Electronic Supplementary Information for Dalton Transactions

Supporting Information

Is Delocalization a Prerequisite for Stability of Ring Systems: A Case Study of Some Inorganic Rings

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Cartesian coordinates of the optimized geometries of the $M_3Z_3R_3$ and $M_3E_3R_3$ rings along with the total energies including zero point vibrational energies of the respective molecules.

1. $B_3N_3H_6$; T. E. = -242.59091

5	1.258607	0.726657	0.000000
7	0.000000	1.411602	0.000000
5	-1.258607	0.726657	0.000000
7	-1.222483	-0.705801	0.000000
5	0.000000	-1.453314	0.000000
7	1.222483	-0.705801	0.000000
1	2.295504	1.325310	0.000000
1	0.000000	2.423744	0.000000
1	-2.295504	1.325310	0.000000
1	-2.099024	-1.211872	0.000000
1	0.000000	-2.650620	0.000000
1	2.099024	-1.211872	0.000000

2. $B_3N_3H_3F_3$, T. E. = -540.55757

5	1.246073	0.719421	0.000000
7	0.000000	1.420870	0.000000
5	-1.246073	0.719421	0.000000
7	-1.230510	-0.710435	0.000000
5	0.000000	-1.438841	0.000000
7	1.230510	-0.710435	0.000000
9	2.415415	1.394541	0.000000
1	0.000000	2.434570	0.000000
9	-2.415415	1.394541	0.000000
1	-2.108399	-1.217285	0.000000
9	0.000000	-2.789081	0.000000

3. $B_3N_3H_3Cl_3$, T. E. = -1621.55959

5	-1.245664	-0.719243	0.000000
7	-1.227381	0.708502	0.000000
5	0.000000	1.438134	0.000000
7	1.227381	0.708502	0.000000
5	1.245664	-0.719243	0.000000
7	0.000000	-1.417312	0.000000
17	-2.792040	-1.611671	0.000000
1	-2.104772	1.215283	0.000000
17	0.000001	3.223573	0.000000
1	2.104772	1.215283	0.000000

17 2.792040 -1.611672 0.000000
1 0.000000 -2.430558 0.000000

4. $B_3N_3H_3(CN)_3$, T. E. = -519.38250

5 -1.248267 -0.720811 0.000000
7 -1.226504 0.708035 0.000000
5 0.000012 1.441342 0.000000
7 1.226515 0.708016 0.000000
5 1.248256 -0.720831 0.000000
7 -0.000012 -1.416439 0.000000
1 -2.104700 1.215031 0.000000
1 2.104719 1.214997 0.000000
1 -0.000020 -2.430465 0.000000
6 -2.590570 -1.495565 0.000000
7 -3.597958 -2.076723 0.000000
6 0.000024 2.991170 0.000000
7 0.000034 4.154172 0.000000
7 2.590545 -1.495607 0.000000
7 3.597924 -2.076782 0.000000

5. $B_3N_3H_3(CF_3)_3$, T. E. = -1253.77522

5 1.411382 -0.266114 0.021283
7 0.471283 -1.337572 0.013195
5 -0.931747 -1.089912 -0.028930
7 -1.387572 0.259852 -0.065111
5 -0.472874 1.352051 -0.029773
7 0.923979 1.072996 0.012039
1 0.807948 -2.295157 0.030186
1 -2.383233 0.446579 -0.131023
1 1.585822 1.842515 0.028823
6 -1.985380 -2.309167 -0.002084
9 -1.507557 -3.430838 -0.612158
9 -2.297620 -2.666265 1.277372
9 -3.162385 -1.997153 -0.615634
6 -1.010629 2.871103 -0.001996
9 -2.223572 3.008391 -0.609725
9 -1.164924 3.318946 1.277652
9 -0.160316 3.741218 -0.617214
6 2.995743 -0.561573 0.002653
9 3.461971 -0.687483 -1.273646
9 3.721564 0.435575 0.583738
9 3.322109 -1.716078 0.650373

6. $B_3P_3H_6$ (Planar), T. E. = -1102.17791

5 1.629840 0.940989 0.000000
15 0.000000 1.799942 0.000000

5 -1.629840 0.940989 0.000000
15 -1.558795 -0.899971 0.000000
5 0.000000 -1.881978 0.000000
15 1.558795 -0.899971 0.000000
1 2.659497 1.535461 0.000000
1 0.000000 3.202369 0.000000
1 -2.659497 1.535461 0.000000
1 -2.773333 -1.601184 0.000000
1 0.000000 -3.070922 0.000000
1 2.773333 -1.601184 0.000000

7. $B_3P_3H_6$ (Puckered), T. E. = -1102.17832

5 0.030032 0.937841 1.596659
15 -0.395947 1.795379 0.000000
5 0.030032 0.937841 -1.596659
15 0.030032 -0.924098 -1.589226
5 0.459263 -1.793980 0.000000
15 0.030032 -0.924098 1.589226
1 0.136900 1.548598 2.613205
1 -0.041502 3.156989 0.000000
1 0.136900 1.548598 -2.613205
1 0.684991 -1.474020 -2.706422
1 0.839333 -2.922410 0.000000
1 0.684991 -1.474020 2.706422

8. $B_3P_3H_3F_3$ (Planar), T. E. = -1400.09289

5 1.635892 0.944482 0.000000
15 0.000000 1.846563 0.000000
5 -1.635892 0.944482 0.000000
15 -1.599170 -0.923281 0.000000
5 0.000000 -1.888965 0.000000
15 1.599170 -0.923281 0.000000
9 2.800717 1.616995 0.000000
1 0.000000 3.247765 0.000000
9 -2.800717 1.616995 0.000000
1 -2.812647 -1.623882 0.000000
9 0.000000 -3.233990 0.000000
1 2.812647 -1.623882 0.000000

9. $B_3P_3H_3F_3$ (Puckered), T. E. = -1400.11134

5 0.001425 1.727481 0.163028
15 -1.650524 0.988997 -0.470197
5 -1.572496 -0.882148 -0.053135
15 -0.001364 -1.807160 0.484475
5 1.570971 -0.884360 -0.053071
15 1.652299 0.986857 -0.470184

9 0.001762 2.898119 0.813994
1 -2.637227 1.481460 0.419359
9 -2.724353 -1.570059 -0.082706
1 -0.002210 -3.082741 -0.123022
9 2.721965 -1.573735 -0.082608
1 2.639396 1.477057 0.420031

10. $B_3P_3H_3Cl_3$ (Planar), T. E. = -2481.11610

5 1.633204 -0.943226 0.000000
15 1.578211 0.911048 0.000000
5 0.000000 1.886096 0.000000
15 -1.578211 0.911049 0.000000
5 -1.633204 -0.943226 0.000000
15 0.000000 -1.823198 0.000000
17 3.171648 -1.830386 0.000000
1 2.791387 1.610937 0.000000
17 0.000001 3.661969 0.000000
1 -2.791386 1.610938 0.000000
17 -3.171648 -1.830385 0.000000
1 -0.000001 -3.223946 0.000000

11. $B_3P_3H_3Cl_3$ (Puckered), T. E. = -2481.12595

5 -0.107367 -0.874769 1.589988
15 -0.507954 0.981607 1.626060
5 0.074903 1.772521 0.000000
15 -0.507954 0.981607 -1.626060
5 -0.107367 -0.874769 -1.589988
15 0.356992 -1.764064 0.000000
17 -0.107367 -1.781127 3.114409
1 0.286141 1.526045 2.660291
17 0.811259 3.381778 0.000000
1 0.286141 1.526045 -2.660291
17 -0.107367 -1.781127 -3.114409
1 -0.130299 -3.086178 0.000000

12. $B_3P_3H_3(CN)_3$ (Planar), T. E. = -1378.96105

5 1.622989 0.937178 0.000000
15 1.570574 -0.906679 0.000000
5 0.000000 -1.874090 0.000000
15 -1.570574 -0.906679 0.000000
5 -1.622989 0.937178 0.000000
15 0.000000 1.813779 0.000000
1 2.783548 -1.606862 0.000000
1 -2.783548 -1.606862 0.000000
1 0.000000 3.214337 0.000000
6 2.943477 1.699305 0.000000

7	3.952934	2.281476	0.000000
6	0.000000	-3.398730	0.000000
7	0.000000	-4.564031	0.000000
6	-2.943477	1.699305	0.000000
7	-3.952934	2.281476	0.000000

13. $B_3P_3H_3(CN)_3$ (Puckered), T. E. = -1378.96328

5	-0.483567	0.769105	1.570189
15	0.081218	-1.017424	1.615426
5	0.815188	-1.620973	0.000000
15	0.081218	-1.017424	-1.615426
5	-0.483567	0.769105	-1.570189
15	-1.255428	1.441535	0.000000
1	0.984079	-1.222953	2.674967
1	0.984079	-1.222953	-2.674967
1	-1.225577	2.848379	0.000000
6	-0.509751	1.596765	2.851823
7	-0.509751	2.237126	3.825938
6	1.848263	-2.743900	0.000000
7	2.653708	-3.586646	0.000000
6	-0.509751	1.596765	-2.851823
7	-0.509751	2.237126	-3.825938

14. $B_3P_3H_3(CF_3)_3$ (Planar), T. E. = -2113.34361

5	1.648036	-0.872298	0.023784
15	0.066001	-1.807642	0.018181
5	-1.579652	-0.991029	-0.025126
15	-1.598466	0.846189	-0.064395
5	-0.068205	1.863086	-0.031759
15	1.532575	0.961712	0.010817
1	0.116268	-3.206554	0.026061
1	-2.834855	1.500998	-0.105911
1	2.717677	1.706788	0.016296
6	-2.942104	-1.845158	0.002077
9	-2.820651	-3.059763	-0.604779
9	-3.346237	-2.092924	1.280694
9	-3.979346	-1.209369	-0.612560
6	-0.127011	3.469823	0.002303
9	-1.223352	3.976576	-0.629770
9	-0.174358	3.932761	1.283732
9	0.958475	4.056150	-0.578049
6	3.069174	-1.624823	-0.001141
9	3.498845	-1.831239	-1.278687
9	4.053997	-0.922406	0.626944
9	3.032407	-2.850115	0.594761

15. $B_3P_3H_3(CF_3)_3$ (Puckered), T. E. = -2113.34406

5	-0.048792	1.826045	-0.171283
15	-1.619341	0.874198	-0.444320
5	-1.561104	-0.953278	-0.109179
15	0.049898	-1.845073	-0.342540
5	1.610873	-0.868521	-0.108819
15	1.570760	0.959990	-0.441264
1	-2.752614	1.503656	0.094293
1	0.083563	-3.115618	0.251102
1	2.668360	1.649438	0.097605
6	-2.922845	-1.781057	0.131363
9	-3.822861	-1.102509	0.896163
9	-3.545316	-2.056722	-1.049846
9	-2.718991	-2.977468	0.750510
6	3.015290	-1.621885	0.130780
9	2.877253	-2.824008	0.756888
9	3.647170	-1.870833	-1.051296
9	3.881094	-0.892580	0.888522
6	-0.092414	3.407114	0.134066
9	-0.123289	3.622206	1.481446
9	0.991176	4.082099	-0.340559
9	-1.188916	4.028653	-0.382050

16. $B_3As_3H_6$ (Planar), T. E. = -6779.44022

5	1.693304	0.977630	0.000000
33	0.000000	1.870511	0.000000
5	-1.693304	0.977630	0.000000
33	-1.619910	-0.935256	0.000000
5	0.000000	-1.955259	0.000000
33	1.619910	-0.935256	0.000000
1	2.721196	1.571083	0.000000
1	0.000000	3.377545	0.000000
1	-2.721196	1.571083	0.000000
1	-2.925040	-1.688773	0.000000
1	0.000000	-3.142167	0.000000
1	2.925040	-1.688773	0.000000

17. $B_3As_3H_6$ (Puckered), T. E. = -6779.44535

5	0.145307	0.984581	1.583449
33	-0.613217	1.870553	0.000000
5	0.145307	0.984581	-1.583449
33	0.145307	-0.978107	-1.702488
5	0.848162	-1.666328	0.000000
33	0.145307	-0.978107	1.702488
1	0.433874	1.633357	2.540038
1	0.034565	3.252239	0.000000
1	0.433874	1.633357	-2.540038

1 1.244193 -1.292865 -2.713555
1 1.561349 -2.620613 0.000000
1 1.244193 -1.292865 2.713555

18. $B_3As_3H_3F_3$ (Planar), T. E. = -7077.36247

5 -0.978984 1.695551 0.000000
33 0.957682 1.658591 0.000000
5 1.958269 -0.000001 0.000000
33 0.957680 -1.658592 0.000000
5 -0.978986 -1.695550 0.000000
33 -1.915315 0.000001 0.000000
9 -1.652142 2.861157 0.000000
1 1.707540 2.960032 0.000000
9 3.304190 -0.000001 0.000000
1 1.707538 -2.960033 0.000000
9 -1.652143 -2.861156 0.000000
1 -3.417273 0.000001 0.000000

19. $B_3As_3H_3F_3$ (Puckered), T. E. = -7077.39264

5 1.600525 0.904181 -0.133879
33 0.001793 1.972372 0.407435
5 -1.598621 0.906994 -0.134361
33 -1.709238 -1.092198 -0.368897
5 -0.001347 -1.631343 0.548816
33 1.706938 -1.094994 -0.369646
9 2.749150 1.574273 -0.297094
1 0.002823 3.115059 -0.604388
9 -2.745790 1.579350 -0.298554
1 -2.713555 -1.346425 0.759801
9 -0.001947 -2.512103 1.552386
1 2.711998 -1.352415 0.757659

20. $B_3As_3H_3Cl_3$ (Planar), T. E. = -8158.39588

5 -0.984776 -1.705192 0.000000
33 0.945033 -1.636752 0.000000
5 1.969747 -0.000029 0.000000
33 0.945081 1.636724 0.000000
5 -0.984725 1.705222 0.000000
33 -1.890922 0.000028 0.000000
17 -1.869358 -3.239126 0.000000
1 1.694474 -2.938302 0.000000
17 3.740346 -0.000056 0.000000
1 1.694562 2.938251 0.000000
17 -1.869262 3.239182 0.000000
1 -3.392944 0.000050 0.000000

21. $B_3As_3H_3Cl_3$ (Puckered), T. E. = -8158.41414

5 0.000640 1.761211 0.187750
33 -1.693860 1.026259 -0.572247
5 -1.628293 -0.902951 -0.052050
33 -0.000658 -1.830206 0.583422
5 1.627295 -0.903633 -0.051894
33 1.695488 1.025823 -0.570981
17 0.000232 3.212571 1.189185
1 -2.738464 1.522252 0.424941
17 -3.146665 -1.809109 -0.085671
1 -0.000652 -3.195031 -0.087205
17 3.144668 -1.811849 -0.086545
1 2.738894 1.520288 0.428344

22. $B_3As_3H_3(CN)_3$ (Planar), T. E. = -7056.25051

5 1.693902 0.977975 0.000000
33 0.000000 1.884422 0.000000
5 -1.693902 0.977975 0.000000
33 -1.631957 -0.942211 0.000000
5 0.000000 -1.955949 0.000000
33 1.631957 -0.942211 0.000000
6 0.000000 -3.474388 0.000000
7 0.000000 -4.640306 0.000000
6 -3.008909 1.737194 0.000000
7 -4.018623 2.320153 0.000000
6 3.008909 1.737194 0.000000
7 4.018623 2.320153 0.000000
1 -2.932248 -1.692934 0.000000
1 0.000000 3.385868 0.000000
1 2.932248 -1.692934 0.000000

23. $B_3As_3H_3(CN)_3$ (Puckered), T. E. = -7056.25927

5 -1.302018 -1.233625 0.083163
33 -1.909322 0.567052 -0.473697
5 -0.417990 1.744481 0.083228
33 1.445749 1.369858 -0.472642
5 1.719503 -0.510809 0.083604
33 0.463844 -1.937656 -0.470224
6 2.992506 -0.888023 0.823091
7 3.977155 -1.179361 1.377189
6 -0.726446 3.033982 0.825751
7 -0.964402 4.031520 1.382301
6 -2.266440 -2.144873 0.824224
7 -3.012987 -2.849087 1.379355
1 2.254228 2.135570 0.562988
1 -2.979072 0.883119 0.559772

1 0.722346 -3.022328 0.563568

24. $B_3As_3H_3(CF_3)_3$ (Planar), T. E. = -7790.63506

5 -1.832222 -0.645644 0.025668
33 -0.345926 -1.849746 0.015595
5 1.474919 -1.264294 -0.027904
33 1.773925 0.624663 -0.076214
5 0.356986 1.908863 -0.026597
33 -1.428393 1.224081 0.019363
6 0.651733 3.483116 0.017177
9 0.762409 3.938963 1.298143
9 1.814796 3.821749 -0.610420
9 -0.334094 4.223363 -0.567421
6 -3.343241 -1.177026 -0.010690
9 -4.220345 -0.318827 0.585611
9 -3.786563 -1.349391 -1.289258
9 -3.496374 -2.381312 0.611840
6 2.691545 -2.305485 0.018414
9 3.081076 -2.564497 1.299738
9 2.379691 -3.512126 -0.536648
9 3.801099 -1.854072 -0.634565
1 3.188122 1.123331 -0.114825
1 -0.621913 -3.323732 0.027284
1 -2.567112 2.200572 0.030585

25. $B_3As_3H_3(CF_3)_3$ (Puckered), T. E. = -7790.63770

5 -0.032459 1.809104 -0.110862
33 1.676889 0.999601 -0.639322
5 1.659069 -0.871476 -0.029716
33 0.036764 -1.762490 0.530692
5 -1.618929 -0.934741 -0.030664
33 -1.706112 0.931126 -0.649261
6 -2.989486 -1.769049 0.030327
9 -3.445278 -2.013335 -1.232097
9 -2.881952 -2.979691 0.645591
9 -3.980426 -1.097358 0.682142
6 -0.072938 3.288244 0.513466
9 -1.122766 4.040226 0.079600
9 -0.198837 3.185508 1.870434
9 1.047523 4.026770 0.282780
6 3.060550 -1.652772 0.028406
9 3.528004 -1.869784 -1.234768
9 4.023556 -0.948242 0.687553
9 2.998614 -2.871043 0.634439
1 0.065854 -3.257092 0.322618
1 2.752710 1.670699 0.193303
1 -2.810508 1.564148 0.176435

26. $B_3O_3H_3$, T. E. = -302.27518

5 1.197083 0.691136 0.000000
8 0.000000 1.374860 0.000000
5 -1.197083 0.691136 0.000000
8 -1.190664 -0.687430 0.000000
5 0.000000 -1.382272 0.000000
8 1.190664 -0.687430 0.000000
1 2.226484 1.285461 0.000000
1 -2.226484 1.285461 0.000000
1 0.000000 -2.570922 0.000000

27. $B_3O_3F_3$, T. E. = -600.24574

5 0.000000 1.370188 0.000000
8 1.193510 0.689073 0.000000
5 1.186617 -0.685094 0.000000
8 0.000000 -1.378146 0.000000
5 -1.186617 -0.685094 0.000000
8 -1.193510 0.689073 0.000000
9 0.000000 2.692764 0.000000
9 2.332002 -1.346382 0.000000
9 -2.332002 -1.346382 0.000000

28. $B_3O_3Cl_3$, T. E. = -1681.23595

5 0.000000 1.374057 0.000000
8 1.190462 0.687313 0.000000
5 1.189968 -0.687028 0.000000
8 0.000000 -1.374627 0.000000
5 -1.189968 -0.687028 0.000000
8 -1.190462 0.687313 0.000000
17 0.000000 3.126285 0.000000
17 2.707443 -1.563143 0.000000
17 -2.707443 -1.563143 0.000000

29. $B_3O_3(CN)_3$, T. E. = -579.04689

5 0.000000 1.372674 0.000000
8 1.190890 0.687561 0.000000
5 1.188771 -0.686337 0.000000
8 0.000000 -1.375122 0.000000
5 -1.188771 -0.686337 0.000000
8 -1.190890 0.687561 0.000000
6 -2.522476 -1.456352 0.000000
7 -3.528756 -2.037328 0.000000
6 2.522476 -1.456352 0.000000
7 3.528756 -2.037328 0.000000

6 0.000000 2.912705 0.000000
7 0.000000 4.074656 0.000000

30. $B_3O_3(CF_3)_3$, T. E. = -1313.43748

5 1.314404 -0.380565 0.015651
8 0.990236 0.951387 -0.001585
5 -0.327577 1.327575 -0.038553
8 -1.318496 0.380444 -0.060563
5 -0.985582 -0.949179 -0.038546
8 0.329659 -1.334139 -0.002497
6 -2.147320 -2.064042 -0.009579
9 -2.471505 -2.344217 1.286286
9 -3.278222 -1.651407 -0.628000
9 -1.767585 -3.226240 -0.589750
6 2.861828 -0.826783 0.011450
9 3.058803 -2.027473 0.603656
9 3.297179 -0.933946 -1.277697
9 3.662221 0.069613 0.633979
6 -0.714655 2.890612 -0.009687
9 -0.833254 3.301904 1.286249
9 0.224522 3.669659 -0.595259
9 -1.893996 3.145506 -0.622654

31. $B_3S_3H_3$, T. E. = -1271.04306

5 0.000000 1.710144 0.000000
16 1.642187 0.948117 0.000000
5 1.481028 -0.855072 0.000000
16 0.000000 -1.896234 0.000000
5 -1.481028 -0.855072 0.000000
16 -1.642187 0.948117 0.000000
1 0.000000 2.899809 0.000000
1 2.511308 -1.449904 0.000000
1 -2.511308 -1.449904 0.000000

32. $B_3S_3F_3$, T. E. = -1568.99018

5 0.000000 1.702816 0.000000
16 1.663795 0.960593 0.000000
5 1.474682 -0.851408 0.000000
16 0.000000 -1.921185 0.000000
5 -1.474682 -0.851408 0.000000
16 -1.663795 0.960593 0.000000
9 0.000000 3.038100 0.000000
9 2.631072 -1.519050 0.000000
9 -2.631072 -1.519050 0.000000

33. $B_3S_3Cl_3$, T. E. = -2649.99267

5	0.000000	1.713931	0.000000
16	1.651652	0.953582	0.000000
5	1.484308	-0.856966	0.000000
16	0.000000	-1.907163	0.000000
5	-1.484308	-0.856966	0.000000
16	-1.651652	0.953582	0.000000
17	0.000000	3.482371	0.000000
17	3.015822	-1.741185	0.000000
17	-3.015822	-1.741185	0.000000

34. $B_3S_3(CN)_3$, T. E. = -1547.81478

5	-0.851634	-1.474906	0.000000
16	0.953013	-1.650696	0.000000
5	1.703226	-0.000002	0.000000
16	0.953016	1.650694	0.000000
5	-0.851632	1.474908	0.000000
16	-1.906271	0.000002	0.000000
6	-1.618487	2.803258	0.000000
7	-2.200444	3.811665	0.000000
6	3.237094	-0.000003	0.000000
7	4.401380	-0.000004	0.000000
6	-1.618492	-2.803255	0.000000
7	-2.200451	-3.811661	0.000000

35. $B_3S_3(CF_3)_3$, T. E. = -2282.19851

5	-1.691639	-0.068485	0.035362
16	-0.883539	-1.682651	0.024828
5	0.902250	-1.430078	-0.053193
16	1.893292	0.076261	-0.140252
5	0.784022	1.497815	-0.053101
16	-1.016217	1.605554	0.025865
6	1.541164	2.931984	0.006103
9	1.779588	3.260048	1.308265
9	2.740170	2.930648	-0.628556
9	0.814170	3.943665	-0.530984
6	-3.312796	-0.133592	-0.000201
9	-3.903500	0.922666	0.612846
9	-3.734677	-0.129096	-1.297243
9	-3.815833	-1.253716	0.576666
6	1.772570	-2.798532	0.006312
9	2.040725	-3.103692	1.308272
9	1.127661	-3.866563	-0.526511
9	2.965544	-2.701964	-0.632276

36. $B_3Se_3H_3$, T. E. = -7274.65706

5 0.000000 1.813915 0.000000
34 1.755125 1.013322 0.000000
5 1.570897 -0.906958 0.000000
34 0.000000 -2.026644 0.000000
5 -1.570897 -0.906958 0.000000
34 -1.755125 1.013322 0.000000
1 0.000000 3.002987 0.000000
1 2.600663 -1.501493 0.000000
1 -2.600663 -1.501493 0.000000

37. $B_3Se_3F_3$, T. E. = -7572.60585

5 0.000000 1.803050 0.000000
34 1.783385 1.029638 0.000000
5 1.561487 -0.901525 0.000000
34 0.000000 -2.059276 0.000000
5 -1.561487 -0.901525 0.000000
34 -1.783385 1.029638 0.000000
9 0.000000 3.141125 0.000000
9 2.720294 -1.570563 0.000000
9 -2.720294 -1.570563 0.000000

38. $B_3Se_3Cl_3$, T. E. = -8653.61659

5 0.000000 1.804090 0.000000
34 1.767946 1.020724 0.000000
5 1.562387 -0.902045 0.000000
34 0.000000 -2.041449 0.000000
5 -1.562387 -0.902045 0.000000
34 -1.767946 1.020724 0.000000
17 0.000000 3.580541 0.000000
17 3.100839 -1.790270 0.000000
17 -3.100839 -1.790270 0.000000

39. $B_3Se_3(CN)_3$, T. E. = -7551.45204

5 -1.548780 0.894279 0.000000
34 -1.768579 -1.020956 0.000000
5 0.000000 -1.788330 0.000000
34 1.768579 -1.020955 0.000000
5 1.548779 0.894280 0.000000
34 0.000000 2.041965 0.000000
6 2.875502 1.660239 0.000000
7 3.884465 2.242398 0.000000
6 0.000001 -3.320408 0.000000
7 0.000001 -4.485278 0.000000
6 -2.875503 1.660238 0.000000
7 -3.884466 2.242396 0.000000

40. $B_3Se_3(CF_3)_3$, T. E. = -8285.84272

5 -0.730120 1.613088 -0.000375
34 1.191898 1.653417 -0.000235
5 1.762064 -0.174268 -0.001892
34 0.835701 -1.858769 -0.005183
5 -1.032131 -1.438644 -0.001725
34 -2.027921 0.205633 -0.000752
6 -2.007562 -2.731797 0.002209
9 -2.827084 -2.724791 -1.086933
9 -1.360183 -3.924934 -0.005445
9 -2.809065 -2.728568 1.104006
6 -1.361944 3.104386 0.000180
9 -2.718858 3.140877 0.002469
9 -0.950357 3.804382 1.094401
9 -0.953920 3.802585 -1.096661
6 3.369737 -0.372807 0.001864
9 3.772781 -1.089353 -1.085162
9 4.079665 0.784136 -0.009595
9 3.768189 -1.065350 1.105611

41. $Al_3N_3H_6$, T. E. = -895.32301

13 1.606600 0.927571 0.000000
7 0.000000 1.751916 0.000000
13 -1.606600 0.927571 0.000000
7 -1.517203 -0.875958 0.000000
13 0.000000 -1.855141 0.000000
7 1.517203 -0.875958 0.000000
1 2.977722 1.719189 0.000000
1 0.000000 2.770020 0.000000
1 -2.977722 1.719189 0.000000
1 -2.398908 -1.385010 0.000000
1 0.000000 -3.438377 0.000000
1 2.398908 -1.385010 0.000000

42. $Al_3N_3H_3F_3$, T. E. = -1193.33869

13 0.912651 1.581153 0.000000
7 -0.879115 1.522770 0.000000
13 -1.825561 0.000000 0.000000
7 -0.879114 -1.522771 0.000000
13 0.912652 -1.581153 0.000000
7 1.757204 0.000000 0.000000
9 1.749774 3.028887 0.000000
1 -1.388125 2.404212 0.000000
9 -3.498248 -0.000001 0.000000
1 -1.388124 -2.404213 0.000000
9 1.749775 -3.028887 0.000000

1 2.775067 0.000001 0.000000

43. $Al_3N_3H_3Cl_3$, T. E. = -2274.37391

13 0.914791 -1.585878 0.000000
7 -0.878220 -1.520473 0.000000
13 -1.831145 0.000000 0.000000
7 -0.878220 1.520473 0.000000
13 0.914791 1.585878 0.000000
7 1.753373 0.000000 0.000000
17 1.973054 -3.413958 0.000000
1 -1.387115 -2.401897 0.000000
17 -3.943468 0.000000 0.000000
1 -1.387116 2.401897 0.000000
17 1.973054 3.413959 0.000000
1 2.771139 0.000000 0.000000

44. $Al_3N_3H_3(CN)_3$, T. E. = -1172.13427

13 1.582198 0.913482 0.000000
7 0.000000 1.757766 0.000000
13 -1.582198 0.913482 0.000000
7 -1.522270 -0.878883 0.000000
13 0.000000 -1.826965 0.000000
7 1.522270 -0.878883 0.000000
1 0.000000 2.776177 0.000000
1 -2.404240 -1.388089 0.000000
1 2.404240 -1.388089 0.000000
6 3.257689 1.880828 0.000000
7 4.267072 2.463595 0.000000
6 -3.257689 1.880828 0.000000
7 -4.267072 2.463595 0.000000
6 0.000000 -3.761655 0.000000
7 0.000000 -4.927190 0.000000

45. $Al_3N_3H_3(CF_3)_3$, T. E. = -1906.48937

13 1.059705 -1.489604 0.011761
7 -0.731852 -1.602101 0.007113
13 -1.821422 -0.175498 -0.014923
7 -1.023289 1.432524 -0.034612
13 0.757000 1.663695 -0.014722
7 1.749007 0.167724 0.007302
1 -1.155094 -2.528518 0.014372
1 -1.615240 2.260976 -0.063477
1 2.762897 0.264714 0.014824
6 -3.838005 -0.368374 0.000377
9 -4.272141 -1.514340 -0.611700
9 -4.349032 -0.407098 1.273304

9	-4.480073	0.664474	-0.629956
6	1.600278	3.505686	0.000421
9	0.841743	4.448334	-0.641638
9	1.792422	3.981429	1.273050
9	2.831108	3.536477	-0.600246
6	2.239366	-3.136591	0.002153
9	2.526040	-3.565885	-1.269286
9	3.449651	-2.932271	0.610415
9	1.671599	-4.207814	0.639441

46. $Al_3P_3H_6$ (Planar), T. E. = -1755.00158

13	2.039721	1.177633	0.000000
15	0.000000	2.173562	0.000000
13	-2.039721	1.177633	0.000000
15	-1.882360	-1.086781	0.000000
13	0.000000	-2.355267	0.000000
15	1.882360	-1.086781	0.000000
1	3.406007	1.966459	0.000000
1	0.000000	3.582068	0.000000
1	-3.406007	1.966459	0.000000
1	-3.102162	-1.791034	0.000000
1	0.000000	-3.932918	0.000000
1	3.102162	-1.791034	0.000000

47. $Al_3P_3H_6$ (Puckered), T. E. = -1755.01507

13	0.292357	1.054437	1.927302
15	-0.215654	2.202655	0.000000
13	0.292357	1.054437	-1.927302
15	0.292357	-1.264179	-1.919718
13	-0.872223	-1.833433	0.000000
15	0.292357	-1.264179	1.919718
1	0.549395	1.854515	3.270477
1	0.535259	3.405012	0.000000
1	0.549395	1.854515	-3.270477
1	-0.643144	-1.515333	-2.961796
1	-2.146065	-2.778554	0.000000
1	-0.643144	-1.515333	2.961796

48. $Al_3P_3H_3F_3$ (Planar), T. E. = -2053.00169

13	1.149942	1.991607	0.000000
15	-1.105375	1.914654	0.000000
13	-2.299849	0.000000	0.000000
15	-1.105375	-1.914654	0.000000
13	1.149942	-1.991607	0.000000
15	2.211030	0.000000	0.000000
9	1.984874	3.438031	0.000000

1	-1.807439	3.131691	0.000000
9	-3.970397	-0.000001	0.000000
1	-1.807438	-3.131691	0.000000
9	1.984875	-3.438030	0.000000
1	3.616062	0.000001	0.000000

49. $Al_3P_3H_3F_3$ (Puckered), T. E. = -2053.02822

13	0.000066	1.978131	0.202780
15	-1.975507	1.216288	-0.735711
13	-1.839781	-1.006003	-0.086348
15	-0.000055	-2.023727	0.857304
13	1.839726	-1.006088	-0.086338
15	1.975440	1.216107	-0.735982
9	0.000190	3.230282	1.316129
1	-2.914404	1.647537	0.243911
9	-3.232255	-1.929058	-0.212170
1	-0.000092	-3.332556	0.309102
9	3.232244	-1.929109	-0.211937
1	2.914587	1.647424	0.243374

50. $Al_3P_3H_3Cl_3$ (Planar), T. E. = -3134.04007

13	2.001987	-1.156170	0.000000
15	1.905258	1.099826	0.000000
13	-0.000001	2.311955	0.000000
15	-1.905259	1.099824	0.000000
13	-2.001985	-1.156172	0.000000
15	0.000001	-2.200719	0.000000
17	3.828227	-2.209410	0.000000
1	3.122508	1.802171	0.000000
17	-0.000003	4.420169	0.000000
1	-3.122510	1.802167	0.000000
17	-3.828225	-2.209414	0.000000
1	0.000002	-3.606130	0.000000

51. $Al_3P_3H_3Cl_3$ (Puckered), T. E. = -3134.06395

13	1.856469	-0.972718	-0.039640
15	1.959439	1.138821	-0.992371
13	0.000000	2.038481	-0.147160
15	-1.959439	1.138820	-0.992371
13	-1.856469	-0.972718	-0.039640
15	0.000000	-1.836693	1.014366
17	3.625675	-2.137142	-0.012535
1	2.925360	1.707235	-0.116126
17	0.000000	3.802381	1.027793
1	-2.925360	1.707235	-0.116126
17	-3.625675	-2.137142	-0.012535

1 0.000000 -3.215946 0.685297

52. $Al_3P_3H_3(CN)_3$ (Planar), T. E. = -2031.80002

13 1.152000 1.995475 0.000000
15 -1.100694 1.906438 0.000000
13 -2.304201 -0.000051 0.000000
15 -1.100609 -1.906488 0.000000
13 1.152090 -1.995424 0.000000
15 2.201243 0.000049 0.000000
1 -1.803429 3.123592 0.000000
1 -1.803290 -3.123673 0.000000
1 3.606711 0.000080 0.000000
6 2.116535 3.665718 0.000000
7 2.699320 4.675404 0.000000
6 -4.232947 -0.000094 0.000000
7 -5.398755 -0.000120 0.000000
6 2.116698 -3.665624 0.000000
7 2.699529 -4.675284 0.000000

53. $Al_3P_3H_3(CN)_3$ (Puckered), T. E. = -2031.81942

13 1.863607 -0.987488 -0.030738
15 -0.000601 -1.905130 0.940097
13 -1.864269 -0.986382 -0.030723
15 -1.960717 1.133456 -0.945437
13 0.000552 2.043377 -0.140228
15 1.961369 1.132368 -0.945309
1 -0.001026 -3.280258 0.599104
1 -2.939225 1.716506 -0.095165
1 2.940114 1.714770 -0.094865
6 3.494577 -2.033112 0.026581
7 4.475438 -2.663295 0.058328
6 -3.495877 -2.031002 0.026752
7 -4.477124 -2.660583 0.058533
6 0.001093 3.708948 0.852580
7 0.001979 4.704734 1.459875

54. $Al_3P_3H_3(CF_3)_3$ (Planar), T. E. = -2766.15688

13 0.437351 2.265270 0.013173
15 2.080720 0.718838 0.009515
13 1.743028 -1.512125 -0.017613
15 -0.417918 -2.162430 -0.039722
13 -2.181124 -0.753919 -0.018744
15 -1.663821 1.442439 0.006830
1 3.409234 1.177594 0.018474
1 -0.684794 -3.541954 -0.080012
1 -2.725758 2.363243 0.016069

6	3.279009	-2.841985	0.003870
9	4.407783	-2.359942	-0.597308
9	3.642256	-3.182752	1.278926
9	2.977134	-4.013488	-0.631919
6	-4.101340	-1.417364	0.004237
9	-4.255766	-2.620809	-0.624863
9	-4.565827	-1.591837	1.279947
9	-4.970388	-0.554208	-0.601902
6	0.822839	4.260168	-0.000277
9	0.923532	4.754142	-1.272933
9	-0.151746	4.993338	0.616723
9	1.995604	4.578175	0.625612

55. $Al_3P_3H_3(CF_3)_3$ (Puckered), T. E. = -2766.17647

13	0.014369	2.057565	-0.460988
15	-1.962054	1.107963	-1.186774
13	-1.871945	-0.918676	-0.070869
15	-0.013922	-1.733714	1.002223
13	1.854112	-0.949789	-0.076197
15	1.967623	1.071247	-1.198657
1	-2.925981	1.771895	-0.379353
1	-0.025996	-3.140801	0.839145
1	2.948089	1.724623	-0.403001
6	-3.590620	-2.005459	0.062430
9	-4.677662	-1.242115	0.392570
9	-3.894477	-2.603326	-1.134408
9	-3.539785	-3.011698	0.984961
6	3.560792	-2.054624	0.062783
9	3.496515	-3.060259	0.985088
9	3.864618	-2.655137	-1.132556
9	4.653384	-1.301146	0.397948
6	0.036383	3.861142	0.490718
9	-0.190071	3.697531	1.836601
9	1.225937	4.525362	0.387407
9	-0.923473	4.728254	0.049103

56. $Al_3As_3H_6$ (Planar), T. E. = -7432.28893

13	-1.220180	-2.113128	0.000000
33	1.102444	-1.908536	0.000000
13	2.441730	0.000002	0.000000
33	1.102441	1.908538	0.000000
13	-1.220183	2.113127	0.000000
33	-2.205323	-0.000001	0.000000
1	-2.007607	-3.478719	0.000000
1	1.858007	-3.223826	0.000000

1 4.018029 0.000003 0.000000
1 1.858003 3.223829 0.000000
1 -2.007611 3.478716 0.000000
1 -3.722123 -0.000002 0.000000

57. $Al_3As_3H_6$ (Puckered), T. E. = -7432.31785

13 1.096503 1.869072 -0.476317
33 -1.312986 1.933182 -0.244046
13 -1.433734 0.014296 1.197247
33 -1.360055 -1.897372 -0.256509
13 1.051456 -1.902886 -0.450558
33 2.304695 -0.025628 0.338126
1 1.888927 3.135986 -1.009098
1 -1.254180 3.052060 0.810900
1 -1.787155 0.011497 2.744479
1 -1.355189 -3.032022 0.783606
1 1.819751 -3.202183 -0.939142
1 3.558345 -0.047608 -0.545402

58. $Al_3As_3H_3F_3$ (Planar), T. E. = -7730.29748

13 -1.180229 -2.043724 0.000000
33 1.132849 -1.961619 0.000000
13 2.361109 -0.000001 0.000000
33 1.132850 1.961618 0.000000
13 -1.180228 2.043725 0.000000
33 -2.266238 0.000001 0.000000
9 -2.013841 -3.488283 0.000000
1 1.884941 -3.270670 0.000000
9 4.029384 -0.000001 0.000000
1 1.884943 3.270669 0.000000
9 -2.013839 3.488284 0.000000
1 -3.775928 0.000001 0.000000

59. $Al_3As_3H_3F_3$ (Puckered), T. E. = -7730.34001

13 -1.810435 1.028527 -0.298285
33 0.000121 2.137571 0.806914
13 1.810631 1.028285 -0.298125
33 2.020466 -1.367587 -0.527122
13 -0.000086 -1.723047 0.726327
33 -2.020777 -1.367338 -0.526854
9 -3.068114 1.977162 -0.866912
1 0.000425 3.475854 0.062074
9 3.068602 1.976693 -0.866479
1 2.989620 -1.470383 0.662434
9 0.000017 -2.305187 2.297470

1 -2.989742 -1.469738 0.662897

60. $Al_3As_3H_3Cl_3$ (Planar), T. E. = -8811.33656

13 -1.189967 -2.060228 0.000000
33 1.126161 -1.950148 0.000000
13 2.380416 -0.000010 0.000000
33 1.126176 1.950139 0.000000
13 -1.189950 2.060238 0.000000
33 -2.253662 0.000009 0.000000
17 -2.240681 -3.882606 0.000000
1 1.878119 -3.258935 0.000000
17 4.483923 -0.000018 0.000000
1 1.878145 3.258920 0.000000
17 -2.240649 3.882624 0.000000
1 -3.763107 0.000015 0.000000

61. $Al_3As_3H_3Cl_3$ (Puckered), T. E. = -8811.37539

13 0.000056 1.980178 0.291723
33 -1.952175 1.256666 -0.904075
13 -1.813806 -1.010979 -0.085720
33 0.000020 -1.885677 1.208269
13 1.813762 -1.011017 -0.085921
33 1.951668 1.256371 -0.904947
17 0.000756 3.358538 1.898801
1 -3.025299 1.648196 0.123856
17 -3.482646 -2.270994 -0.441001
1 -0.000006 -3.338006 0.724518
17 3.482820 -2.270930 -0.440554
1 3.025407 1.648115 0.122244

62. $Al_3As_3H_3(CN)_3$ (Planar), T. E. = -7709.10639

33 2.195810 0.500090 -0.000109
13 0.700681 2.267776 -0.000176
33 -1.531029 1.651433 -0.000112
13 -2.314534 -0.527117 0.000015
33 -0.664713 -2.151320 0.000118
13 1.613771 -1.740720 0.000027
1 3.666032 0.835064 0.000050
1 -2.555349 2.757293 -0.000192
1 -1.109634 -3.592024 0.000216
6 -4.187903 -0.954036 0.000021
7 -5.325047 -1.213225 0.000041
6 2.919962 -3.149936 0.000018
7 3.712805 -4.005314 0.000003
6 1.267821 4.103602 -0.000110

7 1.612024 5.217964 0.000741

63. $Al_3As_3H_3(CN)_3$ (Puckered), T. E. = -7709.13817

13 0.050517 -1.922742 0.131799
33 -1.994689 -1.319904 -0.960967
13 -1.791790 0.915614 -0.066426
33 -0.048633 1.644881 1.388435
13 1.734775 1.014949 -0.063233
33 2.114433 -1.232513 -0.871782
1 -2.907812 -1.742447 0.201374
1 -0.095556 3.149112 1.111243
1 2.966435 -1.563143 0.365573
6 0.037511 -2.821087 1.848652
7 0.030909 -3.399110 2.862091
6 -3.164393 2.204970 -0.519856
7 -4.015804 2.959326 -0.778879
6 2.994884 2.393120 -0.577940
7 3.780141 3.202849 -0.875897

64. $Al3As_3H_3(CF_3)_3$ (Puckered), T. E. = -8443.50671

13 1.762496 0.703213 -0.362059
33 0.000602 2.160590 -1.035680
13 -1.761533 0.703972 -0.360947
33 -2.089259 -1.480287 -1.321466
13 -0.000143 -2.028727 -0.311535
33 2.088627 -1.481107 -1.322825
1 0.000763 3.079891 0.186336
1 -2.929450 -1.938137 -0.122946
1 2.929749 -1.939307 -0.125131
6 -3.283000 1.438958 0.764136
9 -2.887796 2.259500 1.780840
9 -4.108578 2.192522 -0.039563
9 -4.077191 0.483080 1.329287
6 0.000792 -2.225559 1.705659
9 0.001014 -0.861030 2.075109
9 -1.087578 -2.762735 2.309848
9 1.089682 -2.762877 2.308860
6 3.282593 1.439444 0.764193
9 2.883005 2.241473 1.794041
9 4.089655 0.484602 1.312474
9 4.096336 2.212914 -0.032465

65. $Al_3O_3H_3$, T. E. = -955.08139

13 1.534983 0.886223 0.000000
8 0.000000 1.670018 0.000000
13 -1.534983 0.886223 0.000000

8 -1.446278 -0.835009 0.000000
13 0.000000 -1.772446 0.000000
8 1.446278 -0.835009 0.000000
1 2.893615 1.670630 0.000000
1 -2.893615 1.670630 0.000000
1 0.000000 -3.341259 0.000000

66. $Al_3O_3F_3$, T. E. = -1253.08450

13 1.517030 0.875858 0.000000
8 0.000000 1.668242 0.000000
13 -1.517030 0.875858 0.000000
8 -1.444740 -0.834121 0.000000
13 0.000000 -1.751716 0.000000
8 1.444740 -0.834121 0.000000
9 2.952096 1.704393 0.000000
9 -2.952096 1.704393 0.000000
9 0.000000 -3.408786 0.000000

67. $Al_3O_3Cl_3$, T. E. = -2334.11928

13 1.522451 0.878987 0.000000
8 0.000000 1.666755 0.000000
13 -1.522451 0.878987 0.000000
8 -1.443452 -0.833377 0.000000
13 0.000000 -1.757975 0.000000
8 1.443452 -0.833377 0.000000
17 3.330047 1.922604 0.000000
17 -3.330047 1.922604 0.000000
17 0.000000 -3.845208 0.000000

68. $Al_3O_3(CN)_3$, T. E. = -1231.87871

13 1.519004 0.876998 0.000000
8 0.000000 1.668726 0.000000
13 -1.519004 0.876998 0.000000
8 -1.445159 -0.834363 0.000000
13 0.000000 -1.753995 0.000000
8 1.445159 -0.834363 0.000000
6 0.000000 -3.669067 0.000000
7 0.000000 -4.833786 0.000000
6 -3.177505 1.834533 0.000000
7 -4.186181 2.416893 0.000000
6 3.177505 1.834533 0.000000
7 4.186181 2.416893 0.000000

69. $Al_3O_3(CF_3)_3$, T. E. = -1966.23541

13 1.377685 -1.088091 0.021037

8	1.551572	0.617952	0.002540
13	0.251316	1.736121	-0.021574
8	-1.314336	1.035423	-0.025789
13	-1.630738	-0.650371	-0.017718
8	-0.240830	-1.655288	0.006565
6	-3.502076	-1.394859	-0.007084
9	-3.977891	-1.502666	1.275062
9	-4.393054	-0.614111	-0.682146
9	-3.588657	-2.640497	-0.553695
6	2.959632	-2.334372	0.009475
9	2.707153	-3.532432	0.608665
9	3.341093	-2.619917	-1.277095
9	4.058183	-1.816311	0.628576
6	0.542874	3.728815	-0.007282
9	0.658410	4.194029	1.278158
9	1.679840	4.110030	-0.656170
9	-0.479661	4.427233	-0.576895

70. $Al_3S_3H_3$, T. E. = -1923.91852

13	0.000000	2.103110	0.000000
16	1.969450	1.137063	0.000000
13	1.821347	-1.051555	0.000000
16	0.000000	-2.274125	0.000000
13	-1.821347	-1.051555	0.000000
16	-1.969450	1.137063	0.000000
1	0.000000	3.675955	0.000000
1	3.183470	-1.837978	0.000000
1	-3.183470	-1.837978	0.000000

71. $Al_3S_3F_3$, T. E. = -2221.92389

13	0.000000	2.038818	0.000000
16	1.987943	1.147739	0.000000
13	1.765668	-1.019409	0.000000
16	0.000000	-2.295479	0.000000
13	-1.765668	-1.019409	0.000000
16	-1.987943	1.147739	0.000000
9	0.000000	3.703099	0.000000
9	3.206978	-1.851550	0.000000
9	-3.206978	-1.851550	0.000000

72. $Al_3S_3Cl_3$, T. E. = -3302.95805

13	0.000000	2.058986	0.000000
16	1.981437	1.143983	0.000000
13	1.783134	-1.029493	0.000000
16	0.000000	-2.287966	0.000000
13	-1.783134	-1.029493	0.000000

16	-1.981437	1.143983	0.000000
17	0.000000	4.158898	0.000000
17	3.601711	-2.079449	0.000000
17	-3.601711	-2.079449	0.000000

73. $Al_3S_3(CN)_3$, T. E. = -2200.71500

13	-1.023881	-1.773098	0.000000
16	1.144995	-1.983374	0.000000
13	2.047962	-0.000011	0.000000
16	1.145017	1.983362	0.000000
13	-1.023862	1.773109	0.000000
16	-2.290437	0.000012	0.000000
6	-1.986385	3.440230	0.000000
7	-2.568869	4.449658	0.000000
6	3.972868	-0.000021	0.000000
7	5.138301	-0.000028	0.000000
6	-1.986422	-3.440209	0.000000
7	-2.568917	-4.449630	0.000000

74. $Al_3S_3(CF_3)_3$, T. E. = -2935.07216

13	2.047308	-0.100983	0.030419
16	1.243053	1.927132	0.018423
13	-0.935587	1.823072	-0.030942
16	-2.289166	0.112912	-0.084137
13	-1.110491	-1.722426	-0.031651
16	1.047625	-2.040069	0.017878
6	-2.209100	-3.424551	0.004404
9	-2.480465	-3.793999	1.297346
9	-3.414700	-3.304430	-0.621147
9	-1.579528	-4.487135	-0.574171
6	4.070807	-0.200236	0.002433
9	4.568555	-1.321608	0.597095
9	4.531206	-0.212862	-1.289520
9	4.674625	0.858972	0.613726
6	-1.862511	3.624495	0.003846
9	-2.095855	4.019519	1.296601
9	-1.133059	4.620821	-0.574965
9	-3.074707	3.621449	-0.620570

75. $Al_3Se_3H_3$, T. E. = -7927.56986

13	0.000000	2.176129	0.000000
34	2.096463	1.210393	0.000000
13	1.884583	-1.088064	0.000000
34	0.000000	-2.420787	0.000000
13	-1.884583	-1.088064	0.000000
34	-2.096463	1.210393	0.000000

1 0.000000 3.752673 0.000000
1 3.249910 -1.876336 0.000000
1 -3.249910 -1.876336 0.000000

76. $Al_3Se_3F_3$, T. E. = -8225.58570

13 0.000000 2.099701 0.000000
34 2.115608 1.221447 0.000000
13 1.818395 -1.049851 0.000000
34 0.000000 -2.442894 0.000000
13 -1.818395 -1.049851 0.000000
34 -2.115608 1.221447 0.000000
9 0.000000 3.765574 0.000000
9 3.261082 -1.882787 0.000000
9 -3.261082 -1.882787 0.000000

77. $Al_3Se_3Cl_3$, T. E. = -9306.61853

13 1.062584 1.840123 0.000000
34 -1.220155 2.113318 0.000000
13 -2.125181 -0.000008 0.000000
34 -1.220140 -2.113327 0.000000
13 1.062597 -1.840116 0.000000
34 2.440960 0.000009 0.000000
17 2.116191 3.666564 0.000000
17 -4.233739 -0.000015 0.000000
17 2.116217 -3.666549 0.000000

78. $Al_3Se_3(CN)_3$, T. E. = -8204.37857

13 1.828108 -1.055531 0.000000
34 2.113528 1.220160 0.000000
13 0.000101 2.110840 0.000000
34 -2.113411 1.220363 0.000000
13 -1.828210 -1.055355 0.000000
34 -0.000117 -2.440504 0.000000
6 -3.499597 -2.020265 0.000000
7 -4.509581 -2.603050 0.000000
6 0.000194 4.040646 0.000000
7 0.000250 5.206713 0.000000
6 3.499403 -2.020601 0.000000
7 4.509331 -2.603482 0.000000

79. $Al_3Se_3(CF_3)_3$, T. E. = -8938.74253

13 2.056208 -0.446074 0.033692
34 1.646752 1.813097 0.008738
13 -0.640704 2.002699 -0.046737
34 -2.391440 0.517565 -0.062131

13	-1.412100	-1.558980	-0.044917
34	0.748785	-2.333677	0.010889
6	-2.776030	-3.053319	0.008983
9	-3.074676	-3.355292	1.315694
9	-3.960328	-2.740316	-0.590577
9	-2.348315	-4.215031	-0.563565
6	4.034675	-0.872342	0.005514
9	4.355822	-2.051697	0.610445
9	4.461350	-0.979088	-1.296518
9	4.814138	0.084827	0.585429
6	-1.261590	3.928375	0.009872
9	-1.419796	4.321249	1.316956
9	-0.383316	4.809179	-0.549968
9	-2.463309	4.139153	-0.599847

80. $Ga_3N_3H_6$, T. E. = -5936.74669

31	1.654951	0.955486	0.000000
7	0.000000	1.778692	0.000000
31	-1.654951	0.955486	0.000000
7	-1.540392	-0.889346	0.000000
31	0.000000	-1.910973	0.000000
7	1.540392	-0.889346	0.000000
1	3.000254	1.732198	0.000000
1	0.000000	2.795130	0.000000
1	-3.000254	1.732198	0.000000
1	-2.420654	-1.397565	0.000000
1	0.000000	-3.464395	0.000000
1	2.420654	-1.397565	0.000000

81. $Ga_3N_3H_3F_3$, T. E. = -6234.67492

31	1.604298	0.926242	0.000000
7	0.000000	1.818600	0.000000
31	-1.604298	0.926242	0.000000
7	-1.574954	-0.909300	0.000000
31	0.000000	-1.852483	0.000000
7	1.574954	-0.909300	0.000000
9	3.140319	1.813064	0.000000
1	0.000000	2.834163	0.000000
9	-3.140319	1.813064	0.000000
1	-2.454457	-1.417082	0.000000
9	0.000000	-3.626128	0.000000
1	2.454457	-1.417082	0.000000

82. $Ga_3N_3H_3Cl_3$, T. E. = -7315.76827

31	1.614221	0.931971	0.000000
7	0.000000	1.809128	0.000000

31	-1.614221	0.931971	0.000000
7	-1.566751	-0.904564	0.000000
31	0.000000	-1.863942	0.000000
7	1.566751	-0.904564	0.000000
17	3.475789	2.006748	0.000000
1	0.000000	2.824559	0.000000
17	-3.475789	2.006748	0.000000
1	-2.446140	-1.412280	0.000000
17	0.000000	-4.013495	0.000000
1	2.446140	-1.412280	0.000000

83. $Ga_3N_3H_3(CN)_3$, T. E. = -6213.57792

31	1.621770	-0.936297	0.000000
7	1.557406	0.899004	0.000000
31	-0.000034	1.872335	0.000000
7	-1.557439	0.898947	0.000000
31	-1.621736	-0.936356	0.000000
7	0.000033	-1.797837	0.000000
1	2.437515	1.407018	0.000000
1	-2.437566	1.406929	0.000000
1	0.000051	-2.814068	0.000000
6	3.282072	-1.894429	0.000000
7	4.290280	-2.476023	0.000000
6	-0.000069	3.789303	0.000000
7	-0.000090	4.953235	0.000000
6	-3.282003	-1.894548	0.000000
7	-4.290190	-2.476179	0.000000

84. $Ga_3N_3H_3(CF_3)_3$, T. E. = -6947.94276

31	1.686961	-0.825556	0.000677
7	0.129819	-1.800437	0.004361
31	-1.551728	-1.054313	-0.026644
7	-1.618535	0.782171	-0.051607
31	-0.131466	1.864992	-0.026498
7	1.491113	1.004403	-0.010139
1	0.202590	-2.814132	0.008610
1	-2.532252	1.225949	-0.082367
1	2.332149	1.574752	-0.002368
6	-3.210297	-2.171261	0.011211
9	-3.084498	-3.336546	-0.684117
9	-3.550735	-2.520182	1.287594
9	-4.289412	-1.519691	-0.509347
6	-0.285639	3.858729	0.013917
9	-1.290003	4.325678	-0.781493
9	-0.547983	4.319172	1.272950
9	0.856626	4.481248	-0.394336
6	3.493872	-1.679465	0.006450

9 4.207589 -1.382110 -1.118142
9 4.255563 -1.270197 1.062089
9 3.429112 -3.039190 0.077554

85. $Ga_3P_3H_6$, (Planar), T. E. = -6796.51268

31 2.005445 1.157844 0.000000
15 0.000000 2.141255 0.000000
31 -2.005445 1.157844 0.000000
15 -1.854381 -1.070628 0.000000
31 0.000000 -2.315689 0.000000
15 1.854381 -1.070628 0.000000
1 3.347425 1.932637 0.000000
1 0.000000 3.548495 0.000000
1 -3.347425 1.932637 0.000000
1 -3.073086 -1.774247 0.000000
1 0.000000 -3.865274 0.000000
1 3.073086 -1.774247 0.000000

86. $Ga_3P_3H_6$ (Puckered), T. E. = -6796.53047

31 -1.879649 -1.031247 -0.131694
15 -0.009762 -2.044340 0.673121
31 1.869164 -1.047306 -0.131516
15 1.891379 1.198368 -0.611886
31 0.009340 1.929220 0.471348
15 -1.878835 1.214439 -0.611635
1 -3.205225 -1.850404 -0.250586
1 -0.014007 -3.364103 0.153558
1 3.185316 -1.881546 -0.251469
1 2.930174 1.571552 0.286357
1 0.012801 3.027079 1.581779
1 -2.915268 1.599719 0.284073

87. $Ga_3P_3H_3F_3$ (Planar), T. E. = -7094.43281

31 1.114908 1.933340 0.000000
15 -1.110040 1.922229 0.000000
31 -2.231173 -0.000023 0.000000
15 -1.110000 -1.922252 0.000000
31 1.114949 -1.933316 0.000000
15 2.216047 0.000023 0.000000
9 2.009356 3.467355 0.000000
1 -1.811953 3.136355 0.000000
9 -4.007001 -0.000042 0.000000
1 -1.811888 -3.136393 0.000000
9 2.009429 -3.467314 0.000000
1 3.618489 0.000038 0.000000

88. $Ga_3P_3H_3F_3$ (Puckered), T. E = -7094.47812

31 -1.739761 -0.958272 -0.054248
15 -0.000928 -2.050334 0.968011
31 1.738884 -0.959582 -0.054097
15 2.034492 1.231431 -0.727497
31 0.000902 1.921058 0.100821
15 -2.036443 1.234834 -0.721125
9 -3.180552 -1.990483 -0.274372
1 -0.001295 -3.267940 0.237193
9 3.180898 -1.991195 -0.268815
1 2.834129 1.607887 0.389063
9 0.004120 3.283108 1.256071
1 -2.830599 1.608876 0.400199

89. $Ga_3P_3H_3Cl_3$ (Planar), T. E. = -8175.52463

31 1.951181 1.126515 0.000000
15 0.000000 2.195375 0.000000
31 -1.951181 1.126515 0.000000
15 -1.901251 -1.097688 0.000000
31 0.000000 -2.253030 0.000000
15 1.901251 -1.097688 0.000000
17 3.815589 2.202931 0.000000
1 0.000000 3.598347 0.000000
17 -3.815589 2.202931 0.000000
1 -3.116260 -1.799174 0.000000
17 0.000000 -4.405862 0.000000
1 3.116260 -1.799174 0.000000

90. $Ga_3P_3H_3Cl_3$ (Puckered), T. E. = -8175.56419

31 -0.037112 -0.915895 1.759895
15 -1.275764 -1.699510 0.000000
31 -0.037112 -0.915895 -1.759895
15 1.079114 1.094686 -1.970751
31 0.258298 1.946526 0.000000
15 1.079114 1.094686 1.970751
17 -0.037112 -2.182257 3.521991
1 -0.908904 -3.070479 0.000000
17 -0.037112 -2.182257 -3.521991
1 0.134428 1.662476 -2.871672
17 -1.002435 3.708091 0.000000
1 0.134428 1.662476 2.871672

91. $Ga_3P_3H_3(CN)_3$ (Planar), T. E. = -7073.32003

31 1.954916 -1.128776 0.000000
15 1.890312 1.091215 0.000000

31	-0.000005	2.257241	0.000000
15	-1.890317	1.091206	0.000000
31	-1.954911	-1.128785	0.000000
15	0.000005	-2.182716	0.000000
1	3.105779	1.792907	0.000000
1	-3.105787	1.792894	0.000000
1	0.000008	-3.586201	0.000000
6	3.621795	-2.090552	0.000000
7	4.630522	-2.672273	0.000000
6	-0.000009	4.181716	0.000000
7	-0.000012	5.346161	0.000000
6	-3.621786	-2.090568	0.000000
7	-4.630510	-2.672293	0.000000

92. $Ga_3P_3H_3(CN)_3$ (Puckered), T. E. = -7073.35146

31	-1.784601	-0.950169	-0.011403
15	-1.945756	1.129400	-0.987365
31	0.000248	1.971788	-0.121155
15	1.946038	1.128860	-0.987338
31	1.784305	-0.950691	-0.011434
15	-0.000266	-1.815212	1.112632
1	-2.897286	1.658763	-0.071834
1	2.897676	1.657942	-0.071756
1	-0.000482	-3.178419	0.721874
6	-3.394233	-2.036216	-0.009737
7	-4.351983	-2.700025	-0.014248
6	0.000607	3.574056	0.971771
7	0.001031	4.546137	1.614781
6	3.393610	-2.037224	-0.009816
7	4.351159	-2.701323	-0.014353

93. $Ga_3P_3H_3(CF_3)_3$ (Planar), T. E. = -7807.69535

31	-0.138335	2.269095	0.015289
15	1.808838	1.194773	0.008565
31	2.034862	-1.017854	-0.012724
15	0.131050	-2.167150	-0.021595
31	-1.896938	-1.255143	-0.013044
15	-1.940855	0.967685	0.008296
1	2.980241	1.969230	0.011898
1	0.215224	-3.568563	-0.044872
1	-3.197346	1.594146	0.011165
6	3.838538	-1.913341	0.005244
9	4.794935	-1.156376	-0.600143
9	4.272401	-2.150287	1.275404
9	3.824832	-3.115388	-0.634094
6	-3.579020	-2.362075	0.005468
9	-3.418134	-3.556420	-0.628323

9	-3.984612	-2.644209	1.275852
9	-4.618377	-1.729246	-0.605669
6	-0.258825	4.279064	-0.004705
9	-0.291675	4.770823	-1.275534
9	-1.379292	4.735034	0.620361
9	0.802694	4.865474	0.614548

94. $Ga_3P_3H_3(CF_3)_3$ (Puckered), T. E. = -7807.72529

31	-0.067941	1.986192	-0.454735
15	1.910956	1.145424	-1.247408
31	1.803772	-0.787538	0.010468
15	0.053946	-1.458526	1.307291
31	-1.731726	-0.915973	-0.001327
15	-1.952437	0.985326	-1.289510
1	2.828689	1.808425	-0.383045
1	0.105934	-2.873589	1.225777
1	-2.945526	1.586384	-0.464638
6	3.468161	-1.941815	0.041194
9	3.651323	-2.561193	-1.163218
9	4.600188	-1.223434	0.288325
9	3.419215	-2.928511	0.979083
6	-3.324182	-2.167025	0.045486
9	-3.218330	-3.135669	0.997249
9	-4.496298	-1.511933	0.282928
9	-3.470482	-2.812787	-1.149797
6	-0.151200	3.676210	0.650420
9	-0.087433	4.806770	-0.109769
9	-1.302268	3.756196	1.378238
9	0.875196	3.747014	1.547752

95. $Ga_3As_3H_6$ (Planar), T. E. = -12473.80375

33	1.896013	-1.094730	0.000000
31	-0.000059	-2.403457	0.000000
33	-1.895909	-1.094393	0.000000
31	-2.081446	1.201888	0.000000
33	0.000000	2.189029	0.000000
31	2.081345	1.201601	0.000000
1	3.206828	-1.850257	0.000000
1	0.000327	-3.954370	0.000000
1	-3.206420	-1.850424	0.000000
1	-3.424380	1.977887	0.000000
1	0.000752	3.701971	0.000000
1	3.424438	1.977327	0.000000

96. $Ga_3As_3H_6$ (Puckered), T. E. = -12473.83802

31 -0.179830 -1.739346 0.887365
33 -2.049209 -1.140235 -0.455233
31 -1.748295 1.230625 -0.282995
33 0.225366 2.246573 0.548315
31 1.955680 0.880607 -0.317515
33 1.794789 -1.510806 -0.417266
1 -0.262459 -2.443057 2.284080
1 -3.166743 -1.179810 0.601325
1 -2.963254 2.159860 -0.631742
1 0.326872 3.465750 -0.377295
1 3.309118 1.551147 -0.740739
1 2.861037 -1.734925 0.669897

97. $Ga_3As_3H_3F_3$ (Planar), T. E. = -12771.73325

31 1.981240 1.143869 0.000000
33 0.000000 2.284906 0.000000
31 -1.981240 1.143869 0.000000
33 -1.978787 -1.142453 0.000000
31 0.000000 -2.287738 0.000000
33 1.978787 -1.142453 0.000000
9 3.517494 2.030826 0.000000
1 0.000000 3.788762 0.000000
9 -3.517494 2.030826 0.000000
1 -3.281164 -1.894381 0.000000
9 0.000000 -4.061652 0.000000
1 3.281164 -1.894381 0.000000

98. $Ga_3As_3H_3F_3$ (Puckered), T. E. = -12771.79796

31 0.000101 -1.904134 0.408891
33 -2.100598 -1.355635 -0.567548
31 -1.775354 0.969300 -0.088644
33 -0.000065 2.475889 0.459519
31 1.775277 0.969377 -0.088630
33 2.100636 -1.355449 -0.567667
9 0.000020 -2.901649 1.894009
1 -2.956849 -1.609868 0.678197
9 -3.348041 1.823838 -0.132864
1 -0.000153 3.196131 -0.895117
9 3.348017 1.823836 -0.132597
1 2.957197 -1.609815 0.677809

99. $Ga_3As_3H_3Cl_3$ (Planar), T. E. = -13852.82203

33 0.000000 2.255435 0.000000
31 2.015448 1.163620 0.000000
33 1.953264 -1.127718 0.000000
31 0.000000 -2.327239 0.000000

33 -1.953264 -1.127718 0.000000
31 -2.015448 1.163620 0.000000
1 0.000000 3.760749 0.000000
17 3.877778 2.238836 0.000000
1 3.256904 -1.880375 0.000000
17 0.000000 -4.477673 0.000000
1 -3.256904 -1.880375 0.000000
17 -3.877778 2.238836 0.000000

100. $Ga_3As_3H_3Cl_3$ (Puckered), T. E. = -13852.88285

31 -0.000277 1.938839 0.160913
33 2.038761 1.286322 -0.894463
31 1.756771 -0.954346 -0.062657
33 0.000191 -1.906905 1.234072
31 -1.756542 -0.954567 -0.062695
33 -2.038157 1.285498 -0.896179
17 -0.001325 3.237374 1.897018
1 2.967716 1.675026 0.264508
17 3.418106 -2.292876 -0.474081
1 0.000155 -3.293442 0.586678
17 -3.418195 -2.293099 -0.472829
1 -2.968618 1.674758 0.261376

101. $Ga_3As_3H_3(CN)_3$ (Planar), T. E. = -12750.62750

31 1.164683 -2.015952 0.000000
33 -1.117371 -1.935421 -0.000001
31 -2.329310 -0.000149 0.000000
33 -1.117618 1.935279 0.000000
31 1.164425 2.016101 0.000000
33 2.236552 0.000143 0.000000
1 -1.867607 -3.241140 0.000001
1 -1.868021 3.240901 0.000000
1 3.742458 0.000239 0.000000
6 2.120959 3.676251 0.000000
7 2.702283 4.685739 0.000000
6 2.121430 -3.675979 0.000001
7 2.702884 -4.685393 0.000001
6 -4.245252 -0.000272 0.000000
7 -5.410157 -0.000348 0.000001

102. $Ga_3As_3H_3(CN)_3$ (Puckered), T. E. = -12750.67914

31 -0.491497 1.809292 -0.008829
33 1.190869 1.294670 -1.609059
31 1.817824 -0.406011 -0.020013
33 0.418291 -1.437852 1.636954
31 -1.306162 -1.406307 -0.004667

33 -2.582071 0.619400 -0.103576
1 2.291681 2.253330 -1.135634
1 0.975822 -2.845516 1.403815
1 -2.630995 0.584421 -1.637992
6 -0.154074 3.030310 1.454186
7 0.046099 3.800597 2.306248
6 3.658474 -1.000795 -0.074891
7 4.767819 -1.357998 -0.099488
6 -1.693725 -2.943992 -1.109087
7 -1.959576 -3.889277 -1.737503

103. $Ga_3As_3H_3(CF_3)_3$ (Puckered), T. E. = -13485.06537

31 0.002951 -1.969331 -0.051662
33 2.108862 -1.631890 -1.096087
31 1.726399 0.620660 -0.342945
33 -0.004087 1.943743 -1.256374
31 -1.730859 0.616293 -0.342321
33 -2.105960 -1.638356 -1.092454
1 2.924247 -2.000612 0.150845
1 -0.005406 3.064356 -0.220839
1 -2.918262 -2.007897 0.156262
6 3.173266 1.554919 0.694129
9 4.021815 0.708460 1.336804
9 3.939082 2.310970 -0.151652
9 2.672726 2.400353 1.636809
6 -3.178023 1.549340 0.695529
9 -2.677037 2.387405 1.644560
9 -3.938247 2.313221 -0.148174
9 -4.031821 0.702567 1.330740
6 0.006291 -1.660954 1.949909
9 0.011060 -0.240441 1.974422
9 -1.085592 -2.022830 2.655911
9 1.096468 -2.030521 2.654280

104. $Ga_3O_3H_3$, T. E. = -5996.44454

31 1.605463 0.926915 0.000000
8 0.000000 1.757871 0.000000
31 -1.605463 0.926915 0.000000
8 -1.522361 -0.878936 0.000000
31 0.000000 -1.853829 0.000000
8 1.522361 -0.878936 0.000000
1 2.940588 1.697749 0.000000
1 -2.940588 1.697749 0.000000
1 0.000000 -3.395499 0.000000

105. $Ga_3O_3F_3$, T. E. = -6294.35650

31 -0.895659 1.553815 0.000000
8 0.901664 1.561919 0.000000
31 1.792826 -0.000047 0.000000
8 0.901583 -1.561966 0.000000
31 -0.895740 -1.553768 0.000000
8 -1.798628 0.000047 0.000000
9 -1.775954 3.066319 0.000000
9 3.543045 -0.000092 0.000000
9 -1.776114 -3.066226 0.000000

106. $Ga_3O_3Cl_3$, T. E. = -7375.45854

31 1.580119 0.912282 0.000000
8 0.000000 1.766320 0.000000
31 -1.580119 0.912282 0.000000
8 -1.529678 -0.883160 0.000000
31 0.000000 -1.824564 0.000000
8 1.529678 -0.883160 0.000000
17 3.415340 1.971847 0.000000
17 -3.415340 1.971847 0.000000
17 0.000000 -3.943695 0.000000

107. $Ga3O_3(CN)_3$, T. E. = -6273.26194

31 1.579000 0.911636 0.000000
8 0.000000 1.762184 0.000000
31 -1.579000 0.911636 0.000000
8 -1.526096 -0.881092 0.000000
31 0.000000 -1.823272 0.000000
8 1.526096 -0.881092 0.000000
6 0.000000 -3.726525 0.000000
7 0.000000 -4.889501 0.000000
6 -3.227266 1.863263 0.000000
7 -4.234432 2.444750 0.000000
6 3.227266 1.863263 0.000000
7 4.234432 2.444750 0.000000

108. $Ga_3O_3(CF_3)_3$, T. E. = -7007.63625

31 -1.832735 -0.004262 0.034894
8 -0.881797 -1.530380 0.028603
31 0.913480 -1.583518 -0.043382
8 1.751597 0.004204 -0.127798
31 0.905777 1.587881 -0.043410
8 -0.889261 1.526484 0.028660
6 1.911078 3.309748 0.016450
9 2.182519 3.656670 1.306792
9 3.099331 3.236193 -0.632011
9 1.214550 4.335527 -0.531767

6 -3.827334 -0.009218 0.001698
9 -4.356730 1.081474 0.608337
9 -4.281862 -0.010123 -1.283866
9 -4.351314 -1.102745 0.607945
6 1.926926 -3.300638 0.016459
9 2.199096 -3.646953 1.306814
9 1.235738 -4.329476 -0.532779
9 3.115279 -3.221118 -0.631080

109. $Ga_3S_3H_3$, T. E. = -6965.39621

31 0.000000 2.095208 0.000000
16 1.982482 1.144586 0.000000
31 1.814503 -1.047604 0.000000
16 0.000000 -2.289173 0.000000
31 -1.814503 -1.047604 0.000000
16 -1.982482 1.144586 0.000000
1 0.000000 3.646588 0.000000
1 3.158038 -1.823294 0.000000
1 -3.158038 -1.823294 0.000000

110. $Ga_3S_3F_3$, T. E. = -7263.33082

31 0.988961 1.714730 0.000000
16 -1.174853 2.034433 0.000000
31 -1.979404 -0.000006 0.000000
16 -1.174840 -2.034441 0.000000
31 0.988972 -1.714724 0.000000
16 2.346725 0.000007 0.000000
9 1.880289 3.244896 0.000000
9 -3.750257 -0.000012 0.000000
9 1.880309 -3.244884 0.000000

111. $Ga_3S_3Cl_3$, T. E. = -8344.41929

31 0.000000 2.012788 0.000000
16 2.018624 1.165453 0.000000
31 1.743126 -1.006394 0.000000
16 0.000000 -2.330906 0.000000
31 -1.743126 -1.006394 0.000000
16 -2.018624 1.165453 0.000000
17 0.000000 4.162452 0.000000
17 3.604789 -2.081226 0.000000
17 -3.604789 -2.081226 0.000000

112. $Ga_3S_3(CN)_3$, T. E. = -7242.20750

31 0.000000 2.023982 0.000000
16 2.011408 1.161287 0.000000

31	1.752820	-1.011991	0.000000
16	0.000000	-2.322574	0.000000
31	-1.752820	-1.011991	0.000000
16	-2.011408	1.161287	0.000000
6	-3.424135	-1.976925	0.000000
7	-4.432308	-2.558994	0.000000
6	3.424135	-1.976925	0.000000
7	4.432308	-2.558994	0.000000
6	0.000000	3.953851	0.000000
7	0.000000	5.117989	0.000000

113. $Ga_3S_3(CF_3)_3$, T. E. = -7976.58489

31	-0.221875	2.020448	0.016897
16	-2.123673	0.933297	0.001786
31	-1.638898	-1.202954	-0.018088
16	0.253797	-2.306064	-0.013615
31	1.861296	-0.817776	-0.018679
16	1.870721	1.372765	-0.000037
6	3.708024	-1.629202	0.003029
9	4.138936	-1.825780	1.282527
9	3.750166	-2.837920	-0.616748
9	4.629298	-0.836756	-0.605287
6	-0.442990	4.025128	0.003543
9	0.587754	4.664331	0.616544
9	-0.499240	4.500512	-1.274096
9	-1.584811	4.424532	0.622822
6	-3.265490	-2.395785	0.002566
9	-3.645423	-2.680879	1.281622
9	-4.335885	-1.822297	-0.607231
9	-3.043794	-3.584862	-0.616712

114. $Ga_3Se_3H_3$, T. E. = -12969.05273

31	0.000000	2.168687	0.000000
34	2.102975	1.214153	0.000000
31	1.878138	-1.084344	0.000000
34	0.000000	-2.428306	0.000000
31	-1.878138	-1.084344	0.000000
34	-2.102975	1.214153	0.000000
1	0.000000	3.727445	0.000000
1	3.228062	-1.863722	0.000000
1	-3.228062	-1.863722	0.000000

115. $Ga_3Se_3F_3$, T. E. = -13267.00103

31	0.000000	2.035295	0.000000
34	2.151663	1.242263	0.000000
31	1.762617	-1.017648	0.000000

34 0.000000 -2.484526 0.000000
31 -1.762617 -1.017648 0.000000
34 -2.151663 1.242263 0.000000
9 0.000000 3.812333 0.000000
9 3.301577 -1.906166 0.000000
9 -3.301577 -1.906166 0.000000

116. $Ga_3Se_3Cl_3$, T. E. = -14348.08406

31 0.000000 2.078102 0.000000
34 2.137386 1.234021 0.000000
31 1.799689 -1.039051 0.000000
34 0.000000 -2.468041 0.000000
31 -1.799689 -1.039051 0.000000
34 -2.137386 1.234021 0.000000
17 0.000000 4.237677 0.000000
17 3.669936 -2.118839 0.000000
17 -3.669936 -2.118839 0.000000

117. $Ga_3Se_3(CN)_3$, T. E. = -13245.87766

31 0.000000 2.095705 0.000000
34 2.123398 1.225944 0.000000
31 1.814934 -1.047853 0.000000
34 0.000000 -2.451889 0.000000
31 -1.814934 -1.047853 0.000000
34 -2.123398 1.225944 0.000000
6 -3.488013 -2.013805 0.000000
7 -4.496827 -2.596244 0.000000
6 3.488013 -2.013805 0.000000
7 4.496827 -2.596244 0.000000
6 0.000000 4.027611 0.000000
7 0.000000 5.192489 0.000000

118. $Ga_3Se_3(CF_3)_3$, T. E. = -13980.26107

31 2.030170 -0.599676 -0.000508
34 0.606997 -2.399250 -0.001714
31 -1.492631 -1.469086 -0.001615
34 -2.331109 0.658755 -0.000374
31 -0.483945 2.010961 0.000205
34 1.782640 1.680002 0.000568
6 -1.056702 3.940974 -0.000064
9 -1.818595 4.225669 -1.095144
9 -1.821161 4.225346 1.093306
9 -0.019507 4.816958 0.001280
6 3.989590 -1.066317 0.000622
9 4.617088 -0.542506 -1.091260
9 4.613497 -0.547955 1.097286

9	4.234360	-2.401500	-0.002281
6	-2.997349	-2.807597	0.000996
9	-3.804721	-2.641322	-1.085487
9	-2.577618	-4.098601	-0.009527
9	-3.786079	-2.653174	1.103139

Table S1: Summary of QTAIM delocalization index(δ_{AB}), density at AB bond critical point [$\rho(bcp)$] and its laplacian $\nabla^2\rho$ (bcp), total ELF value at the ring bifurcation (ELF_t) and ELF π component ring bifurcation value (ELF_π) for aluminium heterocyclic rings.

Rings	δ_{AB}	$\rho(bcp)$	$\nabla^2\rho$ (bcp)	ELF_t	ELF_π
$Al_3N_3H_6$	0.42	0.09	0.61	0.13	0.01
$Al_3N_3H_3F_3$	0.40	0.09	0.64	0.06	
$Al_3N_3H_3(CN)_3$	0.41	0.09	0.64		
$Al_3N_3H_3Cl_3$	0.42	0.09	0.63	0.13	
$Al_3N_3H_3(CF_3)_3$	0.43	0.09	0.63		0.02
$Al_3P_3H_6$ (planar)	0.51	0.06	0.16	0.30	
$Al_3P_3H_6$ (puckered)	0.52	0.06	0.14		
$Al_3P_3H_3F_3$ (planar)	0.49	0.07	0.16	0.32	0.02
$Al_3P_3H_3F_3$ (puckered)	0.53	0.07	0.11		
$Al_3P_3H_3Cl_3$ (planar)	0.51	0.07	0.16	0.30	0.02
$Al_3P_3H_3Cl_3$ (puckered)	0.54	0.07	0.11	0.29	
$Al_3P_3H_3(CN)_3$ (planar)	0.52	0.07	0.17	0.32	
$Al_3P_3H_3(CN)_3$ (puckered)	0.54	0.07	0.13		
$Al_3P_3H_3(CF_3)_3$ (planar)	0.53	0.07	0.16	0.32	
$Al_3P_3H_3(CF_3)_3$ (puckered)	0.55	0.07	0.12		
$Al_3As_3H_6$ (planar)	0.54	0.06	0.14	0.34	0.02
$Al_3As_3H_6$ (puckered)	0.55	0.06	0.08	0.34	
$Al_3As_3H_3F_3$ (planar)	0.51	0.07	0.14	0.36	0.02
$Al_3As_3H_3F_3$ (puckered)	0.55	0.06	0.09		0.00
$Al_3As_3H_3Cl_3$ (planar)	0.54	0.06	0.14	0.34	
$Al_3As_3H_3Cl_3$ (puckered)	0.57	0.06	0.09	0.90	
$Al_3As_3H_3(CN)_3$ (planar)	0.54	0.07	0.14		
$Al_3As_3H_3(CN)_3$ (puckered)	0.56	0.06	0.09	0.06	
$Al_3As_3H_3(CF_3)_3$ (puckered)	0.57	0.06	0.09		
$Al_3O_3H_3$	0.38	0.09	0.83		0.01
$Al_3O_3F_3$	0.36	0.10	0.86		0.01
$Al_3O_3Cl_3$	0.38	0.10	0.86		0.01
$Al_3O_3(CN)_3$	0.37	0.10	0.86		0.01
$Al_3O_3(CF_3)_3$	0.38	0.10	0.85		0.08
$Al_3S_3H_3$	0.50	0.07	0.23	0.27	0.01

$Al_3S_3F_3$	0.49	0.07	0.23	0.28	0.01
$Al_3S_3Cl_3$	0.51	0.07	0.23	0.27	0.01
$Al_3S_3(CN)_3$	0.51	0.07	0.23	0.28	0.18
$Al_3S_3(CF_3)_3$	0.52	0.07	0.23	0.27	
$Al_3Se_3H_3$	0.53	0.06	0.17	0.29	0.01
$Al_3Se_3F_3$	0.52	0.07	0.17	0.29	0.01
$Al_3Se_3Cl_3$	0.54	0.07	0.17	0.29	0.01
$Al_3Se_3(CN)_3$	0.55	0.07	0.18	0.30	0.19
$Al_3Se_3(CF_3)_3$	0.55	0.07	0.17	0.29	

Table S2: Summary of QTAIM delocalization index(δ_{AB}), density at AB bond critical point [$\rho(bcp)$] and its laplacian $\nabla^2\rho$ (bcp), total ELF value at the ring bifurcation (ELF_t) and ELF π component ring bifurcation value (ELF_π) for gallium heterocyclic rings.

Rings	δ_{AB}	$\rho(bcp)$	$\nabla^2\rho$ (bcp)	ELF_t	ELF_π
$Ga_3N_3H_6$	0.81	0.12	0.56		
$Ga_3N_3H_3F_3$	0.81	0.12	0.56	0.15	
$Ga_3N_3H_3Cl_3$	0.81	0.12	0.56	0.15	0.01
$Ga_3N_3H_3(CN)_3$	0.81	0.12	0.57	0.16	0.00
$Ga_3N_3H_3(CF_3)_3$	0.82	0.12	0.57		
$Ga_3P_3H_6$ (planar)	0.93	0.09	0.07		0.00
$Ga_3P_3H_6$ (puckered)	0.91	0.09	0.05		
$Ga_3P_3H_3F_3$ (planar)	0.92	0.09	0.06		
$Ga_3P_3H_3F_3$ (puckered)	0.89	0.09	0.03		
$Ga_3P_3H_3Cl_3$ (planar)	0.92	0.09	0.06		0.00
$Ga_3P_3H_3Cl_3$ (puckered)	0.89	0.09	0.03	0.26	
$Ga_3P_3H_3(CN)_3$ (planar)	0.93	0.09	0.06		
$Ga_3P_3H_3(CN)_3$ (puckered)	0.88	0.08	0.02		
$Ga_3P_3H_3(CF_3)_3$ (planar)	0.93	0.09	0.07		0.00
$Ga_3P_3H_3(CF_3)_3$ (puckered)	0.89	0.09	0.03		
$Ga_3As_3H_6$ (planar)	0.94	0.08	0.05		
$Ga_3As_3H_6$ (puckered)	0.90	0.08	0.01		
$Ga_3As_3H_3F_3$ (planar)	0.93	0.09	0.04		0.01

$Ga_3As_3H_3F_3$ (puckered)	0.89	0.08	0.00		
$Ga_3As_3H_3Cl_3$ (planar)	0.94	0.09	0.04		
$Ga_3As_3H_3Cl_3$ (puckered)	0.89	0.08	0.00		
$Ga_3As_3H_3(CN)_3$ (planar)	0.95	0.09	0.04		0.01
$Ga_3As_3H_3(CN)_3$ (puckered)	0.89	0.08	0.00		
$Ga_3As_3H_3(CF_3)_3$ (puckered)	0.90	0.08	0.00		
$Ga_3O_3H_3$	0.73	0.12	0.73	0.12	
$Ga_3O_3F_3$	0.75	0.12	0.75		
$Ga_3O_3Cl_3$	0.73	0.12	0.75	0.13	0.00
$Ga_3O_3(CN)_3$	0.73	0.12	0.76	0.13	
$Ga_3O_3(CF_3)_3$	0.73	0.12	0.75	0.12	
$Ga_3S_3H_3$	0.91	0.09	0.15		0.00
$Ga_3S_3F_3$	0.92	0.09	0.14	0.20	
$Ga_3S_3Cl_3$	0.91	0.09	0.14		0.01
$Ga_3S_3(CN)_3$	0.92	0.09	0.14		0.00
$Ga_3S_3(CF_3)_3$	0.92	0.09	0.15		0.00
$Ga_3Se_3H_3$	0.94	0.08	0.09		0.01
$Ga_3Se_3F_3$	0.94	0.09	0.08	0.21	0.00
$Ga_3Se_3Cl_3$	0.94	0.09	0.08	0.22	0.01
$Ga_3Se_3(CN)_3$	0.95	0.09	0.08	0.23	0.01
$Ga_3Se_3(CF_3)_3$	0.96	0.09	0.08		