

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1996 American Chemical Society

Supplementary Material:
Geometries of molecules in Table 1
(cartesian coordinates in Å, xyz format;
E_{tot}(RMP2(fc)/6-31G* in a.u.)

*FILE: 1.xyz

```
6
//RMP2-FC/6-31G* H1P5 C2v -1704.724879
H 1.00000 0.00000 0.00000
P 1.00000 1.40543 0.00000
P -0.82416 2.39749 0.00000
P 2.82416 2.39749 0.00000
P -0.05937 4.37272 0.00000
P 2.05937 4.37272 -0.00000
```

*FILE: 2a.xyz

```
10
//RMP2-FC 6-31G* C4H5P1 Cs -495.6678819
P 0.00000 0.00000 0.00000
C 0.00000 1.26609 -1.28321
C -0.00000 1.26609 1.28321
C -0.23321 2.48836 -0.72594
C -0.23321 2.48836 0.72594
H 1.34922 -0.43384 -0.00000
H 0.01350 1.06248 -2.34815
H 0.01350 1.06248 2.34815
H -0.40140 3.39218 -1.30694
H -0.40140 3.39218 1.30694
```

*FILE: 2b.xyz

```
10
//RMP2-FC 6-31G* C4H5P1 C2v 495.6402047
P 0.00000 0.00000 0.00000
C 0.00000 1.11329 -1.30787
C -0.00000 1.11329 1.30787
C 0.00000 2.37536 -0.70668
C -0.00000 2.37536 0.70668
H 0.00000 -1.39220 -0.00000
H 0.00000 0.89379 -2.36647
H -0.00000 0.89379 2.36647
H -0.00000 3.28782 -1.29508
H -0.00000 3.28782 1.29508
```

*FILE: 3.xyz

```
6
//RMP2-FC/6-31G* H1N5 C2v -273.5378834
H 1.00000 0.00000 0.00000
N 1.00000 1.01723 0.00000
N -0.11512 1.74049 0.00000
N 2.11512 1.74049 0.00000
N 0.32583 2.99206 0.00000
N 1.67417 2.99206 -0.00000
```

*FILE: 4.xyz

```
10
//RMP2-FC/6-31G* C4H5N1 C2v -209.4808411
N 2.00000 -0.78618 0.00000
C 2.00000 1.31860 0.70929
C 2.00000 1.31860 -0.70929
C 2.00000 0.00000 -1.12569
C 2.00000 0.00000 1.12569
H 2.00000 2.18451 1.35801
H 2.00000 2.18451 -1.35801
H 2.00000 -0.43727 -2.11433
H 2.00000 -0.43727 2.11433
H 2.00000 -1.79707 0.00000
```

*FILE: 5.xyz

```
9
//RMP2-FC/6-31G* C1H3P5 C1 -1743.9052619
P 0.00000 0.00000 0.00000
C 1.83610 0.00000 0.00000
P -1.01614 1.81335 0.00000
P -1.02046 -1.81245 -0.01300
P -2.99308 1.06211 -0.01130
P -2.99531 -1.05897 -0.01851
H 2.18154 -1.03492 0.05209
```

```
H 2.21368 0.45908 -0.91499
H 2.20997 0.54590 0.86772
```

*FILE: 6.xyz

```
8
//RMP2-FC/6-31G* H2P6 Cs -2046.1421394
P 0.00000 0.00000 0.00000
P 2.08892 0.00000 0.00000
P -1.05794 1.79965 0.00000
P 2.41392 2.08580 0.00000
P 0.57186 3.13994 0.00000
P -1.21640 -1.81908 -0.00000
H -0.51846 -2.46942 -1.04460
H -0.51846 -2.46942 1.04460
```

*FILE: 7.xyz

```
8
//RMP2-FC/6-31G* H1P7 Cs -2386.377694
P 0.00000 0.00000 0.00000
P 2.09703 0.00000 0.00000
P -1.05768 1.80677 0.00000
P 2.40988 2.08693 0.00000
P 0.56896 3.14833 0.00000
P -1.25405 -1.77162 -0.00000
P 0.16762 -3.26064 -0.00000
H -0.84770 -4.25906 -0.00000
```

*FILE: 8.xyz

```
10
//RMP2-FC/6-31G* P10 D2d -3408.3264297
P 0.000000 0.000000 1.070130
P 0.000000 0.000000 -1.070130
P 0.000000 1.830928 2.084071
P 0.000000 -1.830928 2.084071
P 0.000000 1.063577 4.049122
P 0.000000 -1.063577 4.049122
P 1.830928 0.000000 -2.084071
P -1.830928 0.000000 -2.084071
P 1.063577 0.000000 -4.049122
P -1.063577 0.000000 -4.049122
```

*FILE: 9.xyz

```
10
//RMP2-FC 6-31G* H5P5 Cs -1707.0428776
P 3.31332 0.57922 0.00000
H 2.96546 1.95047 0.00000
P 0.00000 0.00000 -1.12656
P 0.00000 0.00000 1.12656
P 2.11153 0.00000 -1.74893
P 2.11153 0.00000 1.74893
H -0.18485 1.39330 -1.30088
H -0.18485 1.39330 1.30088
H 2.32980 -1.39030 -1.61595
H 2.32980 -1.39030 1.61595
```

*FILE: 10.xyz

```
8
//RMP2-FC 6-31G* H3P5 Cs -1705.870321
P 0.00000 0.00000 0.00000
H -0.11199 1.40846 0.00000
P 3.38649 0.14365 1.02098
P 3.38649 0.14365 -1.02098
P 1.29989 -0.09072 1.76400
P 1.29989 -0.09072 -1.76400
H 1.36316 -1.49797 1.92105
H 1.36316 -1.49797 -1.92105
```

*FILE: 11.xyz

```
10
//RMP2-FC 6-31G* H5N5 Cs -275.7898881
N 2.13769 0.45208 0.00000
H 2.05857 1.47186 0.00000
N 0.00000 0.00000 -0.75812
N 0.00000 0.00000 0.75812
N 1.38707 0.00000 -1.13774
N 1.38707 0.00000 1.13774
H -0.33112 0.93331 -1.02107
H -0.33112 0.93331 1.02107
H 1.63490 -0.98586 -1.23509
H 1.63490 -0.98586 1.23509
```

*FILE: 12.xyz

8

//RMP2-FC/6-31G* H3N5 Cs -274.640761

N	2.20834	0.18047	0.00000
H	2.39339	1.18448	0.00000
N	0.00000	0.00000	-0.62654
N	0.00000	0.00000	0.62654
N	1.35487	0.00000	-1.14073
N	1.35487	0.00000	1.14073
H	1.47624	-0.94095	-1.53320
H	1.47624	-0.94095	1.53320

*FILE: 13.xyz

5

//RMP2-FC/6-31G* P5(1-) D5h -1704.2427595

P	0.00000	1.79640	0.00000
P	0.00000	0.55512	-1.70848
P	0.00000	0.55512	1.70848
P	0.00000	-1.45332	-1.05590
P	0.00000	-1.45332	1.05590

*FILE: 14.xyz

9

//RMP2-FC/6-31G(d) H4P5(1-) -1706.4984632 PG=CS

NImag=0

P	0.723912	0.000000	1.730012
P	-0.142039	-1.124924	-1.485605
P	-0.142039	1.124924	-1.485605
P	-0.196922	-1.643458	0.680428
P	-0.196922	1.643458	0.680428
H	1.258295	-1.300622	-1.638296
H	1.258295	1.300622	-1.638296
H	-1.603218	-1.399070	0.740860
H	-1.603218	1.399070	0.740860

*FILE: 15.xyz

7

//RMP2-FC/6-31G(d) H2P5(1-) -1705.3540388 PG=C01

P	-0.458804	-0.781399	1.560514
P	-0.020467	1.327500	1.222063
P	0.032085	1.598443	-0.976884
P	0.183611	-1.844017	-0.275036
P	0.295637	-0.337014	-1.716786
H	-1.855260	-0.664208	1.302058
H	1.374328	1.211540	1.489875

*FILE: 16.xyz

5

//RMP2-FC 6-31G(d) N5(1-) -273.0197825 PG=D05H

NImag=0

N	0.00000	1.14272	0.00000
N	0.00000	0.35312	-1.08679
N	0.00000	0.35312	1.08679
N	0.00000	-0.92448	-0.67167
N	0.00000	-0.92448	0.67167

*FILE: 18.xyz

7

//RMP2-FC/6-31G(d) H2N5(1-) -274.0707655 PG=C02

NImag=0

N	1.176888	0.000000	0.000000
N	0.497541	0.726917	-0.851338
N	0.497541	-0.726917	0.851338
N	-0.941719	0.589215	-0.401784
N	-0.941719	-0.589215	0.401784
H	-1.009861	1.344419	0.301170
H	-1.009861	-1.344419	-0.301170

*FILE: 19.xyz

9

//RMP2-FC/6-31G(D) C4H4P1(1-) -495.1174855

PG=C02V NIMAG=0

P	0.00000	0.00000	0.00000
C	0.00000	1.24980	-1.24687
C	-0.00000	1.24980	1.24687
C	0.00000	2.54142	-0.70558
C	0.00000	2.54142	0.70558
H	0.00000	1.04615	-2.31721
H	-0.00000	1.04615	2.31721
H	0.00000	3.45408	-1.30595

H	0.00000	3.45408	1.30595
---	---------	---------	---------

*FILE: 20a.xyz

6

//RMP2-FC/6-31G(D) P6 -2044.943012 PG=D02

NIMAG=0

P	0.00000	0.00000	0.00000
P	4.01745	0.00000	-0.00000
P	2.98619	0.41717	-1.79528
P	1.03126	0.41717	1.79528
P	2.98619	-0.41717	1.79528
P	1.03126	-0.41717	-1.79528

*FILE: 20b.xyz

6

//RMP2-FC/6-31G(D) P6 -2044.9383508 PG=D06H

NIMAG=2

P	-1.12422	1.00000	0.00000
P	3.12422	1.00000	0.00000
P	-0.06211	1.00000	1.83963
P	-0.06211	1.00000	-1.83963
P	2.06211	1.00000	1.83963
P	2.06211	1.00000	-1.83963

*FILE: 21a.xyz

6

//RMP2-FC/6-31G(D) N6 -327.4261678 PG=D02

N	0.00000	0.00000	0.00000
N	2.55950	0.00000	-0.00000
N	1.92016	0.22191	-1.14643
N	0.63934	0.22191	1.14643
N	1.92016	-0.22191	1.14643
N	0.63934	-0.22191	-1.14643

*FILE: 21b.xyz

6

//RMP2-FC/6-31G(D) N6 -327.4221701 PG=D06H

NIMAG=2

N	-0.33811	1.00000	0.00000
N	2.33811	1.00000	0.00000
N	0.33095	1.00000	1.15883
N	0.33095	1.00000	-1.15883
N	1.66905	1.00000	1.15883
N	1.66905	1.00000	-1.15883

*FILE: 22a.xyz

6

//RMP2-FC/6-31G(d) H3P3 -1024.1868109 PG=C01

NImag=0

P	0.00000	0.00000	0.00000
P	2.04929	0.00000	0.00000
P	2.49559	2.16135	0.00000
H	-0.09200	-1.41215	-0.13980
H	1.44210	2.66856	0.79929
H	3.45718	2.12782	1.03656

*FILE: 22b.xyz

6

//RMP2-FC/6-31G(D) H3P3 -1024.1536657 PG=CS

NIMAG=1

P	0.00000	0.00000	0.00000
P	2.06437	0.00000	0.00000
P	2.61379	2.01188	0.00000
H	0.01486	-1.42069	-0.00000
H	1.78219	3.13317	0.00000
H	3.96860	2.31908	0.00000

*FILE: 23a.xyz

8

//RMP2-FC/6-31G(d) C2H5P1 -419.681162 PG=CS

NIMAG=0

C	0.00000	0.00000	0.00000
C	1.34101	0.00000	0.00000
H	-0.57066	0.92463	0.00000
H	-0.56787	-0.92621	-0.00000
H	1.87577	0.94783	0.00000
P	2.27250	-1.57686	0.00000
H	3.18631	-1.26470	-1.03801
H	3.18631	-1.26470	1.03801

*FILE: 23b.xyz

8

//RMP2-FC/6-31G(d) C2H5P1 -419.6279955 PG=CS

NImag=1

C	0.00000	0.00000	0.00000
C	1.34473	0.00000	0.00000
H	1.93059	0.00000	0.91350
H	1.88993	0.00000	-0.93658
H	-0.54192	0.00000	-0.94416
P	-1.08399	0.00000	1.39701
H	-2.45342	0.00000	1.20234
H	-0.60553	-0.00000	2.69702

*FILE: 24a.xyz

8

//RMP2-FC/6-31G(d) H3P5 -1705.8315353 PG=CS

NImag=0

P	0.00000	0.00000	0.00000
H	-1.38426	0.27773	0.00000
P	0.00000	-1.22329	-1.82027
P	1.82315	-2.17674	-1.72462
H	1.56723	-2.86511	-2.94452
P	0.00000	-1.22329	1.82027
P	1.82315	-2.17674	1.72462
H	1.56723	-2.86511	2.94452

*FILE: 24b.xyz

8

//RMP2-FC/6-31G(d) H3P5 -1705.8166765 PG=C02V

NImag=1

H	0.00000	0.00000	0.00000
P	1.39669	0.00000	0.00000
P	2.14804	0.00000	1.96769
P	4.21236	-0.00000	1.73833
H	4.34060	0.00000	3.15730
P	2.14804	0.00000	-1.96769
P	4.21236	0.00000	-1.73833
H	4.34060	0.00000	-3.15730

*FILE: 24c.xyz

8

//RMP2-FC/6-31G(D) H3P5 -1705.8284343 PG=CS

NImag=0

P	0.00000	0.00000	0.00000
H	1.33569	0.48887	0.00000
P	0.00000	-1.42887	-1.67233
P	1.71184	-0.87909	-2.66321
H	1.47998	-1.77337	-3.74593
P	0.00000	-1.42887	1.67233
P	1.71184	-0.87909	2.66321
H	1.47998	-1.77337	3.74593

*FILE: 24d.xyz

8

//RMP2-FC/6-31G(D) H3P5 -1705.8099257 PG=C02V

H	0.00000	0.00000	0.00000
P	1.40912	0.00000	0.00000
P	2.48978	0.00000	1.80949
P	0.99801	0.00000	3.23749
H	1.97704	0.00000	4.26853
P	2.48978	0.00000	-1.80949
P	0.99801	0.00000	-3.23749
H	1.97704	0.00000	-4.26853

*FILE: 25a.xyz

12

//RMP2-FC/6-31G(d) C4H7P1 -496.8142115 PG=CS

NImag=0

P	1.00000	0.00000	0.00000
C	2.18252	0.00000	1.39673
C	2.07978	-0.89793	2.38839
H	2.99230	0.72910	1.41636
H	2.78157	-0.91897	3.21796
H	1.28683	-1.64061	2.39971
C	2.18252	0.00000	-1.39673
C	2.07978	-0.89793	-2.38839
H	2.99230	0.72910	-1.41636
H	2.78157	-0.91897	-3.21796
H	1.28683	-1.64061	-2.39971
H	0.72563	1.39409	0.00000

*FILE: 25b.xyz

12

//RMP2-FC/6-31G(D) C4H7P1 -496.7641793 PG=C02V

NImag=1

H	0.00000	0.00000	0.00000
P	1.39081	0.00000	0.00000
C	2.27269	0.00000	1.52780
C	1.76472	0.00000	2.77500
H	3.35272	-0.00000	1.38514
H	2.42485	0.00000	3.63459
H	0.69743	0.00000	2.97256
C	2.27269	0.00000	-1.52780
C	1.76472	0.00000	-2.77500
H	3.35272	0.00000	-1.38514
H	2.42485	0.00000	-3.63459
H	0.69743	0.00000	-2.97256

*FILE: 25c.xyz

12

//RMP2-FC/6-31G(d) C4H7P1 -496.8125445 PG=C01

NImag=0

P	0.00000	0.00000	0.00000
C	1.82109	0.00000	0.00000
C	2.60442	1.09048	0.00000
C	-0.37266	-0.53576	1.71254
C	0.52472	-0.87455	2.65025
H	2.28446	-0.98105	-0.09870
H	3.68444	1.01513	-0.09403
H	2.19291	2.09220	0.08711
H	-1.43347	-0.66104	1.92755
H	0.21069	-1.25978	3.61654
H	1.59303	-0.77282	2.48714
H	-0.18830	1.39818	0.15511

*FILE: 26a.xyz

10

//RMP2-FC/6-31G(D) H3P7 -2387.4769514 PG=C03

P	1.00000	0.00000	0.00000
P	0.12233	2.01150	0.00000
P	0.12233	-1.00575	1.74201
P	0.12233	-1.00575	-1.74201
P	0.56209	2.61514	1.91889
P	0.56209	-2.96938	1.30534
P	0.56209	0.35423	-3.22422
H	-0.07711	-3.42613	2.49268
H	-0.07711	3.87179	1.72078
H	-0.07711	-0.44566	-4.21346

*FILE: 26b.xyz

10

//RMP2-FC/6-31G(D) H3P7 -2387.4671974 PG=C03H

P	1.00000	0.00000	0.00000
P	1.00000	2.13546	0.00000
P	1.00000	-1.06773	1.84936
P	1.00000	-1.06773	-1.84936
P	1.00000	2.62225	2.00869
P	1.00000	-3.05070	1.26659
P	1.00000	0.42845	-3.27528
H	1.00000	-3.44558	2.63429
H	1.00000	4.00416	1.66682
H	1.00000	-0.55857	-4.30111

*FILE: 26c.xyz

10

//RMP2-FC/6-31G(D) H3P7 -2387.4789402 PG=CS

P	0.00000	0.00000	0.00000
P	2.21560	0.00000	0.00000
P	2.48301	2.03634	0.00000
H	3.90568	1.93265	0.00000
P	-0.58406	-1.33224	1.64120
P	-0.58406	-1.33224	-1.64120
P	0.89442	-0.95617	3.02425
P	0.89442	-0.95617	-3.02425
H	0.29747	-1.81873	3.98648
H	0.29747	-1.81873	-3.98648

*FILE: 27a.xyz

16

//RMP2-FC/6-31G(D) C6H9P1 -573.9487772 PG=C03

P	0.000000	0.000000	1.031426
---	----------	----------	----------

C 1.635122 -0.040256 0.216409
C -0.852424 -1.395929 0.216409
C -0.782698 1.436185 0.216409
C 2.043919 0.758396 -0.782960
C -0.365169 -2.149284 -0.782960
C -1.678750 1.390888 -0.782960
H -0.913864 -3.007486 -1.162811
H 3.061491 0.712313 -1.162811
H -2.147627 2.295173 -1.162811
H 2.341366 -0.746991 0.651870
H -1.817597 -1.654187 0.651870
H -0.523770 2.401178 0.651870
H 1.377644 1.479022 -1.246880
H 0.592048 -1.932586 -1.246880
H -1.969693 0.453564 -1.246880

*FILE: 27b.xyz

16

//RMP2-FC/6-31G(D) C6H9P1 -573.9053711 PG=C03

P 0.000000 0.000000 0.117790
C 1.762746 -0.020546 0.163067
C -0.899167 -1.516310 0.163067
C -0.863580 1.536856 0.163067
C 2.566347 0.988239 -0.234128
C -0.427333 -2.716641 -0.234128
C -2.139014 1.728402 -0.234128
H -1.002126 -3.620699 -0.063279
H 3.636680 0.942483 -0.063279
H -2.634554 2.678216 -0.063279
H 2.188028 -0.915092 0.616883
H -1.886507 -1.437342 0.616883
H -0.301521 2.352434 0.616883
H 2.179451 1.880525 -0.716185
H 0.538857 -2.827723 -0.716185
H -2.718308 0.947198 -0.716185

*FILE: 27c.xyz

16

//RMP2-FC/6-31G(D) C6H9P1 -573.9496019 PG=C01

P 0.00000 0.00000 0.00000
C 1.82319 0.00000 0.00000
C -0.33148 1.80323 0.00000
C -0.34135 -0.35140 1.75899
H 2.28153 0.45553 -0.87801
H -1.37812 2.06841 -0.14837
H 0.11605 0.29523 2.50864
C 2.60875 -0.60094 0.90819
C 0.57641 2.78523 0.11956
C -1.14054 -1.36177 2.13603
H 0.28627 3.83171 0.07062
H 3.68853 -0.63196 0.79067
H -1.35300 -1.56487 3.18262
H 2.20025 -1.09085 1.78707
H 1.63137 2.57866 0.27158
H -1.60841 -2.01588 1.40552

*FILE: 28a.xyz

10

//RMP2-FC 6-31G(D) B3H6P1 -418.5642302 PG=C03V

NIMAG=0

P 1.00000 0.00000 0.00000
B 1.26848 1.84197 0.00000
B 1.26848 -0.92099 1.59520
B 1.26848 -0.92099 -1.59520
H 1.34180 2.41983 1.03860
H 1.34180 2.41983 -1.03860
H 1.34180 -2.10937 1.57634
H 1.34180 -0.31046 2.61494
H 1.34180 -0.31046 -2.61494
H 1.34180 -2.10937 -1.57634

*FILE: 28b.xyz

10

//RMP2-FC/6-31G(D) B3H6P1 -418.5636463 PG=D03H

NIMAG=1

P 1.00000 0.00000 0.00000
B 1.00000 1.85915 0.00000
B 1.00000 -0.92958 1.61007

B 1.00000 -0.92958 -1.61007
H 1.00000 2.44171 1.03864
H 1.00000 2.44171 -1.03864
H 1.00000 -2.12034 1.59526
H 1.00000 -0.32137 2.63390
H 1.00000 -0.32137 -2.63390
H 1.00000 -2.12034 -1.59526

*FILE: 29.xyz

6

//RMP2-FC/6-31G(D) H1P5 -1704.6378959 PG=C01

NIMAG=0

H -2.967713 -0.078429 -2.766795
P -2.948432 -0.182433 -1.347916
P -0.903185 0.067979 -1.286181
P -0.663444 0.096556 0.892004
P 1.402293 -0.048380 0.836698
P 3.310615 0.071507 1.089847

*FILE: 30.xyz

6

//RMP2-FC/6-31G(D) H1N5 -273.4802817 PG=CS

NIMAG=0

H 0.00000 0.00000 0.00000
N 1.03260 0.00000 0.00000
N 1.32250 1.22846 0.00000
N 2.74242 1.34627 0.00000
N 3.04167 2.58123 0.00000
N 3.48705 3.64539 -0.00000

*FILE: 31.xyz

4

//RMP2-FC/6-31G(D) H1P3 -1022.9877942 PG=CS

NIMAG=0

P 0.00000 0.00000 0.00000
P 0.00000 1.92280 0.00000
P -0.42930 -2.01866 -0.00000
H 0.96364 -2.31588 -0.00000

*FILE: 32.xyz

4

//RMP2-FC/6-31G(d) H1N3 -164.341068 PG=CS

NIMAG=0

N -0.028771 0.029954 0.099297
N -0.351372 0.029954 1.212703
N 0.315199 -0.163971 -1.087855
H 0.454609 0.728443 -1.569009

*FILE: 33.xyz

6

//RMP2-FC/6-31G(D) B2H3P1 -392.0115946 PG=C02V

NIMAG=0

P 0.00000 0.00000 0.00000
B 1.59760 0.82666 0.00000
B 1.59760 -0.82666 0.00000
H -1.42219 0.00000 -0.00000
H 2.13945 1.88038 0.00000
H 2.13945 -1.88038 0.00000

*FILE: 34.xyz

4

//RMP2-FC/6-31G* H1O2P1 C2v -491.5020559

H 0.000000 0.000000 -1.644174
P 0.000000 0.000000 -0.239623
O 1.367159 0.000000 0.327407
O -1.367159 0.000000 0.327407

*FILE: 35.xyz

8

//RMP2-FC/6-31G* C2H5P1 C2v -419.6154984

P 0.000000 0.000000 -0.293581
C 1.531576 0.000000 0.333963
C -1.531576 0.000000 0.333963
H 1.716523 0.000000 1.399043
H -1.716523 0.000000 1.399043
H 2.363796 0.000000 -0.355704
H -2.363796 0.000000 -0.355704
H 0.000000 0.000000 -1.690523

*FILE: 36.xyz

12

//RMP2-FC/6-31G* C5H6P1(1+) C2v -534.0104202

P 0.000000 0.000000 1.308046
C 0.000000 1.409925 0.364897
C 0.000000 -1.409925 0.364897
C 0.000000 1.243762 -1.024679
C 0.000000 -1.243762 -1.024679
C 0.000000 0.000000 -1.672236
H 0.000000 2.392938 0.827789
H 0.000000 -2.392938 0.827789
H 0.000000 2.144312 -1.634323
H 0.000000 -2.144312 -1.634323
H 0.000000 0.000000 -2.758812
H 0.000000 0.000000 2.701983

*FILE: 37.xyz

11

//RMP2-FC/6-31G* C5H5P1 Cs -533.5769246

P -0.54078 -1.13559 0.00000
C 1.13568 -1.13100 0.00000
C 1.57471 0.22334 0.00000
C -1.42183 0.33127 0.00000
C -0.59673 1.46350 0.00000
C 0.80648 1.40479 0.00000
H -2.50590 0.41289 0.00000
H -1.07083 2.44344 0.00000
H 1.34066 2.35405 0.00000
H 2.65724 0.38002 0.00000
H -1.29939 -2.30792 0.00000

*FILE: 38.xyz

12

//RMP2-FC/6-31G* C3H8P1(1+) C2v -459.2037903

C 0.00000 0.00000 0.00000
P 1.64010 0.00000 0.00000
H -0.55243 0.93520 0.00000
H -0.55243 -0.93520 -0.00000
C 2.57746 1.53920 0.00000
C 2.57746 -1.53920 0.00000
H 1.88201 -2.38163 0.00000
H 1.88201 2.38163 0.00000
H 3.20874 -1.58750 -0.89113
H 3.20874 1.58750 -0.89113
H 3.20874 -1.58750 0.89113
H 3.20874 1.58750 0.89113

*FILE: 39.xyz

12

//RMP2-FC/6-31G* C5H6P1(1+) C2v -533.959632

P 0.00000 0.00000 0.00000
C 0.00000 1.14711 -1.33689
C -0.00000 1.14711 1.33689
C 0.00000 2.36817 -0.74068
C -0.00000 2.36817 0.74068
C 0.00000 -1.64785 -0.00000
H 0.00000 0.91584 -2.39455
H -0.00000 0.91584 2.39455
H -0.00000 3.29674 -1.30465
H -0.00000 3.29674 1.30465
H 0.00000 -2.19643 0.93844
H 0.00000 -2.19643 -0.93844

*FILE: 40.xyz

16

//RMP2-FC/6-31G* C5H10P1(1+) C2 -536.3649364

C 0.000000 0.000000 2.463156
P 0.000000 0.000000 0.821478
C 0.440428 1.333037 -0.332054
C -0.440428 -1.333037 -0.332054
C -0.111506 0.760807 -1.656638
C 0.111506 -0.760807 -1.656638
H 1.530360 1.441024 -0.358463
H 0.000000 2.288590 -0.035947
H -1.530360 -1.441024 -0.358463
H 0.000000 -2.288590 -0.035947
H -1.181705 0.980559 -1.733116
H 1.181705 -0.980559 -1.733116
H 0.386081 1.237454 -2.504466
H -0.386081 -1.237454 -2.504466
H 0.299782 0.887474 3.013594

H -0.299782 -0.887474 3.013594

*FILE: 41.xyz

14

//RMP2-FC/6-31G* C5H8P1(1+) Cs -535.1669427

P -0.619999 0.000000 -0.483429
C -0.619838 0.000000 1.269000
C 1.170859 0.000000 -0.785421
C 0.669595 0.000000 1.674225
C 1.769405 0.000000 0.644825
H -1.498426 0.000000 1.903399
H 1.455315 -0.885205 -1.360555
H 1.455315 0.885205 -1.360555
H 2.407141 -0.877810 0.793929
H 2.407141 0.877810 0.793929
H 0.930720 0.000000 2.730557
C -1.870247 0.000000 -1.544569
H -2.894622 0.000000 -1.183929
H -1.681245 0.000000 -2.613699

*FILE: 42.xyz

8

//RMP2-FC/6-31G* P8 D2h -2726.6403841

P -3.080660 0.000000 0.000000
P 0.000000 0.000000 -1.051833
P 0.000000 0.000000 1.051833
P -1.964715 0.000000 -1.805900
P 1.964715 0.000000 -1.805900
P -1.964715 0.000000 1.805900
P 1.964715 0.000000 1.805900
P 3.080660 0.000000 0.000000

*FILE: 43.xyz

6

//RMP2-FC/6-31G* H1P5 Cs -1704.7107741

P 0.00000 0.00000 0.00000
H -0.32681 -1.38661 -0.00000
P 1.70779 0.00000 -1.45885
P 1.70779 0.00000 1.45885
P 3.10911 -0.94396 -0.00000
P 2.84731 1.24672 -0.00000

*FILE: 44.xyz

6

//RMP2-FC/6-31G* H1P5 Cs -1704.6826792

P 1.99752 0.00000 0.00000
P 0.00000 1.01715 0.00000
P 0.00000 -1.01715 -0.00000
P 2.44629 0.00000 2.17188
P 4.49529 -0.00000 2.01277
H 4.69727 0.00000 3.42185

*FILE: 45.xyz

6

//RMP2-FC/6-31G* H1P5 Cs -1704.6970866

P 0.000000 -0.920069 -1.550897
P 1.116751 -0.844761 0.363051
P -1.116751 -0.844761 0.363051
H 0.000000 -2.343032 -1.658306
P 1.042144 1.382896 0.467675
P -1.042144 1.382896 0.467675