

CHEMPHYSCHEM

Supporting Information

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Electronic Structure of N₂P₂ Four-Membered Rings

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cphc_201301233_sm_miscellaneous_information.pdf

Supporting Information

1 (S_0)

6

scf done: -793.477848

N	-0.712150	0.836054	-0.000065
N	0.834020	2.382262	-0.000065
P	-0.876152	2.546223	0.000005
P	0.998024	0.672093	0.000333
H	1.546905	3.095168	-0.000115
H	-1.425037	0.123151	-0.000115

1 (T_1)

6

scf done: -793.432004

H	-1.405794	3.074923	-0.138843
H	1.526822	0.142729	-0.138240
N	-0.744162	2.415243	0.250773
N	0.867156	0.804214	0.251379
P	-0.853459	0.694617	-0.109305
P	0.975038	2.523275	-0.116664

2 (S_0)

12

scf done: -872.110889

N	-0.720753	0.827374	-0.074115
N	0.842706	2.390876	0.074576
P	-0.869333	2.539391	-0.000273
P	0.991266	0.678790	0.000354
C	-1.746095	-0.197896	-0.002267
H	-1.404326	-1.103242	-0.509071
H	-1.996473	-0.448744	1.032460
H	-2.651647	0.144259	-0.508440
C	1.867964	3.416221	0.002535
H	2.119556	3.665646	-1.032242
H	1.525350	4.322227	0.507586
H	2.772967	3.075030	0.510347

2 (T_1)

12

scf done: -872.064248

C	-1.813844	3.323247	0.045958
H	-1.653692	4.246936	-0.516236
H	-2.818058	2.964724	-0.194725
H	-1.777016	3.558694	1.118325
C	1.944891	-0.095310	0.025011
H	2.182307	-0.042374	1.096269
H	1.681473	-1.127568	-0.219863
H	2.845859	0.154658	-0.541279
N	0.862129	0.788621	-0.371216
N	-0.833892	2.331113	-0.361803
P	0.908643	2.542852	-0.277458
P	-0.797400	0.664206	0.193519

3 (S₀)

6
scf done: -793.382887

N	-0.859356	0.767762	0.246203
N	0.905566	2.532154	0.225533
P	-0.623801	2.304615	0.880894
P	0.670446	0.994860	-0.409658
H	1.620944	0.049727	0.072698
H	-1.574998	3.250481	0.401430

3 (T₁)

6
scf done: -793.327956

N	-0.835243	0.713179	0.486654
N	0.956984	2.505125	0.487006
P	-0.729990	2.399570	0.411020
H	-1.164879	2.834981	-0.898666
P	0.851728	0.818759	0.411322
H	1.287044	0.383341	-0.898223

4 (S₀)

12
scf done: -872.066242

N	-0.852821	0.757161	0.325911
N	0.916886	2.526656	0.305248
P	-0.697293	2.379284	0.976129
P	0.655419	1.012266	-0.213585
C	-1.790891	3.461282	-0.037273
H	-1.625337	3.282716	-1.101648
H	-2.833279	3.250909	0.212330
H	-1.576766	4.506432	0.197141
C	1.943869	-0.276537	-0.173121
H	2.188609	-0.508592	0.865086
H	1.569974	-1.171586	-0.671921
H	2.832977	0.089954	-0.687762

4 (T₁)

12
scf done: -872.011554

N	-0.919516	0.537231	-0.913139
N	0.747252	2.371957	-1.374942
P	-0.918418	2.213108	-1.135054
P	0.747405	0.697329	-1.144066
C	-1.508059	3.125717	0.363810
H	-1.380654	4.196989	0.199161
H	-2.562843	2.897120	0.525548
H	-0.923697	2.812127	1.231803
C	1.721190	0.188628	0.345928
H	1.358897	0.735215	1.219533
H	1.595424	-0.884114	0.502103
H	2.774366	0.418639	0.175850

5 (S0)

6
scf done: -793.407492
N 0.566639 2.436437 -0.132270
P -1.036366 3.043861 0.047441
N 0.671405 1.266932 -0.702289
P -1.044076 1.118288 -1.151111
H 1.436199 2.903190 0.131971
H -1.405601 0.179693 -0.141642

5 (T1)

6
scf done: -793.380538
N 0.614804 2.358951 0.005519
P -0.429225 3.724772 -0.001350
N 0.355522 1.049341 0.001872
P -1.210886 0.542061 -0.009647
H 1.614641 2.537501 0.012858
H -0.862083 -0.840519 -0.009225

6 (S0)

scf done: -872.065474
N 0.596496 2.456726 -0.123795
P -1.022508 3.062263 0.052946
C -1.599650 -0.225862 0.064111
H -1.226985 -1.179591 -0.317518
H -1.245648 -0.080228 1.084259
H -2.691269 -0.264938 0.062036
C 1.844723 3.163814 0.175661
H 2.334504 3.441645 -0.758855
H 1.617823 4.055386 0.758409
H 2.495859 2.497052 0.741680
N 0.668688 1.262254 -0.649704
P -1.040853 1.121409 -1.087780

6 (T1)

12
scf done: -872.025462
N 0.764758 2.518090 0.446813
P -0.964157 2.892436 0.534036
C -1.639371 -0.278550 -0.082873
H -1.171170 -1.264238 -0.159571
H -2.659844 -0.426331 0.281283
H -1.666064 0.178236 -1.072716
C 1.796855 3.303487 -0.208637
H 1.703021 3.269451 -1.300522
H 1.720625 4.337943 0.130516
H 2.772666 2.906942 0.076566
N 0.758282 1.152063 0.196084
P -0.684418 0.720404 1.160469