Supporting Information for

A Theoretical Study of Methylation and CH/π Interactions in DNA Intercalation: Methylated 1,10-Phenanthroline in Adenine-Thymine Base Pairs

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This Supporting Information includes definitions for the R and θ geometrical parameters, the AIM topologies of all the intercalated systems, values of the Energy Decomposition Analysis, values of the energies of frontier molecular orbitals, dipole moment and polarizability of the analyzed systems, values of the electron density (ρ) and Laplacian ($\nabla^2\rho$) of all BCPs corresponding to the studied weak interactions found in all the studied systems, and Cartesian coordinates of all the optimized structures.

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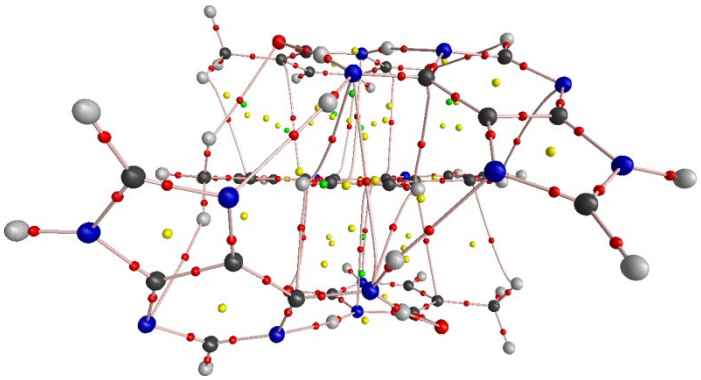
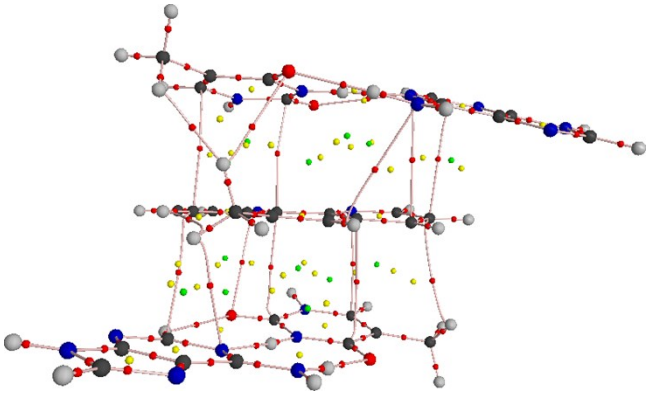
Definitions for the R and *q* parameters.

We defined the xy plane by the two atoms forming the $N_6 \cdots N_7$ hydrogen bond and the third atom for the definition of the xy plane is the C_8 atom of adenine (see Fig. 1). Then, we define the R mean distance between the two base pairs as the difference between the mean z value of the atoms of the upper base pair and the one of the atoms of the lower base pair. The mean distance between phen and base pairs is calculated similarly. We also analyzed the θ angle, defined in Fig. 1. The dashed line joining the C_2 atom of the purine base (adenine) to the C_2 atom of the pyrimidine (thymine) is the long base-pair axis and the θ angle is defined as the rotation of one base pair around the center of its C_2-C_2 axis. Because the base pairs are not strictly planar and parallel after optimization, the θ angle of the optimized systems is defined as the θ angle between the projections on the xy plane of the C_2-C_2 axis of each base pair.

Figures



(AT/4-Mephen/TA)mg



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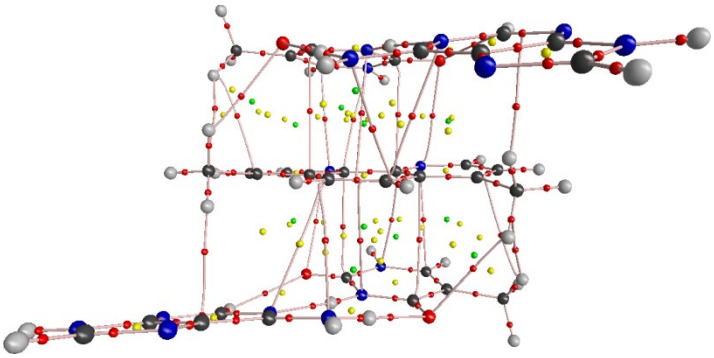

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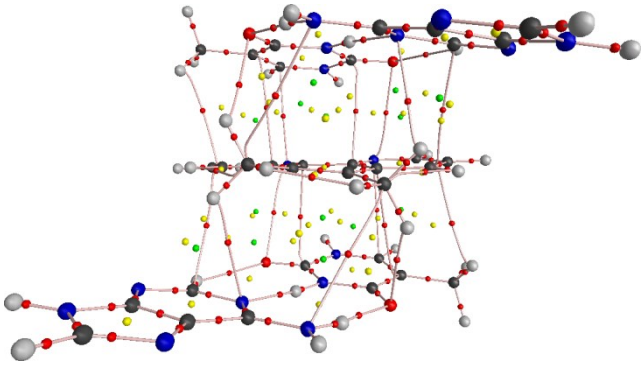

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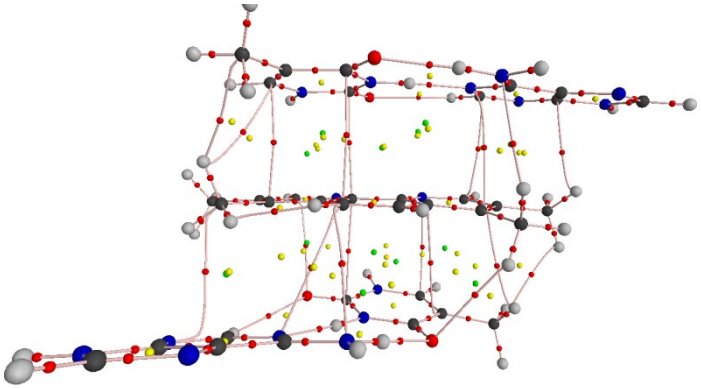

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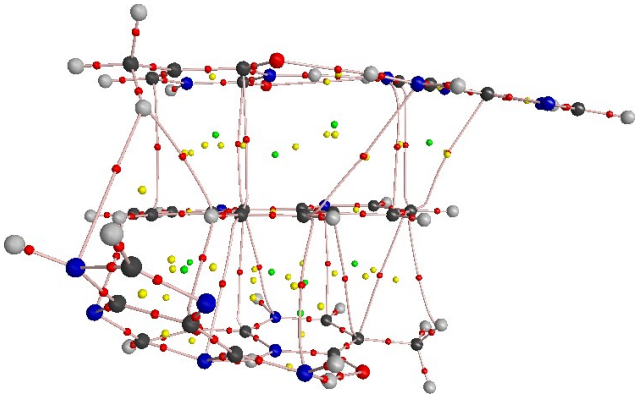
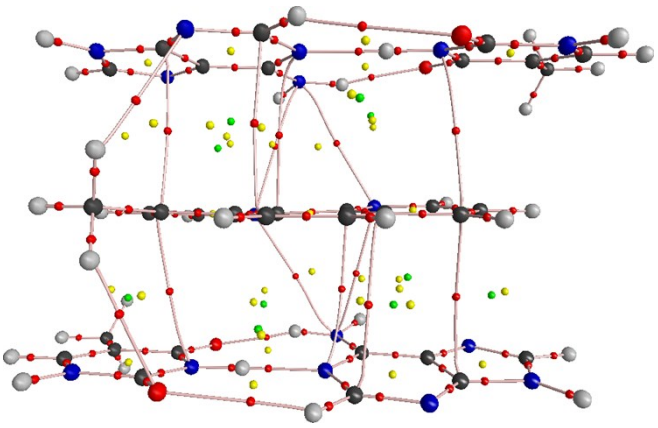
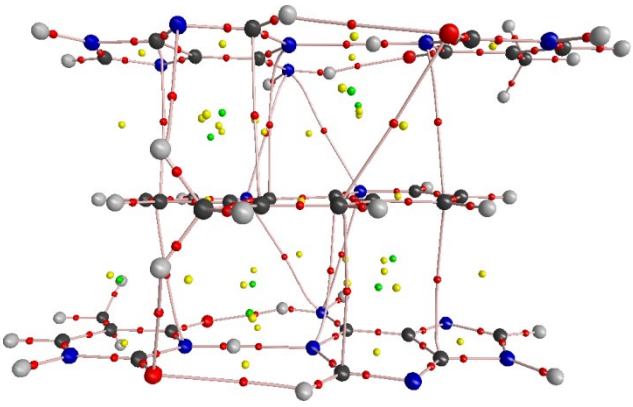


(AT/phen/TA)mg

Figure S1. Topologies of the (AT/4-Mephen/TA)mg, (AT/5-phen/TA)mg, (AT/4,7-Me_2phen/TA)mg, (AT/5,6-Me_2phen/TA)mg, (AT/3,4,7,8-Me_4phen/TA)mg, and (AT/phen/TA)mg systems. Small red spheres correspond to BCPs, yellow spheres to RCPs, and green spheres to CCP. BPs connecting atoms are also shown.



(AT/4-Mephen/TA)MG



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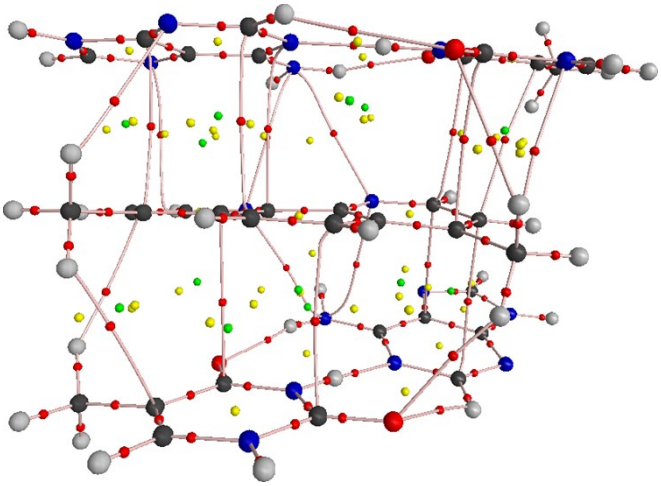

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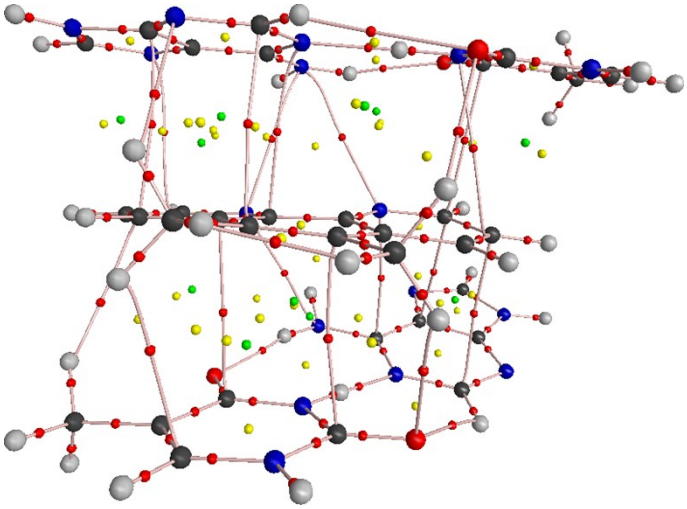
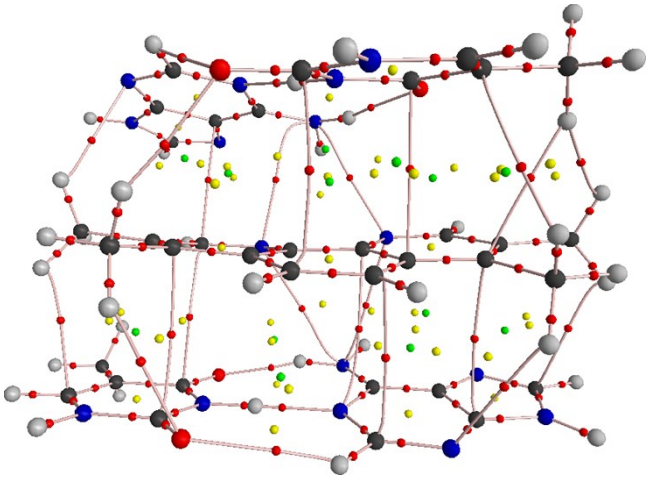
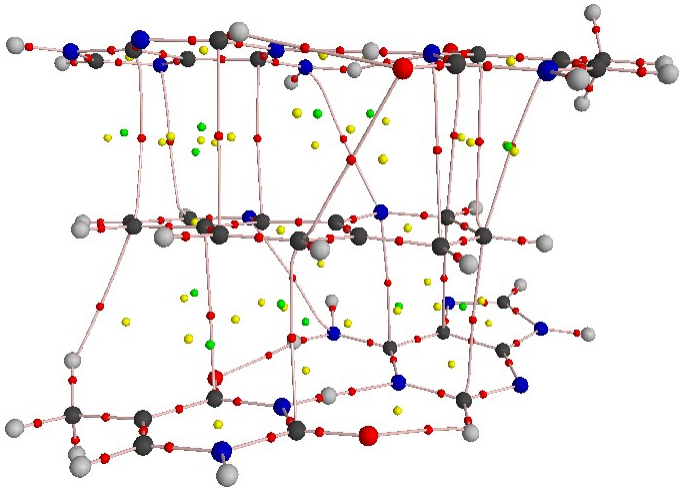


(AT/5,6-Me_2phen/TA)MG



(AT/3,4,7,8-Me$_4$phen/TA)MG



(AT/phen/TA)MG

Figure S2. Topologies of the (AT/4-Mephen/TA)MG, (AT/5-phen/TA)MG, (AT/4,7-Me$_2$phen/TA)MG, (AT/5,6-Me$_2$phen/TA)MG, (AT/3,4,7,8-Me$_4$phen/TA)MG, and (AT/phen/TA)MG systems. Small red spheres correspond to BCPs, yellow spheres to RCPs, and green spheres to CCP. BPs connecting atoms are also shown.

Energy Decomposition Analysis (EDA).

Table S1 and Table S2 give the values of the EDA for (AT/intercalator/TA)mg and (AT/intercalator/TA)MG systems, respectively, with intercalators phen, 4-Mephen, 5-Mephen, 4,7-Me$_2$phen, 5,6-Me$_2$phen and 3,4,7,8-Me$_4$phen. For all the studied systems ΔE_{orb} terms are comparable for both functionals, M06-2X and B3LYP-D3, and the ΔE_{elstat} contribution is also very similar when comparing the results of the two functionals. On the othe hand, as expected, the ΔE_{Pauli} term is larger in the B3LYP-D3 functional with the explicit term for dispersion, but is in most cases nearly compensated by the R^{-6} term after adding the ΔE_{Pauli} and ΔE_{disp} terms with opposite sign (see Table S1 and Table S2).

Table S1. Decomposition of the Interaction Energy (kcal mol^{-1}) between the intercalator[a] and the two pairs of bases (AT/TA) at M06-2X/TZP and B3LYP-D3/TZP levels of calculation when intercalation takes place from the Minor Groove (mg).

Intercalator	**Contribution**	**M06-2X**	**B3LYP-D3**
Phen	ΔE_{Pauli}	18.2	55.3
	ΔE_{elstat}	-24.4	-25.8
	ΔE_{orb}	-13.7	-12.4
	ΔE_{disp}		-46.3
	ΔE_{int}	-19.9	-29.2
4-Mephen	ΔE_{Pauli}	21.9	60.3
	ΔE_{elstat}	-30.0	-31.2
	ΔE_{orb}	-19.1	-14.6
	ΔE_{disp}		-48.6
	ΔE_{int}	-27.3	-34.1
5-Mephen	ΔE_{Pauli}	13.4	56.8
	ΔE_{elstat}	-24.3	-25.9
	ΔE_{orb}	-20.2	-13.1
			-48.3

	ΔE_{disp}	-31.2	-30.5
	ΔE_{int}		
4,7-Me_2phen	ΔE_{Pauli}	15.7	62.9
	ΔE_{elstat}	-31.4	-33.0
	ΔE_{orb}	-18.9	-15.3
	ΔE_{disp}		-51.1
	ΔE_{int}	-34.6	-36.5
5,6-Me_2phen	ΔE_{Pauli}	15.7	62.8
	ΔE_{elstat}	-32.0	-33.2
	ΔE_{orb}	-19.7	-15.5
	ΔE_{disp}		-51.8
	ΔE_{int}	-35.9	-37.7
3,4,7,8-Me_4phen	ΔE_{Pauli}	20.0	63.5
	ΔE_{elstat}	-26.9	-28.0
	ΔE_{orb}	-19.4	-14.9
	ΔE_{disp}		-55.6
	ΔE_{int}	-26.4	-35.0

[a] Intercalator can be: phen, 4-Mephen, 5-Mephen, 4,7-Me_2phen, 5,6-Me_2phen and 3,4,7,8-Me_4phen.

Table S2. Decomposition of the Interaction Energy (kcal mol^{-1}) between the intercalator[a] and the two pairs of bases (AT/TA) at M06-2X/TZP and B3LYP-D3/TZP levels of calculation when intercalation takes place from the Major Groove (MG).

Intercalator	Contribution	M06-2X	B3LYP-D3
Phen	ΔE_{Pauli}	19.4	60.5
	ΔE_{elstat}	-27.2	-29.0
	ΔE_{orb}	-16.2	-12.6
	ΔE_{disp}		-49.4
	ΔE_{int}	-24.0	-30.4
4-Mephen	ΔE_{Pauli}	19.9	62.6
	ΔE_{elstat}	-27.5	-29.5
	ΔE_{orb}	-17.4	-13.4
	ΔE_{disp}		-52.4
	ΔE_{int}	-25.0	-32.6
5-Mephen	ΔE_{Pauli}	20.0	61.1
	ΔE_{elstat}	-27.5	-29.5
	ΔE_{orb}	-16.7	-12.8
	ΔE_{disp}		-51.2
	ΔE_{int}	-24.3	-32.4

4,7-Me_2phen	ΔE_{Pauli}	23.0	68.3
	ΔE_{elstat}	-31.8	-33.7
	ΔE_{orb}	-19.3	-15.0
	ΔE_{disp}		-51.1
	ΔE_{int}	-28.1	-35.5
5,6-Me_2phen	ΔE_{Pauli}	23.1	67.0
	ΔE_{elstat}	-31.4	-33.3
	ΔE_{orb}	-19.0	-14.8
	ΔE_{disp}		-53.7
	ΔE_{int}	-27.2	-34.8
3,4,7,8-Me_4phen	ΔE_{Pauli}	25.3	74.3
	ΔE_{elstat}	-34.2	-36.1
	ΔE_{orb}	-21.6	-17.0
	ΔE_{disp}		-60.1
	ΔE_{int}	-30.4	-38.9

[a] Intercalator can be: phen, 4-Mephen, 5-Mephen, 4,7-Me_2phen, 5,6-Me_2phen and 3,4,7,8-Me_4phen.

Table S3. Energies (eV) of frontier molecular orbitals, dipole moment, μ, (in D) and polarizability, α, (in a. u.$^{-3}$), of the analyzed systems at M06-2X/6-31+G(d,p) level of calculation.

System	HOMO	LUMO	μ	α
Phen	-7.76	-0.85	3.3	152.7
4-Mephen	-7.66	-0.86	3.7	165.8
5-Mephen	-7.61	-0.81	3.7	165.8
4,7-Me2phen	-7.57	-0.87	4.1	179.0
5,6-Me2phen	-7.50	-0.74	4.0	177.8
3,4,7,8-Me4phen	-7.45	-0.79	3.9	207.9
AT	-7.46	-0.30	1.5	170.3
AT/TA	-7.49	-0.21	0.6	332.9
(AT/phen/TA)mg	-7.42	-0.92	2.3	461.9
(AT/4-Mephen/TA)mg	-7.41	-0.79	0.8	472.1
(AT/5-Mephen/TA)mg	-7.26	-0.76	2.3	477.3
(AT/4,7-Me_2phen/TA)mg	-7.32	-0.71	2.4	488.5
(AT/5,6-Me_2phen/TA)mg	-7.27	-0.76	2.1	485.5
(AT/3,4,7,8-Me_4phen/TA)mg	-7.16	-0.78	2.7	515.3
(AT/phen/TA)MG	-7.07	-0.66	3.8	460.7
(AT/4-Mephen/TA)MG	-6.98	-0.59	2.7	470.4

(AT/5-Mephen/TA)MG	-6.94	-0.61	2.6	471.5
(AT/4,7-Me_2phen/TA)MG	-7.00	-0.64	4.0	483.5
(AT/5,6-Me_2phen/TA)MG	-7.00	-0.60	4.1	483.2
(AT/3,4,7,8-Me_4phen/TA)MG	-6.97	-0.63	4.1	508.9

Table S4. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/4-Mephen/TA)mg system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0209	0.0633
N_6-H···O_5 (d)	0.0222	0.0682
N_7···H-N_6 (u)	0.0386	0.0970
N_7···H-N_6 (d)	0.0301	0.0799
C_8-H···O_8 (u)	0.0055	0.0206
C_8-H···O_8 (d)	No BCP	No BCP
N_6(u)-H···N_3(d)	0.0171	0.0506
N_6(d)-H···N_3(u)	0.0179	0.0536
C_3(Tu)···C_{13}(phen)	0.0076	0.0198
N_1(Tu)···C_{12}(phen)	0.0080	0.0242
N_6(Tu)···C_5(phen)	0.0070	0.0183
C_7(Tu)···C_{11}(phen)	0.0081	0.0303
C_5(Au)···H_6(phen)	0.0100	0.0377
N_9(Au)···H_7(phen)	0.0058	0.0182
N_6(Au)···H_5(phen)	0.0070	0.0208
C_5(Ad)···H_5(phen)	0.0082	0.0310
N_6(Ad)···H_6(phen)	0.0086	0.0268
O_8(Td)···C_{13}(phen)	0.0076	0.0241
N_6(Td)···C_6(phen)	0.0076	0.0191
N_1(Td)···C_{11}(phen)	0.0084	0.0249
C_3(Td)···C_{14}(phen)	0.0076	0.0189
N_6(Au)···N_6(Ad)	0.0032	0.0096
C_3-CH_3(Tu)···C_4(phen)	0.0069	0.0222
C_4-CH_3(phen)···O_5(Tu)	0.0072	0.0248
C_4-CH_3(phen)···N_9(Ad)	0.0093	0.0302
C_3-CH_3(Td)···C_7(phen)	0.0062	0.0195

Table S5. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/5-Mephen/TA)mg system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0241	0.0733
N_6-H···O_5 (d)	0.0262	0.0814
N_7···H-N_6 (u)	0.0492	0.1104
N_7···H-N_6 (d)	0.0481	0.1105
C_8-H···O_8 (u)	0.0066	0.0242
C_8-H···O_8 (d)	0.0073	0.0262
C_2(Tu)···C_4(phen)	0.0072	0.0198
C_7(Tu)···C_{12}(phen)	0.0071	0.0261
N_7(Au)···C_7(phen)	0.0079	0.0224
N_9(Au)···C_8(phen)	0.0072	0.0211
N_6(Au)···H_6(phen)	0.0054	0.0152
C_8(Ad)···C_4(phen)	0.0045	0.0136
O_8(Td)···N_1(phen)	0.0084	0.0277
C_7(Td)···C_{12}(phen)	0.0088	0.0345
C_2(Td)···N_{10}(phen)	0.0088	0.0282
C_4(Td)···C_{14}(phen)	0.0066	0.0194
C_3-CH_3(Tu)···H_3C-C_5(phen)	0.0080	0.0282
C_5-CH_3(phen)···O_5(Tu)	0.0083	0.0286
C_5-CH_3(phen)···H_4(phen)	0.0115	0.0494
C_5-CH_3(phen)···N_7(Ad)	0.0084	0.0291
C_3-CH_3(Td)···C_8(phen)	0.0064	0.0199

Table S6. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/4,7-Me_2phen/TA)mg system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0231	0.0692
N_6-H···O_5 (d)	0.0231	0.0692
N_7···H-N_6 (u)	0.0477	0.1099
N_7···H-N_6 (d)	0.0477	0.1099
C_8-H···O_8 (u)	0.0068	0.0249
C_8-H···O_8 (d)	0.0068	0.0250
C_2(Tu)···N_1(phen)	0.0081	0.0257
C_4(Tu)···C_{13}(phen)	0.0075	0.0239
N_1(Tu)···C_{12}(phen)	0.0078	0.0245
C_7(Tu)···C_{11}(phen)	0.0087	0.0339
N_6(Tu)···C_5(phen)	0.0060	0.0160
O_8(Tu)···N_{10}(phen)	0.0080	0.0262
N_7(Au)···C_6(phen)	0.0062	0.0174
N_5(Au)···C_6(phen)	0.0058	0.0171
N_7(Ad)···C_5(phen)	0.0062	0.0174
N_6(Ad)···C_5(phen)	0.0057	0.0169
O_8(Td)···N_1(phen)	0.0079	0.0260
C_7(Td)···C_{12}(phen)	0.0087	0.0337
N_6(Td)···C_6(phen)	0.0060	0.0160
N_1(Td)···C_{11}(phen)	0.0078	0.0245
C_2(Td)···N_{10}(phen)	0.0081	0.0257
C_4(Td)···C_{14}(phen)	0.0075	0.0240
C_5-CH_3(Tu)···C_4(phen)	0.0069	0.0221
C_3-CH_3(Tu)···CH_3-C_4(phen)	0.0065	0.0244
C_4-CH_3(phen)···O_5(Tu)	0.0072	0.0247
C_4-CH_3(phen)···N_9(Ad)	0.0086	0.0310

C_7-CH_3(phen)···N_9(Au)	0.0086	0.0312
C_7-CH_3(phen)···O_5(Td)	0.0072	0.0248
C_3-CH_3(Td)···CH_3-C_7(phen)	0.0065	0.0246
C_3-CH_3(Td)···C_7(phen)	0.0070	0.0224

Table S7. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/5,6-Me_2phen/TA)mg system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0256	0.0789
N_6-H···O_5 (d)	0.0256	0.0789
N_7···H-N_6 (u)	0.0485	0.1104
N_7···H-N_6 (d)	0.0483	0.1102
C_8-H···O_8 (u)	0.0076	0.0270
C_8-H···O_8 (d)	0.0076	0.0269
C_2(Tu)···N_1(phen)	0.0084	0.0272
C_3(Tu)···C_{13}(phen)	0.0069	0.0181
C_4(Tu)···C_{11}(phen)	0.0087	0.0340
O_5(Tu)···N_{10}(phen)	0.0085	0.0279
C_8(Au)···C_7(phen)	0.0049	0.0148
N_6(Au)···CH_3-C_5(phen)	0.0052	0.0158
C_8(Ad)···C_4(phen)	0.0048	0.0144
N_6(Ad)···CH_3-C_6(phen)	0.0053	0.0160
O_8(Td)···N_1(phen)	0.0085	0.0279
C_7(Td)···C_{12}(phen)	0.0088	0.0341
C_2(Td)···N_{10}(phen)	0.0084	0.0272
C_3(Td)···C_{14}(phen)	0.0069	0.0181
C_3-CH_3(Tu)···C_4(phen)	0.0063	0.0194
C_5-CH_3(phen)···O_5(Tu)	0.0092	0.0316
C_5-CH_3(phen)···N_7(Ad)	0.0092	0.0312
C_6-CH_3(phen)···N_7(Au)	0.0092	0.0314
C_6-CH_3(phen)···O_5(Td)	0.0091	0.0314
C_3-CH_3(Td)···C_7(phen)	0.0063	0.0192

Table S8. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/3,4,7,8-Me_4phen/TA)mg system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0270	0.0837
N_6-H···O_5 (d)	0.0243	0.0738
N_7···H-N_6 (u)	0.0517	0.1130
N_7···H-N_6 (d)	0.0471	0.1098
C_8-H···O_8 (u)	0.0073	0.0266
C_8-H···O_8 (d)	0.0061	0.0227
C_2(Tu)···C_4(phen)	0.0080	0.0242
C_7(Tu)···C_{12}(phen)	0.0068	0.0247
C_4(Tu)···C_5(phen)	0.0062	0.0205
C_8(Au)···C_9(phen)	0.0072	0.0225
N_7(Au)···C_7(phen)	0.0069	0.0191
N_9(Ad)···CH_3-C_4(phen)	0.0075	0.0264
N_7(Ad)···C_5(phen)	0.0056	0.0158
N_5(Ad)···C_5(phen)	0.0055	0.0161
O_8(Td)···C_2(phen)	0.0081	0.0271
C_7(Td)···C_{12}(phen)	0.0086	0.0331
C_2(Td)···N_{10}(phen)	0.0082	0.0259
C_3(Td)···C_{14}(phen)	0.0071	0.0192
C_4-CH_3(phen)···C_2(Tu)	0.0065	0.0206
C_4-CH_3(phen)···CH_3-C_3(Tu)	0.0060	0.0219
C_7-CH_3(phen)···N_6(Au)	0.0093	0.0268
C_7-CH_3(phen)···O_5(Td)	0.0071	0.0245
C_8-CH_3(phen)···C_{10}(Au)	0.0086	0.0324
C_3-CH_3(Td)···C_7(phen)	0.0072	0.0235

Table S9. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/phen/TA)mg system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0260	0.0804
N_6-H···O_5 (d)	0.0259	0.0816
N_7···H-N_6 (u)	0.0490	0.1100
N_7···H-N_6 (d)	0.0395	0.0992
C_8-H···O_8 (u)	0.0066	0.0244
C_8-H···O_8 (d)	0.0060	0.0220
CH_3(Tu)···H-C_5(phen)	0.0035	0.0120
CH_3(Tu)···N_1(Ad)	0.0016	0.0056
CH_3(Td)···C_8(phen)	0.0064	0.0200
C_2(Tu)···C_4(phen)	0.0084	0.0252
C_7(Tu)···C_{12}(phen)	0.0066	0.0232
C_4(Tu)···C_5(phen)	0.0076	0.0256
N_6(Au)···C_6(phen)	0.0038	0.0108
N_7(Au)···C_7(phen)	0.0081	0.0240
C_8(Au)···C_8(phen)	0.0068	0.0208

C_{10}(Au)···C_8(phen)	0.0059	0.0184
N_9(Ad)···H_4(phen)	0.0073	0.0232
C_4(Ad)···H_5(phen)	0.0065	0.0208
N_7(Ad)···C_5(phen)	0.0083	0.0240
N_6(Ad)···C_6(phen)	0.0041	0.0116
C_7(Td)···C_{12}(phen)	0.0085	0.0324
N_1(Td)···C_{12}(phen)	0.0084	0.0276
C_3(Td)···C_{14}(phen)	0.0061	0.0152
C_2(Td)···N_{10}(phen)	0.0086	0.0276
C_3(Td)···C_8(phen)	0.0060	0.0160

Table S10. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/4-Mephen/TA)MG system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0228	0.0707
N_6-H···O_5 (d)	0.0232	0.0721
N_7···H-N_6 (u)	0.0520	0.1101
N_7···H-N_6 (d)	0.0526	0.1103
C_8-H···O_8 (u)	0.0069	0.0249
C_8-H···O_8 (d)	0.0070	0.0252
C_{10}(Au)···C_4(phen)	0.0083	0.0245
C_8(Au)···C_5(phen)	0.0066	0.0201
N_6(Au)···N_1(phen)	0.0066	0.0190
N_6(Au)···N_{10}(phen)	0.0050	0.0141
N_7(Au)···C_{12}(phen)	0.0074	0.0224
N_6(Tu)···C_7(phen)	0.0085	0.0243
N_6(Td)···C_4(phen)	0.0080	0.0222
N_6(Ad)···N_1(phen)	0.0044	0.0129
N_6(Ad)···N_{10}(phen)	0.0069	0.0194
N_7(Ad)···C_{11}(phen)	0.0075	0.0217
C_8(Ad)···C_{14}(phen)	0.0063	0.0195
C_{10}(Ad)···C_7(phen)	0.0078	0.0225
C_4-CH_3(phen)···N_9(Au)	0.0082	0.0259
C_4-CH_3(phen)···O_8(Td)	0.0101	0.0343

Table S11. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/5-Mephen/TA)MG system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0230	0.0715
N_6-H···O_5 (d)	0.0232	0.0727
N_7···H-N_6 (u)	0.0515	0.1098
N_7···H-N_6 (d)	0.0521	0.1095
C_8-H···O_8 (u)	0.0068	0.0246
C_8-H···O_8 (d)	0.0068	0.0246
C_{10}(Au)···C_4(phen)	0.0080	0.0235
N_6(Au)···N_1(phen)	0.0066	0.0192
N_6(Au)···N_{10}(phen)	0.0049	0.0140
N_7(Au)···C_{12}(phen)	0.0075	0.0229
C_8(Au)···C_5(phen)	0.0070	0.0217
O_8(Tu)···C_6(phen)	0.0052	0.0173
N_6(Tu)···C_7(phen)	0.0086	0.0243
N_6(Td)···C_4(phen)	0.0084	0.0235
N_6(Ad)···N_1(phen)	0.0045	0.0132
N_6(Ad)···N_{10}(phen)	0.0069	0.0193
N_7(Ad)···C_{11}(phen)	0.0076	0.0222
C_8(Ad)···C_6(phen)	0.0065	0.0197
C_{10}(Ad)···C_7(phen)	0.0078	0.0226
C_5-CH_3(phen)···N_9(Au)	0.0062	0.0190
C_5-CH_3(phen)···O_8(Td)	0.0097	0.0335

Table S12. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/4,7-Me_2phen/TA)MG system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0232	0.0724
N_6-H···O_5 (d)	0.0220	0.0674
N_7···H-N_6 (u)	0.0502	0.1088
N_7···H-N_6 (d)	0.0508	0.1088
C_8-H···O_8 (u)	0.0063	0.0232
C_8-H···O_8 (d)	0.0066	0.0238
C_{10}(Au)···C_4(phen)	0.0083	0.0247
N_3(Au)···C_2(phen)	0.0070	0.0205
N_6(Au)···N_1(phen)	0.0067	0.0194
N_6(Au)···N_{10}(phen)	0.0052	0.0150
N_7(Au)···C_{12}(phen)	0.0076	0.0234
C_8(Au)···C_5(phen)	0.0070	0.0215
C_4(Tu)···C_9(phen)	0.0072	0.0251
C_3(Tu)···C_8(phen)	0.0067	0.0171
C_7(Tu)···C_7(phen)	0.0078	0.0276
N_1(Tu)···CH_3-C_7(phen)	0.0064	0.0214
C_4(Td)···C_{13}(phen)	0.0072	0.0244
C_7(Td)···C_6(phen)	0.0080	0.0276
N_6(Ad)···N_1(phen)	0.0068	0.0205
N_6(Ad)···N_{10}(phen)	0.0087	0.0266

C_4(Ad)···C_9(phen)	0.0087	0.0258
C_8(Ad)···C_8(phen)	0.0072	0.0215
C_4-CH_3(phen)···N_9(Au)	0.0078	0.0247
C_4-CH_3(phen)···C_3(Td)	0.0066	0.0196
C_7-CH_3(phen)···O_8(Tu)	0.0091	0.0309
C_7-CH_3(phen)···O_8(Td)	0.0114	0.0393
C_3-CH_3(Td)···C_4(phen)	0.0073	0.0224

Table S13. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/5,6-Me_2phen/TA)MG system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0231	0.0722
N_6-H···O_5 (d)	0.0221	0.0673
N_7···H-N_6 (u)	0.0499	0.1082
N_7···H-N_6 (d)	0.0508	0.1089
C_8-H···O_8 (u)	0.0064	0.0236
C_8-H···O_8 (d)	0.0066	0.0242
C_{10}(Au)···C_4(phen)	0.0078	0.0225
N_3(Au)···C_2(phen)	0.0068	0.0200
N_6(Au)···N_1(phen)	0.0070	0.0200
N_6(Au)···N_{10}(phen)	0.0052	0.0152
N_7(Au)···C_{12}(phen)	0.0078	0.0235
C_8(Au)···C_5(phen)	0.0070	0.0216
N_6(Tu)··C_8(phen)	0.0076	0.0204
C_4(Tu)···C_9(phen)	0.0076	0.0276
C_4(Td)···C_{13}(phen)	0.0070	0.0239
C_7(Td)···C_6(phen)	0.0078	0.0280
N_6(Ad)···N_1(phen)	0.0078	0.0228
C_5(Ad)···N_{10}(phen)	0.0086	0.0303
C_4(Ad)···C_9(phen)	0.0080	0.0238

C_5-CH_3(phen)···N_9(Au)	0.0084	0.0256
C_6-CH_3(phen)···O_8(Tu)	0.0122	0.0412
C_5-CH_3(phen)···C_2(Td)	0.0073	0.0222
C_6-CH_3(phen)···O_8(Td)	0.0111	0.0367
C_3-CH_3(Td)···C_4(phen)	0.0070	0.0219

Table S14. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/3,4,7,8-Me_4phen/TA)MG system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0215	0.0654
N_6-H···O_5 (d)	0.0243	0.0766
N_7···H-N_6 (u)	0.0518	0.1100
N_7···H-N_6 (d)	0.0522	0.1107
C_8-H···O_8 (u)	0.0063	0.0232
C_8-H···O_8 (d)	0.0064	0.0234
C_4(Au)···C_2(phen)	0.0089	0.0267
N_6(Au)···N_1(phen)	0.0088	0.0284
N_6(Au)···N_{10}(phen)	0.0083	0.0249
C_4(Tu)···C_{14}(phen)	0.0072	0.0248
C_7(Tu)···C_5(phen)	0.0076	0.0261
C_7(Td)···C_4(phen)	0.0077	0.0273
C_4(Td)···C_2(phen)	0.0072	0.0255
N_6(Ad)···N_1(phen)	0.0048	0.0139
N_6(Ad)···N_{10}(phen)	0.0070	0.0198
C_{10}(Ad)···C_7(phen)	0.0081	0.0237
C_8(Ad)···C_6(phen)	0.0069	0.0215
N_7(Ad)···C_{11}(phen)	0.0077	0.0228

C_3-CH_3(phen)···N_9(Au)	0.0107	0.0339
C_4-CH_3(phen)···O_8(Tu)	0.0118	0.0403
C_7-CH_3(phen)···C_3(Tu)	0.0070	0.0215
C_3-CH_3(Tu)···C_7(phen)	0.0070	0.0215
C_8-CH_3(phen)···C_2(Ad)	0.0069	0.0244
C_7-CH_3(phen)···N_9(Ad)	0.0079	0.0247
C_4-CH_3(phen)···O_8(Td)	0.0092	0.0308
C_3-CH_3(phen)···C_2(Td)	0.0087	0.0302

Table S15. Electron Density (ρ) and Laplacian ($\nabla^2\rho$) in a.u. on all BCPs corresponding to weak interactions found in (AT/phen/TA)MG system.

BCP's	ρ	$\nabla^2\rho$
N_6-H···O_5 (u)	0.0226	0.0704
N_6-H···O_5 (d)	0.0226	0.0692
N_7···H-N_6 (u)	0.0500	0.1084
N_7···H-N_6 (d)	0.0498	0.1080
C_8-H···O_8 (u)	0.0064	0.0232
C_8-H···O_8 (d)	0.0060	0.0224
CH_3(Td)···C_4(phen)	0.0067	0.0208
C_{10}(Au)···C_4(phen)	0.0077	0.0220
N_3(Au)···C_2(phen)	0.0069	0.0204
C_5(Au)···C_{12}(phen)	0.0078	0.0264
C_8(Au)···C_5(phen)	0.0069	0.0216

N_6(Au)···N_{10}(phen)	0.0058	0.0164
O_8(Tu)···C_6(phen)	0.0064	0.0216
N_6(Tu)···C_7(phen)	0.0083	0.0236
O_5(Tu)···C_9(phen)	0.0068	0.0232
C_4(Tu)···C_8(phen)	0.0070	0.0216
C_3(Tu)···C_8(phen)	0.0069	0.0180
C_4(Td)···C_{13}(phen)	0.0072	0.0252
C_7(Td)···C_6(phen)	0.0084	0.0304
N_6(Ad)···N_1(phen)	0.0073	0.0212
C_5(Ad)···N_{10}(phen)	0.0087	0.0304
C_4(Ad)···C_9(phen)	0.0082	0.0240
C_8(Ad)···C_8(phen)	0.0070	0.0212

Table S16. Cartesian coordinates of: phen (M06-2X/6-31+G(d,p)), 4-Mephen (M06-2X/6-31+G(d,p)), 5-Mephen (M06-2X/6-31+G(d,p)), 4,7-Me_2phen (M06-2X/6-31+G(d,p)), 5,6-Me_2phen (M06-2X/6-31+G(d,p)), 3,4,7,8-Me_4phen (M06-2X/6-31+G(d,p)), AT/TA (M06-2X/6-31+G(d,p)), (AT/phen/TA)mg (M06-2X/6-31+G(d,p)), (AT/4-Mephen/TA)mg (M06-2X/6-31+G(d,p)), (AT/5-Mephen/TA)mg (M06-2X/6-31+G(d,p)), (AT/4,7-Me_2phen/TA)mg (M06-2X/6-31+G(d,p)), (AT/5,6-Me_2phen/TA)mg (M06-2X/6-31+G(d,p)), (AT/3,4,7,8-Me_4phen/TA)mg (M06-2X/6-31+G(d,p)), (AT/phen/TA)MG (M06-2X/6-31+G(d,p)), (AT/4-Mephen/TA)MG (M06-2X/6-31+G(d,p)), (AT/5-Mephen/TA)MG (M06-2X/6-31+G(d,p)), (AT/4,7-Me_2phen/TA)MG (M06-2X/6-31+G(d,p)), (AT/5,6-Me_2phen/TA)MG (M06-2X/6-31+G(d,p)), (AT/3,4,7,8-Me_4phen/TA)MG (M06-2X/6-31+G(d,p)).

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

```
C 0.103853 -3.707595 2.989506
N -1.142123 -3.381993 3.262126
C -1.442085 -2.068561 3.342469
C -0.481545 -1.045417 3.147531
C  0.856885 -1.424109 2.854326
C  1.135339 -2.772512 2.778200
C -2.821596 -1.698229 3.644619
C -3.160716 -0.327054 3.734099
C -2.157424  0.678258 3.529348
C -0.875396  0.334485 3.248758
N -3.728388 -2.680883 3.828793
C -4.970988 -2.337691 4.101466
C -5.416761 -1.004032 4.213693
C -4.500261  0.003909 4.027472
C  1.930709 -0.392549 2.635067
H -4.787807  1.049571 4.101973
H -5.673539 -3.156516 4.243587
H -6.456094 -0.793403 4.440875
H  0.320680 -4.772510 2.930125
H  2.140582 -3.118784 2.557324
H -0.130229  1.108370 3.097227
H -2.447592  1.722853 3.604144
H  2.887136 -0.874351 2.423948
H  1.685643  0.260942 1.791699
H  2.056947  0.241437 3.518503
```

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

```
C  0.799566  0.926761 2.981966

C -0.528087  0.259866 3.222630

C -0.613022 -1.186937 3.260672
```

C -1.852699 -1.837901 3.486357

C -3.055003 -1.033226 3.681532

C -2.936663 0.374482 3.637872

C -1.659336 0.989172 3.406778

N -4.230072 -1.658756 3.895073

C -5.305756 -0.916104 4.068620

C -5.302813 0.493313 4.044803

C -4.106715 1.137895 3.827457

C 0.521020 -2.006369 3.076661

C 0.387083 -3.375979 3.121921

C -0.892997 -3.912978 3.353305

N -1.974253 -3.179784 3.529384

H -1.614414 2.075938 3.381352

H 1.493170 -1.557138 2.900373

H -6.236656 -1.453306 4.238385

H -6.225464 1.043229 4.195034

H -1.032338 -4.991360 3.395120

H 1.239292 -4.032503 2.983906

H -4.047722 2.222938 3.799218

H 0.686901 2.012603 2.984221

H 1.526083 0.660135 3.756973

H 1.224527 0.632499 2.016416

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4,7-Me$_2$phen (M06-2X/6-31+G(d,p))

N -3.737823 -2.572862 3.630952

C -2.832354 -1.575464 3.535788

C -3.191417 -0.206321 3.578647

C -4.564906 0.129460 3.728834

C -5.466718 -0.908689 3.823846

C -5.002775 -2.237738 3.769345

C -1.426729 -1.940430 3.382581

C -0.453118 -0.917351 3.279438

C -0.863193 0.458012 3.327580

C -2.170202 0.797379 3.470458

N -1.114804 -3.253869 3.346155

C 0.153495 -3.576448 3.208190

C 1.199530 -2.639435 3.096773

C 0.910390 -1.292137 3.130982

C 1.996753 -0.256873 3.016019

C -5.016825 1.564067 3.782105

H -5.712508 -3.059650 3.843609

H -6.528352 -0.711924 3.939856

H 0.378684 -4.641051 3.181781

H 2.223249 -2.984061 2.985009

H -0.111778 1.236755 3.247970

H -2.452497 1.844547 3.504152

H 2.971914 -0.735371 2.908252

H 1.837141 0.389730 2.147206

H 2.028210 0.383886 3.903072

H -6.100514 1.620090 3.900400

H -4.555118 2.093588 4.621656

H -4.746396 2.098522 2.865785

28

5,6-Me$_2$phen (M06-2X/6-31+G(d,p))

C 4.633663 0.018446 3.764780

C 3.260331 -0.276362 3.613994

C 2.901905 -1.644432 3.616309

N 3.796729 -2.642409 3.753095

C 5.069317 -2.328120 3.891690

C 5.544694 -1.005263 3.904355

C 1.496696 -2.000649 3.463576

C 0.544881 -0.964760 3.318499

C 0.941136 0.435683 3.319639

C 2.260042 0.770041 3.463479

N 1.170757 -3.307990 3.468547

C -0.098110 -3.637830 3.331329

C -1.131972 -2.697508 3.179469

C -0.803649 -1.359779 3.173676

H -1.584231 -0.616381 3.057941

H 5.761908 -3.160374 3.999598

H 6.604093 -0.804157 4.021532

H -0.322639 -4.702487 3.340361

H -2.160060 -3.025476 3.069959

C -0.168469 1.446032 3.156906

C 2.769583 2.190854 3.477949

H 4.977209 1.046650 3.771449

H 0.185061 2.473414 3.165772

H -0.903847 1.345973 3.962304

H -0.697721 1.290245 2.210798

H 3.286032 2.406917 4.419243

H 1.980118 2.928669 3.364116

H 3.488037 2.352346 2.667246

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3,4,7,5-Me$_2$phen (M06-2X/6-31+G(d,p))

C -3.919461 2.893299 3.500863

C -3.996209 1.393424 3.627407

C -2.822503 0.606546 3.469036

C -2.920643 -0.799009 3.592758

N -4.088846 -1.419452 3.855758

C -5.158016 -0.668531 3.997052

C -5.189787 0.742028 3.896911

C -1.725562 -1.620757 3.432940

C -0.484605 -1.001021 3.156265

C -0.429722 0.430237 3.038374

C -1.542071 1.195098 3.187260

N -1.851610 -2.957741 3.556729

C -0.768138 -3.686910 3.410725

C 0.526112 -3.188146 3.133453

C 0.670820 -1.815621 3.003373

C 2.005503 -1.180934 2.708016

H -6.087691 -1.197362 4.208890

C -6.500962 1.461617 4.085033

H -0.900397 -4.764067 3.516096

C 1.671840 -4.157836 2.994249

H 0.520263 0.908982 2.825909

H -1.463055 2.272765 3.091407

H 2.795093 -1.926471 2.617839

H 1.971047 -0.614478 1.771594

H 2.292059 -0.483686 3.502154

H -4.892663 3.360559 3.648994

H -3.229866 3.313943 4.240054

H -3.555156 3.184617 2.510216

H 2.454083 -3.968642 3.736212

H 1.320670 -5.182488 3.136125

H 2.133647 -4.098834 2.003561

H -7.301185 0.745497 4.285457

H -6.461680 2.160444 4.926650

H -6.780723 2.031940 3.193599

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

N	-2.821481	0.226632	-6.277781
C	-3.846066	1.137828	-6.410718
N	-3.424857	2.396208	-6.798274
C	-2.110525	2.702386	-7.056344
C	-1.116197	1.795372	-6.945515
C	-1.470746	0.467860	-6.444173
O	-5.015788	0.866960	-6.200895
O	-0.645892	-0.405512	-6.169075
C	0.320537	2.080612	-7.257003
H	-3.091725	-0.707089	-5.906637
H	-1.925003	3.729473	-7.353077
H	0.464401	3.140857	-7.480446
H	-4.125955	3.123381	-6.739489
H	0.958141	1.811739	-6.410327
H	0.657252	1.490046	-8.114873
N	-2.770151	-4.162312	-1.963126
C	-3.319419	-3.518717	-3.055538
C	-4.709790	-3.568604	-3.020456
N	-5.002500	-4.288196	-1.887986
C	-3.804660	-4.607668	-1.298030
N	-5.563700	-2.995394	-3.879782
C	-4.914807	-2.333908	-4.831470
N	-3.586776	-2.216124	-5.001283
C	-2.740612	-2.795557	-4.126437
N	-1.421573	-2.638910	-4.276245
H	-5.521096	-1.795931	-5.556587
H	-0.778192	-2.993766	-3.573634
H	-1.082576	-1.990957	-4.988107
H	-5.928794	-4.510316	-1.553984
H	-3.756057	-5.165150	-0.372936
C	2.056926	-1.137431	-1.233056
N	2.339726	-0.014026	-0.558970
C	1.249079	0.497143	0.000000
N	0.000000	0.000000	0.000000
C	-0.248231	-1.169873	-0.622404
C	0.819524	-1.763902	-1.337766
N	0.885503	-2.865201	-2.169605
C	2.137150	-2.907346	-2.547200
N	-1.470151	-1.706784	-0.565674
N	2.896878	-1.898082	-2.008618
H	1.369321	1.443888	0.519924
H	-1.652551	-2.611019	-0.990298
H	-2.217495	-1.197613	-0.092681
H	3.877832	-1.718986	-2.165369
H	2.560106	-3.642835	-3.217320

N	-2.287124	1.872145	-0.119567
C	-2.033792	3.126344	-0.635495
N	-3.174793	3.879859	-0.845970
C	-4.440646	3.428968	-0.558373
C	-4.676923	2.199583	-0.052451
C	-3.529662	1.306766	0.110183
O	-0.914691	3.534801	-0.886482
O	-3.623771	0.120196	0.423671
C	-6.036586	1.678023	0.295946
H	-1.464739	1.257754	0.000000
H	-5.240963	4.128039	-0.777892
H	-6.811444	2.389205	-0.001472
H	-6.221039	0.726619	-0.210210
H	-6.119086	1.493953	1.371699
H	-3.035705	4.737522	-1.365308
C	-0.990466	4.447120	-4.316069
N	-2.236930	4.058611	-4.128543
C	-2.439371	2.771668	-3.765191
C	-1.380373	1.852158	-3.574522
C	-0.049755	2.291759	-3.812717
C	0.129486	3.606658	-4.182502
C	-3.812042	2.322379	-3.560610
C	-4.040377	0.997594	-3.121537
C	-2.935834	0.118173	-2.883963
C	-1.661912	0.518071	-3.122318
N	-4.822266	3.186623	-3.804581
C	-6.058169	2.755386	-3.634540
C	-6.395037	1.454601	-3.208083
C	-5.374175	0.573500	-2.946878
C	1.108333	1.349468	-3.655827
H	-5.570959	-0.446080	-2.622143
H	-6.848190	3.472341	-3.852409
H	-7.435743	1.168061	-3.102220
H	-0.850130	5.491065	-4.593170
H	1.125146	4.000748	-4.363736
H	-0.839453	-0.171489	-2.966146
H	-3.145227	-0.874361	-2.498546
H	2.044593	1.837708	-3.936115
H	1.197406	1.027822	-2.613555
H	0.970751	0.459026	-4.281607

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

C	1.299151	-0.246413	6.449449
N	2.328951	-1.163341	6.405149
C	2.216553	-2.531628	6.336004
N	0.911377	-2.984969	6.306069
C	-0.171493	-2.143574	6.379603
C	-0.050364	-0.803173	6.497041
O	3.181269	-3.277929	6.294877
C	-1.206801	0.138773	6.630813
O	1.542105	0.963093	6.444540
H	3.308220	-0.794752	6.341945
H	-1.138820	-2.633086	6.333914
H	-2.153324	-0.385174	6.472409
H	-1.124391	0.947290	5.899836
H	-1.221821	0.600111	7.623477
H	0.796157	-3.952932	6.033186
N	4.943416	-0.244563	6.107113

C	5.901032	-1.181697	5.995792
N	7.183171	-1.000133	5.701647
C	7.466596	0.300934	5.535723
C	6.582143	1.373012	5.619165
C	5.235679	1.051868	5.903039
N	7.214572	2.571247	5.361906
C	8.455377	2.231931	5.135468
N	8.672939	0.875673	5.223868
N	4.257895	1.965545	5.946529
H	5.558486	-2.202801	6.154976
H	4.494741	2.937398	5.822502
H	3.295096	1.684726	6.148964
H	9.544550	0.383833	5.094103
H	9.256362	2.919191	4.900838
N	0.000000	0.000000	0.000000
C	-1.225403	-0.554776	0.000000
N	-2.391132	0.055294	0.174132
C	-2.228138	1.368496	0.383056
C	-1.027534	2.072431	0.430478
C	0.146844	1.316310	0.222869
N	-3.190697	2.318382	0.620798
C	-2.533257	3.515201	0.795759
N	-1.235401	3.411153	0.691948
N	1.377551	1.848347	0.270527
H	-1.238747	-1.632322	-0.148223
H	1.468125	2.847667	0.368461
H	2.196829	1.276984	0.053243
H	-4.186526	2.155799	0.644181
H	-3.070537	4.431544	0.997490
N	2.934391	-3.880873	0.274965
C	1.848244	-3.021423	0.216113
N	2.198475	-1.704674	0.023587
C	3.467555	-1.201912	-0.170656
C	4.550169	-2.186469	-0.198037
C	4.223938	-3.474194	0.048296
O	0.698444	-3.401909	0.323327
C	5.944119	-1.722870	-0.494329
O	3.645050	0.010012	-0.315295
H	1.388298	-1.035907	0.000000
H	4.971302	-4.260669	0.082998
H	6.634236	-2.569844	-0.521132
H	2.712589	-4.842499	0.492486
H	5.981332	-1.208825	-1.459117
H	6.298655	-1.011537	0.257293
H	0.003754	1.374263	3.207283
C	4.872430	0.054305	2.842834
C	3.546251	-0.616778	3.077263
C	3.452243	-2.058571	3.204808
C	2.189713	-2.699694	3.316662
C	0.975330	-1.892301	3.277560
C	1.107178	-0.486586	3.213117
C	2.403073	0.119569	3.120910
N	-0.224517	-2.510064	3.326521
C	-1.307056	-1.757946	3.295611
C	-1.290019	-0.347524	3.256875
C	-0.072176	0.288986	3.229784
C	4.597567	-2.883427	3.248617
C	4.454688	-4.240816	3.422026
C	3.154222	-4.764455	3.548834

N	2.059223	-4.033756	3.490206
H	2.453024	1.204143	3.055477
H	5.587068	-2.444871	3.158914
H	-2.259558	-2.285521	3.308653
H	-2.223219	0.206900	3.246397
H	3.011998	-5.830958	3.716586
H	5.317312	-4.895695	3.487480
H	4.794804	1.124404	3.051989
H	5.162445	-0.054136	1.792206
H	5.672741	-0.357128	3.463155

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(AT/4,7-Me$_2$phen/TA)mg (M06-2X/6-31+G(d,p))

C	2.460175	-2.967853	-6.289555
N	2.188910	-1.620457	-6.228985
C	0.952293	-1.017339	-6.321444
C	-0.168638	-1.905284	-6.625681
C	0.080383	-3.233163	-6.638170
N	1.339661	-3.755254	-6.472291
O	0.839032	0.199621	-6.146613
C	-1.520365	-1.305256	-6.863077
O	3.585815	-3.425486	-6.184201
H	-0.707879	-3.965090	-6.780635
H	-2.281472	-2.086547	-6.935866
H	-1.792799	-0.628503	-6.049163
H	-1.528564	-0.718666	-7.787254
H	1.476281	-4.745467	-6.316382
H	3.018637	-1.019926	-6.006971
N	4.446176	-0.124039	-5.553963
C	5.646601	-0.722789	-5.658967
N	6.827156	-0.239130	-5.294183
C	6.708674	0.981650	-4.752894
C	5.536908	1.713251	-4.568132
C	4.344434	1.107333	-5.023944
N	5.791168	2.933180	-3.976414
C	7.085933	2.937942	-3.805299
N	3.141901	1.693056	-4.937654
N	7.698555	1.789894	-4.253202
H	5.620073	-1.725381	-6.080597
H	3.083821	2.634679	-4.582223
H	2.318634	1.240716	-5.340500
H	8.683013	1.568893	-4.228226
H	7.652168	3.744446	-3.360380
N	0.000000	0.000000	0.000000
C	0.714202	1.135540	-0.088630
C	-0.008793	2.344136	-0.205149
C	-1.398039	2.235408	-0.177793
N	-2.122935	1.112336	-0.074847
C	-1.344956	0.040055	-0.000000
N	-1.844208	3.528624	-0.284405
C	-0.727520	4.328669	-0.367575
N	0.392661	3.658653	-0.322641
N	2.053279	1.077401	-0.077308
H	-1.829453	-0.932600	0.052812
H	2.577778	1.938143	-0.096794
H	2.528867	0.185425	0.073768
H	-2.810627	3.819316	-0.296212
H	-0.807139	5.402930	-0.460336
N	0.939702	-4.733149	-0.627082

C	0.342095	-3.502114	-0.436367
N	1.219750	-2.509574	-0.065837
C	2.581625	-2.629944	0.113965
C	3.121933	-3.983917	0.003131
C	2.276988	-4.955019	-0.407338
O	-0.852766	-3.310982	-0.589310
C	4.571514	-4.209126	0.305729
O	3.268931	-1.631236	0.347563
H	0.792819	-1.554701	-0.000000
H	2.612466	-5.970938	-0.588341
H	4.864233	-5.230721	0.049509
H	0.366392	-5.425650	-1.090988
H	5.198361	-3.515238	-0.260314
H	4.778281	-4.039378	1.367157
C	3.083609	-2.367857	-3.005359
C	2.120084	-3.360113	-3.307083
N	2.447352	-4.655271	-3.522660
C	3.723593	-4.976921	-3.452462
C	4.752588	-4.075992	-3.119860
C	4.444111	-2.756673	-2.868540
C	2.674227	-1.003016	-2.842710
C	1.376394	-0.638866	-2.993311
C	0.360560	-1.614363	-3.263742
C	0.713158	-2.978853	-3.397078
C	-1.004923	-1.245225	-3.405463
C	-1.918659	-2.260863	-3.586163
C	-1.468221	-3.592040	-3.665224
N	-0.202491	-3.953951	-3.601465
C	-1.411579	0.201831	-3.418646
C	5.481459	-1.771475	-2.406910
H	-2.191517	-4.395428	-3.797676
H	-2.978702	-2.043313	-3.679699
H	3.969035	-6.017283	-3.661099
H	5.777717	-4.428635	-3.052386
H	3.418076	-0.248445	-2.608546
H	1.098587	0.405479	-2.894799
H	6.476488	-2.221877	-2.418307
H	5.506662	-0.880566	-3.041043
H	5.246347	-1.443346	-1.386521
H	-2.498131	0.299249	-3.472758
H	-1.069264	0.727775	-2.522925
H	-0.961441	0.701021	-4.285951

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(AT/5,6-Me$_2$phen/TA)mg (M06-2X/6-31+G(d,p))

N	-1.581869	1.990797	-6.439359
C	-2.495214	3.013113	-6.334062
N	-1.925594	4.248651	-6.090141
C	-0.568602	4.439801	-5.997839
C	0.323018	3.435917	-6.146073
C	-0.211691	2.088645	-6.327872
O	-3.698761	2.844445	-6.439792
O	0.491019	1.074707	-6.381065
C	1.809121	3.612959	-6.098182
H	-1.999453	1.034305	-6.547478
H	-0.259041	5.459604	-5.793818
H	2.068238	4.631993	-5.798861
H	-2.572081	4.972051	-5.802688
H	2.252393	2.913698	-5.384198

H	2.258331	3.407140	-7.074939
N	-2.392969	-4.187087	-6.288426
C	-2.788142	-2.871541	-6.411730
C	-4.175567	-2.753001	-6.409787
N	-4.629103	-4.042075	-6.287553
C	-3.516506	-4.849677	-6.220658
N	-4.893510	-1.622088	-6.486170
C	-4.108587	-0.556518	-6.591210
N	-2.763980	-0.525470	-6.605421
C	-2.058549	-1.664649	-6.495876
N	-0.721320	-1.612445	-6.450392
H	-4.586473	0.419159	-6.659599
H	-0.203191	-2.472230	-6.359967
H	-0.238521	-0.711684	-6.473302
H	-5.597026	-4.326119	-6.256197
H	-3.601829	-5.923039	-6.122916
H	2.279745	-1.309373	-0.286156
N	2.393779	0.020201	-0.146721
C	1.206184	0.595233	-0.000000
N	0.000000	0.000000	0.000000
C	-0.099390	-1.329517	-0.172808
C	1.104771	-2.056169	-0.306814
N	1.361527	-3.397527	-0.498801
C	2.663263	-3.461036	-0.585038
N	3.276764	-2.234747	-0.465246
N	-1.309359	-1.900142	-0.231302
H	1.179349	1.676789	0.120274
H	-1.371737	-2.896835	-0.367632
H	-2.153954	-1.327639	-0.169489
H	4.265813	-2.036809	-0.499325
H	3.234290	-4.366968	-0.733939
N	-2.214759	1.689294	-0.072642
C	-1.879810	3.021777	-0.126411
N	-2.959598	3.861780	-0.323902
C	-4.251756	3.406349	-0.420688
C	-4.575457	2.098525	-0.322744
C	-3.475675	1.145860	-0.193001
O	-0.733920	3.425577	-0.016565
O	-3.628202	-0.079461	-0.189831
C	-5.975038	1.568875	-0.376218
H	-1.400982	1.031209	-0.000000
H	-5.000541	4.174340	-0.584788
H	-6.679928	2.362480	-0.637923
H	-6.051485	0.771402	-1.120109
H	-6.267497	1.141412	0.588142
H	-2.724991	4.813444	-0.575252
C	-4.589967	1.072239	-3.612531
C	-3.219753	1.355872	-3.412543
C	-2.860151	2.722071	-3.339407
N	-3.748625	3.731141	-3.465072
C	-5.013672	3.422728	-3.676241
C	-5.490006	2.103644	-3.755064
C	-1.460511	3.063464	-3.126059
C	-0.504907	2.020525	-3.106784
C	-0.894343	0.625303	-3.249919
C	-2.223864	0.298192	-3.322826
N	-1.143132	4.363940	-2.948396
C	0.122229	4.671998	-2.738177
C	1.159155	3.724908	-2.711514

C	0.841755	2.400021	-2.906217
H	1.625705	1.650422	-2.889702
H	-5.700353	4.258830	-3.798164
H	-6.542838	1.910797	-3.932063
H	0.341507	5.725712	-2.573732
H	2.182576	4.037706	-2.533339
C	0.227023	-0.380072	-3.336403
C	-2.747576	-1.116134	-3.289620
H	-4.934359	0.045185	-3.669960
H	-0.127731	-1.407577	-3.386223
H	0.812509	-0.179863	-4.241961
H	0.906631	-0.302966	-2.483495
H	-3.381354	-1.334070	-4.153580
H	-1.954698	-1.860846	-3.262548
H	-3.362012	-1.244616	-2.390312

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(AT/3,4,7,8-Me$_4$phen/TA)mg (M06-2X/6-31+G(d,p))

N	-2.707020	0.225913	6.371767
C	-2.787695	-1.135252	6.558683
N	-1.554210	-1.766209	6.581919
C	-0.363949	-1.092303	6.467798
C	-0.297805	0.248066	6.318908
C	-1.562445	0.981952	6.252118
O	-3.837201	-1.732486	6.701056
O	-1.628116	2.204271	6.104757
C	0.974512	1.026487	6.187241
H	-3.638245	0.712609	6.306978
H	0.525641	-1.715112	6.500971
H	1.846055	0.376104	6.300002
H	-1.585510	-2.774416	6.639245
H	1.025815	1.518614	5.209750
H	1.023466	1.815759	6.942610
N	-7.122036	4.443841	5.273853
C	-6.633425	3.204557	5.635134
C	-7.664750	2.295727	5.861245
N	-8.811155	3.017314	5.640914
C	-8.419629	4.289429	5.289664
N	-7.549908	1.001579	6.185347
C	-6.276186	0.643677	6.305007
N	-5.190062	1.421185	6.152023
C	-5.321276	2.713330	5.808796
N	-4.226681	3.469211	5.634217
H	-6.062423	-0.395067	6.548666
H	-4.345844	4.456688	5.469135
H	-3.294994	3.086119	5.815204
H	-9.753364	2.662773	5.712973
H	-9.141413	5.061024	5.060070
C	2.592812	0.464268	0.220818
N	2.249446	-0.825559	0.095393
C	0.933673	-0.966949	-0.000000
N	0.000000	0.000000	0.000000
C	0.359901	1.291249	0.108649
C	1.739208	1.565724	0.248391
N	2.441038	2.745206	0.386606
C	3.689312	2.365981	0.443578
N	3.848742	1.001940	0.349344
N	-0.582242	2.243566	0.094054

H	0.539937	-1.979215	-0.071989
H	-0.295749	3.209725	0.118649
H	-1.559230	1.995890	-0.079761
H	4.714029	0.482653	0.361197
H	4.537001	3.028126	0.553125
N	-2.680551	-0.787752	0.059331
C	-2.853584	-2.097283	0.444691
N	-4.175417	-2.456639	0.624118
C	-5.220191	-1.602830	0.370329
C	-5.040150	-0.336359	-0.064417
C	-3.666552	0.151815	-0.153050
O	-1.923652	-2.868047	0.616758
O	-3.367238	1.324468	-0.399085
C	-6.155622	0.599309	-0.413066
H	-1.683650	-0.474179	-0.000000
H	-6.207633	-2.017621	0.544256
H	-7.121572	0.168988	-0.134044
H	-6.030346	1.554974	0.103810
H	-6.164196	0.813280	-1.486715
H	-4.325730	-3.328646	1.115399
C	-4.997983	2.963334	2.286196
C	-5.110833	1.538925	2.761254
C	-3.930338	0.775653	2.990862
C	-4.049941	-0.598752	3.303227
N	-5.249899	-1.197317	3.462786
C	-6.324187	-0.452424	3.312459
C	-6.334999	0.913343	2.941984
C	-2.846375	-1.420649	3.409836
C	-1.570926	-0.819130	3.256741
C	-1.499946	0.596381	3.014778
C	-2.620331	1.350975	2.875288
N	-3.003022	-2.746537	3.610579
C	-1.916424	-3.484347	3.671375
C	-0.595591	-3.002222	3.546737
C	-0.414980	-1.644484	3.330386
C	0.980118	-1.088148	3.210502
H	-7.279561	-0.952140	3.481274
C	-7.661084	1.598553	2.728708
H	-2.071653	-4.554049	3.818950
C	0.558293	-3.966095	3.617249
H	-0.533680	1.081604	2.930414
H	-2.522297	2.412544	2.675184
H	1.632106	-1.777203	2.669058
H	1.012519	-0.131621	2.686435
H	1.415706	-0.932702	4.205834
H	-5.976535	3.409788	2.106633
H	-4.477524	3.581771	3.024217
H	-4.427225	2.995032	1.350346
H	1.307141	-3.655866	4.354890
H	0.210496	-4.966585	3.885489
H	1.067689	-4.038697	2.649666
H	-8.463022	1.015287	3.190741
H	-7.679275	2.601423	3.164633
H	-7.889926	1.702993	1.661640

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

N	-3.211581	2.778926	6.174430
C	-2.356389	1.699989	6.259869
C	-3.056429	0.506284	6.403896
N	-4.377027	0.878027	6.398620
C	-4.401238	2.248710	6.261052
N	-2.545628	-0.729542	6.513534
C	-1.219298	-0.705690	6.481775
N	-0.417357	0.365629	6.352328
C	-0.946306	1.598772	6.219902
N	-0.143546	2.655160	6.072251
N	2.305658	-0.139640	6.336490
C	3.181947	0.929024	6.321895
C	4.610235	0.595466	6.271835
C	4.943589	-0.707958	6.191269
N	3.996710	-1.706546	6.149690
C	2.632626	-1.464128	6.205916
O	2.764633	2.083186	6.351609
O	1.812276	-2.365524	6.142602
C	5.593568	1.724125	6.281101
C	1.033079	-0.707258	3.216772
C	0.090603	-1.785310	3.285922
C	-1.243632	-1.539860	3.297239
C	-1.750748	-0.197170	3.219595
C	-0.852606	0.894239	3.115745
C	0.583838	0.633973	3.164331
N	1.438455	1.682532	3.152874
C	2.732742	1.430726	3.157623
C	3.285466	0.131629	3.157140
C	2.424686	-0.940186	3.186864
C	-3.146005	0.078083	3.264441
C	-3.538287	1.393970	3.135780
C	-2.564103	2.400742	2.984854
N	-1.266278	2.175366	2.986143
C	-4.148129	-1.025242	3.469429
H	2.786634	-1.966235	3.193103
N	0.000000	0.000000	0.000000
C	0.970591	0.935563	0.003495
C	2.306775	0.473840	-0.021710
C	2.482811	-0.906221	-0.023989
N	1.528997	-1.848920	-0.007330
C	0.318164	-1.306920	0.000000
N	3.843973	-1.079280	-0.038318
C	4.403177	0.179444	-0.048587
N	3.516335	1.137397	-0.037964
N	0.648342	2.231139	0.016048
N	-2.693981	0.627717	0.003011
C	-3.080898	1.950038	-0.107107
C	-4.524324	2.210312	-0.050154
C	-5.341134	1.156551	0.146356

N	-4.861522	-0.125631	0.293086
C	-3.514259	-0.444050	0.237041
O	-2.246303	2.839460	-0.244829
O	-3.113808	-1.588476	0.386163
C	-4.985890	3.627817	-0.186493
H	-0.534547	-1.982335	0.021036
H	1.376491	2.903145	0.203441
H	-0.327199	2.518039	0.089464
H	4.324113	-1.966240	-0.063061
H	5.474947	0.322171	-0.068957
H	-1.657169	0.412163	0.000000
H	-6.419755	1.260959	0.208734
H	-6.075250	3.692307	-0.131753
H	-4.552905	4.248030	0.604346
H	-4.652076	4.051984	-1.137535
H	-5.484389	-0.906284	0.442269
H	-0.698353	-1.658286	6.554048
H	-0.552203	3.529056	5.778013
H	0.864757	2.525256	5.999082
H	-5.165054	0.255945	6.499446
H	-5.332361	2.798065	6.236312
H	1.269689	0.075228	6.339442
H	5.975410	-1.041533	6.143384
H	6.619810	1.350329	6.249748
H	4.259588	-2.679442	6.087516
H	3.391039	2.297527	3.154479
H	4.363174	0.001425	3.133504
H	-2.873283	3.438432	2.870619
H	-4.590931	1.665295	3.159822
H	-1.946207	-2.363893	3.357121
H	0.472769	-2.800432	3.341078
H	5.428465	2.380878	5.421237
H	5.466425	2.339211	7.176223
H	-4.071810	-1.774774	2.674168
H	-3.966767	-1.528158	4.426697
H	-5.163394	-0.617520	3.473219

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

N	-3.224075	2.674205	6.198370
C	-2.360523	1.599796	6.256561
C	-3.050816	0.398145	6.377669
N	-4.373815	0.760486	6.389344
C	-4.409223	2.133418	6.281288
N	-2.529560	-0.835883	6.455636
C	-1.203514	-0.800022	6.422112
N	-0.409809	0.280563	6.316708
C	-0.949637	1.511414	6.212654
N	-0.157048	2.578202	6.086820
N	2.322208	-0.194997	6.319399
C	3.184616	0.884998	6.317871
C	4.617119	0.570368	6.266680
C	4.967448	-0.727530	6.171353
N	4.033505	-1.737718	6.116740
C	2.666302	-1.513232	6.169859
C	5.585399	1.711697	6.287407
O	2.752462	2.033284	6.360518
O	1.857597	-2.423697	6.089722
C	-2.562643	2.368035	2.981609

C	-3.515056	1.337244	3.102804
C	-3.064536	0.040497	3.207152
C	-1.677274	-0.221315	3.189732
C	-0.808146	0.896546	3.101821
N	-1.259508	2.164865	2.985798
C	0.634349	0.677660	3.147951
C	1.107694	-0.653604	3.193419
C	0.190496	-1.753096	3.267431
C	-1.156642	-1.570248	3.279719
C	2.503649	-0.856990	3.158498
C	3.341844	0.233522	3.128385
C	2.763491	1.520923	3.133569
N	1.463577	1.744872	3.134878
H	0.606250	-2.755576	3.334098
C	-2.104245	-2.731308	3.394992
N	0.599019	2.245047	0.005745
C	0.949774	0.956898	-0.008410
N	0.000000	0.000000	0.000000
C	0.348427	-1.299381	-0.000000
N	1.570877	-1.813849	-0.018914
C	2.503076	-0.849990	-0.048202
C	2.295733	0.525660	-0.047008
N	3.867421	-0.992218	-0.079019
C	4.397741	0.278943	-0.099797
N	3.489631	1.216483	-0.080720
N	-2.713060	0.559870	-0.010259
C	-3.125320	1.874785	-0.122258
C	-4.574428	2.105739	-0.088773
C	-5.372717	1.035188	0.092146
N	-4.869203	-0.236861	0.248583
C	-3.514882	-0.527588	0.212629
O	-2.307140	2.781458	-0.243160
O	-3.093813	-1.663340	0.370116
C	-5.062101	3.513814	-0.232217
H	-3.764323	-0.785389	3.299196
H	2.887740	-1.875110	3.159637
H	-0.488287	-1.994497	0.030502
H	1.313552	2.933385	0.186211
H	-0.382076	2.509512	0.085916
H	4.367276	-1.868112	-0.106373
H	5.465647	0.445846	-0.133894
H	-1.671573	0.367514	-0.000000
H	-6.454202	1.117198	0.134580
H	-6.153421	3.555891	-0.199238
H	-4.657994	4.141304	0.568134
H	-4.717965	3.946347	-1.175748
H	-5.477679	-1.031872	0.379599
H	-0.674452	-1.750038	6.472036
H	-0.574414	3.457013	5.821032
H	0.852957	2.461010	6.014818
H	-5.156041	0.130468	6.484225
H	-5.344350	2.676435	6.274824
H	1.284156	0.006792	6.315309
H	6.003509	-1.047236	6.120863
H	6.616533	1.351908	6.252674
H	4.308827	-2.706121	6.040059
H	3.403512	2.401118	3.128253
H	4.421913	0.125175	3.099907
H	-2.888423	3.401909	2.882929

H	-4.574702	1.574835	3.113157
H	5.411196	2.374045	5.433558
H	5.449974	2.316698	7.188166
H	-1.546356	-3.668143	3.452999
H	-2.714425	-2.640484	4.301615
H	-2.767041	-2.775244	2.524147

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(AT/4,7-Me$_2$phen/TA)MG (M06-2X/6-31+G(d,p))

C	-0.655166	0.537529	-6.417594
N	0.136267	-0.594916	-6.365006
C	-0.300399	-1.891026	-6.275004
N	-1.677986	-2.028050	-6.314821
C	-2.541254	-0.960270	-6.405859
C	-2.104280	0.313477	-6.462164
O	0.443673	-2.854143	-6.170117
C	-2.996124	1.513779	-6.530595
O	-0.150022	1.656393	-6.423941
H	1.181758	-0.460975	-6.298097
H	-3.596435	-1.214199	-6.419681
H	-4.047787	1.218826	-6.561189
H	-2.832929	2.159649	-5.662124
H	-2.769030	2.113628	-7.416288
H	-2.020391	-2.976115	-6.253748
N	2.893544	-0.290884	-6.163401
C	3.481508	0.897519	-5.915728
C	4.888782	0.900391	-5.772565
C	5.522552	-0.333744	-5.875452
N	4.949738	-1.526969	-6.097620
C	3.634255	-1.410084	-6.232872
N	5.793711	1.913846	-5.534367
C	6.947776	1.305478	-5.490903
N	6.852839	-0.055043	-5.687206
N	2.738641	2.002573	-5.827512
H	3.066146	-2.321752	-6.406421
H	3.164519	2.834114	-5.447287
H	1.721827	1.940834	-5.874056
H	7.606577	-0.725257	-5.715422
H	7.901391	1.787472	-5.324567
N	0.000000	0.000000	0.000000
C	0.134277	1.324383	-0.206220
C	-1.054096	2.064284	-0.412592
C	-2.244838	1.344897	-0.381477
N	-2.394034	0.027286	-0.175619
C	-1.221021	-0.564938	0.000000
N	-3.218053	2.278596	-0.637336
C	-2.574272	3.484875	-0.805616
N	-1.277630	3.398299	-0.680276
N	1.349250	1.881679	-0.204006
H	-1.223733	-1.643446	0.146517
H	1.450763	2.783302	-0.647384
H	2.172958	1.283293	-0.151244
H	-4.210749	2.101595	-0.671866
H	-3.121059	4.393379	-1.017204
C	3.431020	-1.234310	0.219115
N	2.160709	-1.744705	0.018359
C	1.828496	-3.059615	-0.169014

N	2.902728	-3.929965	-0.114946
C	4.194225	-3.517384	0.123008
C	4.515623	-2.220148	0.301959
O	0.686701	-3.450821	-0.363299
O	3.609694	-0.024972	0.325708
C	5.897840	-1.722154	0.589029
H	1.353848	-1.061922	0.000000
H	4.936232	-4.309057	0.161636
H	6.620116	-2.542751	0.580059
H	2.677830	-4.904341	-0.254008
H	6.193193	-0.973669	-0.152602
H	5.932689	-1.230900	1.565979
C	3.248695	-2.340815	-3.146042
C	3.816611	-1.037636	-2.937873
C	2.969889	0.095514	-2.893573
C	1.535303	-0.082576	-3.095492
C	1.008148	-1.395292	-3.171673
C	1.904280	-2.515161	-3.230250
C	-0.404470	-1.557317	-3.199833
C	-1.170323	-0.410404	-3.254661
C	-0.538319	0.848113	-3.291538
N	0.764246	1.022997	-3.194246
C	5.215177	-0.843243	-2.766328
C	5.652712	0.437433	-2.507950
C	4.722387	1.493556	-2.458492
N	3.429670	1.346421	-2.658215
C	-1.032470	-2.922327	-3.148314
C	6.178232	-1.993022	-2.878641
H	5.069725	2.505928	-2.261603
H	6.709308	0.644202	-2.357869
H	-1.136942	1.753756	-3.392112
H	-2.255439	-0.468557	-3.267375
H	1.490982	-3.509620	-3.362253
H	3.910733	-3.197882	-3.223969
H	7.204675	-1.648395	-2.727398
H	5.963463	-2.763774	-2.129569
H	6.101195	-2.458474	-3.868542
H	-0.698875	-3.537232	-3.991835
H	-0.742594	-3.430063	-2.222460
H	-2.122045	-2.839204	-3.177577

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(AT/5,6-Me$_2$phen/TA)MG (M06-2X/6-31+G(d,p))

C	-0.760436	0.244187	-6.375602
N	0.057748	-0.870882	-6.361996
C	-0.348174	-2.178110	-6.321622
N	-1.722170	-2.347292	-6.343803
C	-2.611167	-1.297479	-6.390312
C	-2.204539	-0.012693	-6.408502
O	0.420518	-3.126728	-6.273701
C	-3.124664	1.167955	-6.431478
O	-0.281541	1.373849	-6.357150
H	1.100832	-0.716458	-6.299419
H	-3.660253	-1.575403	-6.401963
H	-4.169514	0.849467	-6.457569
H	-2.965382	1.792742	-5.547021
H	-2.922746	1.797605	-7.302471
H	-2.040007	-3.305544	-6.327545

N	2.813051	-0.516787	-6.175803
C	3.380459	0.686056	-5.951745
C	4.790966	0.723150	-5.851923
C	5.451926	-0.494501	-5.974348
N	4.900803	-1.701669	-6.176021
C	3.579117	-1.617762	-6.266837
N	5.677367	1.759917	-5.645377
C	6.847342	1.181021	-5.641682
N	6.780128	-0.181350	-5.834168
N	2.616162	1.774867	-5.845755
H	3.028315	-2.543744	-6.422758
H	3.037061	2.618684	-5.487790
H	1.600086	1.690581	-5.852671
H	7.548685	-0.832947	-5.884647
H	7.793532	1.687283	-5.508520
N	0.000000	0.000000	0.000000
C	0.224851	1.299902	-0.272649
C	-0.906993	2.105551	-0.537497
C	-2.143369	1.468567	-0.494083
N	-2.382885	0.174955	-0.230227
C	-1.255210	-0.483900	0.000000
N	-3.048252	2.450336	-0.812525
C	-2.322719	3.601915	-1.027533
N	-1.037063	3.436521	-0.874246
N	1.474955	1.774891	-0.275580
H	-1.331967	-1.551517	0.194553
H	1.640932	2.637599	-0.773693
H	2.253461	1.121766	-0.192603
H	-4.049730	2.337099	-0.858254
H	-2.804545	4.532751	-1.293045
C	3.946758	-3.792390	0.075024
C	4.363343	-2.520810	0.241424
C	3.351977	-1.460097	0.173355
N	2.044874	-1.878501	0.000914
C	1.614774	-3.167669	-0.172411
N	2.626720	-4.112510	-0.143395
O	0.443711	-3.475551	-0.337058
O	3.618962	-0.265478	0.268402
C	5.783017	-2.124258	0.503420
H	1.285642	-1.143317	0.000000
H	4.631122	-4.634734	0.102068
H	6.449499	-2.988385	0.437458
H	2.331286	-5.069051	-0.275371
H	6.102609	-1.365404	-0.216050
H	5.881659	-1.678850	1.498148
N	3.382755	1.101491	-2.725810
C	2.973207	-0.168441	-2.937620
C	3.857939	-1.270111	-2.979530
C	5.231798	-0.986410	-2.806635
C	5.642318	0.305966	-2.573770
C	4.669204	1.320544	-2.541102
C	3.374473	-2.626664	-3.182142
C	2.026770	-2.869382	-3.234932
C	1.094577	-1.753485	-3.177064
C	1.548911	-0.414026	-3.117576
C	-0.304239	-1.946305	-3.192653
C	-1.145486	-0.855550	-3.232753
C	-0.573495	0.428448	-3.283309
N	0.724933	0.650330	-3.210886

H	-0.715472	-2.949401	-3.171821
H	5.962794	-1.787469	-2.849053
H	4.965475	2.353271	-2.368849
H	6.689467	0.549516	-2.423684
H	-1.206254	1.310701	-3.379693
H	-2.224556	-0.972226	-3.229022
C	1.426557	-4.246509	-3.376345
C	4.425898	-3.696069	-3.347680
H	4.001511	-4.679508	-3.534973
H	5.067831	-3.447764	-4.201107
H	5.063134	-3.768455	-2.458202
H	2.175685	-5.035124	-3.346808
H	0.718353	-4.431751	-2.561434
H	0.890795	-4.323935	-4.328327

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(AT/3,4,7,8-Me$_4$phen/TA)MG (M06-2X/6-31+G(d,p))

N	-0.401592	-0.819439	6.340723
C	0.903285	-0.364322	6.397240
C	1.939832	-1.397068	6.512682
C	1.543709	-2.685686	6.491524
N	0.219846	-3.045963	6.386028
C	-0.811484	-2.125577	6.319081
O	1.149665	0.837318	6.359181
O	-1.982596	-2.469707	6.254045
C	3.360766	-0.949466	6.650578
H	2.247016	-3.509862	6.561312
H	4.043532	-1.803090	6.666802
H	-0.063103	-4.014900	6.367348
H	-1.170186	-0.093632	6.320128
H	3.627878	-0.291925	5.818285
H	3.494698	-0.370033	7.568905
N	-3.659945	4.321105	5.131293
C	-3.460991	3.051473	5.629992
C	-4.669317	2.405511	5.872007
N	-5.627894	3.317565	5.507790
C	-4.958695	4.441208	5.073875
N	-4.846577	1.155842	6.329198
C	-3.685126	0.546686	6.520539
N	-2.449882	1.044296	6.331234
C	-2.286268	2.304367	5.884498
N	-1.054763	2.793819	5.706491
H	-3.714954	-0.488950	6.853511
H	-0.952440	3.571141	5.068810
H	-0.258857	2.164581	5.805761
H	-6.625794	3.180775	5.567622
H	-5.489409	5.318300	4.730095
N	0.000000	0.000000	0.000000
C	0.629992	1.189854	0.087058
C	2.042241	1.163955	0.140145
C	2.638455	-0.092440	0.125693
N	2.025694	-1.284225	0.063937
C	0.706894	-1.142156	-0.000000
N	3.985301	0.164240	0.197823
C	4.124683	1.534783	0.239018
N	2.984930	2.169555	0.212211
N	-0.078426	2.320400	0.103826
H	0.107120	-2.049036	-0.043267

H	0.392883	3.172853	0.365364
H	-1.097657	2.286141	0.130311
H	4.719461	-0.527858	0.178350
H	5.098369	2.002885	0.290186
N	-2.757269	-0.231804	-0.004621
C	-3.518837	0.913581	-0.144343
C	-4.973463	0.729396	-0.133568
C	-5.443094	-0.521836	0.037100
N	-4.608166	-1.600707	0.219244
C	-3.225725	-1.501573	0.207428
O	-2.985284	2.011446	-0.274540
O	-2.506289	-2.475342	0.369870
C	-5.835392	1.944003	-0.282397
H	-1.704852	-0.126071	-0.000000
H	-6.505245	-0.745032	0.061805
H	-6.894886	1.678197	-0.248380
H	-5.622860	2.659608	0.518605
H	-5.626206	2.456209	-1.225684
H	-4.973987	-2.532345	0.354186
C	1.070362	-0.464655	3.223054
C	0.473311	-1.772493	3.182430
C	-0.875638	-1.934044	3.192107
C	-1.762707	-0.803566	3.189483
C	-1.214181	0.497447	3.097252
C	0.232119	0.673357	3.192233
N	0.721921	1.931425	3.262955
C	2.023867	2.071255	3.377856
C	2.964557	1.015226	3.403862
C	2.479717	-0.279529	3.304735
C	-3.175958	-0.951536	3.268125
C	-3.957244	0.191624	3.153800
C	-3.290707	1.421991	2.941486
N	-1.985630	1.593178	2.932339
C	-3.773044	-2.316669	3.482748
C	3.391960	-1.477958	3.264633
H	2.392209	3.095425	3.440525
C	4.426840	1.355172	3.543051
H	-3.888504	2.322753	2.783840
C	-5.460220	0.183483	3.265166
H	-1.298800	-2.932865	3.182830
H	1.115868	-2.646815	3.154083
H	4.440221	-1.192144	3.364373
H	3.158168	-2.174978	4.077050
H	3.261158	-2.016657	2.318032
H	-3.502205	-2.985840	2.657666
H	-3.386169	-2.745858	4.412610
H	-4.860342	-2.272401	3.554740
H	-5.864379	1.155841	2.964741
H	-5.914608	-0.578789	2.626124
H	-5.772047	-0.006451	4.297766
H	4.576659	2.430678	3.419437
H	4.814600	1.078414	4.530324
H	5.041297	0.844780	2.796000