The $P(^4S)$ + $NH(^3\Sigma^-)$ and $N(^4S)$ + $PH(^3\Sigma^-)$ reactions as sources of interstellar phosphorus nitride

Supplementary Information

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Part I

Structures and frequencies ($1^2A'$) obtained at the M06-2X/AVTZ+d level

(Coordinates in Angstroms and frequencies in cm^{-1})

1) HNP

P	-4.2676572413	2.2151160767	-0.0091065209
N	-2.8426455607	1.6455824756	-0.0432598066
H	-1.9911471981	2.1918784477	0.0539416353

Frequencies:

1	699.66
2	1228.39
3	3522.30

2) HPN

P	-1.9607814421	2.2190762485	0.0350110579
H	-0.8582036377	3.1439712769	0.0505195529
N	-3.1206709202	3.2490774747	0.0045431543

Frequencies:

1	746.08
2	1121.07
3	2233.01

3) TS_HNP →HPN

H	0.0000000000	1.2070809159	0.3120020739
P	0.0000000000	-0.0308742902	-0.5062140212
N	0.0000000000	-0.0204906257	1.0667539473

Frequencies:

1	1899.71i
2	1126.23
3	2212.33

4) TS_HNP →H+PN

H	0.0000000000	1.3208749848	-2.1677707808
N	0.0000000000	-0.1736495223	-0.9578886517
P	0.0000000000	0.0334955375	0.5065684325

Frequencies:

1	823.75i
2	297.52
3	1412.41

Part II

Structures and frequencies ($1^2A'$) obtained at the CAS/AVTZ+d level

(Coordinates in Angstroms and frequencies in cm^{-1})

1) HNP

P	-4.2657491264	2.2344168292	-0.0064908471
N	-2.8278972401	1.6032030375	-0.0484530131
H	-2.0078036337	2.2149571333	0.0565191680

Frequencies:

1	775.95
2	1099.19
3	3360.33

2) HPN

P	-1.9577007255	2.2327257058	0.0349762020
H	-0.8153435465	3.1336489922	0.0514493971
N	-3.1666117281	3.2457503021	0.0036481660

Frequencies:

1	731.07
2	1041.25
3	1960.64

3) TS_HNP →HPN

H	0.0000000000	1.2091174680	0.3052003464
P	0.0000000000	-0.0266474724	-0.5240336495
N	0.0000000000	-0.0267539957	1.0913753031

Frequencies:

1	1787.43i
2	998.29
3	2173.17

4) TS_HNP →H+PN

H	0.0000000000	1.1835586268	-2.0247965229
N	0.0000000000	-0.1469645574	-1.0106312510
P	0.0000000000	0.0422906906	0.5009598439

Frequencies:

1	1578.19i
2	449.83
3	1218.40

Part III

Structures and frequencies ($1^2A'$) obtained at the CCSD(T)/AVTZ+d level

(Coordinates in Angstroms and frequencies in cm^{-1})

1) HNP

P	-4.2732152263	2.2244167099	-0.0080347213
N	-2.8320790863	1.6274642774	-0.0453563586
H	-1.9961556874	2.2006950127	0.0549660799

Frequencies:

1	728.75
2	1130.06
3	3488.39

2) HPN

P	-1.9544833567	2.2178292140	0.0351457208
H	-0.8447514320	3.1411758243	0.0508087126
N	-3.1404212113	3.2531189617	0.0041195667

Frequencies:

1	722.54
2	1053.87
3	2180.16

3) TS_HNP →HPN

H	0.0000000000	1.2056497903	0.3109007220
P	0.0000000000	-0.0294243349	-0.5210567214
N	0.0000000000	-0.0205094554	1.0826979994

Frequencies:

1	1858.01i
2	1024.00
3	2170.93

Part IV

Search for intersystem crossing regions between $1^2A'$ and $1^4A'$ potential energies surfaces

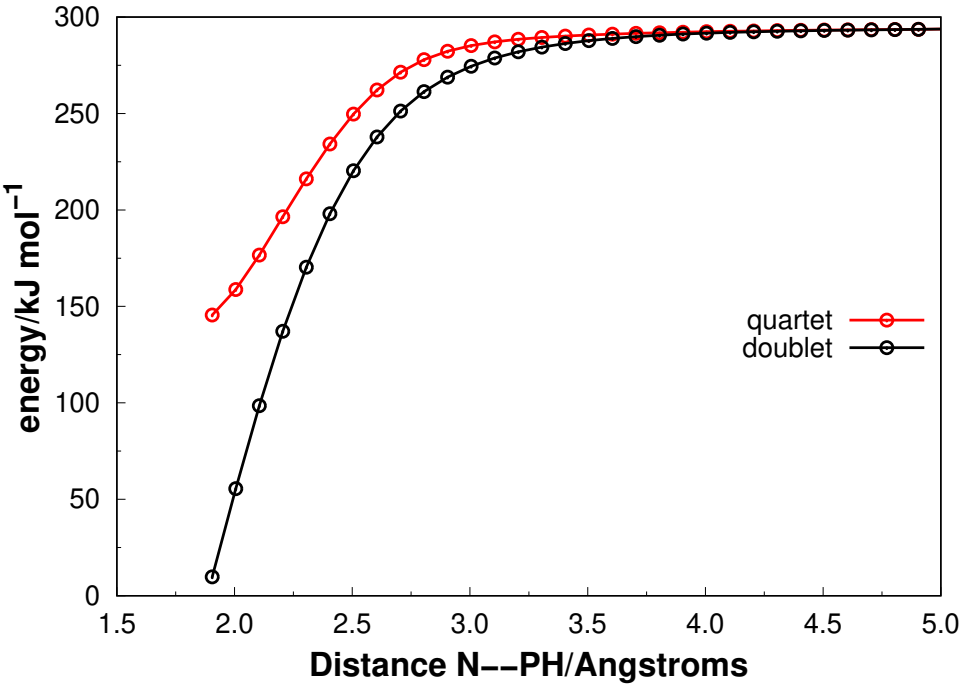

Figure S1: Search for intersystem crossing regions between doublet and quartet potential energies surfaces (N+PH). Energies are given relative to the H(^{2}S)+PN($^1\Sigma^+$) channel.

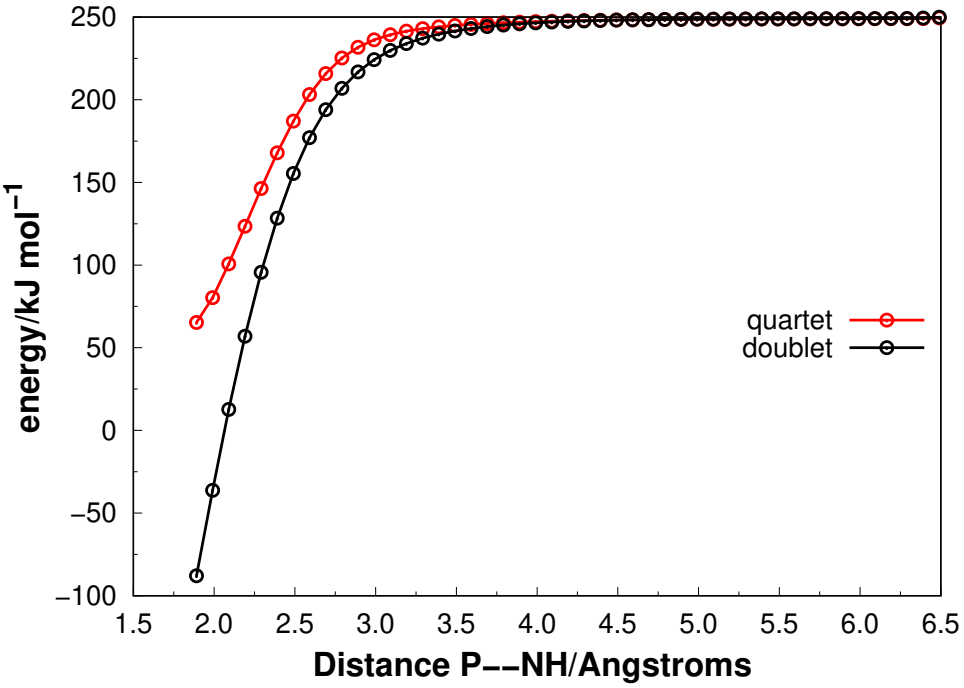

Figure S2: Search for intersystem crossing regions between doublet and quartet potential energies surfaces (P+NH). Energies are given relative to the H(^{2}S)+PN($^1\Sigma^+$) channel.

Part V

Minimum energy path from HPN towards the H+PN channel

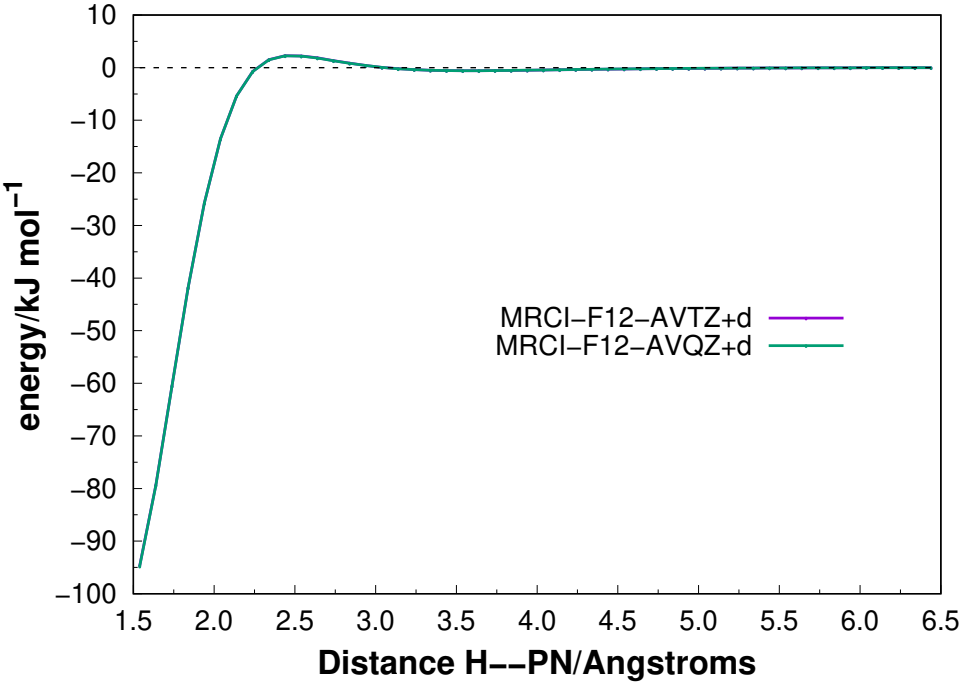

Figure S3: Minimum energy path from HPN towards the H+PN channel.