	0.942626	-0.262595

Energia *single-point*:

CCSD/6–311++G(d,p) : E = -56,394582 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = -56,476665789 u. a.

^{1}PH

CCSD/6–311++G(d,p)

1	15	0	0.000000	0.000000	0.088868
2	1	0	0.000000	0.000000	-1.333017

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –341,331357 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –341,38198379 u. a.

^{3}PH

CCSD/6–311++G(d,p)

1	15	0	0.000000	0.000000	0.089029
2	1	0	0.000000	0.000000	-1.335438

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –341,384588 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –341,42645706 u. a.

$^{2}PH_{2}$

CCSD/6–311++G(d,p)

1	15	0	0.000000	0.000000	0.116015
2	1	0	0.000000	1.019302	-0.870111
3	1	0	0.000000	-1.019302	-0.870111

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –341,995085 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –342,05238277 u. a.

PH_{3}

CCSD/6–311++G(d,p)

1	15	0	0.105196	-0.015063	-0.066930
2	1	0	-1.157159	0.165691	-0.677726
3	1	0	-0.063525	1.055809	0.840841
4	1	0	-0.357256	-0.995559	0.840841

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –342,615841 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –342,68976067 u. a.

^{1}PN

CCSD/6–311++G(d,p)

1	15	0	0.000000	0.000000	0.475176
2	7	0	0.000000	0.000000	-1.018235

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –395,458222 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –395,54477575 u. a.

^{3}PN

CCSD/6–311++G(d,p)

1	15	0	0.000000	0.000000	0.495423
2	7	0	0.000000	0.000000	-1.061621

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –395,306462 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –395,39318076 u. a.

^{2}HPN

CCSD/6–311++G(d,p)

1	15	0	0.061919	-0.470592	0.000000
2	1	0	-1.362222	-0.676409	0.000000
3	7	0	0.061919	1.105040	0.000000

Energia s*ingle-point*:

CCSD/6–311++G(d,p) : E = –395,1987640 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,08072068 u. a.

^{2}PNH

CCSD/6–311++G(d,p)

1	7	0	0.036858	0.990284	0.000000
2	1	0	-0.810881	1.555130	0.000000
3	15	0	0.036858	-0.565808	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,020853 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,12178529 u. a.

cis-^{1}HPNH

CCSD/6–311++G(d,p)

1	7	0	0.096169	1.050143	0.000000
2	15	0	0.096169	-0.531822	0.000000
3	1	0	-0.812839	1.510472	0.000000
4	1	0	-1.302882	-0.884146	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,621412 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,73716259 u. a.

trans-^{1}HPNH

CCSD/6–311++G(d,p)

1	7	0	0.018477	1.055085	0.000000
2	15	0	0.018477	-0.535562	0.000000
3	1	0	0.984375	1.390991	0.000000
4	1	0	-1.390868	-0.743151	0.000000

/

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,623321 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,73905498 u. a.

^1H_2PN

CCSD/6–311++G(d,p)

1	15	0	0.000006	0.370572	0.000000
2	1	0	-0.000069	1.235537	1.113362
3	1	0	-0.000069	1.235537	-1.113362
4	7	0	0.000006	-1.147094	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,557887 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,67450761 u. a.

^3H_2PN

CCSD/6–311++G(d,p)

1	15	0	0.077614	-0.491752	0.000000
2	1	0	-0.853754	-0.670808	1.053332
3	1	0	-0.853754	-0.670808	-1.053332
4	7	0	0.077614	1.245414	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,549131 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,64923750 u. a.

$^1PNH_2$

CCSD/6–311++G(d,p)

1	7	0	-0.000027	-0.979918	0.000000
2	1	0	0.000302	-1.540850	0.844609
3	1	0	0.000302	-1.540850	-0.844609
4	15	0	-0.000027	0.662742	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,603110 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,71916748 u. a.

$^{3}PNH_{2}$

CCSD/6–311++G(d,p)

1	7	0	-1.030321	-0.000087	-0.079587
2	1	0	-1.520752	0.833614	0.216297
3	1	0	-1.522791	-0.832373	0.216671
4	15	0	0.683719	-0.000042	0.008276

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,610856 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,72001940 u. a.

$^{2}PNH_{3}$

CCSD/6–311++G(d,p)

1	7	0	1.145479	0.001085	-0.006265
2	1	0	1.539237	-0.801213	-0.492036
3	1	0	1.460150	-0.058835	0.960804
4	1	0	1.550614	0.847695	-0.398305
5	15	0	-0.837890	0.000317	-0.001774

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,153588 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,28242874 u. a.

$^{2}H_{3}PN$

CCSD/6–311++G(d,p)

1	15	0	-0.373371	-0.004300	0.000005
2	1	0	-1.104295	-0.559769	1.075980
3	1	0	-1.104142	-0.561783	-1.075024
4	1	0	-0.820377	1.327061	-0.001225
5	7	0	1.232769	-0.020144	0.000028

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,122321 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,25008416 u. a.

$^2HPNH_2$

CCSD/6–311++G(d,p)

1	15	0	-0.646714	-0.098144	0.010909
2	1	0	-0.851824	1.302479	-0.053315
3	7	0	1.059847	0.018952	-0.066463
4	1	0	1.542140	0.853795	0.229986
5	1	0	1.591458	-0.816773	0.124933

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,221101 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,34578669 u. a.

^2H_2PNH

CCSD/6–311++G(d,p)

1	7	0	1.141042	-0.144641	0.058961
2	1	0	1.598541	0.765495	-0.035132
3	15	0	-0.511501	0.018070	-0.116629
4	1	0	-0.978720	-1.082684	0.623014
5	1	0	-0.934601	1.058623	0.748832

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,185247 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,30981499 u. a.

H_2PNH_2

CCSD/6–311++G(d,p)

1	7	0	1.111103	0.040242	-0.080087
2	1	0	1.545938	0.839846	0.357849
3	1	0	1.614100	-0.803708	0.150227
4	15	0	-0.603955	-0.122019	-0.023731
5	1	0	-0.941269	0.502301	1.207685
6	1	0	-0.937169	1.010154	-0.799181

Energia *single-point*:

CCSD/6–311++G(d,p) :E = –397,833060 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,97316181 u. a.

$^{1}HPNH_3$

CCSD/6–311++G(d,p)

1	15	0	-0.795911	-0.089110	0.000003
2	1	0	-0.819300	1.329941	0.000002
3	7	0	1.163728	0.004942	0.000008
4	1	0	1.517163	-0.949515	-0.000262
5	1	0	1.547268	0.461008	-0.824219
6	1	0	1.547430	0.460619	0.824377

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,776550 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,91962553 u. a.

^{2}SH

CCSD/6–311++G(d,p)

1	16	0	0.000000	0.000000	0.078978
2	1	0	0.000000	0.000000	-1.263646

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –398,220262 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –398,28137787 u. a.

H_2S

CCSD/6–311++G(d,p)

1	16	0	0.000000	0.000000	0.103104
2	1	0	0.000000	0.963282	-0.824828
3	1	0	0.000000	-0.963282	-0.824828

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –398,853981 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –398,93151868 u. a.

^{2}NS

CCSD/6–311++G(d,p)

1	7	0	0.000000	0.000000	-1.047806
2	16	0	0.000000	0.000000	0.458415

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –452,223615 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –452,32685207 u. a.

^{1}HNS

CCSD/6–311++G(d,p)

1	7	0	0.040475	1.037911	0.000000
2	1	0	-0.930925	1.376679	0.000000
3	16	0	0.040475	-0.540129	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –452,816047 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –452,93372130 u. a.

^{3}HNS

CCSD/6–311++G(d,p)

1	7	0	0.034372	1.016891	0.000000
2	1	0	-0.790550	1.608570	0.000000
3	16	0	0.034372	-0.545426	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –452,810454 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –452,92561514 u. a.

^{1}NSH

CCSD/6–311++G(d,p)

1	16	0	0.055525	-0.415417	0.000000
2	1	0	-1.277076	-0.895505	0.000000
3	7	0	0.055525	1.077453	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –452,779256 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –452,89875682 u. a.

^{3}NSH

CCSD/6–311++G(d,p)

1	16	0	0.055771	-0.481473	0.000000
2	1	0	-1.282733	-0.623833	0.000000
3	7	0	0.055771	1.189629	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 452,779882 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 452,88561872 u. a.

^{2}NSH$_2$

CCSD/6–311++G(d,p)

1	16	0	-0.386932	-0.000149	-0.106230
2	1	0	-1.024196	0.987863	0.602222
3	1	0	-1.027977	-0.984481	0.604476
4	7	0	1.177583	-0.000143	0.070425

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –453,321434 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –453,45679184 u. a.

^2H_2NS

CCSD/6–311++G(d,p)

1	7	0	0.000347	1.010595	0.000000
2	1	0	-0.003991	1.537073	0.859168
3	1	0	-0.003991	1.537073	-0.859168
4	16	0	0.000347	-0.634269	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –453,436222 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –453,56439444 u. a.

cis-^{2}HNSH

CCSD/6–311++G(d,p)

1	7	0	0.091057	1.123368	0.000000
2	1	0	-0.873593	1.462606	0.000000
3	16	0	0.091057	-0.529784	0.000000
4	1	0	-1.220710	-0.849631	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –453,406721 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –453,53586851 u. a.

trans-^{2}HNSH

CCSD/6–311++G(d,p)

1	7	0	0.013481	1.125802	0.000000
2	1	0	1.008214	1.376834	0.000000
3	16	0	0.013481	-0.535626	0.000000
4	1	0	-1.318279	-0.687430	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –453,410680 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –453,53918908 u. a.

$^1NSH_3$

CCSD/6–311++G(d,p)

1	16	0	0.307070	0.000004	0.000000
2	1	0	1.074815	1.160275	-0.087516
3	1	0	1.074790	-0.655958	-0.961064
4	1	0	1.074792	-0.504371	1.048583
5	7	0	-1.162502	-0.000001	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –453,856270 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –454,02303543 u. a.

^1H_3NS

CCSD/6–311++G(d,p)

1	7	0	1.099371	0.000000	0.000006
2	1	0	1.468675	0.829906	-0.459269
3	1	0	1.468675	-0.812656	-0.489143
4	1	0	1.468940	-0.017247	0.948266
5	16	0	-0.756368	0.000000	0.000007

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –454,012602 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –454,16121395 u. a.

$^1HNSH_2$

CCSD/6–311++G(d,p)

1	16	0	-0.456051	-0.123023	-0.000294
2	1	0	-1.038907	0.651117	-0.957686
3	1	0	-1.039456	0.646456	0.960531
4	7	0	1.120558	0.200500	0.000521
5	1	0	1.531270	-0.732706	-0.001795

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –453,962417 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –454,11783288 u. a.

cis-$^{1}H_2NSH$

CCSD/6–311++G(d,p)

1	7	0	1.100339	-0.089590	0.000000
2	1	0	1.499914	0.331126	0.828313
3	1	0	1.499916	0.331138	-0.828308
4	16	0	-0.614157	-0.079827	0.000000
5	1	0	-0.875700	1.242102	0.000006

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –454,041388 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –454,18535445 u. a.

t*rans*-$^{1}H_2NSH$

CCSD/6–311++G(d,p)

1	7	0	-1.101081	0.133163	0.000000
2	1	0	-1.517996	-0.283577	-0.822709
3	1	0	-1.517997	-0.283574	0.822709
4	16	0	0.612914	-0.097872	0.000000
5	1	0	0.936936	1.200964	-0.000002

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –454,042366 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –454,18571643 u. a.

Coordenadas Cartesianas dos Estados de Transição

Sistema PN:

TS1 = $^1HPNH_3 \rightarrow H_2PNH_2$

CCSD/6–311++G(d,p)

1	15	0	0.751719	-0.090265	-0.041942
2	7	0	-1.201997	0.014231	0.027848
3	1	0	0.814240	1.319196	0.069890
4	1	0	-1.618983	0.831744	-0.398204
5	1	0	-1.636495	-0.849492	-0.268376
6	1	0	-0.420563	-0.047087	1.030876

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –398,421961 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,87654194 u. a.

TS2 = $H_2PNH_2 \rightarrow H_2PN + H_2$

CCSD/6–311++G(d,p)

1	15	0	0.586403	-0.060853	-0.000052
2	7	0	-1.019507	-0.338711	0.000038
3	1	0	1.033149	0.731747	-1.078472
4	1	0	-1.863152	0.911583	0.401305
5	1	0	-1.862923	0.909705	-0.401297
6	1	0	1.033432	0.730732	1.078985

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –398,357810 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,80529089 u. a.

TS3 = H_2PNH_2 → cis-HPNH + H_2

CCSD/6–311++G(d,p)

1	15	0	0.617587	0.048133	-0.018838
2	7	0	-0.989062	-0.159315	0.012815
3	1	0	-0.422325	1.884749	0.105986
4	1	0	-1.256903	0.941812	-0.008876
5	1	0	-1.473179	-1.053209	-0.095869
6	1	0	0.812034	-1.380139	0.191629

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –398,374829 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,82694375 u. a.

TS4 = $H_2PNH_2 \rightarrow {}^1PNH_2 + H_2$

CCSD/6–311++G(d,p)

1	15	0	0.551452	-0.267093	0.000000
2	7	0	-1.072565	0.086254	0.000000
3	1	0	1.223772	1.470328	-0.398756
4	1	0	-1.605683	0.230980	0.845047
5	1	0	-1.605683	0.230980	-0.845047
6	1	0	1.223772	1.470327	0.398756

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –398,434253 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,88824474 u. a.

TS5 = cis-^{1}HPNH → trans-^{1}HPNH

CCSD/6–311++G(d,p)

1	15	0	-0.527102	-0.108851	0.000007
2	7	0	0.992775	0.043541	-0.000042
3	1	0	1.990119	0.068999	0.000179
4	1	0	-1.033008	1.258983	0.000009

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,267071 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,71465526 u. a.

TS6 = *trans*-^{1}HPNH → ^1H_2PN

CCSD/6–311++G(d,p)

1	15	0	-0.466298	0.036014	-0.107357
2	7	0	1.139654	-0.104977	0.008395
3	1	0	0.122129	1.062819	0.730836
4	1	0	-1.105233	-0.868195	0.820762

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,167265 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,61143212 u. a.

TS7 = *trans*-^{1}HPNH → $^1PNH_2$

CCSD/6–311++G(d,p)

1	15	0	0.637849	-0.012693	0.019100
2	1	0	-1.585501	0.446484	0.563524
3	7	0	-1.069308	-0.175264	-0.071950
4	1	0	-0.497073	0.970752	-0.346370

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,173473 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,62316319 u. a.

TS8 = ^1H_2PN→ ^1PN+ H_2

CCSD/6–311++G(d,p)

1	15	0	0.083792	-0.368840	0.000000
2	1	0	-0.370348	-1.718350	0.000000
3	1	0	-1.473067	-0.966318	0.000000
4	7	0	0.083792	1.173896	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,111982 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,55759098 u. a.

TS9 = $^{1}PNH_2 \rightarrow {}^{1}PN + H_2$

CCSD/6–311++G(d,p)

1	15	0	0.656806	0.051902	0.000000
2	7	0	-0.835087	-0.225385	-0.000003
3	1	0	-1.844821	-0.319855	0.000012
4	1	0	-2.161653	1.119019	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,167679 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,61335543 u. a.

TS10 = $^{2}PNH_3 \rightarrow {}^{2}HPNH_2$

CCSD/6–311++G(d,p)

1	15	0	-0.779012	0.024296	-0.025724
2	1	0	1.594450	-0.587456	-0.662443
3	7	0	1.147296	0.009767	0.020656
4	1	0	1.639279	0.883690	0.172158
5	1	0	0.420388	-0.729039	0.731549

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,796737 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,24178558 u. a.

TS11 = $^{2}H_2PNH \rightarrow {}^{2}H_3PN$

CCSD/6–311++G(d,p)

1	15	0	0.418480	-0.004671	-0.041374
2	1	0	1.229575	-0.799926	0.796130
3	1	0	1.237464	1.151496	-0.146824
4	1	0	-0.424675	-0.977466	-0.748329
5	7	0	-1.188510	0.099422	0.102805

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,749814 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,20178008 u. a.

TS12 = $^2HPNH_2 \rightarrow {}^2H_2PNH$

CCSD/6–311++G(d,p)

1	15	0	0.601664	-0.113363	-0.033034
2	1	0	-0.363731	0.033567	1.121412
3	1	0	0.938922	1.260102	-0.011005
4	7	0	-1.148185	0.168083	-0.084277
5	1	0	-1.562859	-0.769808	-0.024955

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,810833 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,26023944 u. a.

TS13 = $^2H_2PNH \rightarrow {}^2HPN + H_2$

CCSD/6–311++G(d,p)

1	15	0	0.449587	-0.148085	-0.108540
2	7	0	-1.173990	-0.048830	0.054671
3	1	0	0.991563	-0.218992	1.209092
4	1	0	-0.241026	1.242522	0.045517
5	1	0	0.723589	1.539549	-0.009212

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,718576 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,16522453 u. a.

TS14 = $^2H_2PNH \rightarrow {}^2PNH + H_2$

CCSD/6–311++G(d,p)

1	15	0	0.482602	-0.208695	0.000000
2	1	0	1.053865	1.252375	0.471590
3	1	0	1.053864	1.252377	-0.471588
4	7	0	-1.102619	-0.029898	0.000000
5	1	0	-1.628431	0.834964	-0.000004

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –397,802672 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –397,24620129 u. a.

TS15 = ^{2}HPN→ ^{2}PNH

CCSD/6–311++G(d,p)

1	15	0	0.052782	-0.524358	0.000000
2	7	0	0.052782	1.076050	0.000000
3	1	0	-1.161206	0.333019	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,607357 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,04541776 u. a.

TS16 = ^{2}PNH → ^{1}PN + H

CCSD/6–311++G(d,p)

1	15	0	0.066492	-0.564368	0.000000
2	7	0	0.066492	0.938794	0.000000
3	1	0	-1.462820	1.893970	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = –396,603948 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –396,03677269 u. a.

Sistema NS

TS1 = *cis*-^{2}HNSH→ *trans*-^{2}HNSH

CCSD/6–311++G(d,p)

1	7	0	1.044807	0.041388	-0.114648
2	16	0	-0.508733	-0.095672	0.014652
3	1	0	1.806361	0.048493	0.543541
4	1	0	-0.980286	1.192549	0.024558

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,374405 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –453,50542765 u. a.

TS2 = *trans*-^{2}HNSH → ^2H_2NS

CCSD/6–311++G(d,p)

1	7	0	1.146279	0.039562	-0.119297
2	16	0	-0.614709	-0.038989	-0.004546
3	1	0	1.505892	-0.672185	0.529150
4	1	0	0.305494	1.019078	0.378663

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,345468 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 453,47207387 u. a.

TS3 = ^2H_2NS→ $^2NS + H_2$

CCSD/6–311++G(d,p)

1	7	0	0.940609	-0.322073	-0.000014
2	1	0	1.687678	0.762633	0.431444
3	1	0	1.687632	0.762816	-0.431385
4	16	0	-0.622473	0.045566	0.000003

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,304610 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 453,42861564 u. a.

TS4 = ^{2}NSH → ^{2}NS + H_2

CCSD/6–311++G(d,p)

1	16	0	0.357733	-0.182644	0.000000
2	1	0	1.182678	0.945667	-0.605942
3	1	0	1.182655	0.945649	0.605953
4	7	0	-1.155580	0.147284	0.000000

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,279771 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 453,40975887 u. a.

TS5 = ^1H_2NSH→ $^1HNSH_2$

CCSD/6–311++G(d,p)

1	16	0	-0.579870	-0.030681	-0.101745
2	7	0	1.240160	-0.080055	0.003193
3	1	0	1.529708	0.896497	-0.135111
4	1	0	-1.047647	0.842084	0.829968
5	1	0	0.114739	-0.687296	0.910718

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,912894 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = –454,06051028 u. a.

TS6 = ^1H_2NSH → *trans*-^1H_2NSH

CCSD/6–311++G(d,p)

1	7	0	1.138993	-0.003647	-0.131055
2	1	0	1.453478	0.871651	0.279025
3	1	0	1.500829	-0.716876	0.497425
4	16	0	-0.631170	-0.085187	0.003025
5	1	0	-0.828547	1.233752	0.092528

Energia *single-point*:

CCSD/6–311++G(d,p) :E = – 454,031089 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 454,17419703 u. a.

TS7 = $^1HNSH_2 \rightarrow {}^1NSH_3$

CCSD/6–311++G(d,p)

1	16	0	-0.373399	0.017073	-0.066437
2	1	0	-1.292029	0.306525	0.925944
3	1	0	-1.010223	-1.274745	-0.135768
4	1	0	-0.007003	1.354389	-0.285140
5	7	0	1.183377	-0.094192	0.079708

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,787878 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 453,95091677 u. a.

TS8 = $^1NSH_3 \rightarrow {}^1NSH + H_2$

CCSD/6–311++G(d,p)

1	16	0	0.273141	0.000029	-0.124453
2	7	0	-1.185996	-0.000038	0.134708
3	1	0	1.186516	1.027067	-0.037940
4	1	0	1.186612	-1.026976	-0.038349
5	1	0	1.558593	-0.000288	1.124576

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,798440 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 453,96123121 u. a.

TS9 = $^1HNSH_2 \rightarrow {}^1HNS + H_2$

CCSD/6–311++G(d,p)

1	7	0	-0.974601	-0.350167	0.103369
2	1	0	-1.818518	0.975558	0.244562
3	1	0	-1.813070	0.679761	-0.517921
4	16	0	0.590583	0.027452	-0.100142
5	1	0	1.004470	0.356618	1.152046

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,895666 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 454,03443078 u. a.

TS10 = *trans*-$^1H_2NSH \rightarrow {}^1NSH + H_2$

CCSD/6–311++G(d,p)

1	16	0	0.422335	-0.192409	0.019215
2	7	0	-1.114855	0.115708	-0.146070
3	1	0	-1.513110	0.250973	0.784681
4	1	0	1.286311	1.057916	0.482184
5	1	0	1.273424	0.959697	-0.551819

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,910995 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 454,06072462 u. a.

TS11 = $^1H_3NS \rightarrow$ *trans*-^1H_2NSH

CCSD/6–311++G(d,p)

1	16	0	0.725209	0.000021	-0.036800
2	1	0	-1.554023	0.847457	-0.351726
3	7	0	-1.165114	-0.000015	0.039523
4	1	0	-1.553982	-0.847122	-0.352555
5	1	0	-0.339539	-0.000559	1.016417

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,969708 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 454,11318960 u. a.

TS12 = *trans*-$^1HNSH_2 \rightarrow$ *cis*-$^1HNSH_2$

CCSD/6–311++G(d,p)

1	16	0	0.469240	-0.004699	-0.117461
2	1	0	0.975490	-0.839065	0.836939
3	1	0	1.005979	1.031131	0.607981
4	7	0	-1.136834	-0.131231	0.043152
5	1	0	-1.531476	0.801733	0.132396

Energia *single-point*:

CCSD/6–311++G(d,p) : E = – 453,947729 u. a.

CCSD(T)/6–311++G(3df,3pd) : E = – 454,10190516 u. a.

TS13 = ^{1}NSH→ ^{1}HNS

CCSD/6–311++G(d,p)

1	16	0	0.049019	-0.511946	0.000000
2	7	0	0.049019	1.136254	0.000000
3	1	0	-1.127428	0.237364	0.000000

Energia *single-point*:

CCSD/6−311++G(d,p) : E = – 452,707007 u. a.

CCSD(T)/6−311++G(3df,3pd) : E = – 452,82758732 u. a.