Supporting Information for

Effects of the Oxygenation in the Intercalation of 1,10-phenanthroline-5,6/4,7-dione between DNA Base Pairs: A Computational Study

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This Supporting Information includes the frontier orbitals from HOMO-5 to LUMO+5 and Cartesian coordinates of the optimized structures for all the studied systems.

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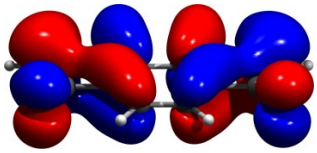
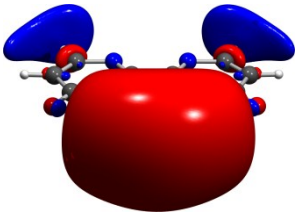
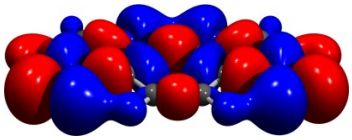


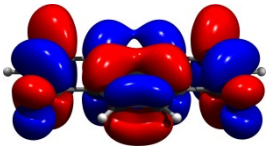
HOMO -0.29968 a.u. (-8.15 eV)



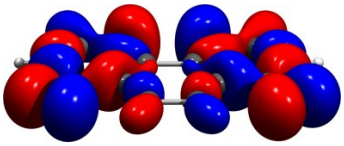
LUMO+5 0.01758 a.u. (0.48 eV)



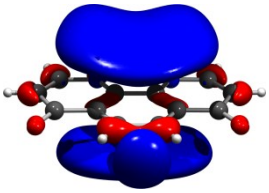
HOMO-1 -0.34535 a.u. (-9.40 eV)



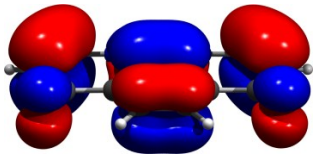
LUMO+4 0.01255 a.u. (0.34 eV)



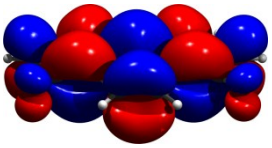
HOMO-2 -0.34884 a.u. (-9.49 eV)



LUMO+3 0.00748 a.u. (0.20 eV)



HOMO-3 -0.35288 a.u. (-9.60 eV)



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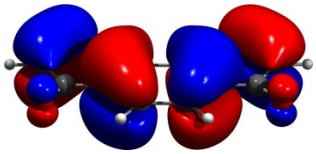
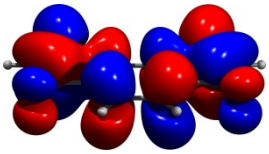
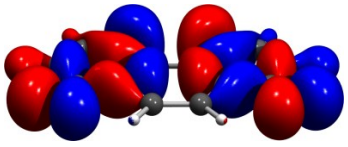


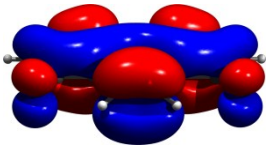
HOMO-4 -0.35752 a.u. (-9.73 eV)



LUMO+1 -0.04820 a.u. (-1.31 eV)



HOMO-5 -0.36103 a.u. (-9.82 eV)



LUMO -0.15238 a.u. (-4.15 eV)

4,7-O_2phen

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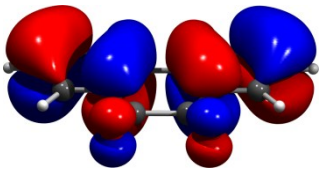
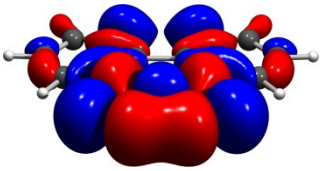
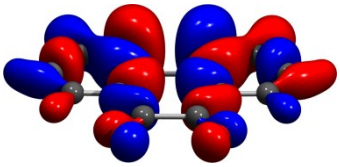


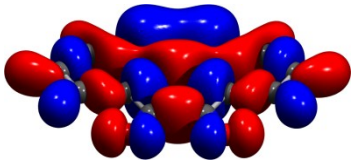
HOMO – 0.31781 a.u. (-8.65 eV)



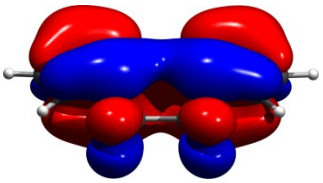
HOMO-1 -0.33350 a.u. (-9.08 eV)



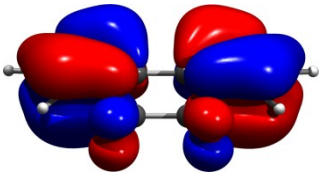
HOMO-2 -0.33720 a.u. (-9.18 eV)



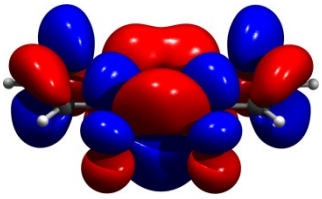
HOMO-3 -0.35663 a.u. (-9.70 eV)



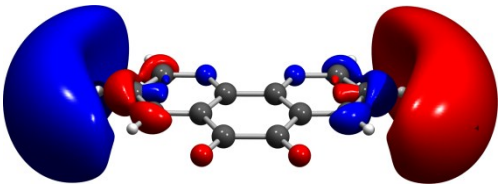
HOMO-4 -0.36411 a.u. (-9.91 eV)



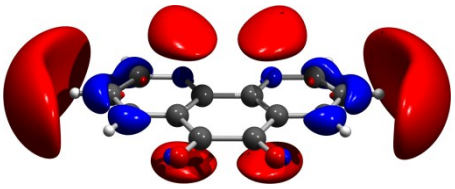
HOMO-5 -0.36455 a.u. (-9.92 eV)



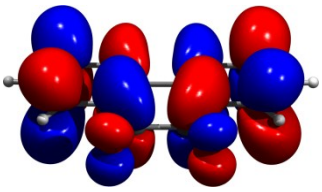
LUMO+5 0.01889 a.u. (0.51 eV)



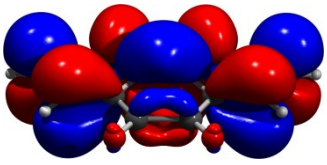
LUMO+4 0.01228 a.u. (0.33 eV)



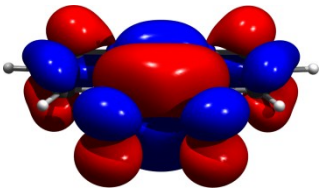
LUMO+3 0.00768 a.u. (0.21 eV)



LUMO+2 -0.02857 a.u. (-0.78 eV)



LUMO+1 -0.04663 a.u. (-1.27 eV)



LUMO -0.09721 a.u. (-2.64 eV)

5,6-O_2phen

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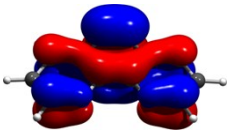
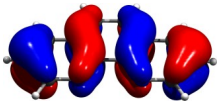
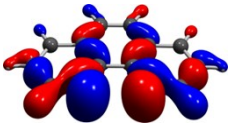


HOMO -0.28519 a.u. (-7.76 eV)



HOMO-1 -0.29881 a.u. (-8.13 eV)



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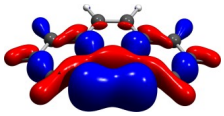
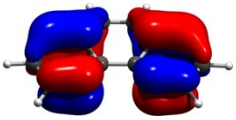
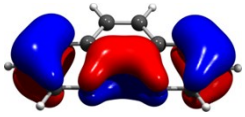


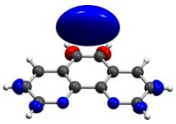
HOMO-3 -0.32991 a.u. (-8.98 eV)



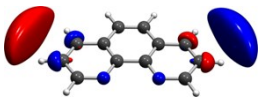
HOMO-4 -0.35618 a.u. (-9.69 eV)



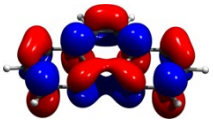
HOMO-5 -0.36389 a.u. (-9.90 eV)



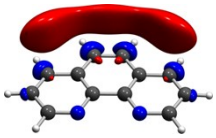
LUMO+5 0.02521 a.u. (0.68 eV)



LUMO+4 0.01784 a.u. (0.48 eV)



LUMO+3 0.01202 a.u. (0.33 eV)



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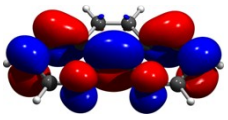
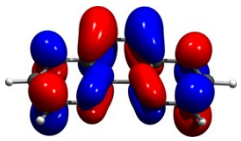


LUMO+1 -0.02846 a.u. (-0.77 eV)



LUMO -0.03123 a.u. (-0.85 eV)

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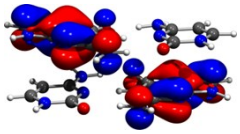
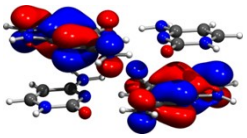
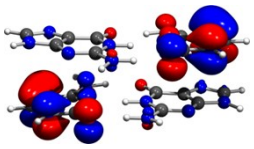


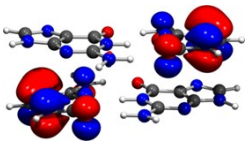
HOMO -0.24452 a.u. (-6.65 eV)



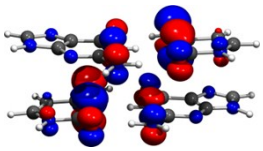
HOMO-1 -0.25033 a.u. (-6.81 eV)



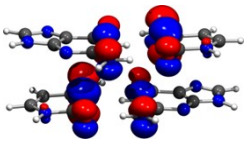
HOMO-2 -0.29700 a.u. (-8.08 eV)



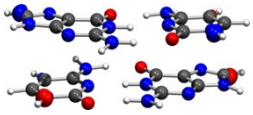
HOMO-3 -0.29795 a.u. (-8.11 eV)



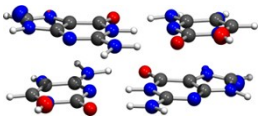
HOMO-4 -0.30504 a.u. (-8.30 eV)



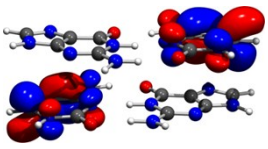
HOMO-5 -0.30906 a.u. (-8.41 eV)



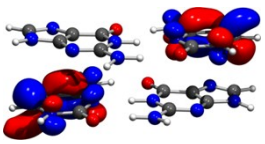
LUMO+5 0.01510 a.u. (0.41 eV)



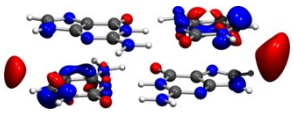
LUMO+4 0.01333 a.u. (0.36 eV)



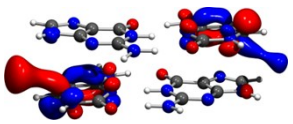
LUMO+3 -0.00825 a.u. (-0.22 eV)



LUMO+2 -0.00914 a.u. (-0.25 eV)



LUMO+1 -0.01205 a.u. (-0.33 eV)



LUMO -0.01271 a.u. (-0.34 eV)

GC/CG

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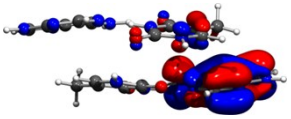
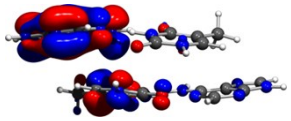
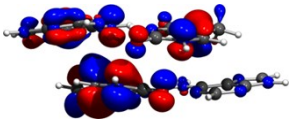


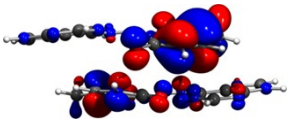
HOMO -0.27540 a.u. (-7.49 eV)



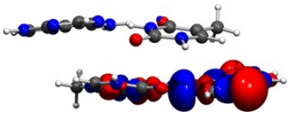
HOMO-1 -0.27862 a.u. (-7.58 eV)



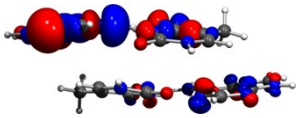
HOMO-2 -0.28712 a.u. (-7.81 eV)



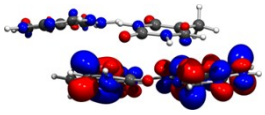
HOMO-3 -0.29013 a.u. (-7.89 eV)



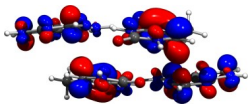
HOMO-4 -0.32667 a.u. (-8.89 eV)



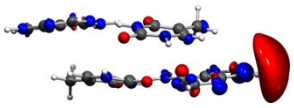
HOMO-5 -0.33071 a.u. (-9.00 eV)



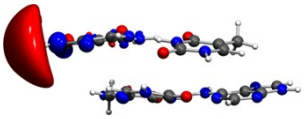
LUMO+5 0.00388 a.u. (0.10 eV)



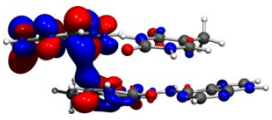
LUMO+4 0.00164 a.u. (0.04 eV)



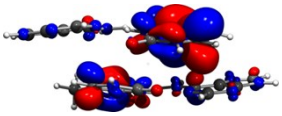
LUMO+3 0.00019 a.u. (0.00 eV)



LUMO+2 -0.00158 (-0.04 eV)



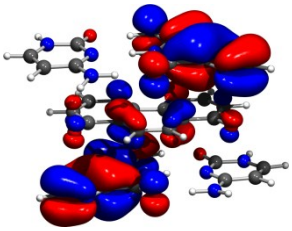
LUMO+1 -0.00537 (-0.15 eV)



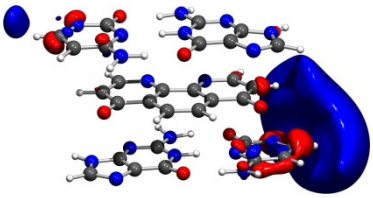
LUMO -0.00788 (-0.21 eV)

AT/TA

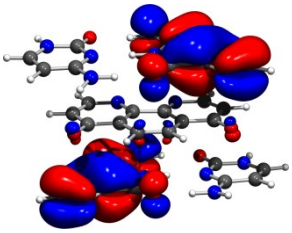
(continued)



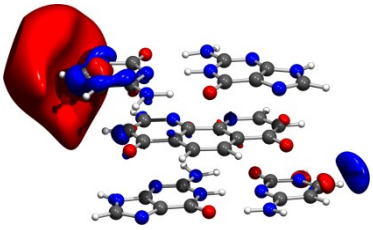
HOMO -0.24136 a.u. (-6.57 eV)



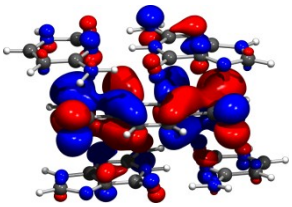
LUMO+5 -0.01084 a.u. (-0.29 eV)



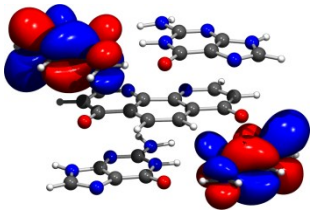
HOMO-1 -0.24996 a.u. (-6.80 eV)



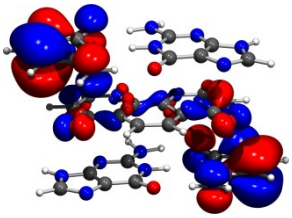
LUMO+4 -0.01099 a.u. (-0.30 eV)



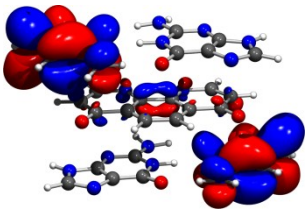
HOMO-2 -0.27692 a.u. (-7.54 eV)



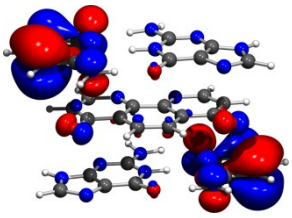
LUMO+3 -0.01856 a.u. (-0.50 eV)



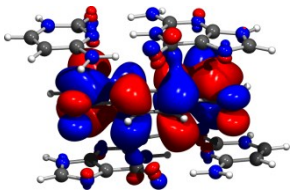
HOMO-3 -0.30644 a.u. (-8.34 eV)



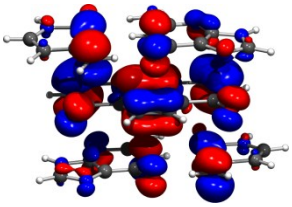
LUMO+2 –0.01984 a.u. (-0.54 eV)



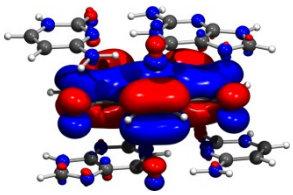
HOMO-4 -0.30661 a.u. (-8.34 eV)



LUMO+1 -0.02617 a.u. (-0.71 eV)



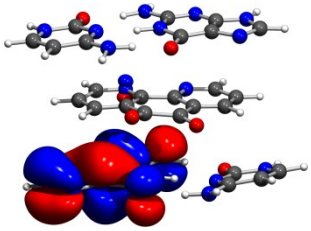
HOMO-5 -0.31280 a.u. (-8.51 eV)



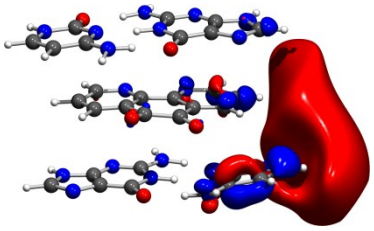
LUMO -0.12102 a.u. (-3.29 eV)

(GC/4,7-O_2phen/CG)mg

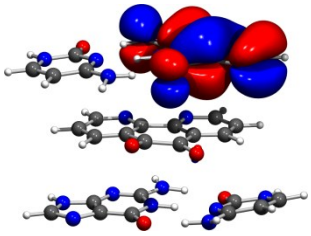
(continued)



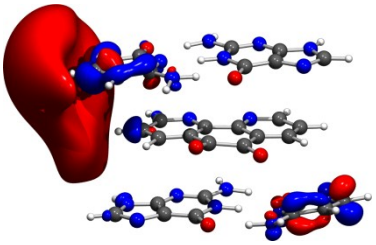
HOMO -0.24540 a.u. (-6.68 eV)



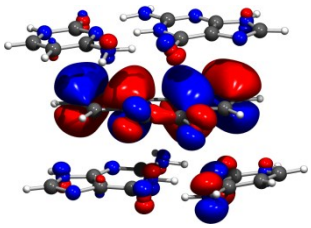
LUMO+5 -0.01221 a.u. (-0.33 eV)



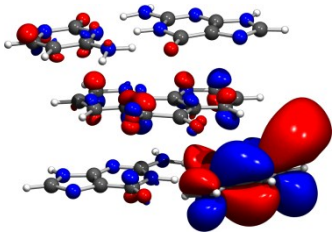
HOMO-1 -0.25010 a.u. (-6.80 eV)



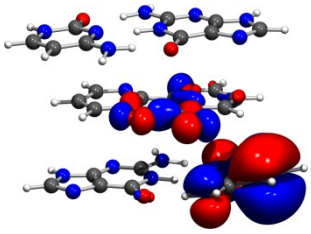
LUMO+4 -0.01495 a.u. (-0.41 eV)



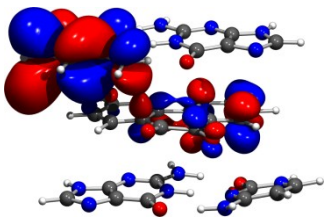
HOMO-2 -0.29369 a.u. (-7.99 eV)



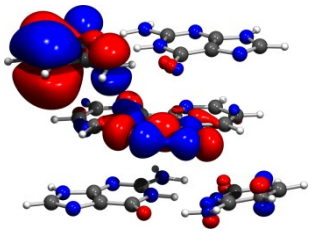
LUMO+3 -0.01710 a.u. (-0.46 eV)



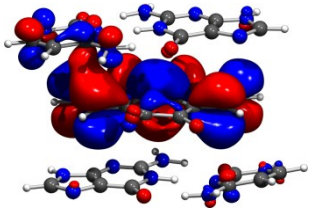
HOMO-3 -0.30479 a.u. (-8.29 eV)



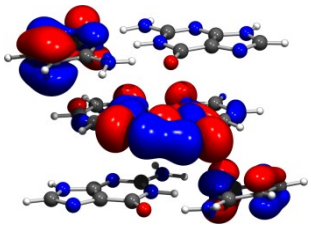
LUMO+2 -0.02270 a.u. (-0.62 eV)



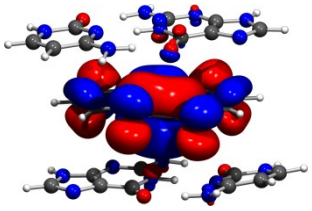
HOMO-4 -0.31023 a.u. (-8.44 eV)



LUMO+1 -0.03118 a.u. (-0.85 eV)



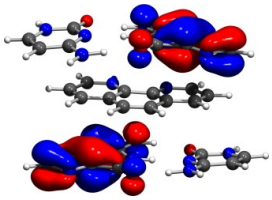
HOMO-5 -0.31187 a.u. (-8.49 eV)



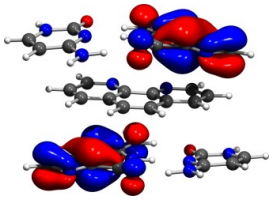
LUMO -0.07214 a.u. (-1.96 eV)

(GC/5,6-O_2phen/CG)mg

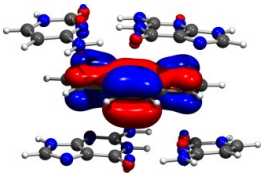
(continued)



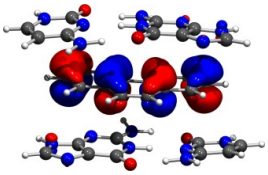
HOMO -0.24304 a.u. (-6.61 eV)



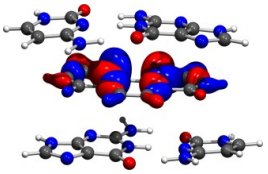
HOMO-1 -0.24395 a.u. (-6.64 eV)



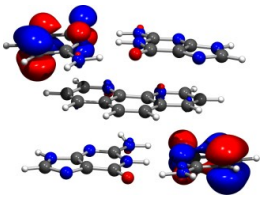
HOMO-2 -0.26867 a.u. (-7.31 eV)



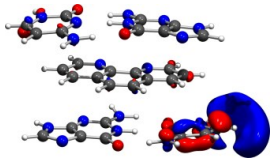
HOMO-3 -0.28834 a.u. (-7.85 eV)



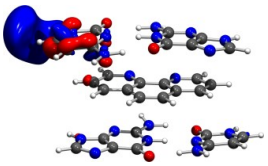
HOMO-4 -0.30522 a.u. (-8.30 eV)



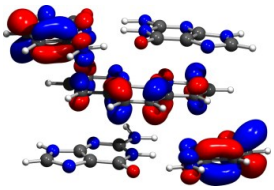
HOMO-5 -0.30780 a.u. (-8.38 eV)



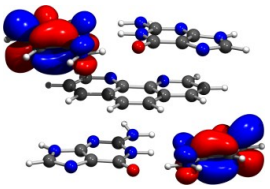
LUMO+5 -0.01458 a.u. (-0.40 eV)



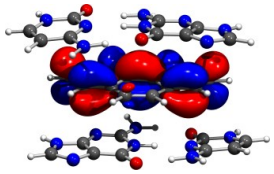
LUMO+4 -0.01474 a.u. (-0.40 eV)



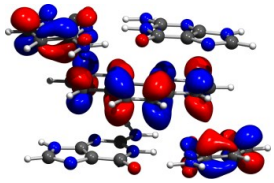
LUMO+3 -0.01755 a.u. (-0.48 eV)



LUMO+2 -0.02117 (-0.58 eV)



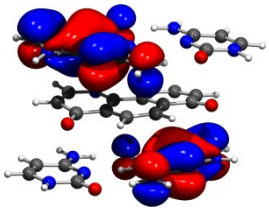
LUMO+1 -0.02428 (-0.66 eV)



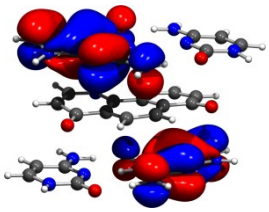
LUMO -0.02670 (-0.73 eV)

(GC/phen/CG)mg

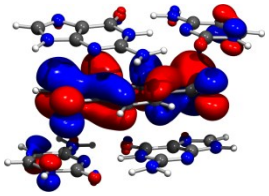
(continued)



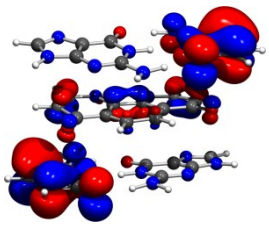
HOMO -0.25146 a.u. (-6.84 eV)



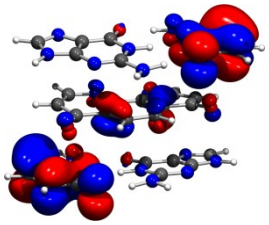
HOMO-1 -0.25189 a.u. (-6.85 eV)



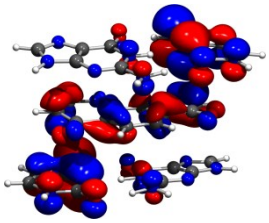
HOMO-2 -0.27489 a.u. (-7.48 eV)



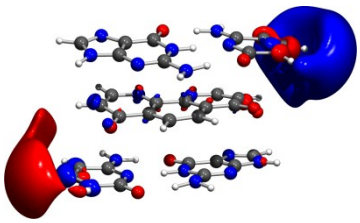
HOMO-3 -0.30426 a.u. (-8.28 eV)



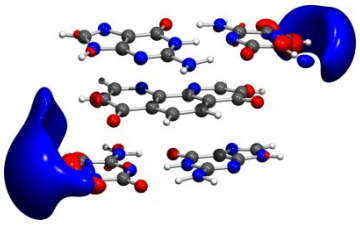
HOMO-4 -0.30692 a.u. (-8.35 eV)



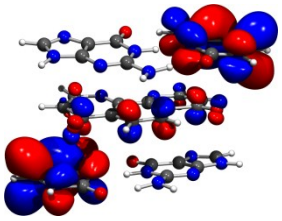
HOMO-5 -0.31792 a.u. (-8.65 eV)



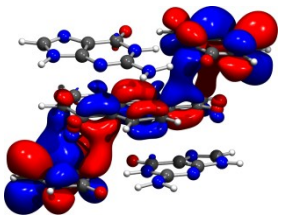
LUMO+5 -0.00835 a.u. (-0.23 eV)



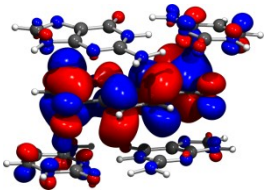
LUMO+4 -0.00851 a.u. (-0.23 eV)



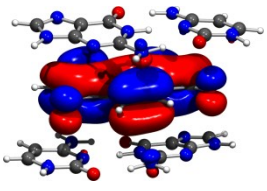
LUMO+3 -0.01617 a.u. (-0.44 eV)



LUMO+2 -0.02174 a.u. (-0.59 eV)



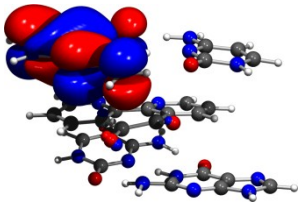
LUMO+1 -0.03110 a.u. (-0.85 eV)



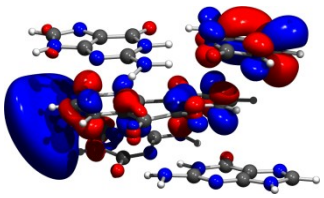
LUMO -0.12671 a.u. (-3.45 eV)

(GC/4,7-O_2phen/CG)MG

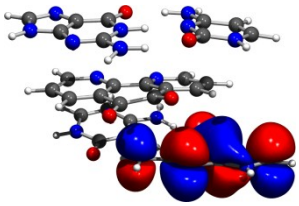
(continued)



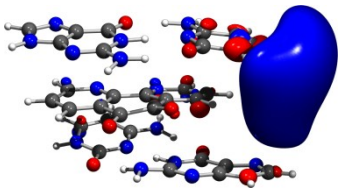
HOMO -0.24750 a.u. (-6.73 eV)



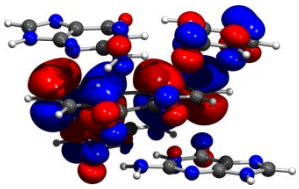
LUMO+5 -0.01082 a.u. (-0.29 eV)



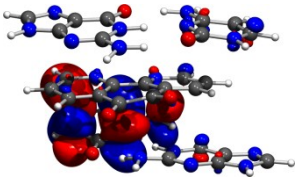
HOMO-1 -0.25528 a.u. (-6.95 eV)



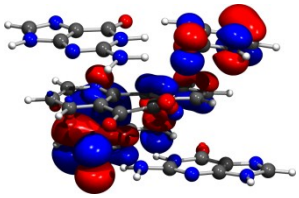
LUMO+4 -0.01284 a.u. (-0.35 eV)



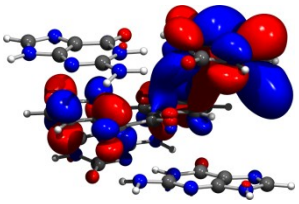
HOMO-2 -0.29383 a.u. (-8.00 eV)



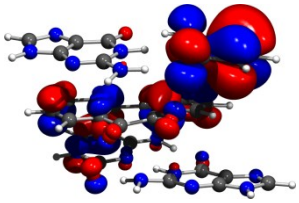
LUMO+3 -0.01446 a.u. (-0.39 eV)



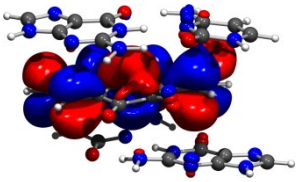
HOMO-3 -0.30285 a.u. (-8.24 eV)



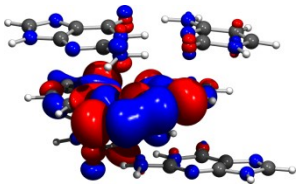
LUMO+2 -0.02308 a.u. (-0.63 eV)



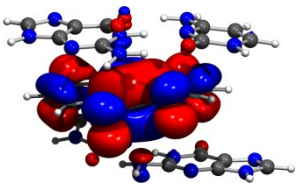
HOMO-4 -0.30789 a.u. (-8.38 eV)



LUMO+1 -0.03241 a.u. (-0.88 eV)



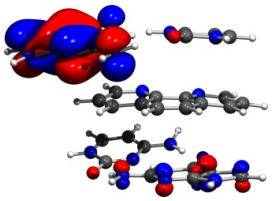
HOMO-5 -0.31389 a.u. (-8.54 eV)



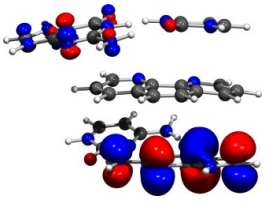
LUMO -0.07507 a.u. (-2.04 eV)

(GC/5,6-O_2phen/CG)MG

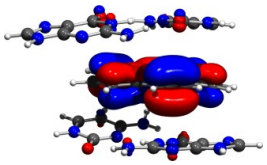
(continued)



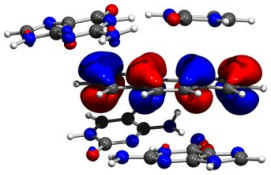
HOMO -0.24812 a.u. (-6.75 eV)



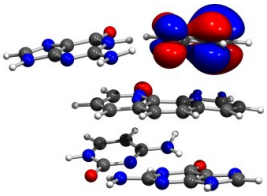
HOMO-1 -0.25120 a.u. (-6.84 eV)



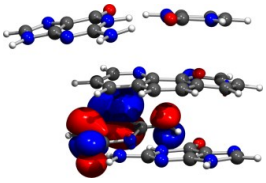
HOMO-2 -0.27463 a.u. (-7.47 eV)



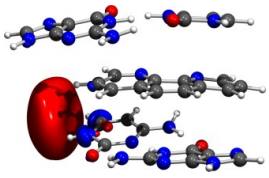
HOMO-3 -0.29041 a.u. (-7.90 eV)



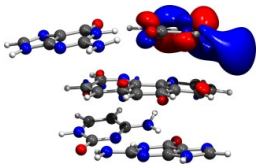
HOMO-4 -0.29930 a.u. (-8.14 eV)



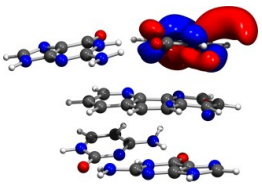
HOMO-5 -0.30780 a.u. (-8.38 eV)



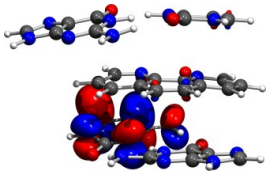
LUMO+5 -0.00522 a.u. (-0.14 eV)



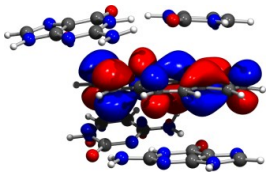
LUMO+4 -0.00789 a.u. (-0.21 eV)



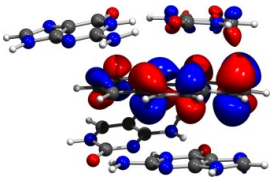
LUMO+3 -0.01007 a.u. (-0.27 eV)



LUMO+2 -0.01176 (-0.32 eV)



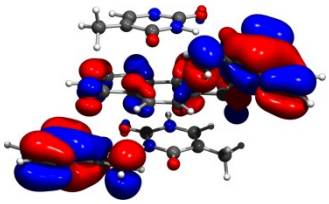
LUMO+1 -0.02679 (-0.73 eV)



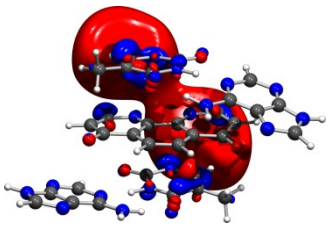
LUMO -0.02943 (-0.80 eV)

(GC/phen/CG)MG

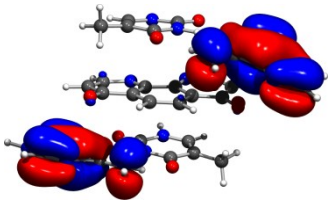
(continued)



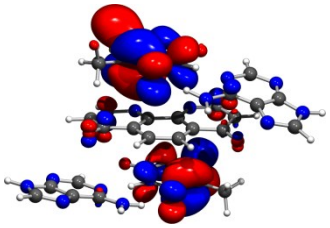
HOMO -0.26916 a.u. (-7.32 eV)



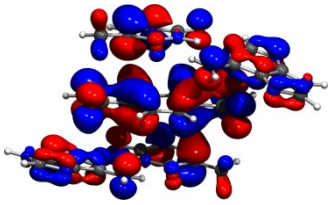
LUMO+5 -0.00234 a.u. (-0.06 eV)



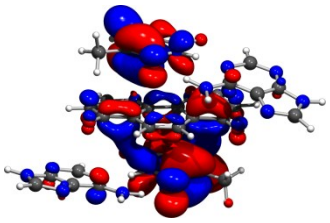
HOMO-1 -0.27220 a.u. (-7.41 eV)



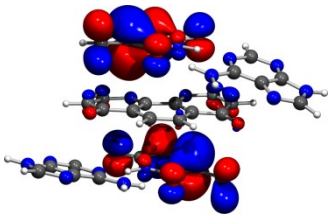
LUMO+4 -0.01029 a.u. (-0.28 eV)



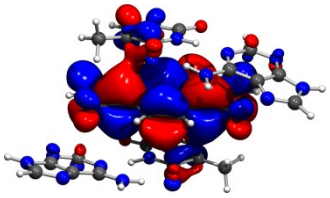
HOMO-2 -0.28638 a.u. (-7.79 eV)



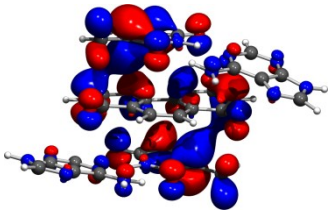
LUMO+3 -0.01108 a.u. (-0.30 eV)



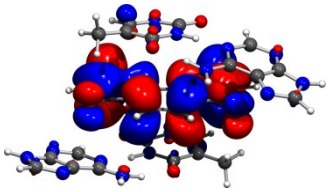
HOMO-3 -0.29458 a.u. (-8.02 eV)



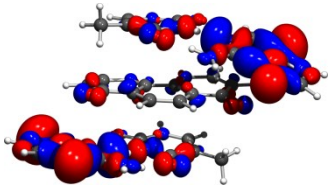
LUMO+2 -0.01828 a.u. (-0.50 eV)



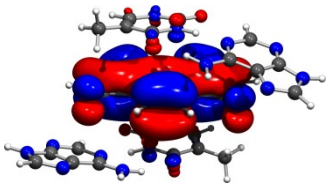
HOMO-4 -0.29720 a.u. (-8.09 eV)



LUMO+1 -0.03705 a.u. (-1.01 eV)



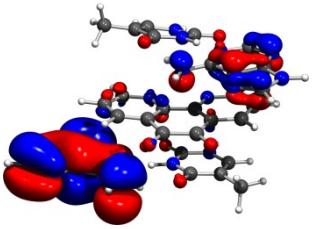
HOMO-5 -0.32506 a.u. (-8.84 eV)



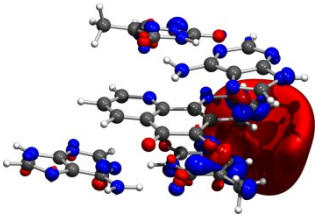
LUMO -0.13670 a.u. (-3.72 eV)

(AT/4,7-O_2phen/TA)mg

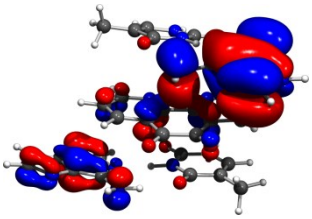
(continued)



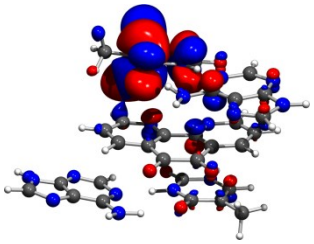
HOMO -0.27577 a.u. (-7.50 eV)



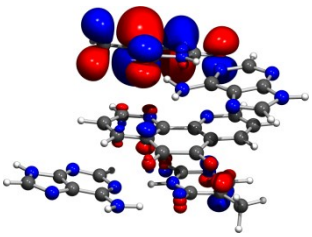
LUMO+5 -0.00378 a.u. (-0.10 eV)



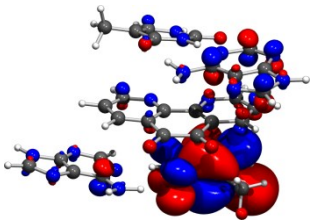
HOMO-1 -0.27809 a.u. (-7.57 eV)



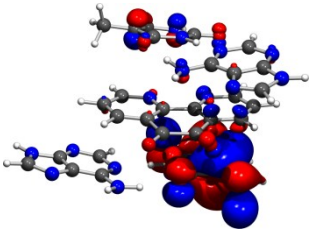
LUMO+4 -0.00661 a.u. (-0.18 eV)



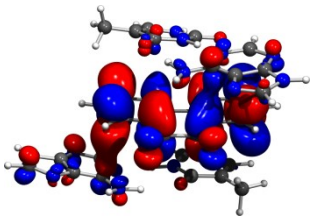
HOMO-2 -0.28920 a.u. (-7.87 eV)



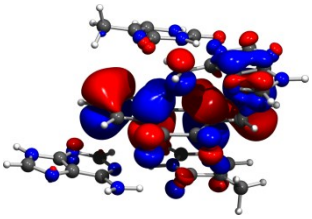
LUMO+3 -0.00862 a.u. (-0.23 eV)



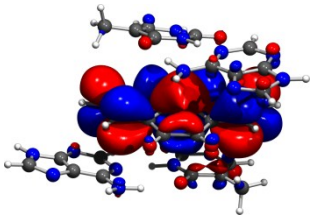
HOMO-3 -0.29067 a.u. (-7.91 eV)



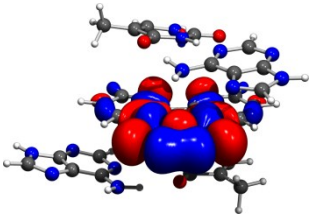
LUMO+2 -0.01622 a.u. (-0.44 eV)



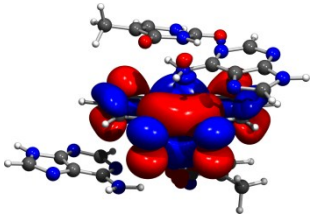
HOMO-4 -0.30148 a.u. (-8.20 eV)



LUMO+1 -0.03505 a.u. (-0.95 eV)



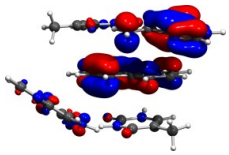
HOMO-5 -0.31407 a.u. (-8.55 eV)



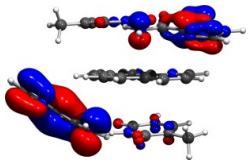
LUMO -0.07420 a.u. (-2.02 eV)

(AT/5,6-O_2phen/TA)mg

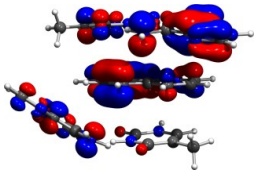
(continued)



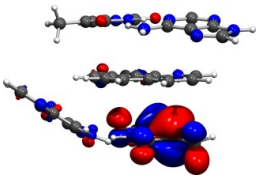
HOMO -0.27268 a.u. (-7.42 eV)



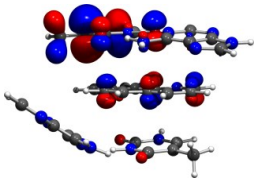
HOMO-1 -0.27862 a.u. (-7.58 eV)



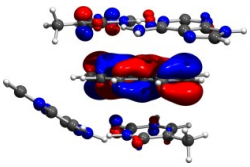
HOMO-2 -0.28256 a.u. (-7.69 eV)



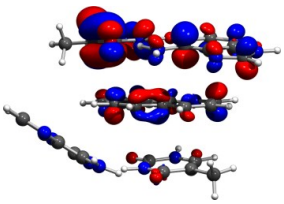
HOMO-3 -0.28420 a.u. (-7.73 eV)



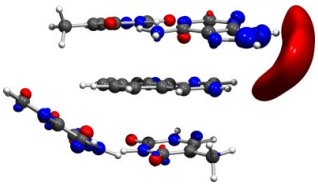
HOMO-4 -0.28924 a.u. (-7.87 eV)



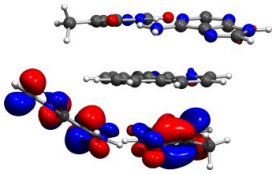
HOMO-5 -0.29454 a.u. (-8.01 eV)



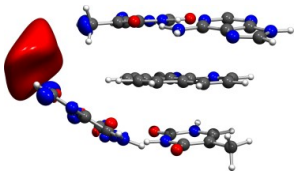
LUMO+5 -0.00163 a.u. (-0.04 eV)



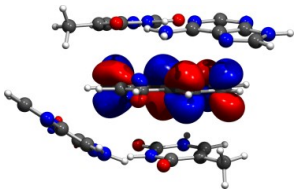
LUMO+4 -0.00225 a.u. (-0.06 eV)



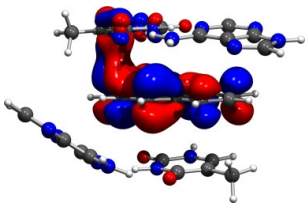
LUMO+3 -0.00421 a.u. (-0.11 eV)



LUMO+2 -0.00636 (-0.17 eV)



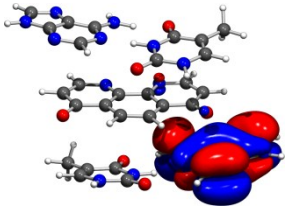
LUMO+1 -0.02897 (-0.79 eV)



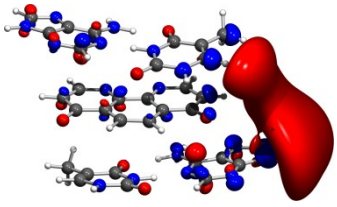
LUMO -0.03379 (-0.92 eV)

(AT/phen/TA)mg

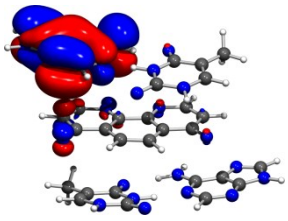
(continued)



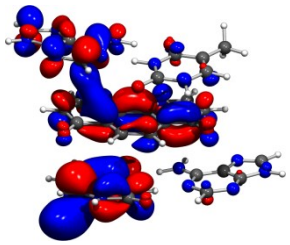
HOMO -0.27414 a.u. (-7.46 eV)



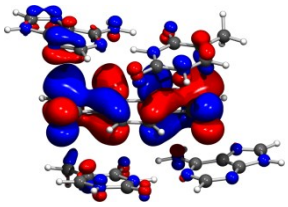
LUMO+5 -0.00179 a.u. (-0.05 eV)



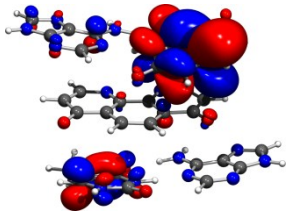
HOMO-1 -0.27524 a.u. (-7.49 eV)



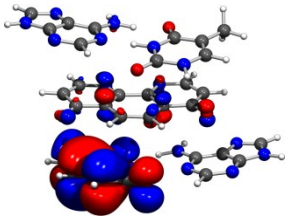
LUMO+4 -0.00382 a.u. (-0.10 eV)



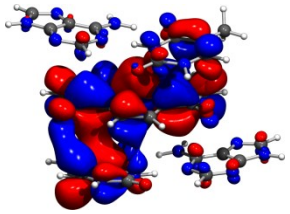
HOMO-2 -0.28337 a.u. (-7.71 eV)



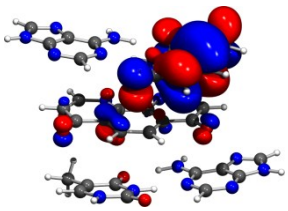
LUMO+3 -0.01038 a.u. (-0.28 eV)



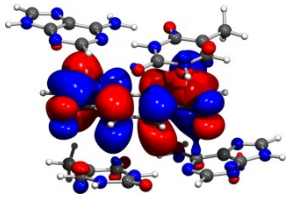
HOMO-3 -0.29338 a.u. (-7.98 eV)



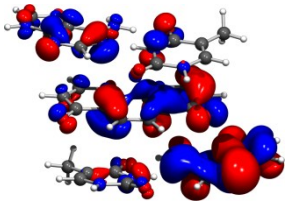
LUMO+2 -0.02009 a.u. (-0.55 eV)



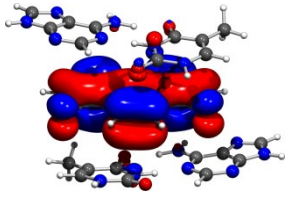
HOMO-4 -0.29539 a.u. (-8.04 eV)



LUMO+1 -0.03575 a.u. (-0.97 eV)



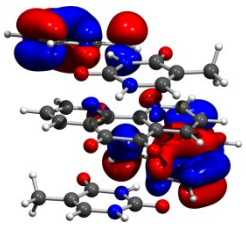
HOMO-5 -0.32221 a.u. (-8.77 eV)



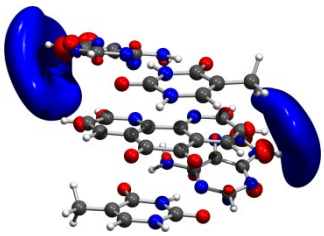
LUMO -0.13260 a.u. (-3.61 eV)

(AT/4,7-O_2phen/TA)MG

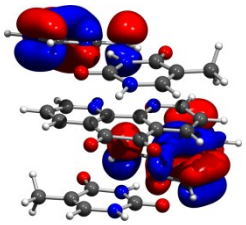
(continued)



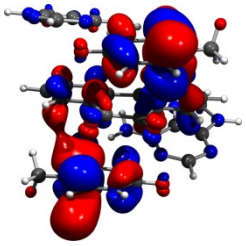
HOMO -0.27157 a.u. (-7.39 eV)



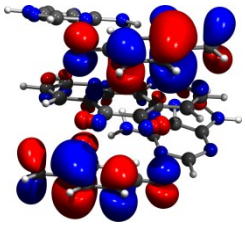
LUMO+5 0.00005 a.u. (0.00 eV)



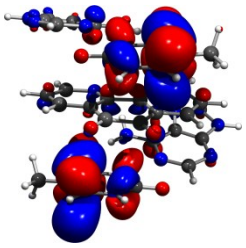
HOMO-1 -0.27390 a.u. (-7.45 eV)



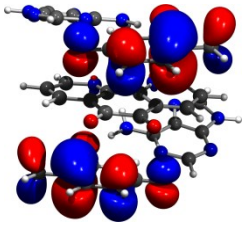
LUMO+4 -0.00296 a.u. (-0.08 eV)



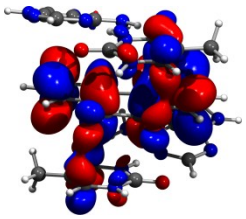
HOMO-2 -0.29135 a.u. (-7.93 eV)



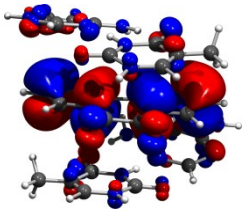
LUMO+3 -0.00757 a.u. (-0.20 eV)



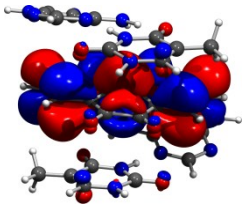
HOMO-3 -0.29330 a.u. (-7.98 eV)



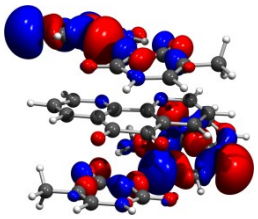
LUMO+2 -0.02505 a.u. (-0.68 eV)



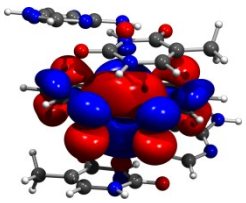
HOMO-4 -0.30185 a.u. (-8.21 eV)



LUMO+1 -0.03654 a.u. (-0.99 eV)



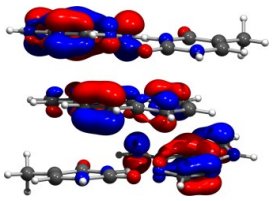
HOMO-5 -0.32527 a.u. (-8.85 eV)



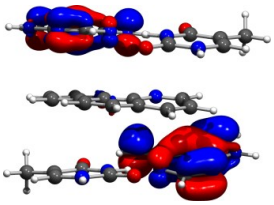
LUMO -0.09336 a.u. (-2.54 eV)

(AT/5,6-O_2phen/TA)MG

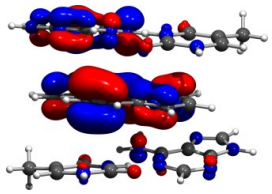
(continued)



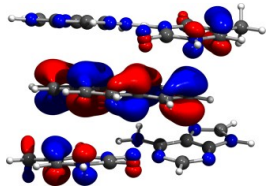
HOMO -0.25985 a.u. (-7.07 eV)



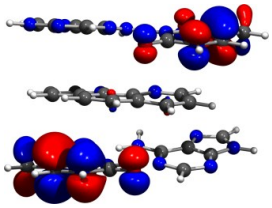
HOMO-1 -0.26596 a.u. (-7.24 eV)



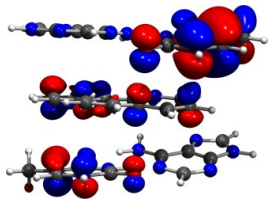
HOMO-2 -0.27775 a.u. (-7.56 eV)



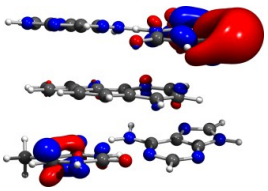
HOMO-3 -0.28479 a.u. (-7.75 eV)



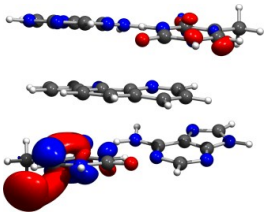
HOMO-4 -0.29200 a.u. (-7.94 eV)



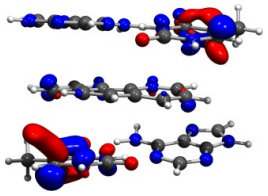
HOMO-5 -0.29359 a.u. (-7.99 eV)



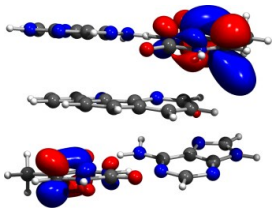
LUMO+5 -0.00368 a.u. (-0.10 eV)



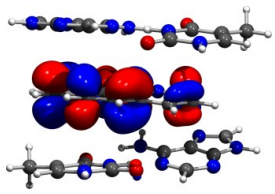
LUMO+4 -0.00379 a.u. (-0.10 eV)



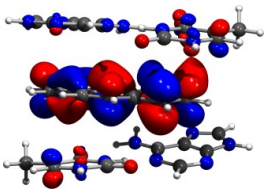
LUMO+3 -0.00760 a.u. (-0.21 eV)



LUMO+2 -0.00861 a.u. (-0.23 eV)



LUMO+1 -0.02214 a.u. (-0.60 eV)



LUMO -0.02439 a.u. (-0.66 eV)

(AT/phen/TA)MG

Figure S1. Frontier Molecular Orbitals (from HOMO-5 to LUMO+5) for 4,7-O_2phen, 5,6-O_2phen, phen, AT/TA, GC/CG, (GC/4,7-O_2phen/CG)mg, (GC/5,6-O_2phen/CG)mg, (GC/phen/CG)mg, (GC/4,7-O_2phen/CG)MG, (GC/5,6-O_2phen/CG)MG, (GC/phen/CG)MG, (AT/4,7-O_2phen/TA)mg, (AT/5,6-O_2phen/TA)mg, (AT/phen/TA)mg, (AT/4,7-O_2phen/TA)MG, (AT/5,6-O_2phen/TA)MG, and (AT/phen/TA)mg systems calculated at M06-2X/6-31+G(d,p) level of theory.

Table S1. Cartesian coordinates of the optimized structures, at M06-2X/6-31+G(d,p) level, corresponding to: phen, 4,7-O_2phen, 5,6-O_2phen, GC/CG, (GC/phen/CG)mg, (GC/4,7-O_2phen/CG)mg, (GC/5,6-O_2phen/CG)mg, (GC/phen/CG)MG, (GC/4,7-O_2phen/CG)MG, (GC/5,6-O_2phen/CG)MG, AT/TA, (AT/phen/TA)mg, (AT/4,7-O_2phen/TA)mg, (AT/5,6-O_2phen/TA)mg, (AT/phen/TA)MG, (AT/4,7-O_2phen/TA)MG and (AT/5,6-O_2phen/TA)MG.

22

phen (M06-2X/6-31+G(d,p))

```
C   -5.088753   0.053182   1.700749
C   -4.737382  -1.311917   1.744765
N   -3.496367  -1.755479   1.730055
C   -2.497779  -0.850526   1.669292
C   -2.736317   0.544554   1.620874
C   -4.076880   0.982714   1.638353
C   -1.637785   1.469323   1.556388
C   -0.357603   1.024403   1.540871
C   -0.068078  -0.382837   1.588557
C   -1.119225  -1.329657   1.652953
N   -0.895856  -2.659254   1.699031
C    0.352765  -3.080985   1.683618
C    1.473796  -2.227662   1.621736
C    1.255283  -0.870575   1.573898
H   -4.290926   2.047840   1.602361
H    2.082747  -0.167373   1.525166
H   -5.516354  -2.070073   1.794433
H   -6.132115   0.348525   1.716485
H    0.494694  -4.159161   1.722243
H    2.475529  -2.643047   1.612572
H    0.473942   1.722189   1.492624
H   -1.858450   2.532661   1.520504
```

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4,7-O_2phen (M06-2X/6-31+G(d,p))

```
N  0.015655 0.000000 -0.016377
C 0.007996 0.000000 1.377079
H 0.979141 0.000000 1.829655
C -1.111757 0.000000 -0.650568
C -1.105766 0.000000 -2.143863
C -2.409668 0.000000 0.023907
C -3.566174 0.000000 -0.684743
C -2.440381 0.000000 1.517885
C -3.560253 0.000000 -2.129453
C -1.118336 0.000000 2.147470
O -3.489699 0.000000 2.142839
H -1.067503 0.000000 3.230493
C -2.398108 0.000000 -2.828644
N 0.026870 0.000000 -2.769022
C 0.014210 0.000000 -4.162808
C -1.089988 0.000000 -4.941802
H 1.004916 0.000000 -4.607449
```

H -1.030699 0.000000 -6.024414
C -2.416913 0.000000 -4.322714
O -3.461284 0.000000 -4.956039
H -4.497027 0.000000 -2.680967
H -4.507454 0.000000 -0.140954

22

5,6-O_2phen (M06-2X/6-31+G(d,p))

C -2.326602 0.000000 -4.257574
C -2.367289 0.000000 -2.862010
C -1.158462 0.000000 -2.144696
N 0.029710 0.000000 -2.753710
C 0.051505 -0.000000 -4.083887
C -1.092834 -0.000000 -4.887176
C -3.687519 -0.000000 -2.180385
C -3.693699 -0.000000 -0.634733
C -2.378957 -0.000000 0.057427
C -1.164417 -0.000000 -0.650198
C -2.349457 -0.000000 1.453256
C -1.120774 0.000000 2.092722
C 0.029957 0.000000 1.298643
N 0.018839 0.000000 -0.031678
H -3.288844 -0.000000 1.996685
H -3.261604 0.000000 -4.808509
H 1.013895 0.000000 1.761846
H -1.042285 0.000000 3.173998
H 1.039125 -0.000000 -4.539194
H -1.005667 -0.000000 -5.967789
O -4.735942 0.000000 -2.780458
O -4.746890 -0.000000 -0.043068

58

GC/CG (M06-2X/6-31+G(d,p))

N -2.007835 1.234334 -0.007559
C -2.757137 0.099465 -0.027219
H -3.833586 0.230103 -0.037213
C -2.160774 -1.112483 -0.033858
H -2.731147 -2.030667 -0.060240
C -0.716504 -1.126753 -0.038680
N -0.065171 -2.287305 -0.071545
H 0.960322 -2.296298 -0.136609
H -0.565303 -3.125908 -0.324657
N 0.000000 0.000000 0.000000
C -0.609709 1.211931 0.000000
O -0.006628 2.287563 0.003313
H -2.426261 2.153050 -0.049096
N 6.856555 -0.132779 0.379375

C	7.021050	-1.505029	0.381475
H	7.997939	-1.959161	0.473009
N	5.893286	-2.148365	0.267884
C	4.934788	-1.157252	0.202358
C	3.506207	-1.232944	0.083837
O	2.800301	-2.237141	0.001054
N	2.928046	0.041393	0.063417
H	1.893924	0.056511	0.000000
C	3.609794	1.231945	0.084720
N	2.870632	2.350089	0.022521
H	1.850746	2.333755	-0.056186
H	3.375492	3.214455	-0.087568
N	4.928428	1.316459	0.176909
C	5.514211	0.105978	0.253649
H	7.567075	0.574768	0.489073
N	6.154414	1.218376	-2.935267
C	6.902522	0.083246	-2.897392
H	7.979156	0.212835	-2.894996
C	6.304902	-1.127706	-2.864452
H	6.874471	-2.045849	-2.823086
C	4.860728	-1.140196	-2.853293
N	4.208592	-2.299395	-2.796170
H	3.183363	-2.306037	-2.726678
H	4.709143	-3.133504	-2.529255
N	4.145253	-0.013578	-2.910543
C	4.756131	1.197507	-2.936969
O	4.154100	2.273422	-2.959995
H	6.574177	2.137222	-2.916233
N	-2.710286	-0.152841	-3.294883
C	-2.872728	-1.525215	-3.270371
H	-3.848751	-1.982478	-3.355476
N	-1.744426	-2.164388	-3.140631
C	-0.787614	-1.170636	-3.092179
C	0.640587	-1.241597	-2.967698
O	1.346961	-2.242936	-2.859077
N	1.217523	0.033454	-2.975794
H	2.251672	0.050526	-2.911986
C	0.534492	1.222335	-3.026801
N	1.272831	2.342379	-2.992850

H	2.292223	2.327909	-2.909026
H	0.767545	3.209104	-2.905992
N	-0.784198	1.303024	-3.121472
C	-1.368489	0.090382	-3.171634
H	-3.421152	0.551124	-3.423996

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(GC/phen/CG)mg (M06-2X/6-31+G(d,p))

C	3.326747	-1.402255	-3.127548
C	3.485747	-1.2378	0.052145
C	4.91586	-1.180376	0.010283
C	5.488288	-0.178822	-3.17317
C	4.076684	-0.179887	-3.190711
C	5.510193	0.076916	-0.06198
N	6.852989	-0.175675	-0.093824
C	7.004435	-1.549799	-0.055942
N	5.866934	-2.181546	0.004717
N	4.934028	1.290908	-0.131868
C	3.614554	1.223238	-0.107581
N	2.922365	0.040586	-0.004395
C	3.416297	1.071684	-3.252645
C	6.159142	1.016934	-3.255822
O	2.759638	-2.234004	0.117682
N	4.086055	2.243977	-3.338904
N	2.881891	2.349175	-0.169945
C	5.402051	2.205208	-3.349819
C	1.970795	-1.380564	-3.125515
C	1.259874	-0.133957	-3.16424
C	1.959301	1.096699	-3.206674
N	1.326696	2.29281	-3.217604
O	-0.04117	2.284771	0.087739
C	-0.622429	1.206309	0.000000
N	0.000000	0.000000	0.000000
N	-2.022131	1.210254	-0.107777
C	-2.743314	0.075581	-0.296826
C	-2.122264	-1.124774	-0.35822
C	-0.685815	-1.122589	-0.196776
C	-0.784035	1.128936	-3.198822

N	0.43448	1.105831	-6.331647
C	-0.163086	-0.099498	-6.30319
C	-0.151294	-0.089883	-3.180919
C	0.010379	2.296568	-3.203887
C	0.408952	-1.368868	-6.275862
C	1.837737	-1.454735	-6.316413
N	2.423641	-0.186095	-6.361656
C	1.752572	1.013073	-6.352119
N	-1.510067	-0.325087	-6.249528
C	-1.685566	-1.694998	-6.177883
N	-0.55942	-2.349481	-6.189536
O	2.545987	-2.465745	-6.306172
N	2.504952	2.12726	-6.380608
N	-0.003329	-2.266807	-0.260744
O	5.427885	1.990463	-6.638968
C	5.988977	0.912677	-6.459843
N	7.388459	0.900086	-6.348726
C	8.089193	-0.229057	-6.07074
C	7.446339	-1.409121	-5.914236
C	6.009824	-1.3932	-6.074046
N	5.344424	-0.277955	-6.361548
N	5.307009	-2.515716	-5.915346
H	-3.81721	0.192268	-0.391634
H	-2.674634	-2.042433	-0.509704
H	1.020822	-2.267555	-0.113039
H	-0.489139	-3.141257	-0.377077
H	-2.456893	2.122665	-0.088563
H	7.981228	-2.013021	-0.063779
H	1.888687	0.067879	0.000000
H	1.86308	2.327159	-0.205578
H	3.359162	3.171278	-0.506533
H	7.574866	0.526833	-0.146556
H	9.165152	-0.124782	-5.985166
H	7.982051	-2.321751	-5.689997
H	4.282405	-2.511119	-6.059643
H	5.778047	-3.386217	-5.729153
H	7.839814	1.79979	-6.441987
H	-2.670263	-2.138844	-6.131827
H	3.457703	-0.177144	-6.370233

H	3.52336	2.091335	-6.346346
H	2.042669	2.982026	-6.11136
H	-2.219475	0.391916	-6.25257
H	-0.710026	-1.024736	-3.192688
H	6.017372	-1.126358	-3.081351
H	-0.466803	3.274832	-3.201896
H	-1.867332	1.205886	-3.217912
H	5.909716	3.16452	-3.432021
H	7.244402	1.060501	-3.241907
H	3.869443	-2.342254	-3.074357
H	1.398435	-2.304004	-3.10045

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(GC/4,7-O_2phen/CG)mg (M06-2X/6-31+G(d,p))

C	2.168223	1.093029	-0.093407
C	0.725221	1.120140	-0.036830
N	0.000000	0.000000	0.000000
C	0.601088	-1.217738	-0.000000
N	1.999242	-1.250222	0.018792
C	2.757113	-0.121412	-0.054166
N	0.077604	2.281882	-0.023119
O	-0.009975	-2.286003	-0.028682
O	-2.735523	2.256568	-0.029151
C	-3.470419	1.265717	0.047386
C	-4.896430	1.229627	0.101239
C	-5.512701	-0.019519	0.067961
N	-4.950948	-1.244936	0.043709
C	-3.631068	-1.195814	0.031798
N	-2.918953	-0.018968	0.023911
N	-6.850027	0.260679	0.037328
C	-6.972077	1.638508	0.044594
N	-5.823019	2.248843	0.085729
N	-2.911111	-2.331075	0.029675
C	-3.430570	1.895803	-2.977378
C	-1.986357	1.925706	-2.961355
C	-1.254238	0.780830	-3.009741
C	-1.909565	-0.525598	-3.076799
C	-3.404558	-0.554951	-3.122227
C	-4.114074	0.722477	-3.050967
N	-4.000537	-1.703311	-3.202246
C	-5.389893	-1.721425	-3.197892
C	-6.188543	-0.635061	-3.101256
C	-5.603631	0.703406	-3.028652
C	0.234885	0.826072	-3.026180
C	0.875588	-0.487661	-3.082076
C	0.122985	-1.610171	-3.107823
N	-1.265883	-1.649973	-3.115786
H	-1.467162	2.880414	-2.936949
H	-3.989951	2.824823	-2.900584
C	-1.924755	1.564003	-6.037088
C	-0.498469	1.582520	-6.094283
C	0.160757	0.357579	-6.174694

N	-0.358036	-0.883699	-6.260275
C	-1.678969	-0.881956	-6.244357
N	-2.431328	0.263868	-6.130697
N	1.487757	0.680458	-6.120353
C	1.561975	2.056835	-6.004251
N	0.392212	2.627891	-5.988697
O	-2.693081	2.517510	-5.870428
N	-2.358779	-2.037215	-6.344955
N	-5.506052	2.447835	-5.875999
C	-6.113026	1.268487	-5.975598
N	-5.349346	0.182511	-6.115365
C	-5.907980	-1.049673	-6.232931
N	-7.304139	-1.128286	-6.260812
C	-8.100725	-0.038272	-6.084236
C	-7.554235	1.186508	-5.927693
O	-5.260369	-2.094310	-6.301311
H	3.832133	-0.259760	-0.080408
H	2.745075	2.004299	-0.170120
H	-0.952320	2.294451	-0.023947
H	0.580921	3.134463	-0.210030
H	2.414834	-2.171293	0.025558
H	-7.938978	2.119878	0.010716
H	-1.883874	-0.057495	-0.000000
H	-1.897649	-2.324950	-0.098256
H	-3.421369	-3.175997	-0.172087
H	-7.589939	-0.423718	0.001063
H	-9.170318	-0.215388	-6.075470
H	-8.162353	2.066019	-5.767364
H	-4.477325	2.495923	-5.871780
H	-6.038739	3.261304	-5.612158
H	-7.687528	-2.058388	-6.356077
H	2.511769	2.566757	-5.929052
H	-3.464574	0.188004	-6.115766
H	-3.370801	-2.076922	-6.212265
H	-1.819437	-2.877437	-6.209648
H	2.251082	0.021818	-6.147798
O	0.868867	1.874943	-2.976266
O	-6.280915	1.724835	-2.975051
H	0.590068	-2.590840	-3.127603
H	1.960937	-0.522052	-3.090138
H	-5.815912	-2.717577	-3.277864
H	-7.271397	-0.716083	-3.090367

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(GC/5,6-O_2phen/CG)mg (M06-2X/6-31+G(d,p))

N	0.000000	0.000000	0.000000
C	-1.107992	0.781262	0.000000
N	-2.348149	0.149763	-0.170254
C	-2.466040	-1.189871	-0.372036
C	-1.363916	-1.971309	-0.407974
C	-0.091827	-1.313908	-0.213394
O	-1.092048	2.005914	0.129688
N	1.033063	-2.023765	-0.242421
O	3.448310	-0.597761	-0.338298
C	3.631373	0.593414	-0.047081
C	4.867562	1.279768	0.149656
C	4.811446	2.655063	0.369342

N	3.738909	3.461722	0.452733
C	2.601939	2.803385	0.305561
N	2.539185	1.450211	0.080225
N	6.173468	0.831032	0.124385
C	6.887391	1.900353	0.326409
N	6.118713	3.041095	0.475370
N	1.428360	3.448061	0.402271
C	4.048756	-0.986210	-3.169011
C	2.571281	-1.414052	-3.086387
C	1.546008	-0.337411	-3.113466
C	1.892587	1.020150	-2.999949
C	3.328788	1.432447	-2.979215
C	4.344766	0.467212	-3.080838
N	0.972150	1.987769	-2.931132
C	-0.307826	1.639505	-3.025267
C	-0.749777	0.325253	-3.206509
C	0.199810	-0.682166	-3.244457
N	3.593204	2.736797	-2.863061
C	4.868437	3.115842	-2.845089
C	5.948191	2.234389	-2.934751
C	5.675351	0.881588	-3.045261
C	2.174896	-1.530687	-6.345013
C	0.744238	-1.468195	-6.404583
C	0.148582	-0.210671	-6.371678
N	0.719974	1.004611	-6.256846
C	2.037493	0.935848	-6.191119
N	2.736581	-0.248059	-6.231544
N	-1.192331	-0.458818	-6.450717
C	-1.342761	-1.832967	-6.517547
N	-0.205530	-2.466522	-6.491111
O	2.905383	-2.519840	-6.368947
N	2.766147	2.055898	-6.060697
N	5.712489	-2.591659	-6.021262
C	6.337626	-1.425424	-5.885290
N	5.650060	-0.309518	-6.138422
C	6.243175	0.907501	-6.065886
N	7.608610	0.945119	-5.756904
C	8.323070	-0.175803	-5.463121
C	7.731142	-1.389625	-5.502681
O	5.654788	1.975432	-6.242786
H	9.365631	-0.031313	-5.202802
H	8.275177	-2.294545	-5.269186
H	4.693266	-2.598810	-6.166169
H	6.142281	-3.425101	-5.652308
H	8.022216	1.866322	-5.720591
H	-2.317538	-2.293571	-6.597200
H	3.772715	-0.223375	-6.223983
H	3.787419	2.053043	-6.086375
H	2.261441	2.918077	-5.930218
H	-1.914248	0.245388	-6.464906
H	-3.471327	-1.575898	-0.499564
H	-1.428002	-3.038893	-0.570053
H	1.937177	-1.531102	-0.219007
H	1.020860	-2.978748	-0.567096
H	-3.154575	0.758466	-0.145653
H	7.966506	1.934482	0.384597
H	1.613251	0.995165	-0.000000
H	0.539134	2.981777	0.221022
H	1.470279	4.452903	0.442770

H	6.435838	3.980833	0.659905
H	6.457529	0.127014	-3.083830
H	-0.065180	-1.729005	-3.377204
H	5.039698	4.185452	-2.739269
H	6.966479	2.608104	-2.895705
H	-1.025791	2.453708	-2.951667
H	-1.808913	0.107743	-3.306200
O	2.283342	-2.585650	-3.000758
O	4.909571	-1.823939	-3.308174

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(GC/phen/CG)MG (M06-2X/6-31+G(d,p))

C	-0.098708	1.639355	3.305106
C	-1.285865	0.831405	3.257075
C	-1.194604	-0.578408	3.144096
C	0.121996	-1.201889	3.231029
C	1.263100	-0.369829	3.336873
C	1.127509	1.060938	3.324946
N	0.000000	0.000000	0.000000
C	0.114004	-1.325672	0.120150
C	2.517784	-0.986402	3.521220
C	2.120122	0.810515	6.405776
C	0.960287	-0.033275	6.421850
C	1.919977	2.187787	6.398672
N	3.177770	2.722088	6.340816
C	4.062692	1.661263	6.308717
N	3.464464	0.503630	6.340505
C	2.592414	-2.357442	3.578821
N	0.764722	2.881201	6.402753
C	-0.292917	2.089541	6.417712
N	-0.218324	0.721988	6.454472
O	0.905893	-1.263469	6.393812
N	0.210613	-2.553050	3.246128
C	1.098588	0.794696	-0.000000
N	2.346833	0.174205	0.116558
C	2.487805	-1.174870	0.223488
C	1.399101	-1.973643	0.223128
C	1.402141	-3.093975	3.420993
N	-2.282614	-1.362474	2.976024
O	-3.503292	-0.737652	-0.199906
C	-3.675329	0.460838	0.023199
N	-2.576897	1.326309	0.096188
C	-2.625709	2.650678	0.442384
N	-3.748334	3.304610	0.682226
C	-4.834022	2.511811	0.570964
C	-4.905890	1.157667	0.259289
N	-6.128909	2.884256	0.803737
C	-6.907038	1.754094	0.634431
N	-6.207166	0.702573	0.315352
N	-1.481182	-2.719011	5.811432
C	-3.468785	-0.782666	2.973247
C	-3.675751	0.595066	3.191000
C	-2.656685	-2.097114	5.880504
N	-2.674501	-0.825833	6.286375
C	-3.841266	-0.138751	6.361397
N	-5.019650	-0.825786	6.052168
C	-5.027283	-2.127278	5.652556

C	-3.867185	-2.809835	5.545143
C	-2.572418	1.406472	3.322109
O	-3.923510	1.050682	6.678006
N	-1.530588	2.623381	6.366238
N	-0.999284	-2.054133	0.133001
O	1.062903	2.024424	-0.091725
N	-1.441483	3.284160	0.566184
H	-5.995375	-2.558742	5.424928
H	-3.839209	-3.839688	5.216989
H	-0.618939	-2.194284	6.005005
H	-1.401247	-3.543997	5.235904
H	-5.870530	-0.284549	6.117803
H	5.131817	1.816224	6.269045
H	-1.101657	0.177852	6.437477
H	-2.371159	2.061684	6.528880
H	-1.581114	3.623832	6.474978
H	3.393763	3.707660	6.331783
H	3.500104	-1.551617	0.315271
H	1.481261	-3.047702	0.317697
H	-1.916673	-1.594304	0.074871
H	-0.961351	-3.008934	0.454970
H	3.143900	0.795168	0.125064
H	-7.980684	1.782485	0.756529
H	-1.647768	0.874601	-0.000000
H	-0.559115	2.851891	0.278623
H	-1.485242	4.281768	0.698688
H	-6.434656	3.814202	1.048062
H	3.399726	-0.366961	3.663581
H	-2.670422	2.480952	3.454249
H	1.434993	-4.182477	3.447000
H	3.531332	-2.868855	3.760389
H	-4.322210	-1.432608	2.788944
H	-4.684324	0.995514	3.221393
H	-0.210944	2.719369	3.338841
H	2.030077	1.665985	3.376256

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(GC/4,7-O_2phen/CG)MG (M06-2X/6-31+G(d,p))

N	1.150529	-2.255900	-3.479851
C	1.795449	-1.150901	-3.281692
C	1.142941	0.150130	-3.125104
C	-0.348433	0.197715	-3.128079
C	-0.988436	-1.088705	-3.395389
C	-0.235103	-2.199653	-3.560488
C	3.286788	-1.192103	-3.234014
C	4.004138	0.083271	-3.191637
C	3.326887	1.257466	-3.101377
C	1.878430	1.288919	-3.036791
N	3.874872	-2.345267	-3.210268
C	5.261244	-2.371440	-3.127019
C	6.069810	-1.287410	-3.122504
C	5.495994	0.055173	-3.187192
O	6.178447	1.073916	-3.224706
C	3.442322	-1.304552	0.060296
C	4.875410	-1.261973	0.061203
C	5.487259	-0.014077	-0.026525

N	4.924121	1.210882	-0.085486
C	3.608078	1.155210	-0.075642
N	2.894940	-0.014446	-0.016817
N	5.812200	-2.272077	0.124819
C	6.958185	-1.654726	0.068770
N	6.826110	-0.282994	-0.027392
N	2.886242	2.293655	-0.181223
O	2.701612	-2.285854	0.109115
N	-0.101357	-2.276087	-0.144567
C	-0.735518	-1.104444	-0.136183
C	-2.168648	-1.046915	-0.288957
C	-2.733376	0.183260	-0.285175
N	-1.970373	1.289242	-0.103751
C	-0.579079	1.228600	0.000000
N	0.000000	0.000000	0.000000
O	0.050834	2.282933	0.094255
C	1.648366	-0.754903	-6.554592
C	0.219263	-0.640475	-6.543172
C	-0.329150	0.608599	-6.263257
N	0.294810	1.780206	-6.020049
C	1.606390	1.660344	-6.043333
N	2.259817	0.478912	-6.282992
N	-0.767061	-1.580446	-6.756546
C	-1.880636	-0.921919	-6.602101
N	-1.679863	0.410575	-6.298046
O	2.338829	-1.753216	-6.756162
N	2.384388	2.731305	-5.767798
N	5.137404	-1.923398	-6.513413
C	5.829964	-0.797886	-6.344627
N	5.151673	0.350127	-6.307164
C	5.792065	1.533472	-6.121806
N	7.184245	1.507181	-6.015447
C	7.889706	0.349359	-6.008247
C	7.263564	-0.836832	-6.190440
O	5.216633	2.620305	-6.051382
H	1.362455	2.241217	-2.940863
H	-3.797531	0.345492	-0.413397
H	-2.759701	-1.943019	-0.421804
H	0.925970	-2.312292	-0.061073
H	-0.613266	-3.128843	-0.301161
H	-2.356209	2.218856	-0.196115
H	7.929803	-2.128449	0.093945
H	1.858151	0.026359	0.000000
H	1.876095	2.305118	-0.010970
H	3.410130	3.149528	-0.085114
H	7.555989	0.407992	-0.119231
H	8.960198	0.436126	-5.860901
H	7.808083	-1.771408	-6.198475
H	4.109854	-1.894378	-6.597534
H	5.604898	-2.814870	-6.491076
H	7.616137	2.391031	-5.783353
H	-2.874815	-1.336649	-6.695326
H	3.297419	0.469489	-6.297086
H	3.394637	2.717377	-5.937453
H	1.904938	3.617250	-5.729894
H	-2.374254	1.115311	-6.098554
H	5.677494	-3.372157	-3.049582
H	-2.070761	-1.114762	-3.468634
H	3.890248	2.186167	-3.052145

H	-0.700604	-3.154560	-3.788841
O	-0.979183	1.231582	-2.932410
H	7.149175	-1.378450	-3.058074

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(GC/5,6-O_2phen/CG)MG (M06-2X/6-31+G(d,p))

O	1.974338	-4.574984	3.894098
C	1.265151	-3.653366	3.559549
C	-0.239306	-3.884609	3.327505
O	-0.675252	-5.012678	3.282146
C	-2.478250	-2.838891	3.142363
C	-1.095028	-2.679016	3.195078
C	3.163142	-2.087144	3.263392
C	1.783816	-2.281562	3.331216
C	1.960674	-3.189270	0.342292
N	2.910102	-4.092134	0.477183
C	4.142688	-3.563612	0.333595
C	4.508714	-2.245953	0.078137
C	3.461600	-1.278521	-0.064088
N	2.198818	-1.869010	0.063452
N	5.324956	-4.238270	0.451655
C	6.333355	-3.310511	0.271881
N	5.881573	-2.108131	0.051835
O	3.560081	-0.063274	-0.250559
N	0.667095	-3.541528	0.544857
N	1.435378	1.771210	0.140907
C	0.186608	1.306146	0.184166

C	-0.914890	2.213322	0.393971
C	-2.157295	1.687383	0.325935
N	-2.325881	0.360158	0.083783
C	-1.249619	-0.525938	-0.000000
N	0.000000	0.000000	0.000000
O	-1.488050	-1.733919	-0.081642
C	-2.781268	-2.821493	6.277347
C	-2.169691	-1.570848	6.303739
C	-0.739167	-1.533060	6.337403
N	-0.190393	-2.825251	6.355618
C	-0.904005	-4.002661	6.349392
N	-2.223567	-4.047930	6.282822
N	-4.120566	-2.552280	6.239473
C	-4.253033	-1.175135	6.253926
N	-3.107126	-0.557581	6.287440
O	0.003208	-0.549869	6.337905
N	-0.190581	-5.136740	6.413147
N	2.796248	-0.531838	6.269783
C	3.437240	-1.698986	6.319257
N	2.711894	-2.801242	6.499692
C	3.299726	-4.026412	6.557768
N	4.690271	-4.080899	6.379283
C	5.449597	-2.969652	6.199142
C	4.873345	-1.746090	6.169699

O	2.692671	-5.073425	6.758900
H	-3.059148	2.275783	0.452380
H	-0.753737	3.264793	0.588454
H	2.221064	1.129554	-0.031302
H	1.613400	2.750554	0.289147
H	-3.240264	-0.070382	0.094504
H	7.376150	-3.592693	0.310684
H	1.391769	-1.215998	0.000000
H	-0.096835	-2.926491	0.245087
H	0.494277	-4.536861	0.569873
H	5.416060	-5.226411	0.634576
H	6.516695	-3.123321	6.082331
H	5.457272	-0.846894	6.025929
H	1.765583	-0.507523	6.315100
H	3.301709	0.313016	6.058616
H	5.094982	-5.006695	6.404897
H	-5.223887	-0.699583	6.241496
H	0.843044	-2.861065	6.442988
H	0.831068	-5.142929	6.425538
H	-0.689526	-5.991882	6.227036
H	-4.853920	-3.245094	6.242469
C	-3.274967	-1.707211	3.078443
C	3.645239	-0.817910	2.993723
C	-2.641908	-0.462908	3.074739

C	2.712020	0.206875	2.805971
N	1.393160	0.040154	2.866346
C	-0.553109	-1.382398	3.134857
N	-1.322486	-0.292647	3.070345
H	-2.888498	-3.843932	3.181030
H	-4.357961	-1.773481	3.062245
C	0.927228	-1.188431	3.118033
H	3.821194	-2.942822	3.397716
H	4.707277	-0.622380	2.882974
H	3.052191	1.212688	2.566577
H	-3.233875	0.451450	3.073752

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AT/TA (M06-2X/6-31+G(d,p))

C	2.186042	-1.653973	2.656962
C	0.784687	-1.469258	3.026988
N	-0.043589	-2.559200	2.824804
C	0.288634	-3.732699	2.195938
N	1.629579	-3.857030	1.907866
C	2.528312	-2.831542	2.092492
O	0.333073	-0.426457	3.499238
O	-0.535628	-4.598054	1.926633
C	3.139900	-0.533073	2.932191
N	-2.757130	-2.293280	3.505208
C	-3.323258	-1.082543	3.671563
C	-4.735675	-1.031972	3.715589
C	-5.403608	-2.235594	3.510838
N	-4.854667	-3.444018	3.308948

C	-3.529762	-3.380116	3.337039
N	-6.733835	-1.901649	3.551802
C	-6.794867	-0.544959	3.780627
N	-5.618956	0.013651	3.881243
N	-2.551925	0.004680	3.762662
C	-3.289079	-0.555704	0.471157
C	-2.053168	0.217763	0.349491
N	-0.912688	-0.514285	0.082868
C	-0.810744	-1.878645	-0.000000
N	-1.992100	-2.552707	0.224599
C	-3.185841	-1.902394	0.440447
O	-1.991721	1.441654	0.467337
O	0.247066	-2.448948	-0.234785
C	-4.571715	0.189551	0.673279
N	1.569934	0.729927	-0.000000
C	1.747168	2.000722	0.404853
C	3.079465	2.463110	0.507117
C	4.076963	1.548675	0.178296
N	3.914991	0.278813	-0.224358
C	2.630477	-0.045970	-0.285818
N	5.248355	2.236867	0.368441
C	4.902362	3.500960	0.790468
N	3.612221	3.676967	0.887296
N	0.683430	2.760880	0.687964
H	-2.984830	-4.309794	3.183814
H	-2.988676	0.910264	3.841717
H	-1.533952	-0.071611	3.702634
H	-7.506852	-2.543611	3.456301
H	-7.740286	-0.026964	3.862899
H	-1.048473	-2.458431	3.101267
H	3.541018	-3.035735	1.759949
H	4.121470	-0.740097	2.499777
H	2.758464	0.402496	2.512068

H	3.246573	-0.376188	4.010186
H	1.868658	-4.655113	1.336552
H	2.379383	-1.059871	-0.590385
H	0.831280	3.702865	1.014181
H	-0.261532	2.379537	0.620900
H	6.177366	1.874837	0.212883
H	5.651705	4.248531	1.010682
H	0.000000	0.000000	0.000000
H	-4.045260	-2.550086	0.591491
H	-5.403542	-0.502900	0.833497
H	-4.794789	0.816385	-0.195639
H	-4.503148	0.852931	1.540369
H	-1.898649	-3.555502	0.356562

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(AT/phen/TA)mg (M06-2X/6-31+G(d,p))

N	1.475444	3.345550	0.522028
C	1.173283	2.014519	0.319298
C	2.322880	1.229772	0.280659
N	3.351429	2.120917	0.462242
C	2.779170	3.365795	0.598540
C	-0.053232	1.331559	0.170581
N	0.000000	0.000000	0.000000
C	1.185592	-0.636027	0.000000
N	2.392867	-0.099395	0.129175
N	-1.243697	1.947452	0.229193
N	-2.301306	-1.566059	0.046091
C	-2.043313	-2.913316	0.159009
N	-3.186175	-3.692961	0.245273
C	-4.455460	-3.171431	0.206150
C	-4.694863	-1.849184	0.075713
C	-3.537366	-0.958024	-0.011065
O	-0.921540	-3.382992	0.173860
O	-3.630679	0.265464	-0.123963
C	-6.061203	-1.236538	0.068938
C	-2.856329	-4.827831	3.588057
N	-1.836509	-3.997695	3.505257
C	-2.101706	-2.681980	3.335396
C	-3.421793	-2.177063	3.265350
C	-4.488812	-3.097730	3.350813
C	-4.209502	-4.433552	3.508078
C	-0.986299	-1.744371	3.266944
C	-1.265750	-0.356992	3.189944
C	-2.620936	0.110957	3.105618
C	-3.655009	-0.767087	3.126875

C	-0.172722	0.536688	3.199998
C	1.105182	0.032706	3.237735
C	1.270915	-1.367390	3.277925
N	0.273647	-2.229614	3.311250
N	-5.020871	-0.079857	5.930424
C	-5.877705	-1.063027	5.608164
N	-6.948706	-0.990352	4.824526
C	-7.127455	0.253896	4.356104
C	-6.322653	1.364182	4.596846
C	-5.193958	1.153156	5.420947
N	-8.109088	0.717180	3.516163
C	-7.847683	2.051882	3.299290
N	-6.783884	2.477436	3.925189
N	-4.304695	2.117104	5.694686
N	-2.381901	-0.986231	6.477411
C	-1.381539	-0.032511	6.504279
C	-0.013098	-0.542084	6.505067
C	0.152619	-1.875760	6.369538
N	-0.901501	-2.754061	6.314497
C	-2.221932	-2.349967	6.375123
O	-1.665551	1.166405	6.524209
C	1.111524	0.440681	6.614082
O	-3.157771	-3.130570	6.334027
H	-5.634406	-2.037790	6.026879
H	-4.417022	3.011751	5.243045
H	-3.409175	1.873038	6.122382
H	-8.876800	0.175221	3.148256
H	-8.481891	2.656447	2.665900
H	-3.363469	-0.645781	6.423388
H	1.134615	-2.330589	6.291942
H	2.071864	-0.048117	6.428888
H	0.981016	1.248810	5.889586
H	1.135337	0.898133	7.608271
H	-0.756949	-3.714751	6.028385
H	1.123538	-1.716932	-0.107494
H	-1.263646	2.953836	0.286422
H	-2.106902	1.423363	0.068128
H	4.334358	1.892039	0.474721
H	3.380482	4.251254	0.751591
H	-1.446395	-0.956192	0.000000
H	-5.257671	-3.895938	0.304954
H	-6.833199	-2.007187	0.138348
H	-3.026355	-4.679235	0.396154
H	-0.360221	1.607543	3.163050
H	-5.512297	-2.730201	3.308525
H	2.273805	-1.791551	3.287740
H	1.973939	0.684021	3.229529
H	-2.607946	-5.876977	3.740348
H	-4.998215	-5.172757	3.601195
H	-4.682838	-0.419051	3.043255
H	-2.797138	1.179202	3.010683
H	-6.174123	-0.547068	0.913276
H	-6.222467	-0.652163	-0.841315

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(AT/4,7-O_2phen/TA)mg (M06-2X/6-31+G(d,p))

N	-3.460075	1.909908	-0.573019

C	-2.388250	1.086203	-0.349788
C	-1.288317	1.938242	-0.353999
N	-1.660779	3.245962	-0.576446
C	-2.959361	3.185364	-0.702831
C	-0.026944	1.330558	-0.190584
N	0.000000	0.000000	0.000000
C	-1.151179	-0.701516	0.000000
N	-2.381054	-0.244197	-0.174487
N	1.124320	2.018604	-0.239935
N	2.330664	-1.506891	-0.107325
C	2.130964	-2.861018	-0.235562
N	3.295194	-3.574420	-0.456095
C	4.541295	-2.996025	-0.470141
C	4.734336	-1.670613	-0.285592
C	3.540357	-0.838463	-0.132575
O	1.030968	-3.384292	-0.178329
O	3.568530	0.389651	-0.045427
C	6.078027	-1.008254	-0.230865
C	5.328282	-3.168330	-3.816453
N	3.950735	-3.153717	-3.617409
C	3.373533	-2.009185	-3.428634
C	4.094068	-0.738926	-3.390243
C	5.580840	-0.766614	-3.485799
C	6.145064	-2.092830	-3.743851
C	3.430313	0.438199	-3.247078
C	1.988832	0.477249	-3.145004
C	1.253414	-0.665325	-3.132748
C	1.894362	-1.974046	-3.237507
N	1.247090	-3.094814	-3.174902
C	-0.129304	-3.046256	-2.973731
C	-0.878018	-1.921207	-2.925384
C	-0.232589	-0.611912	-3.036064
C	0.684394	-2.544122	-6.286928
C	0.585385	-1.196294	-6.319096
C	1.835459	-0.438372	-6.380177
N	2.995604	-1.182504	-6.487774
C	3.099854	-2.553306	-6.512699
N	1.886984	-3.203121	-6.371419
C	-0.707710	-0.438726	-6.291994
O	1.893875	0.790388	-6.321929
O	4.160619	-3.143122	-6.630166
N	5.424417	0.171755	-6.436462
C	6.526766	-0.600348	-6.512231
N	7.782763	-0.247842	-6.287382
C	7.876584	1.052337	-5.968247
C	6.835509	1.970205	-5.872930
C	5.537919	1.469112	-6.101836
N	7.291405	3.217997	-5.507698
C	8.581903	3.057632	-5.385978
N	8.998518	1.773605	-5.654718
N	4.435704	2.224329	-5.979458
H	-1.029565	-1.772923	0.148105
H	1.083303	3.021421	-0.332496
H	2.014335	1.544484	-0.086299
H	-4.423585	1.619296	-0.643484
H	-3.608010	4.030878	-0.885322
H	1.457905	-0.923549	0.000000
H	5.367842	-3.678033	-0.645115
H	6.864832	-1.699930	-0.544262

H	6.104796	-0.128788	-0.879190
H	6.295040	-0.667020	0.786447
H	3.167407	-4.548045	-0.694918
H	6.336227	-1.639007	-6.776035
H	4.543452	3.203896	-5.767814
H	3.515917	1.829413	-6.175366
H	9.940027	1.413460	-5.614581
H	9.283102	3.833184	-5.110516
H	3.905949	-0.651512	-6.533176
H	-0.188475	-3.182062	-6.187233
H	-1.541573	-1.102023	-6.046418
H	-0.900935	0.022767	-7.265725
H	-0.670777	0.366571	-5.554024
H	1.944370	-4.204147	-6.245894
H	-0.589720	-4.022819	-2.855186
H	-1.952446	-1.948360	-2.775583
O	-0.850767	0.444690	-3.049849
H	5.728067	-4.152534	-4.043392
H	7.216156	-2.169317	-3.900404
O	6.262451	0.242007	-3.356371
H	4.006073	1.359423	-3.214482
H	1.471643	1.430225	-3.070901

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(AT/5,6-O_2phen/TA)mg (M06-2X/6-31+G(d,p))

N	1.106849	-1.708475	-2.983977
C	1.491793	-0.430417	-3.022239
C	0.573865	0.626193	-3.145527
C	-0.787600	0.331495	-3.207752
C	-1.187043	-0.994781	-3.150491
C	-0.196161	-1.974494	-3.036654
C	1.014294	2.046004	-3.196150
C	2.525035	2.328815	-3.044335
C	3.427127	1.164385	-2.839162
C	2.952331	-0.156083	-2.884447
N	3.762858	-1.212631	-2.770496
C	5.057639	-0.985939	-2.568224
C	5.616565	0.288100	-2.434046
C	4.782398	1.382678	-2.587232
O	0.236375	2.961393	-3.328012
O	2.930247	3.467942	-3.083077
C	4.131910	-3.647385	-0.080973
C	4.440920	-2.384830	0.280254
C	3.362221	-1.396650	0.250708
N	2.098190	-1.885774	-0.007241
C	1.768533	-3.173700	-0.353077
N	2.853385	-4.029138	-0.407789
O	3.538983	-0.192854	0.445501
C	5.811680	-1.927727	0.673411
O	0.627154	-3.545779	-0.569770
N	0.000000	0.000000	0.000000
C	-1.254414	-0.484746	0.000000
N	-2.390177	0.191110	-0.115532
C	-2.165110	1.507564	-0.227566
C	-0.927905	2.151482	-0.229968
C	0.206126	1.322246	-0.123616
N	-3.077801	2.522557	-0.356416

C	-2.357921	3.697520	-0.414999
N	-1.068607	3.518686	-0.339922
N	1.465747	1.795688	-0.203662
C	0.315618	-1.580787	-6.335153
N	1.361003	-2.462427	-6.204836
C	2.677860	-2.065674	-6.039751
N	2.833828	-0.698593	-5.976248
C	1.838807	0.249633	-6.045589
C	0.485611	-0.241779	-6.294587
O	2.105705	1.444971	-5.882279
O	3.601789	-2.854382	-5.974944
C	-0.614094	0.760339	-6.468101
N	5.449094	0.271519	-5.743307
C	6.378058	-0.686600	-5.570793
N	7.638236	-0.541802	-5.181758
C	7.931551	0.747866	-4.958905
C	7.079659	1.840390	-5.091575
C	5.757675	1.560389	-5.505933
N	7.707256	3.016709	-4.736482
C	8.914782	2.644374	-4.406486
N	9.114423	1.286451	-4.518326
N	4.824004	2.507219	-5.649089
H	6.028365	-1.699376	-5.763841
H	5.033015	3.446911	-5.346017
H	3.852196	2.234572	-5.801051
H	9.963269	0.773782	-4.331708
H	9.702141	3.307119	-4.074599
H	3.817253	-0.343716	-5.875283
H	-0.660850	-2.033865	-6.476172
H	-1.592502	0.274099	-6.426488
H	-0.563439	1.527522	-5.689918
H	-0.519146	1.277357	-7.428392
H	1.209136	-3.460603	-6.201144
H	-1.326139	-1.566911	0.090797
H	1.590796	2.797868	-0.156768
H	2.240861	1.180694	0.058727
H	-4.080857	2.416318	-0.380935
H	-2.849247	4.655630	-0.514259
H	1.311784	-1.196628	0.000000
H	4.878972	-4.433400	-0.128524
H	6.539799	-2.735260	0.562241
H	5.821751	-1.586616	1.713252
H	6.123012	-1.077303	0.059729
H	2.645700	-4.974313	-0.694668
H	5.688265	-1.870727	-2.497651
H	6.679378	0.405056	-2.245933
H	5.152010	2.403479	-2.534614
H	-0.463709	-3.025697	-2.957367
H	-2.235765	-1.272258	-3.162686
H	-1.497959	1.150691	-3.287609

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(AT/phen/TA)MG (M06-2X/6-31+G(d,p))

C	-3.061042	-1.830308	0.300914
N	-2.732801	-0.530220	0.015202
C	-3.610744	0.530027	-0.115059

C	-5.038408	0.200787	-0.041947
C	-5.371700	-1.083623	0.194562
N	-4.424726	-2.067730	0.364896
O	-3.193324	1.672555	-0.281165
C	-6.022810	1.318079	-0.194121
O	-2.239974	-2.714910	0.484151
N	0.000000	0.000000	0.000000
C	0.513264	1.244962	0.067421
C	1.922981	1.358038	0.105889
C	2.638990	0.165211	0.090606
N	2.142758	-1.080978	0.047357
C	0.817069	-1.068222	-0.000000
N	3.954248	0.552219	0.137429
C	3.960729	1.929156	0.174639
N	2.764027	2.450454	0.157841
N	-0.302439	2.301462	0.086841
N	0.705643	2.151027	3.221773
C	0.250752	0.878665	3.171006
C	1.115729	-0.240431	3.214719
C	2.502199	0.003613	3.301758
C	2.955467	1.299417	3.368742
C	2.005780	2.341104	3.325472
C	0.585733	-1.576177	3.185464
C	-0.753217	-1.790009	3.186931
C	-1.667640	-0.682042	3.176647
C	-1.186721	0.647097	3.084398
N	-2.009996	1.706289	2.928437
C	-3.310737	1.486026	2.938131
C	-3.895419	0.217917	3.141612
C	-3.062494	-0.872685	3.250296
C	-3.517287	3.265544	5.611528
C	-2.357121	2.493371	5.853932
N	-2.541958	1.212496	6.228360
C	-3.786697	0.717004	6.350146
N	-4.937869	1.345453	6.154773
C	-4.737574	2.619647	5.784589
N	-5.677432	3.566896	5.462942
C	-4.986688	4.708477	5.119471
N	-3.690968	4.568291	5.194180

N	-1.118347	2.980803	5.732837
N	-0.463171	-0.639316	6.289696
C	0.836767	-0.174364	6.373331
C	1.880621	-1.197094	6.504444
C	1.494745	-2.488922	6.474068
N	0.176620	-2.860766	6.341674
C	-0.862585	-1.950393	6.242992
C	3.294909	-0.738488	6.680605
O	1.073996	1.030073	6.339706
O	-2.025946	-2.302046	6.127061
H	0.307950	-2.029573	-0.027483
H	0.082201	3.198034	0.343347
H	-1.312559	2.167064	0.112498
H	4.751325	-0.066119	0.126289
H	4.884788	2.489755	0.209401
H	-1.699413	-0.313102	-0.000000
H	-6.403397	-1.410604	0.276218
H	-7.048779	0.947779	-0.130179
H	-5.867467	2.070291	0.585917
H	-5.886475	1.825686	-1.153020
H	-4.687979	-3.023263	0.558013
H	-3.833750	-0.334949	6.623987
H	-0.996658	3.816040	5.178626
H	-0.323218	2.349400	5.825691
H	-6.677840	3.439962	5.494908
H	-5.500102	5.613105	4.824286
H	-1.238117	0.076469	6.249494
H	2.203206	-3.307136	6.556567
H	3.983913	-1.586888	6.687987
H	-0.094891	-3.832365	6.301738
H	3.187445	-0.841676	3.321024
H	-3.450723	-1.877673	3.395828
H	2.339667	3.375885	3.365814
H	4.012727	1.532031	3.447663
H	-3.943989	2.359991	2.787807
H	-4.974312	0.121593	3.207529
H	-1.165789	-2.794799	3.181567
H	1.287115	-2.407037	3.172991
H	3.574550	-0.052599	5.876158

H	3.405577	-0.186726	7.619085

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(AT/4,7-O_2phen/TA)MG (M06-2X/6-31+G(d,p))

N	3.983747	0.086030	-0.296182
C	2.634707	-0.146541	-0.204006
C	2.061084	1.120893	-0.214845
N	3.019296	2.108662	-0.307984
C	4.147504	1.451366	-0.355182
C	0.651592	1.174204	-0.114431
N	0.000000	0.000000	0.000000
C	0.690214	-1.157479	-0.000000
N	2.001343	-1.323560	-0.100852
N	-0.036123	2.318011	-0.121896
N	-2.786614	-0.219548	-0.026088
C	-3.266672	-1.482650	0.208728
N	-4.644233	-1.574872	0.178837
C	-5.467145	-0.505959	-0.087355
C	-4.987589	0.730198	-0.339849
C	-3.538704	0.920255	-0.269727
C	-5.842201	1.921330	-0.644851
O	-2.546920	-2.440535	0.453011
O	-2.985903	2.009607	-0.399190
C	-4.828696	0.311194	2.948017
C	-3.399262	-0.091479	3.080707
C	-2.367360	0.942042	2.977447
N	-2.633035	2.195825	2.794781
C	-3.968009	2.577732	2.704125
C	-5.034160	1.748857	2.780707
C	-3.066239	-1.398152	3.229872
C	-1.682195	-1.819524	3.237559
C	-0.668523	-0.921442	3.165208
C	-0.939705	0.511469	3.056041
C	0.748677	-1.381710	3.214933
C	1.730817	-0.305350	3.091910
C	1.314908	0.979865	3.007502
N	-0.009089	1.408970	3.000771
N	-2.557531	-2.008108	6.229189
C	-2.595402	-3.354127	5.954368
N	-1.349576	-3.956683	5.933785
C	-0.173536	-3.265608	6.115834
C	-0.146611	-1.939459	6.361669
C	-1.422125	-1.229831	6.366122
O	-3.626395	-3.965833	5.728137
C	1.108919	-1.141644	6.526285
O	-1.517362	-0.005190	6.456565
N	-5.001712	-0.665945	6.016901
C	-5.106837	0.673293	5.946095
C	-6.392711	1.211538	5.723696
C	-7.429324	0.293486	5.583365
N	-7.344015	-1.041375	5.646704
C	-6.097751	-1.434257	5.858763
N	-8.541068	1.064024	5.355762
C	-8.124053	2.375412	5.363559
N	-6.842158	2.508737	5.579305
N	-4.007664	1.434781	6.041834

H	-5.913172	-2.505367	5.911222
H	-4.105216	2.436968	5.991002
H	-3.097007	1.009849	6.221967
H	-9.476147	0.717521	5.202539
H	-8.816546	3.191025	5.206955
H	-3.482745	-1.503736	6.191274
H	0.733152	-3.852989	6.019165
H	1.987600	-1.753876	6.309369
H	1.102845	-0.281222	5.849658
H	1.190591	-0.743059	7.542297
H	-1.346053	-4.941176	5.707562
H	0.079436	-2.053104	0.103142
H	0.466367	3.191310	-0.139014
H	-1.053721	2.313387	-0.059430
H	4.703002	-0.621336	-0.325022
H	5.127856	1.900588	-0.435597
H	-1.738358	-0.117447	-0.000000
H	-6.529890	-0.721828	-0.060977
H	-6.902520	1.668196	-0.569947
H	-5.638874	2.297426	-1.652015
H	-5.620135	2.735917	0.050786
H	-5.029305	-2.474138	0.431790
H	-4.109533	3.644334	2.553419
H	2.037944	1.787823	2.925285
O	-5.740544	-0.508570	2.942702
H	-6.052990	2.116575	2.709578
H	2.782564	-0.571745	3.083222
O	1.048674	-2.558410	3.376850
H	-3.856952	-2.141191	3.320835
H	-1.441565	-2.878849	3.294639

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(AT/5,6-O_2phen/TA)MG (M06-2X/6-31+G(d,p))

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C	4.806334	0.693471	-2.621083
N	3.479776	0.690545	-2.736917
C	2.875554	-0.475816	-2.974771
C	3.591408	-1.683710	-3.066150
C	4.983446	-1.655826	-2.985124
C	5.610182	-0.440385	-2.765230
C	1.392003	-0.464599	-3.134315
C	0.674451	-1.673370	-3.196717
C	1.359680	-2.984271	-3.240655
C	2.904383	-2.988658	-3.188563
C	-0.717532	-1.633468	-3.273368
C	-1.342596	-0.399061	-3.337060
C	-0.537173	0.742816	-3.336363
N	0.789437	0.723315	-3.222184
O	3.488731	-4.049531	-3.219952
O	0.773867	-4.039766	-3.343877
N	1.808529	-2.120563	-0.059150
C	1.193166	-3.335170	-0.255979
N	2.074628	-4.397107	-0.342027
C	3.433548	-4.262657	-0.178114
C	4.023505	-3.073955	0.072537
C	3.165642	-1.888329	0.099943
O	-0.013215	-3.461929	-0.377616

C	5.494892	-2.892595	0.286559
O	3.585081	-0.739678	0.227004
N	0.000000	0.000000	0.000000
C	0.392670	1.265389	-0.241726
C	-0.622682	2.217185	-0.492066
C	-1.932354	1.747369	-0.455386
N	-2.339647	0.492726	-0.211384
C	-1.308913	-0.314384	-0.000000
N	-0.576478	3.559723	-0.804505
C	-1.830133	3.895498	-0.948671
N	-2.700095	2.845645	-0.752321
N	1.694229	1.570496	-0.234622
C	0.241495	-2.653768	-6.485632
C	0.830102	-3.865261	-6.387236
N	2.188938	-4.020848	-6.242183
C	3.071537	-2.957509	-6.193396
N	2.457581	-1.727047	-6.235803
C	1.100711	-1.475091	-6.363572
C	-1.229797	-2.445103	-6.673988
O	0.682450	-0.319150	-6.344384
O	4.277722	-3.099870	-6.088180
N	4.269101	0.381359	-6.024550
C	5.577669	0.068154	-6.064398
N	6.609219	0.840919	-5.752510
C	6.203200	2.054974	-5.351590
C	4.894005	2.517735	-5.255633
C	3.877711	1.606355	-5.624478
N	4.849199	3.810013	-4.775872
C	6.103197	4.123540	-4.590493
N	6.972069	3.106057	-4.918134
N	2.576460	1.911207	-5.592932
H	-1.525141	-1.365603	0.178610
H	1.977590	2.434044	-0.674002
H	2.385430	0.826177	-0.145670
H	-3.707975	2.866581	-0.795696
H	-2.186283	4.886765	-1.193362
H	1.153228	-1.296637	0.000000
H	4.003975	-5.180521	-0.275087
H	6.029705	-3.831408	0.123422
H	5.889305	-2.134145	-0.395606
H	5.698676	-2.542922	1.303284
H	1.665373	-5.280042	-0.615121
H	5.792840	-0.952199	-6.374729
H	2.293739	2.712471	-5.047868
H	1.884611	1.184810	-5.775548
H	7.979969	3.120315	-4.872615
H	6.460353	5.075519	-4.222392
H	3.113933	-0.903135	-6.190029
H	0.258617	-4.787376	-6.406516
H	-1.765956	-3.396123	-6.628419
H	-1.433972	-1.971113	-7.638956
H	-1.622018	-1.776946	-5.902069
H	2.597115	-4.931549	-6.081933
H	-0.987846	1.730505	-3.421286
H	5.258509	1.661722	-2.411572
H	-1.267118	-2.570555	-3.284494
H	-2.422048	-0.308908	-3.388448
H	6.689740	-0.358818	-2.702839
H	5.531731	-2.587510	-3.093035