

Electronic Supporting Information for the

Externally controlling tautomeric distributions and inter-conversions: New insights into the realm of catalyzed tautomerization

Biman Bandyopadhyay^a and Partha Biswas^b

^aDepartment of Basic Science & Humanities, Institute of Engineering & Management, Salt Lake Electronics Complex, Sector-5, Kolkata 700091, India.

^b*Department of Chemistry, Scottish Church College, 1 & 3 Urquhart Square, Kolkata-700006, India.*

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Computational details:

Molecular geometries of both amide and imidic acid tautomers of all four isomeric compounds, their hydrogen bonded complexes with the catalyst molecules and all the transition states were optimized at the M06-2X/aug-cc-pVTZ level of theory. Transition state optimizations were carried out using the QST2/QST3 method. Basis set superposition errors (BSSEs) for all reactant and product complexes and the associated transition states for tautomeric conversion were corrected using the single point counterpoise method proposed by Boys and Bernardi¹. Normal mode frequencies were calculated for all the species to ascertain that optimized geometries corresponded to minima in the potential energy surfaces and transition states corresponded to first-order saddle points characterized by a single imaginary frequency. To ensure that the optimized transition states connect the corresponding reactants and products, intrinsic reaction coordinate (IRC) calculations were performed. Single-point energy calculations at MP2/aug-cc-pVTZ level were carried out using geometries optimized at M06-2X/aug-cc-pVTZ level. The calculations were carried out using two other DFT methods namely B3LYP and B97D at 6-311++G(d,p) basis set and also at M06-2X/6-311++G(d,p) level to check whether the results depend on functional and/or basis sets or not. To limit integration errors, ultrafine grid was used for all calculation done using M06-2X functional. All calculations reported here were carried out with Gaussian 09 program package². All the values reported here are calculated at M06-2X/aug-cc-pVTZ level of theory, unless mentioned otherwise.

References:

1. F. Boys and F. Bernardi, *Mol. Phys.* **19**, 1970, 553-566
2. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, J. A. Pople, Gaussian, Inc., Wallingford CT, 2009.

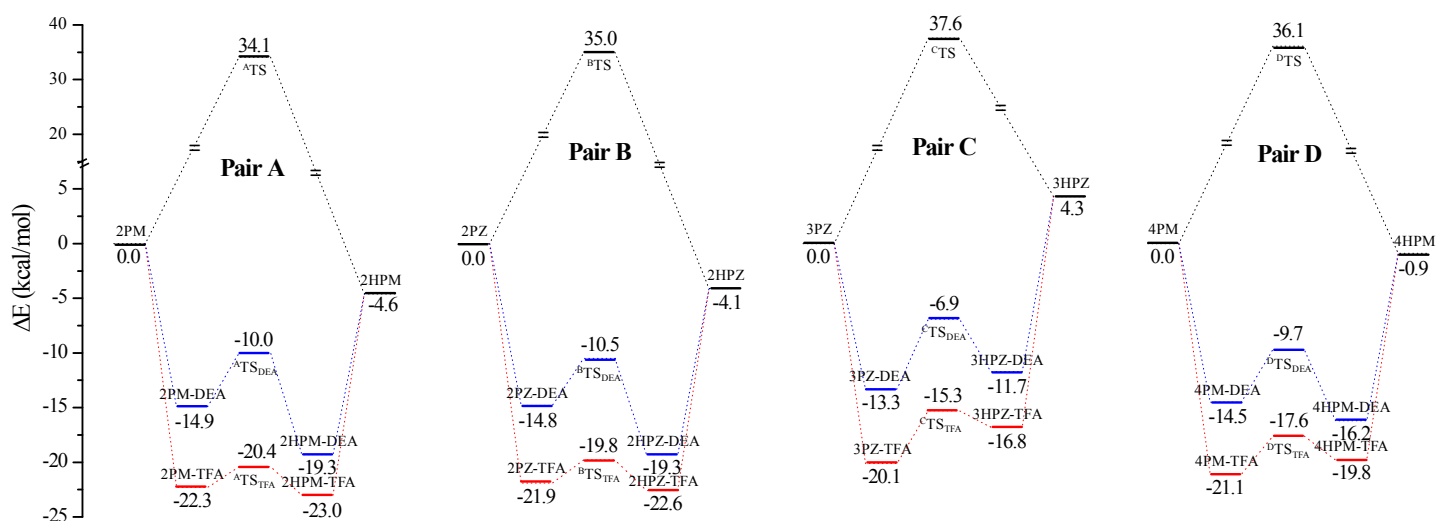


Fig. S1 Tautomeric behaviour of four sets of tautomeric pairs (Black) and effects of TFA (Red) and DEA (Blue) on them as predicted by calculations performed at MP2/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ level.

^XTS_Y stands for transition state for 'Pair X' with catalyst 'Y'.

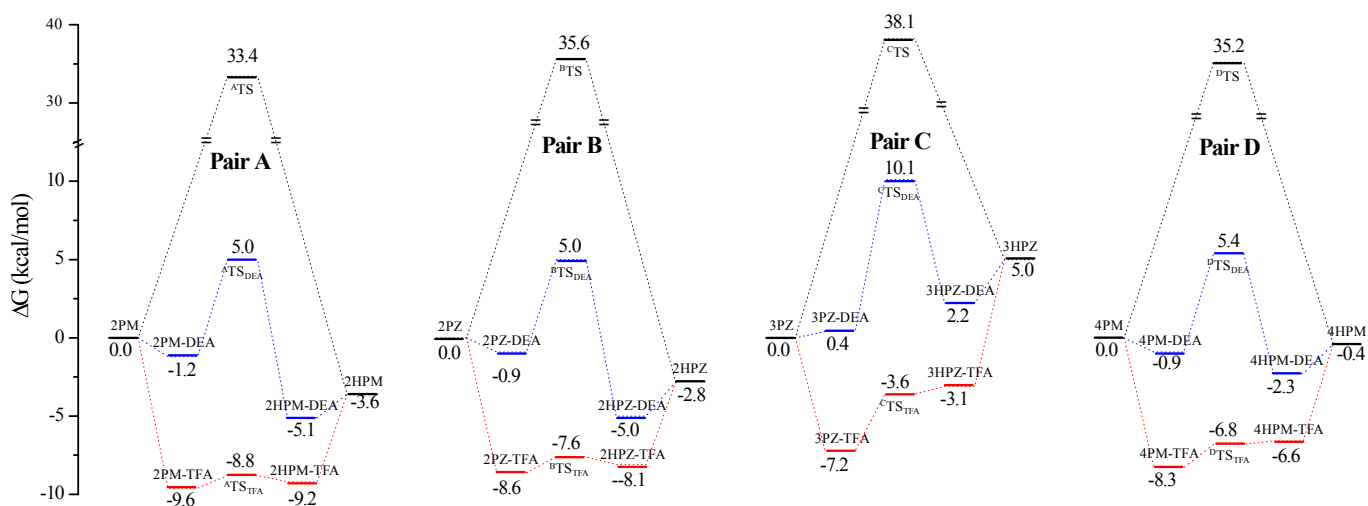
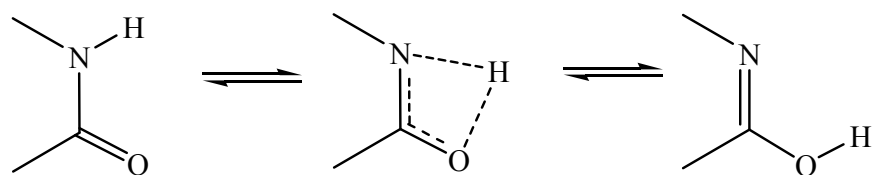
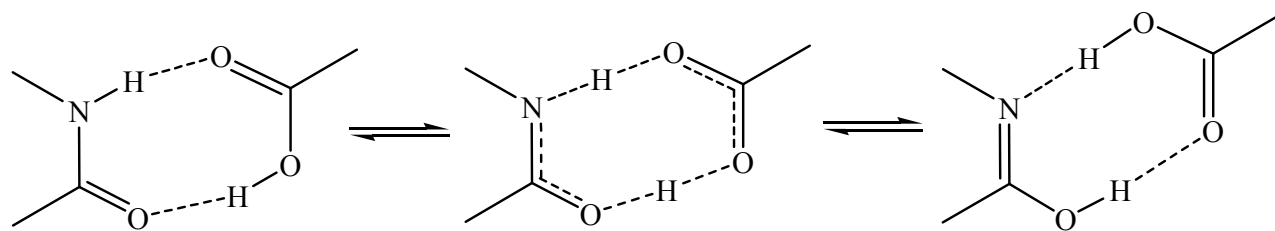


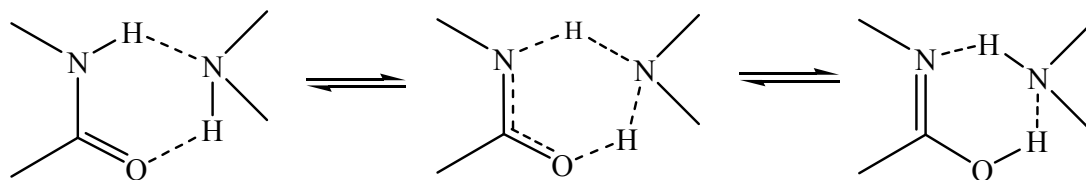
Fig. S2 Free energy profile (at 298 K) of four sets of tautomeric pairs (Black) and effects of TFA (Red) and DEA (Blue) on them as predicted by calculations performed at M06-2X/aug-cc-pVTZ level. ^XTS_Y stands for transition state for 'Pair X' with catalyst 'Y'.



Uncatalyzed Tautomerization



Carboxylic Acid Catalyzed Tautomerization



Amine Base Catalyzed Tautomerization

Fig. S3 Schematic representation of reaction centre for amide-imidic acid tautomerization under uncatalyzed, carboxylic acid catalyzed and amine base catalyzed conditions

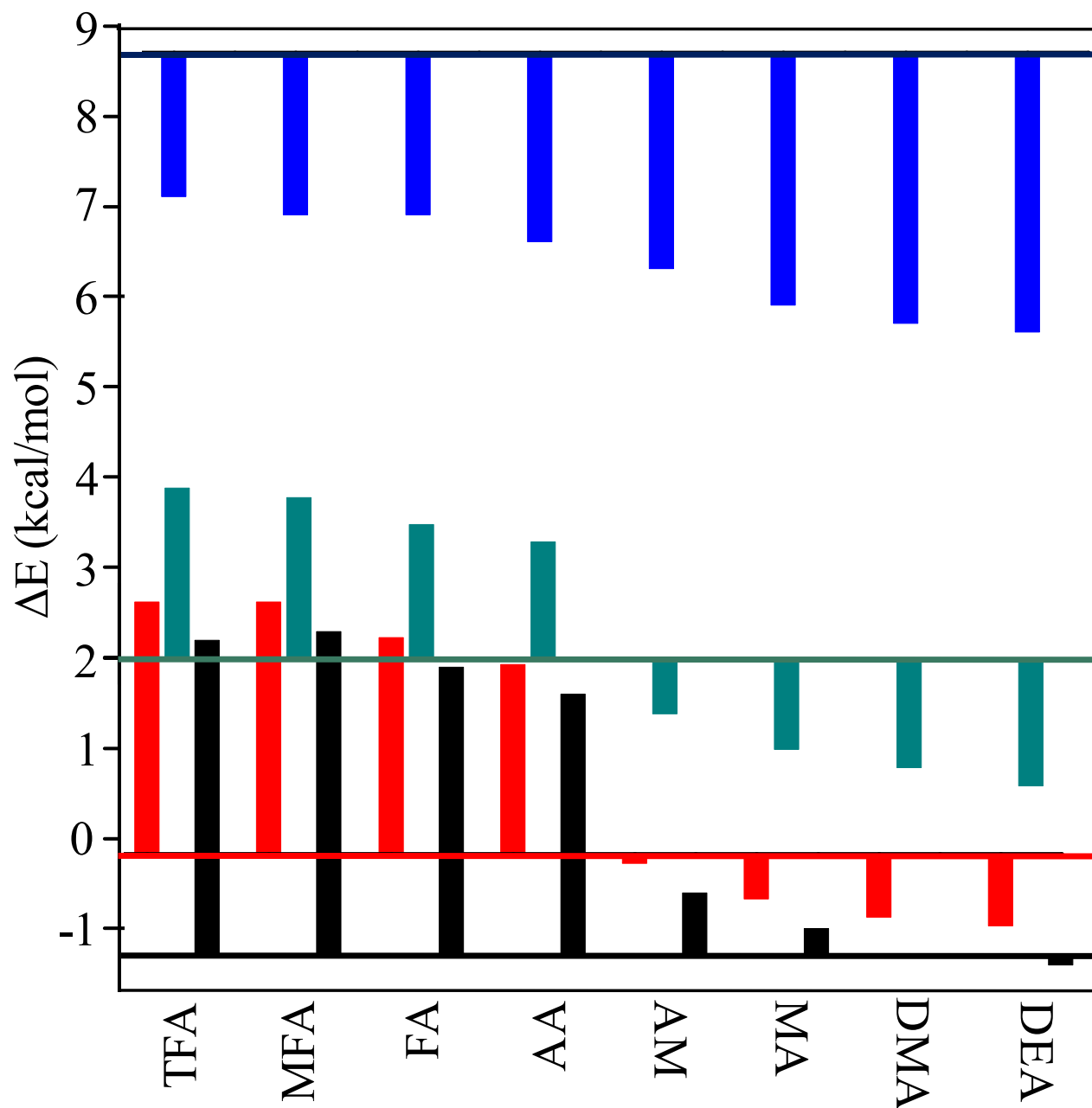


Fig. S4 Effect of catalysts on the relative energies ($\Delta E = E_{\text{imidic acid}} - E_{\text{amide}}$) for the four sets of tautomeric pairs calculated by B3LYP/6-311++G(d,p) level of theory; Black: Pair A; Red: Pair B; Blue: Pair C; Green: Pair D. Horizontal lines of corresponding colours represent the respective ΔE in absence of catalysts.

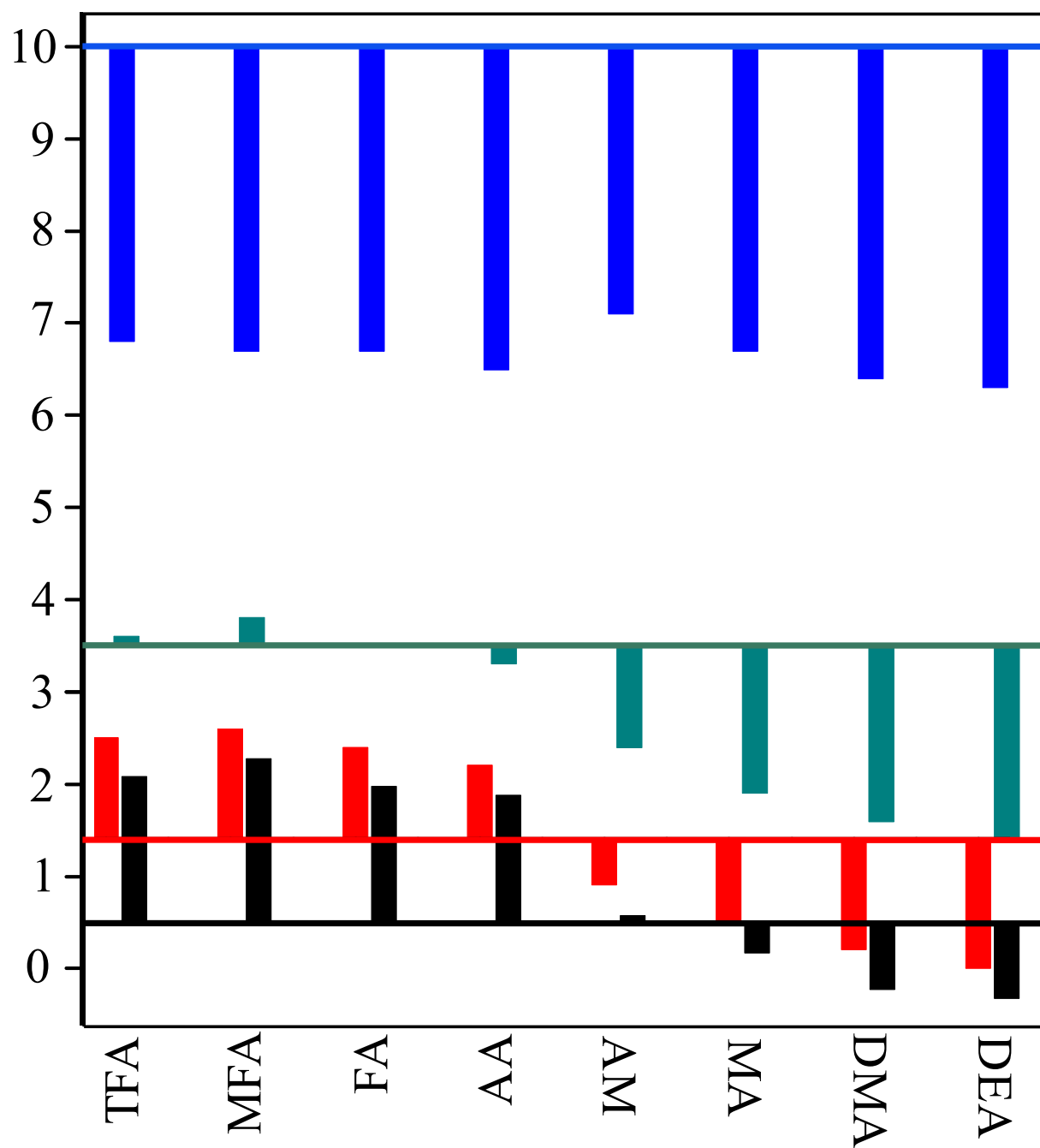


Fig. S5 Effect of catalysts on the relative energies ($\Delta E = E_{\text{imidic acid}} - E_{\text{amide}}$) for the four sets of tautomeric pairs calculated by B97D/6-311++G(d,p) level of theory; Black: Pair A; Red: Pair B; Blue: Pair C; Green: Pair D. Horizontal lines of corresponding colours represent the respective ΔE in absence of catalysts.

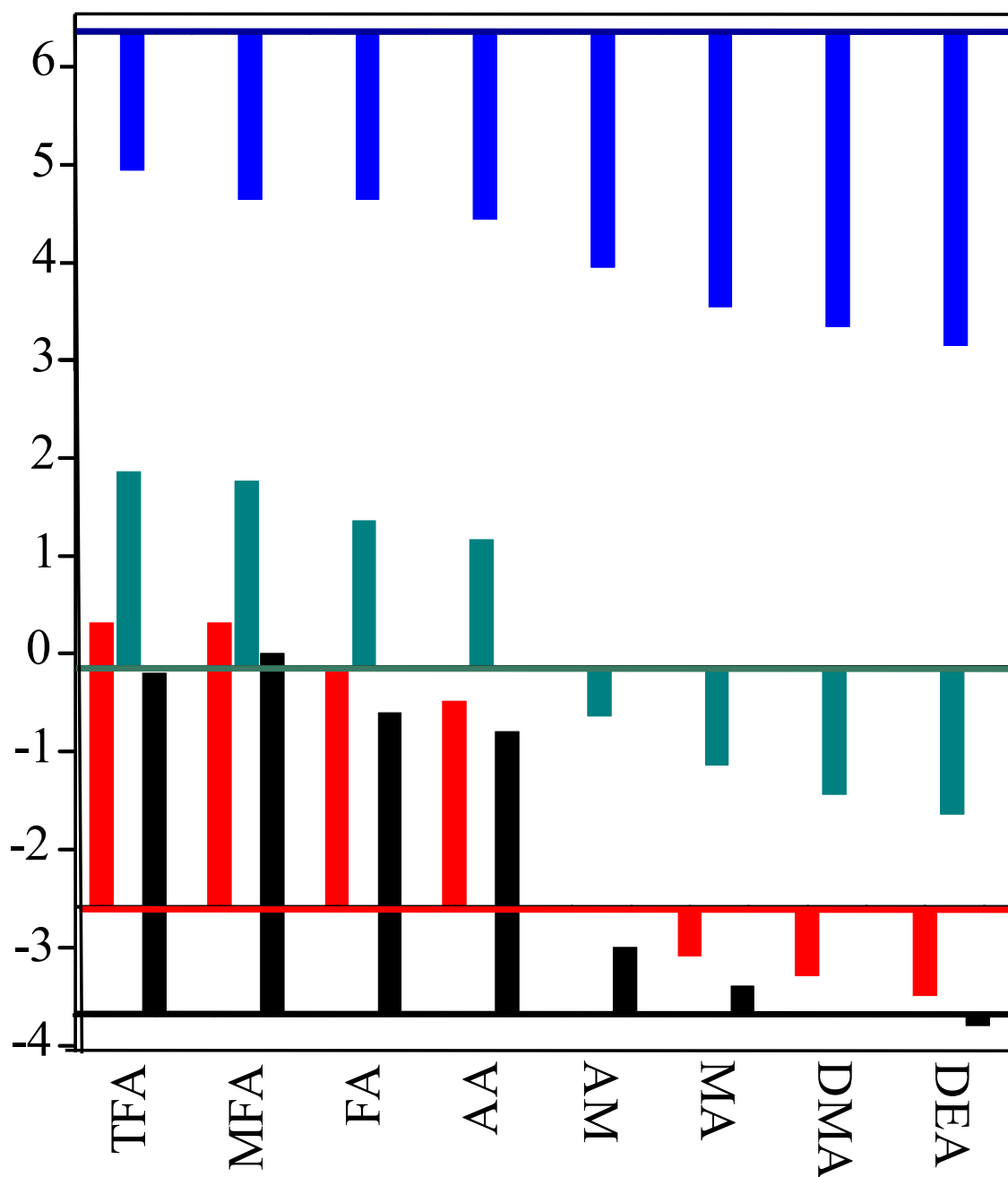


Fig. S6 Effect of catalysts on the relative energies ($\Delta E = E_{\text{imidic acid}} - E_{\text{amide}}$) for the four sets of tautomeric pairs calculated by M06-2X/6-311++G(d,p) level of theory; Black: Pair A; Red: Pair B; Blue: Pair C; Green: Pair D. Horizontal lines of corresponding colours represent the respective ΔE in absence of catalysts.

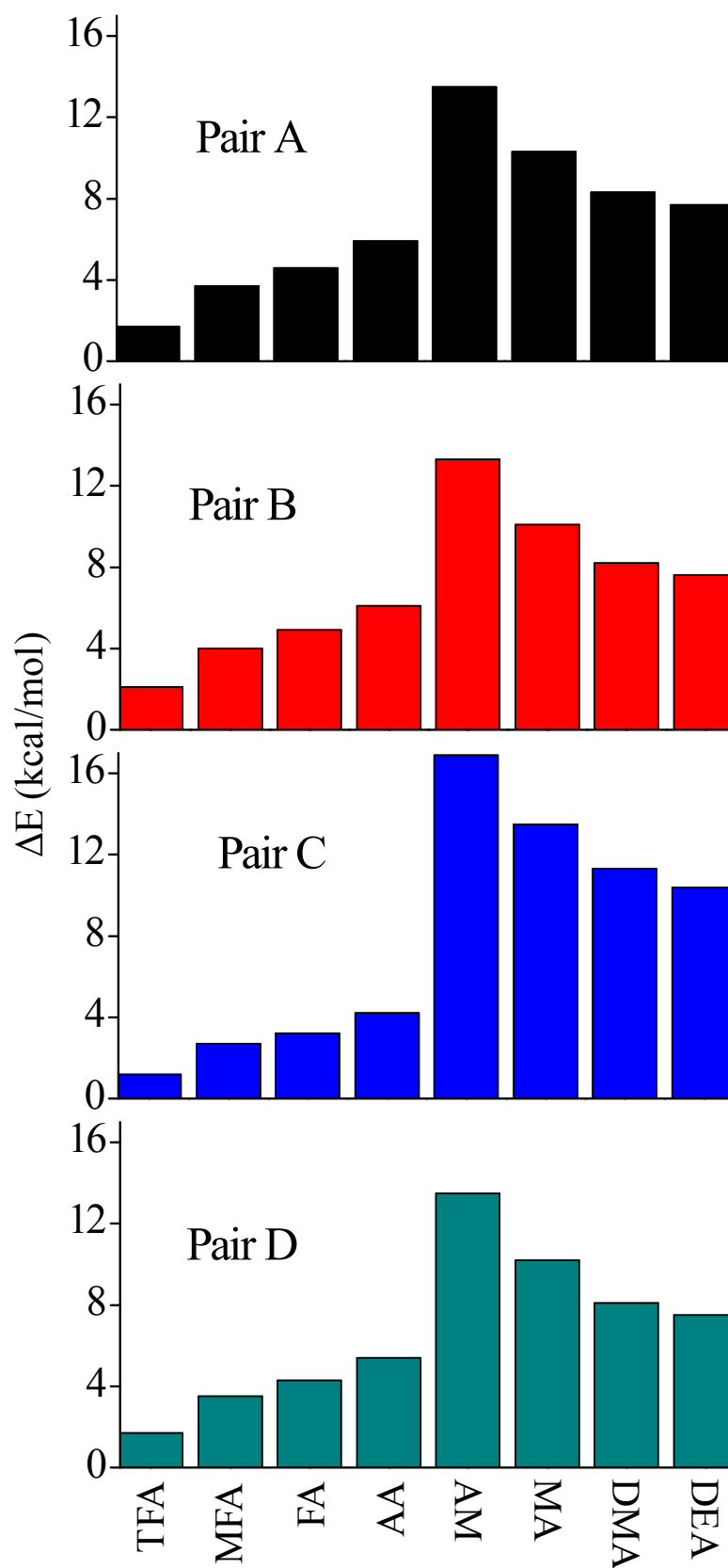


Fig. S7 Activation energies of tautomerization in presence of catalysts for the four sets of tautomeric pairs calculated by B3LYP/6-311++G(d,p) level of theory. Barrier heights for acid and base catalysts have been calculated with respect to imidic acid and amide forms, respectively.

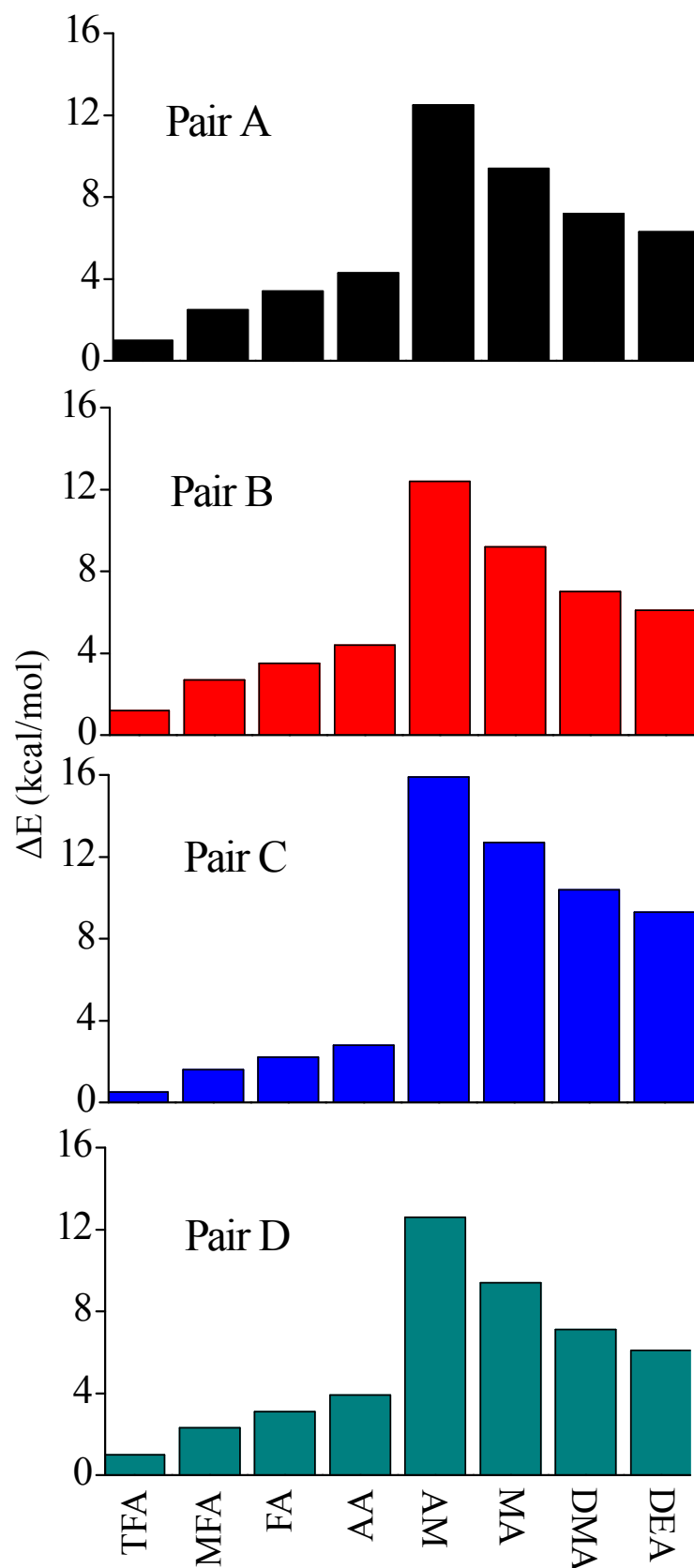


Fig. S8 Activation energies of tautomerization in presence of catalysts for the four sets of tautomeric pairs calculated by B97D/6-311++G(d,p) level of theory. Barrier heights for acid and base catalysts have been calculated with respect to imidic acid and amide forms, respectively.

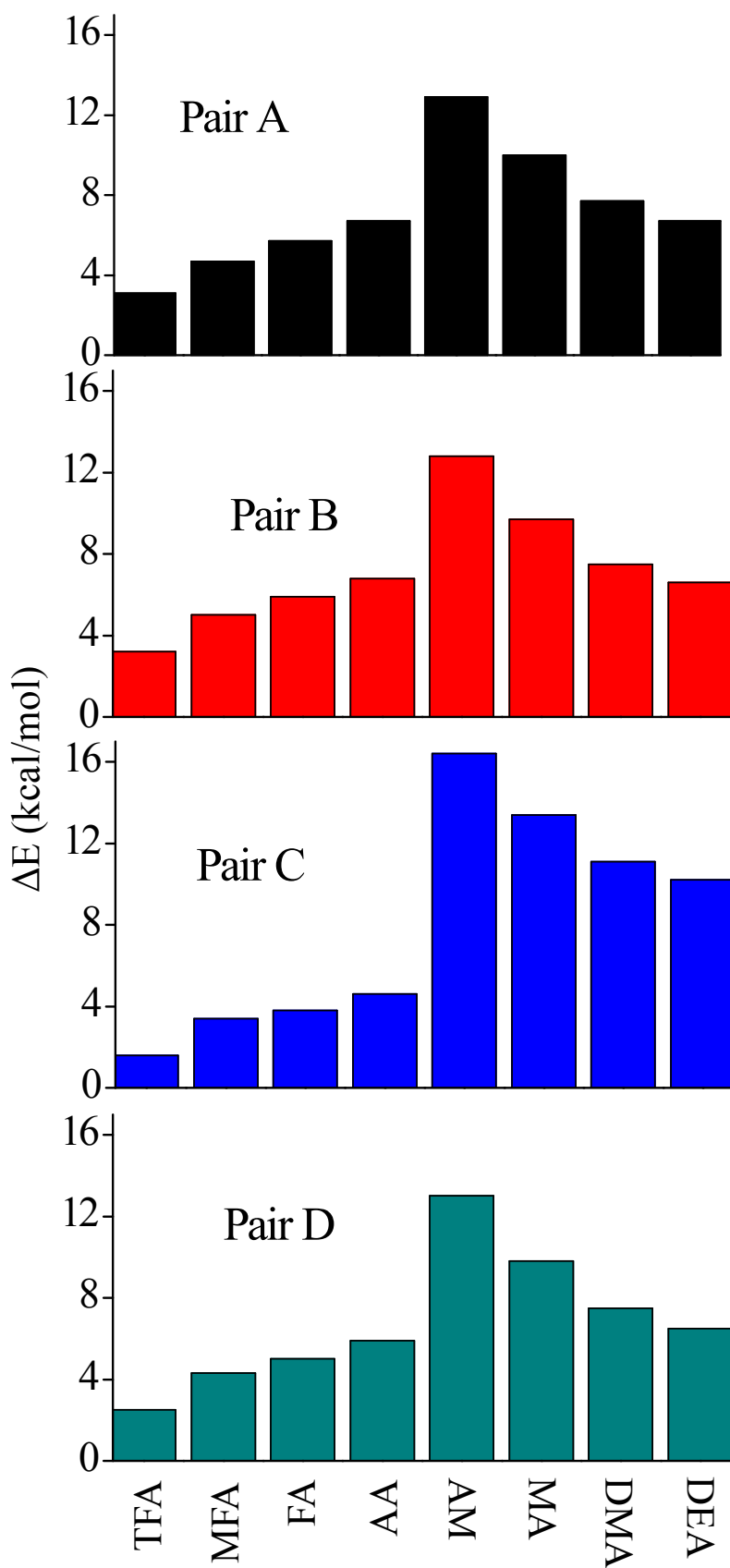


Fig. S9 Activation energies of tautomerization in presence of catalysts for the four sets of tautomeric pairs calculated by M06-2X /6-311++G(d,p) level of theory. Barrier heights for acid and base catalysts have been calculated with respect to imidic acid and amide forms, respectively.

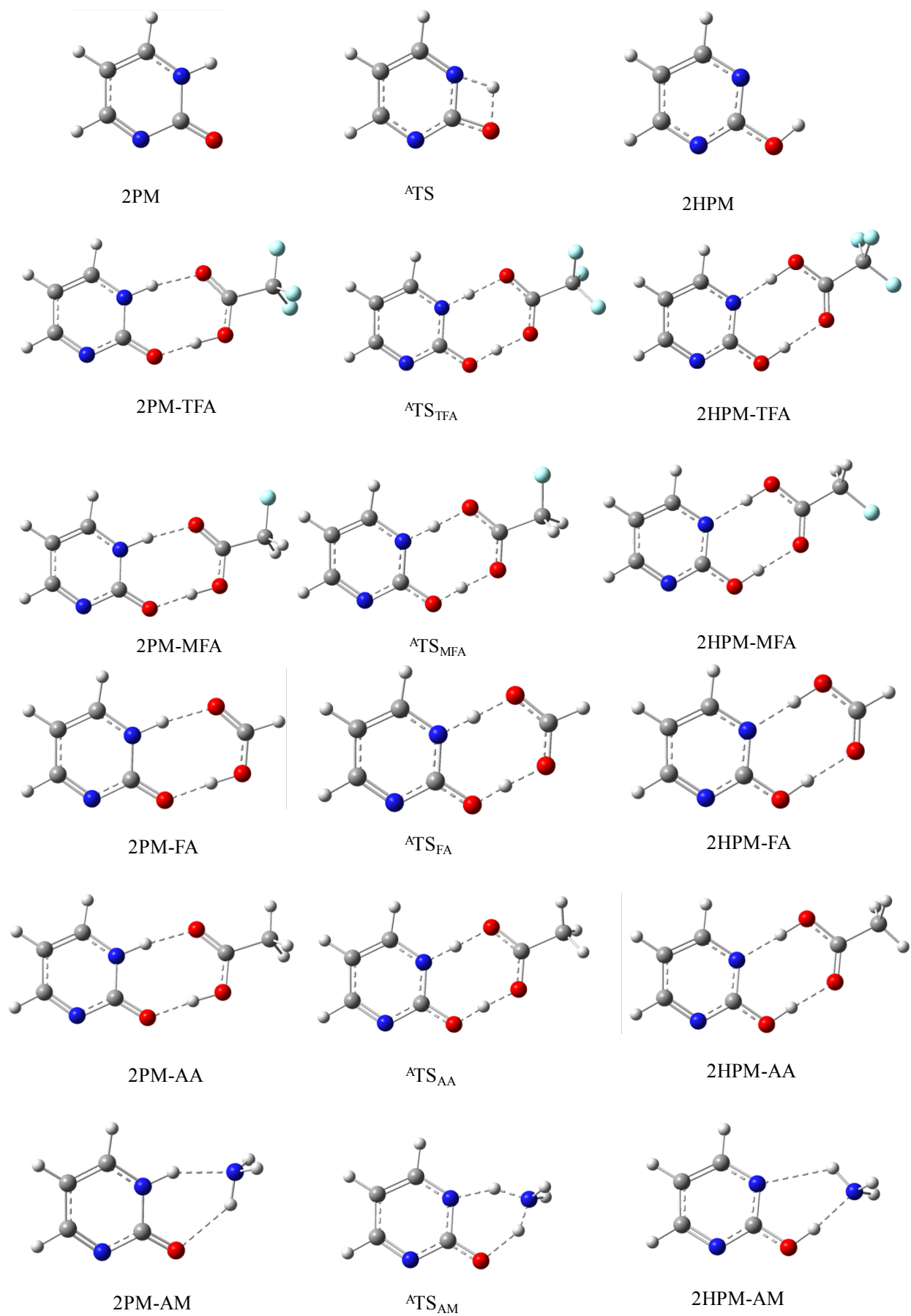


Fig. S10 Optimized geometries of all species calculated at M06-2X/aug-cc-pVTZ level of theory

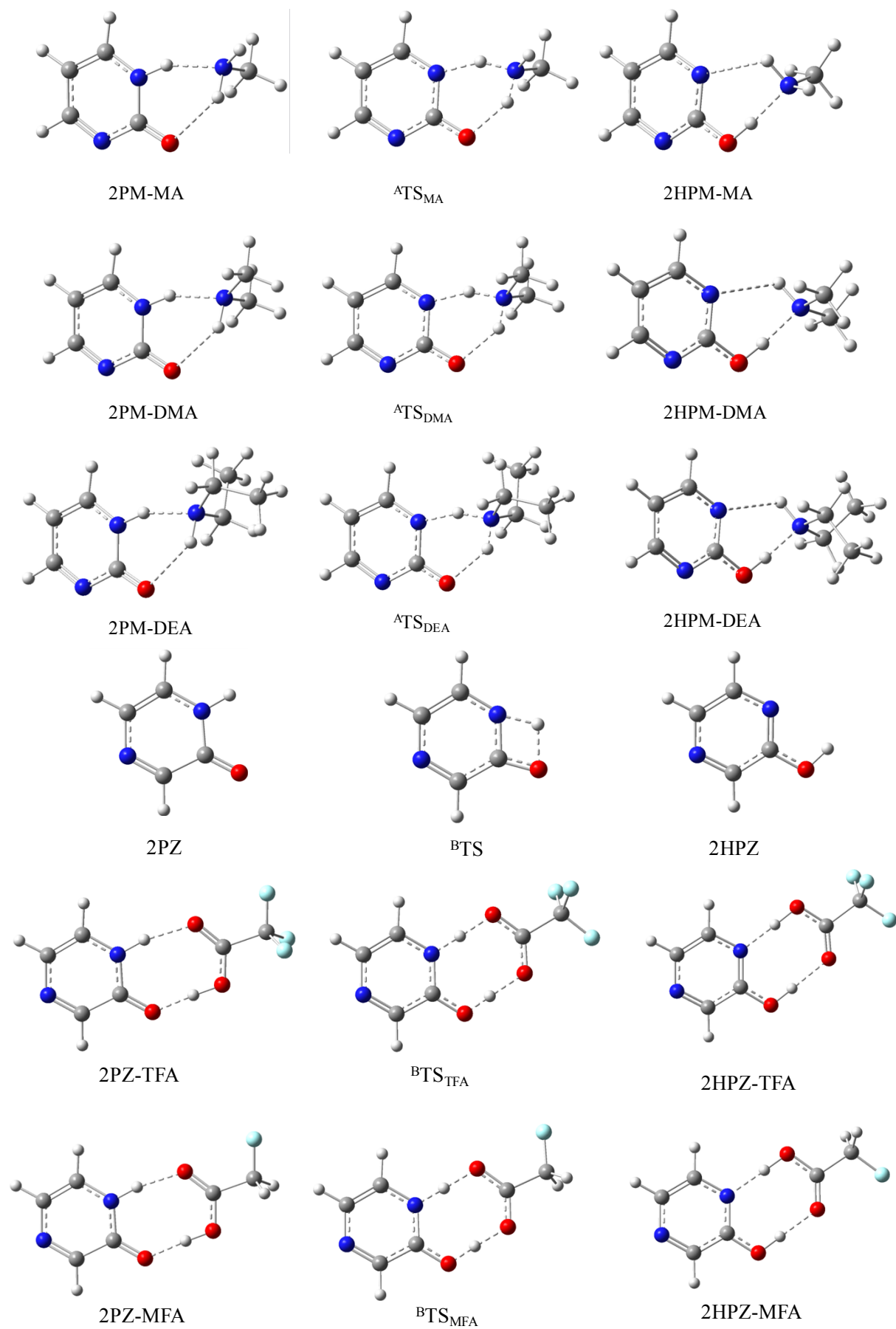


Fig. S10 (Continued)

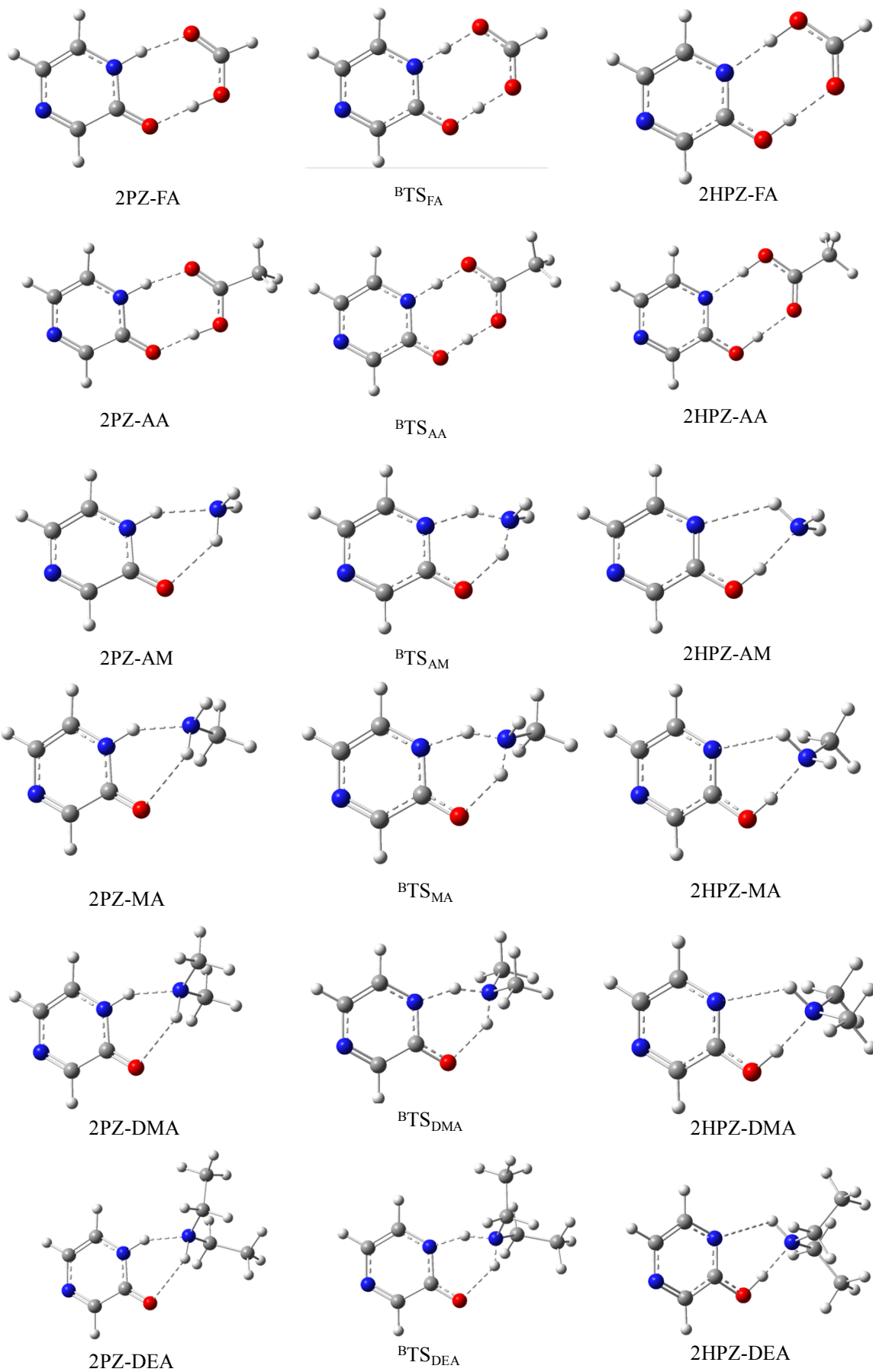


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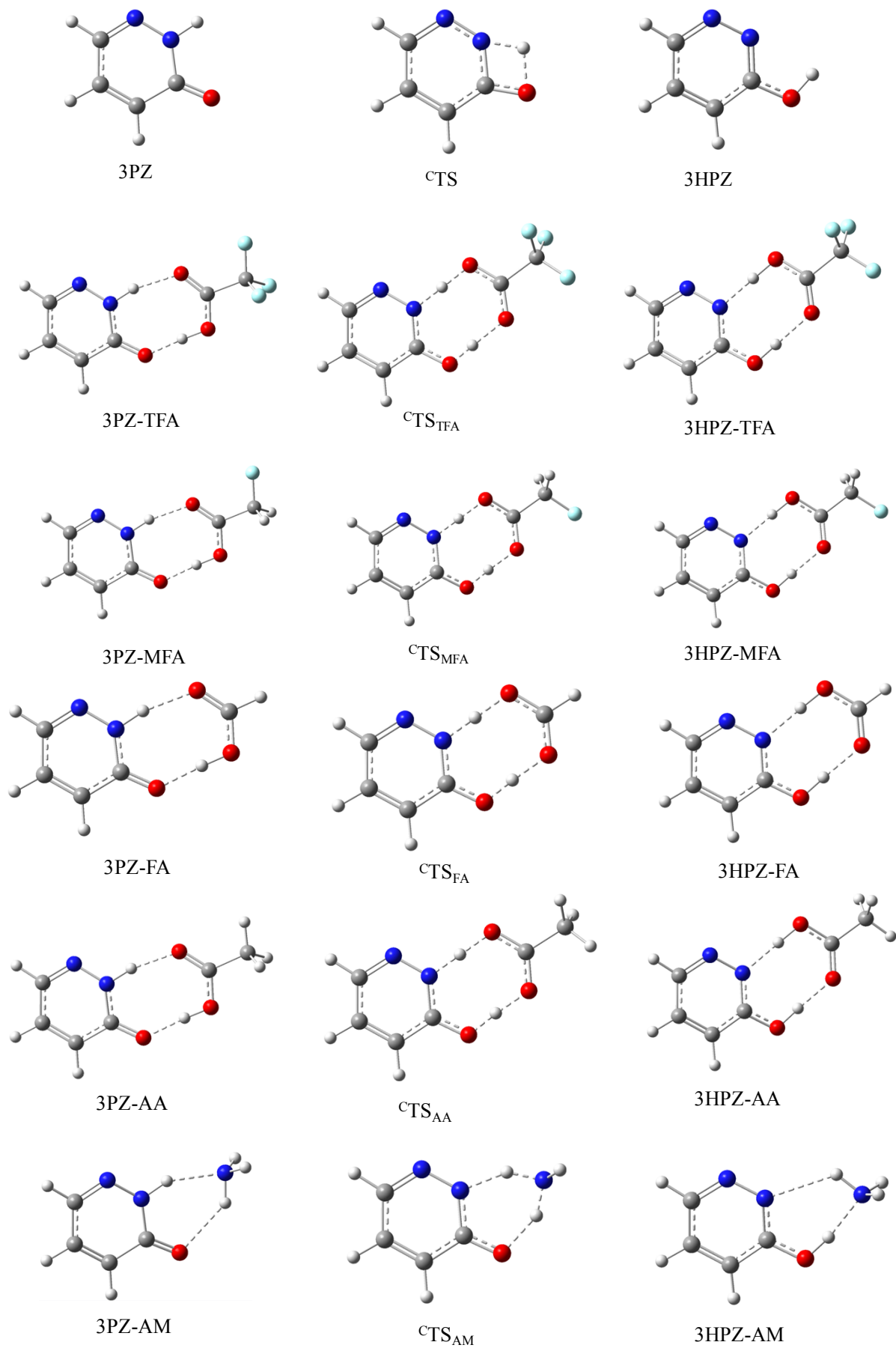


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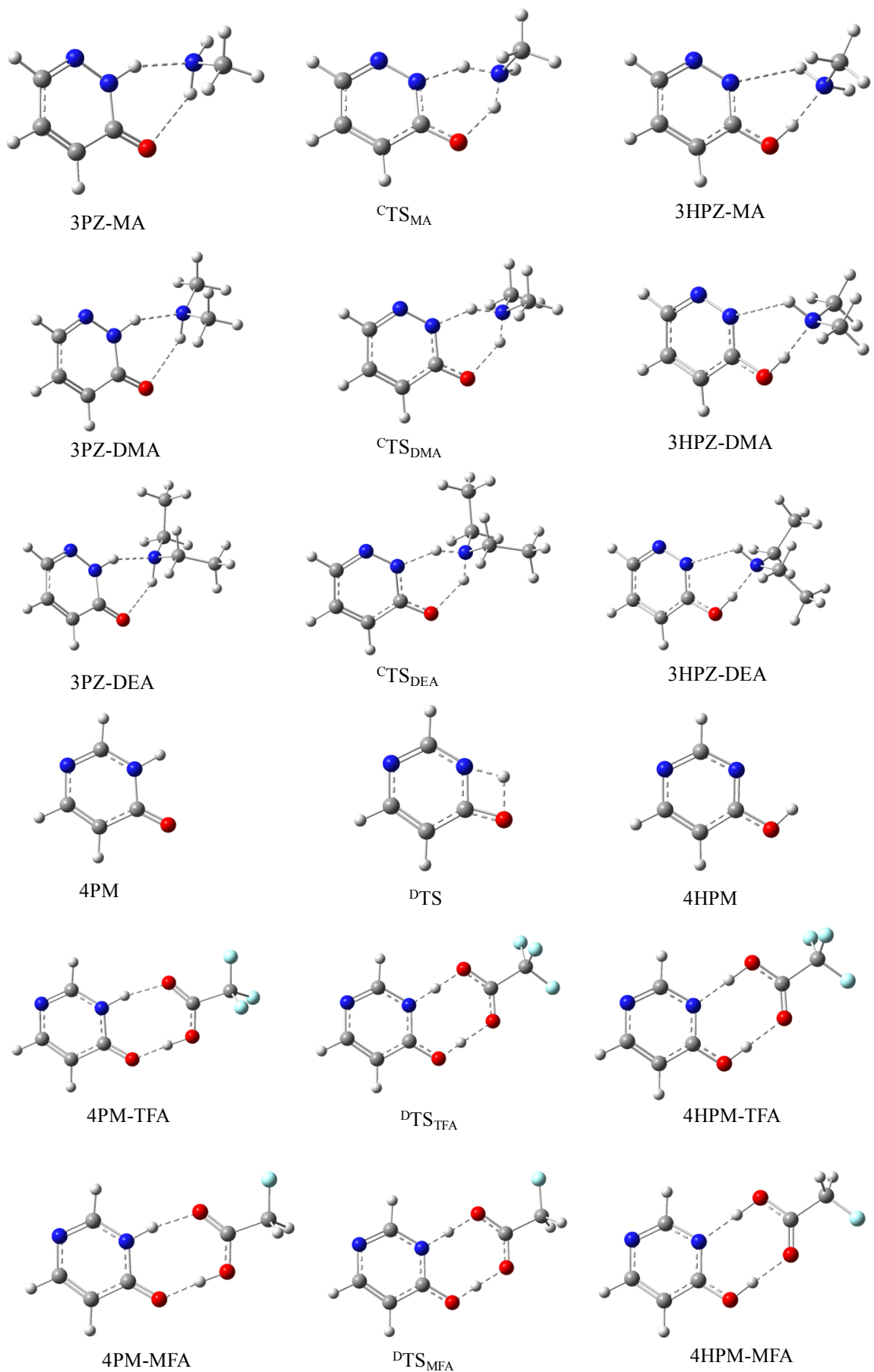


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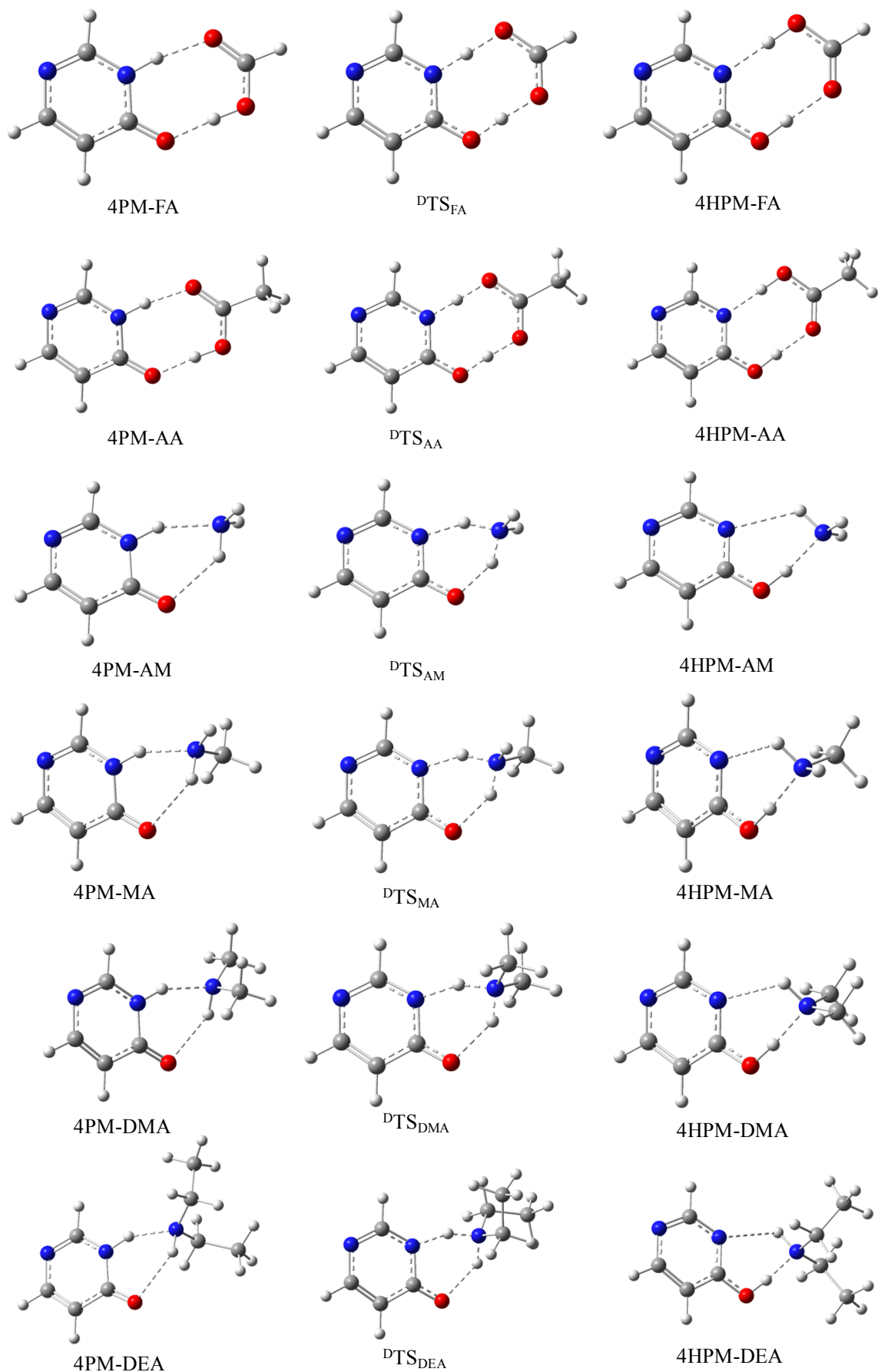


Fig. S10 (Continued)

Table S1 Relative energies (kcal/mol) of the imidic acid forms with respect to amide forms for the four tautomeric pairs calculated at different levels of theory

	Pair A	Pair B	Pair C	Pair D
B3LYP/6-311++G(d,p)	-1.3	-0.2	8.7	2.0
B97D/6-311++G(d,p)	0.5	1.4	10.0	3.5
M06-2X/6-311++G(d,p)	-3.7	-2.6	6.3	-0.2
M06-2X/aug-cc-pVTZ	-3.8	-2.8	5.5	-0.4
MP2/aug-cc-pVTZ// M06-2X/aug-cc-pVTZ	-4.6	-4.1	4.3	-0.9
M06-2X/aug-cc-pVTZ ^a	-3.6	-2.8	5.0	-0.4

^a Relative free energies(kcal/mol) of the imidic acid forms with respect to amide forms at 298 K

Table S2 Barrier for tautomerization (kcal/mol) with respect to both amide and imidic acid forms for the four tautomeric pairs calculated at four different levels of theory

		B3LYP/ 6-311++G(d,p)	B97D/ 6-311++G(d,p)	M06-2X/ 6-311++G(d,p)	M06-2X/ Aug-cc-pVTZ
Pair	E _{TS} - E _{2PM}	37.4	35.0	37.2	36.3
A	E _{TS} - E _{2HPM}	38.7	34.5	40.9	40.1
Pair	E _{TS} - E _{2PZ}	39.6	37.0	39.7	38.7
B	E _{TS} - E _{2HPZ}	39.8	35.6	42.3	41.5
Pair	E _{TS} - E _{3PZ}	42.7	39.7	42.8	41.4
C	E _{TS} - E _{3HPZ}	34.0	29.7	36.5	36.0
Pair	E _{TS} - E _{4PM}	39.3	36.8	39.3	38.3
D	E _{TS} - E _{4HPM}	37.3	33.3	39.5	38.7

Table S3 List of pK_a values of the catalysts at 298 K

Catalyst	TFA	MFA	FA	AA	AM	MA	DMA	DEA
pK _a	0.52	2.59	3.75	4.76	9.25	10.66	10.73	10.84

Reference: David R. Lide, ed., CRC Handbook of Chemistry and Physics, Internet Version 2005, , CRC Press, Boca Raton, FL, 2005

Table S4 Relative energies (kcal/mol) of the imidic acid forms with respect to amide forms for the four tautomeric pairs with all eight catalysts calculated at M06-2X/aug-cc-pVTZ level

	Pair A	Pair B	Pair C	Pair D
TFA	0.1	0.4	4.5	1.8
MFA	0.2	0.2	4.1	1.6
FA	-0.3	-0.2	4.1	1.3
AA	-0.6	-0.5	3.8	1.0
AM	-3.1	-2.9	3.2	-1.0
MA	-3.6	-3.4	2.7	-1.6
DMA	-3.9	-3.6	2.5	-1.8
DEA	-4.1	-3.8	2.4	-2.0

Table S5 Barrier for tautomerization (kcal/mol) in presence of all eight catalysts calculated at M06-2X/aug-cc-pVTZ level. Barriers are calculated with respect to the imidic acid forms for the acidic catalysts and with respect to amide forms for the basic catalysts

	Pair A	Pair B	Pair C	Pair D
TFA	2.0	2.4	1.2	1.8
MFA	3.7	4.2	2.8	3.5
FA	4.6	4.9	3.2	4.1
AA	5.5	5.8	3.9	4.9
AM	13.2	13.1	16.6	13.4
MA	10.2	10.0	13.3	10.2
DMA	8.0	7.8	11.0	7.9
DEA	7.1	6.9	10.0	6.9

Table S6 Relative free energies at 298 K (kcal/mol) of the imidic acid forms with respect to amide forms for the four tautomeric pairs with all eight catalysts calculated at M06-2X/aug-cc-pVTZ level

	Pair A	Pair B	Pair C	Pair D
TFA	0.4	0.5	4.1	1.7
MFA	0.2	0.1	3.6	1.5
FA	0.2	-0.2	3.7	1.3
AA	-0.9	-0.9	3.0	0.6
AM	-3.3	-3.1	3.0	-0.9
MA	-3.5	-3.4	2.4	-1.2
DMA	-3.8	-4.0	2.4	-1.8
DEA	-3.9	-4.1	1.8	-1.4

Table S7 Free energies of activation at 298 K (kcal/mol) in presence of all eight catalysts calculated at M06-2X/aug-cc-pVTZ level. Barriers are calculated with respect to the imidic acid forms for the acidic catalysts and with respect to amide forms for the basic catalysts

	Pair A	Pair B	Pair C	Pair D
TFA	0.4	0.5	-0.5	-0.2
MFA	1.4	1.7	0.3	0.9
FA	1.6	2.1	0.4	1.3
AA	2.7	2.3	0.6	1.4
AM	11.9	12.0	15.4	12.3
MA	8.9	8.8	12.5	9.4
DMA	6.9	6.2	10.1	7.0
DEA	6.2	5.9	9.7	6.3

Table S8 Relative energies (kcal/mol) of the imidic acid forms with respect to amide forms for the four tautomeric pairs with all eight catalysts calculated at B3LYP/6-311++G(d,p)

	Pair A	Pair B	Pair C	Pair D
TFA	2.2	2.6	7.1	3.9
MFA	2.3	2.6	6.9	3.8
FA	1.9	2.2	6.9	3.5
AA	1.6	1.9	6.6	3.3
AM	-0.6	-0.3	6.3	1.4
MA	-1.0	-0.7	5.9	1.0
DMA	-1.3	-0.9	5.7	0.8
DEA	-1.4	-1.0	5.6	0.6

Table S9 Relative energies (kcal/mol) of the imidic acid forms with respect to amide forms for the four tautomeric pairs with all eight catalysts calculated at B97D/6-311++G(d,p)

	Pair A	Pair B	Pair C	Pair D
TFA	2.1	2.5	6.8	3.6
MFA	2.3	2.6	6.7	3.8
FA	2.0	2.4	6.7	3.5
AA	1.9	2.2	6.5	3.3
AM	0.6	0.9	7.1	2.4
MA	0.2	0.5	6.7	1.9
DMA	-0.2	0.2	6.4	1.6
DEA	-0.3	0.0	6.3	1.4

Table S10 Relative energies (kcal/mol) of the imidic acid forms with respect to amide forms for the four tautomeric pairs with all eight catalysts calculated at M06-2X/6-311++G(d,p)

	Pair A	Pair B	Pair C	Pair D
TFA	-0.2	0.3	4.9	1.8
MFA	0.0	0.3	4.6	1.7
FA	-0.6	-0.2	4.6	1.3
AA	-0.8	-0.5	4.5	1.1
AM	-3.0	-2.6	3.9	-0.7
MA	-3.4	-3.1	3.5	-1.2
DMA	-3.7	-3.3	3.3	-1.5
DEA	-3.8	-3.5	3.1	-1.7

Table S11 Barrier for tautomerization (kcal/mol) in presence of all eight catalysts calculated at B3LYP/6-311++G(d,p) level. Barriers are calculated with respect to the imidic acid forms for the acidic catalysts and with respect to amide forms for the basic catalysts.

	Pair A	Pair B	Pair C	Pair D
TFA	1.7	2.1	1.2	1.7
MFA	3.7	4.0	2.7	3.5
FA	4.6	4.9	3.2	4.3
AA	5.9	6.1	4.2	5.4
AM	13.5	13.3	16.9	13.5
MA	10.3	10.1	13.5	10.2
DMA	8.3	8.2	11.3	8.1
DEA	7.7	7.6	10.4	7.5

Table S12 Barrier for tautomerization (kcal/mol) in presence of all eight catalysts calculated at B97D/6-311++G(d,p) level. Barriers are calculated with respect to the imidic acid forms for the acidic catalysts and with respect to amide forms for the basic catalysts.

	Pair A	Pair B	Pair C	Pair D
TFA	1.0	1.2	0.5	1.0
MFA	2.5	2.7	1.6	2.3
FA	3.4	3.5	2.2	3.1
AA	4.3	4.4	2.8	3.9
AM	12.5	12.4	15.9	12.6
MA	9.4	9.2	12.7	9.4
DMA	7.2	7.0	10.4	7.1
DEA	6.3	6.1	9.3	6.1

Table S13 Barrier for tautomerization (kcal/mol) in presence of all eight catalysts calculated at M06-2X/6-311++G(d,p) level. Barriers are calculated with respect to the imidic acid forms for the acidic catalysts and with respect to amide forms for the basic catalysts.

	Pair A	Pair B	Pair C	Pair D
TFA	3.1	3.2	1.6	2.5
MFA	4.7	5.0	3.4	4.3
FA	5.7	5.9	3.8	5.0
AA	6.7	6.8	4.6	5.9
AM	12.9	12.8	16.4	13.0
MA	10.0	9.7	13.4	9.8
DMA	7.7	7.5	11.1	7.5
DEA	6.7	6.6	10.2	6.5

Table S14 Optimized geometries in Cartesian Coordinates and normal mode frequencies of all species calculated at M06-2X/aug-cc-pVTZ level of theory

Species	Cartesian coordinate (Å)				Vibrational frequencies (cm ⁻¹)			
2PM	C	0.004615	-0.000033	0.004216	134.1255	400.8841	492.1750	499.7613
	N	0.006691	-0.000026	1.300810	576.5410	634.8212	724.40	785.6599
	C	1.160650	0.000004	-0.824329	827.4988	855.1517	1003.4657	1007.0330
	C	2.350230	0.000007	-0.178424	1028.3735	1034.6936	1130.45	1163.7166
	C	1.214702	0.000068	1.977724	1226.0209	1388.4542	1452.7094	1503.4889
	N	2.369174	0.000021	1.168567	1605.1682	1715.5355	1824.9591	3152.2649
	O	1.337392	-0.000103	3.177579	3222.4952	3272.4118	3623.7466	
	H	-0.974182	-0.000045	-0.468283				
	H	1.094764	0.000001	-1.898835				
	H	3.308872	0.0000	-0.678145				
	H	3.240127	0.000004	1.678050				
^a TS	C	0.008150	-0.000107	0.004806	-1835.3757	170.2548	411.4050	501.5306
	N	0.007228	-0.000228	1.331229	559.3456	609.1123	703.6991	798.3703
	C	1.148255	0.000143	-0.804089	806.8212	934.0899	1019.6431	1021.3587
	C	2.374237	0.000314	-0.165661	1039.3997	1084.9432	1127.0252	1131.5091
	C	1.223260	-0.000098	1.879018	1218.9273	1310.2909	1416.7890	1495.1128
	N	2.386833	0.000223	1.156147	1579.4611	1635.3839	1713.1949	2183.0891
	O	1.586643	-0.000236	3.096197	3181.5989	3218.6975	3265.1221	
	H	-0.971124	-0.000216	-0.461500				
	H	1.072681	0.000214	-1.878574				
	H	3.321469	0.000541	-0.688050				
	H	2.746739	0.000070	2.366687				
2HPM	C	0.006026	-0.000031	0.002927	196.2423	423.6794	463.6188	526.9827
	N	0.007073	0.000088	1.329487	562.3934	604.7484	651.7980	824.4078
	C	1.169217	-0.000022	-0.751560	849.0984	905.9850	1019.2522	1031.6460
	C	2.355006	0.000181	-0.038400	1034.0171	1105.5752	1113.3418	1207.8477
	C	1.204069	0.000187	1.898148	1253.0468	1365.9747	1392.2761	1493.7466
	N	2.386106	0.000305	1.289258	1512.5750	1657.4677	1672.6839	3186.3684
	O	1.210560	0.000549	3.235168	3189.6325	3252.4118	3843.9408	
	H	-0.968176	-0.000174	-0.472220				
	H	1.150932	-0.000148	-1.829761				
	H	3.315405	0.000216	-0.540256				
	H	2.133276	0.000728	3.515427				

2PM-AM	C	2.185902	-0.383880	-0.000048	61.4954	125.4435	139.4953	150.0410
	N	1.224841	-1.258851	0.000031	179.6508	292.2339	408.4507	456.6196
	C	2.015103	1.023026	0.000051	515.2918	521.5595	582.6978	638.6486
	C	0.729609	1.459088	-0.000075	789.4920	830.9657	867.8946	966.8401
	C	-0.083505	-0.817204	0.000107	1004.2647	1030.9657	1033.8654	1046.4201
	N	-0.276643	0.571323	-0.000070	1119.3102	1137.6834	1174.5160	1261.4627
	O	-1.051014	-1.553281	-0.000090	1403.8426	1474.5971	1521.4280	1616.1446
	H	3.194658	-0.788573	0.000206	1651.8798	1674.6295	1710.5529	1791.9547
	H	2.850436	1.702255	0.000153	3151.9625	3215.4774	3219.5684	3267.6092
	H	0.449275	2.503676	-0.000120	3457.5130	3586.4076	3629.4351	
	H	-1.262836	0.867122	-0.000148				
	N	-3.165396	0.591927	0.000034				
	H	-2.901870	-0.392485	-0.000266				
	H	-3.742322	0.758809	-0.814729				
	H	-3.741503	0.758475	0.815448				
^{AT} S _{AM}	C	0.014063	0.000895	0.013424	-759.1643	80.7061	158.3572	334.1397
	N	0.017419	0.000204	1.324035	389.4217	406.2977	416.2553	444.3676
	C	1.165919	0.000295	-0.783181	540.1355	585.0467	614.0933	678.8473
	C	2.353977	-0.001113	-0.095586	794.9519	815.3065	856.2579	897.1416
	C	1.225437	-0.001199	1.959482	1014.4738	1017.4403	1030.3909	1076.7162
	N	2.402955	-0.001855	1.233085	1134.6465	1186.7224	1294.7414	1343.7125
	O	1.290387	-0.001920	3.212575	1424.6639	1498.3783	1542.3246	1564.3237
	H	-0.965079	0.002007	-0.457707	1604.2729	1605.8836	1661.0622	1689.6571
	H	1.122982	0.000897	-1.859883	1900.4085	2572.2950	3152.6141	3171.0222
	H	3.307858	-0.001683	-0.612278	3257.1028	3553.7126	3643.0849	
	H	3.480945	-0.003260	2.211430				
	N	3.833388	-0.004128	3.324828				
	H	2.797270	-0.003413	3.639470				
	H	4.330890	0.827245	3.616417				
	H	4.329485	-0.836638	3.615563				

2HPM-AM	C	0.015824	-0.000248	0.009738	59.4418	110.3350	114.9048	186.1160
	N	0.008909	-0.000432	1.332639	208.9604	273.2329	393.9484	425.4632
	C	1.181860	0.000402	-0.742563	540.5782	547.2083	606.2332	656.2625
	C	2.359742	0.000811	-0.019817	815.6098	853.6792	908.5946	1008.5091
	C	1.202337	0.000042	1.928425	1015.3759	1027.6704	1030.5913	1088.2807
	N	2.389624	0.000627	1.307914	1106.2816	1117.4566	1227.1306	1296.3374
	O	1.186065	-0.000222	3.247209	1406.4305	1441.4220	1505.4121	1529.9605
	H	-0.956190	-0.000617	-0.471346	1639.7494	1655.8226	1664.7569	1676.5643
	H	1.170374	0.000567	-1.820770	3140.3995	3176.6363	3179.1227	3252.5032
	H	3.322172	0.001314	-0.519272	3491.1138	3613.3194	3638.4330	
	H	4.087330	-0.001007	3.053083				
	N	3.813442	-0.001235	4.030843				
	H	2.115598	0.000112	3.606526				
	H	4.210282	0.816209	4.475923				
	H	4.207889	-0.820479	4.474750				
2PM-MA	C	0.139857	-0.284294	0.114093	47.0305	74.6519	99.3284	112.0734
	N	0.195432	-0.343713	1.411386	159.2665	176.9870	198.1584	409.0440
	C	1.239385	-0.033739	-0.744239	450.8529	516.74	520.9437	582.4808
	C	2.434904	0.154502	-0.128675	638.0501	787.7487	832.5969	868.3868
	C	1.411440	-0.150891	2.038036	911.9244	982.0802	1001.2185	1004.4011
	N	2.513951	0.095679	1.209116	1030.0658	1047.0184	1062.6491	1076.6297
	O	1.571842	-0.185266	3.242737	1137.0788	1175.3884	1195.8156	1262.3076
	H	-0.841468	-0.442804	-0.325549	1351.7104	1404.2953	1456.0204	1475.7003
	H	1.133525	0.005031	-1.814995	1506.7029	1523.1733	1532.2214	1619.4382
	H	3.357447	0.354898	-0.656759	1631.3322	1709.0052	1792.9208	3048.6545
	H	3.405083	0.238830	1.718043	3092.7357	3114.3126	3144.6780	3150.9614
	N	4.529239	0.209866	3.195561	3214.2292	3268.5625	3508.9131	3604.3814
	H	3.764638	0.543011	3.774829				
	H	5.359901	0.735037	3.434267				
	C	4.720640	-1.222531	3.441925				
	H	3.782304	-1.733592	3.231241				
	H	5.484928	-1.609941	2.769900				
	H	5.009478	-1.458704	4.468270				

ATS _{MA}	C	0.047165	-0.100621	0.048207	-492.7865	52.2280	79.2888	117.5224
	N	0.066231	-0.103224	1.357539	164.5658	180.1726	328.7098	424.6112
	C	1.186876	-0.026196	-0.763881	435.1795	538.5189	566.3451	599.0473
	C	2.380868	0.045685	-0.090555	673.1501	780.4804	790.2639	855.4709
	C	1.282011	-0.028463	1.982968	891.9324	975.2431	1012.1773	1015.3173
	N	2.448694	0.044648	1.237248	1030.3627	1065.2133	1072.4647	1079.7939
	O	1.364232	-0.026358	3.229504	1135.6492	1181.0053	1290.8973	1325.2407
	H	-0.935862	-0.161129	-0.411578	1341.1537	1423.1998	1466.9143	1498.4567
	H	1.130177	-0.025740	-1.839970	1512.9615	1517.4263	1561.0834	1587.8286
	H	3.325738	0.106542	-0.620829	1625.9794	1635.7164	1691.6957	1938.2470
	H	3.543213	0.128433	2.211173	2966.0352	3088.9147	3147.6807	3166.0137
	N	3.956789	0.070749	3.290890	3167.9872	3171.1350	3256.6313	3577.9758
	H	2.993097	0.172566	3.699209				
	H	4.578776	0.822414	3.560548				
	C	4.492190	-1.269519	3.570806				
	H	3.746860	-1.991387	3.244877				
	H	5.413238	-1.428592	3.016276				
	H	4.677112	-1.404203	4.633419				
2HPM-MA	C	0.118254	-0.133442	0.120273	46.4911	66.8814	97.1890	112.6388
	N	0.075360	0.027533	1.432571	182.8399	195.9436	233.0856	420.3227
	C	1.304043	-0.235769	-0.593543	425.6641	544.3981	547.6006	606.4975
	C	2.462109	-0.159610	0.157225	656.0513	816.4012	853.9492	886.8569
	C	1.252546	0.089027	2.058369	909.2260	984.5971	1014.3565	1026.7681
	N	2.456625	0.001374	1.475254	1031.4501	1072.8367	1090.7766	1106.1898
	O	1.205853	0.248382	3.364891	1116.9840	1193.1198	1227.4826	1299.0639
	H	-0.840314	-0.182828	-0.384894	1343.6161	1407.4942	1454.3674	1457.2717
	H	1.321332	-0.366142	-1.663796	1506.0348	1511.7885	1525.2930	1538.6671
	H	3.437497	-0.229901	-0.311499	1633.0543	1651.1731	1674.5191	2971.6135
	H	4.162736	0.602408	3.370507	3055.2404	3122.8985	3151.4583	3175.1199
	N	3.763812	0.197780	4.209597	3177.3556	3250.5682	3525.7461	3612.4205
	H	2.137311	0.292733	3.742190				
	H	4.144259	0.683226	5.011149				
	C	4.054173	-1.237686	4.263059				
	H	3.625157	-1.704311	3.377953				
	H	5.120407	-1.470015	4.297826				
	H	3.574379	-1.668221	5.139680				

2PM-DMA	C	0.003164	-0.180381	0.079165	40.7648	46.2958	76.9378	102.8632
	N	0.034645	-0.031085	1.370092	125.1540	159.6439	188.0098	224.8052
	C	1.136779	-0.223928	-0.770151	297.5579	406.4401	409.1591	514.5706
	C	2.339359	-0.096586	-0.152537	522.3480	581.8279	637.4428	788.0213
	C	1.258124	0.099149	1.997980	832.7922	868.0363	900.2161	964.3693
	N	2.393913	0.057266	1.178812	991.6102	1003.2796	1032.3980	1038.9597
	O	1.398058	0.243160	3.197439	1047.2314	1064.5625	1107.2080	1137.0184
	H	-0.985297	-0.277632	-0.362314	1174.8090	1191.5002	1213.8443	1261.9607
	H	1.049889	-0.349440	-1.835960	1272.4235	1404.7079	1438.9868	1466.3907
	H	3.286719	-0.110654	-0.674580	1474.2877	1477.3958	1492.9806	1507.4913
	H	3.291156	0.163142	1.691170	1519.5106	1522.6820	1527.6054	1622.2566
	N	4.390032	0.251184	3.177362	1708.2758	1789.6085	3007.1495	3015.2535
	H	3.638454	0.734122	3.660683	3045.8618	3091.3358	3095.3604	3140.4139
	C	4.403240	-1.132197	3.639554	3141.8939	3151.4616	3215.1922	3268.6011
	H	3.403906	-1.552122	3.535428	3516.2465			
	H	5.098616	-1.711350	3.030251				
	H	4.711650	-1.224302	4.687197				
	C	5.662151	0.922958	3.396423				
	H	6.432649	0.441864	2.792904				
	H	5.590456	1.964595	3.088981				
	H	5.985170	0.887598	4.443635				
ATS _{DMA}	C	0.019010	-0.130668	0.014761	-403.3783	36.3963	56.7313	100.1639
	N	0.035038	-0.167951	1.322700	167.0355	185.9451	225.9261	230.8796
	C	1.157756	-0.004308	-0.793829	273.7332	405.7890	424.9074	502.8309
	C	2.348436	0.081018	-0.117003	538.8250	560.6753	616.2152	672.2053
	C	1.248807	-0.077110	1.956106	785.4755	854.7914	886.4632	946.9585
	N	2.413714	0.046813	1.210657	1010.3125	1012.5175	1028.8017	1034.7170
	O	1.333236	-0.104444	3.197689	1064.0115	1073.9121	1085.4732	1135.6168
	H	-0.961116	-0.205461	-0.449877	1176.0144	1181.6105	1255.7511	1297.1915
	H	1.102337	0.020690	-1.869711	1340.9792	1420.6616	1447.2201	1479.8378
	H	3.292656	0.179296	-0.643383	1488.2851	1500.4356	1502.3819	1518.7027
	H	3.485528	0.115530	2.168995	1522.3533	1526.0726	1576.5767	1617.2046
	N	3.973950	0.096327	3.233752	1636.8680	1691.2630	1875.6455	3067.1691
	H	3.051667	0.144254	3.708583	3072.7683	3142.7250	3149.3334	3153.0915
	C	4.584440	-1.212266	3.482783	3158.4776	3160.3473	3170.0141	3188.6866
	H	3.855181	-1.981140	3.237289	3235.2115			
	H	5.464049	-1.328987	2.851913				
	H	4.876459	-1.308438	4.527966				
	C	4.833329	1.242038	3.530485				
	H	5.725011	1.197094	2.907273				
	H	4.290260	2.158823	3.313984				
	H	5.132024	1.237664	4.578450				

2HPM-DMA	C	-0.027525	-0.1515	0.043782	41.4201	42.7841	69.6184	104.2127
	N	0.064183	-0.569095	1.295544	129.3134	195.3758	208.7690	222.2905
	C	1.021527	0.454249	-0.633441	306.1191	406.9977	425.1457	532.1665
	C	2.192318	0.600585	0.086574	547.8716	605.7099	655.4090	815.6854
	C	1.240494	-0.378291	1.897198	854.1462	871.0780	909.7990	955.9075
	N	2.320277	0.193645	1.343897	1013.9897	1027.5451	1030.6394	1039.8441
	O	1.329245	-0.7932	3.143070	1083.8119	1106.55	1117.1601	1118.6754
	H	-0.984859	-0.308471	-0.441408	1196.8982	1216.3381	1227.9875	1269.5418
	H	0.929711	0.788948	-1.654359	1300.8179	1407.8764	1440.4609	1459.9647
	H	3.067233	1.062510	-0.357534	1467.9188	1473.3253	1495.0262	1508.3694
	H	4.212851	-0.203466	3.072031	1512.5741	1519.7862	1522.0336	1544.7953
	N	3.786798	-0.141373	3.989961	1650.7134	1674.6210	2868.8733	3022.5803
	H	2.255960	-0.609210	3.504596	3027.1174	3103.1656	3105.6773	3146.8946
	C	4.551248	-0.897953	4.972187	3147.5451	3175.1077	3176.9494	3251.4049
	H	4.666938	-1.926722	4.637412	3539.4021			
	H	5.543137	-0.469778	5.154732				
	H	4.006989	-0.906263	5.916356				
	C	3.638493	1.264909	4.348438				
	H	4.600708	1.762537	4.510654				
	H	3.100472	1.777952	3.553281				
	H	3.055726	1.338202	5.266707				

2PM-DEA	C	-0.010975	-0.046620	0.047330	28.9361	33.7820	59.8505	82.2848
	C	0.087081	-0.308644	2.810388	92.8176	117.6980	129.1617	160.3018
	N	1.170071	0.109577	2.068253	178.8954	250.4570	301.3669	323.5148
	O	0.140623	-0.421773	4.028089	409.9408	475.8347	507.5282	515.9735
	H	-0.072649	0.047965	-1.025149	522.6664	582.2820	637.6199	777.6449
	H	2.023490	0.324176	2.625066	785.4663	805.6685	833.3463	848.0990
	C	-1.090580	-0.592632	1.991439	868.8284	911.2808	923.7201	992.7895
	H	-1.975485	-0.927132	2.520981	1002.7545	1029.5105	1041.5477	1047.2390
	C	1.127465	0.240201	0.719264	1064.2090	1076.4990	1099.6926	1136.7965
	H	2.032319	0.576720	0.234387	1164.2688	1174.8412	1196.7671	1212.5697
	N	-1.133088	-0.469840	0.707815	1265.6107	1307.1908	1331.3705	1379.6406
	N	3.072231	0.350688	4.137130	1397.7743	1405.9877	1410.1472	1414.4063
	H	2.233775	0.510480	4.689754	1476.8437	1488.3374	1491.8456	1496.2540
	C	4.118974	1.295633	4.526154	1503.4731	1504.7107	1515.9221	1527.8486
	H	3.706352	2.297916	4.408142	1534.8501	1623.4637	1707.9414	1789.7862
	H	4.395867	1.189225	5.581238	2982.1906	3030.6661	3059.1101	3060.5251
	C	3.417797	-1.069039	4.264846	3070.9955	3098.5296	3102.3058	3127.0433
	H	2.512744	-1.626071	4.018438	3133.3572	3136.6431	3142.7280	3149.0354
	H	4.162537	-1.312862	3.504933	3209.4624	3268.9580	3507.8032	
	C	3.917781	-1.494413	5.639722				
	H	4.056181	-2.574541	5.673793				
	H	4.872833	-1.029754	5.886105				
	H	3.195314	-1.221230	6.410076				
	C	5.360400	1.151790	3.662338				
	H	6.070487	1.946601	3.885260				
	H	5.863199	0.200730	3.837366				
	H	5.099073	1.208608	2.605054				

ATS _{DEA}	C	0.080858	-0.369957	-0.065969	-227.3343	28.7283	37.0240	71.8826
	N	0.065024	-0.413302	1.241362	86.2089	97.8286	160.8004	168.7652
	C	1.219477	-0.109408	-0.843364	209.8002	256.0710	291.2046	315.3326
	C	2.373446	0.108090	-0.133004	423.9800	426.5479	509.1703	536.3112
	C	1.244388	-0.188856	1.910014	551.0972	584.4208	664.2324	677.0829
	N	2.406827	0.073232	1.195230	783.4741	789.1959	805.4253	854.3373
	O	1.302599	-0.216387	3.150488	865.1429	886.9184	925.2675	1008.6180
	H	-0.871301	-0.552684	-0.558079	1013.0173	1027.8485	1035.2745	1044.2103
	H	1.189549	-0.082157	-1.920195	1070.8660	1078.3935	1097.3955	1132.9994
	H	3.313666	0.319077	-0.633673	1174.1074	1180.1726	1196.2552	1236.9134
	H	3.438326	0.273174	2.196413	1313.3908	1319.8715	1358.8979	1392.8502
	N	3.934469	0.274235	3.248929	1408.8704	1417.6157	1424.0828	1429.3332
	H	3.048725	0.344284	3.770421	1486.5353	1494.3639	1495.5199	1503.9672
	C	4.472575	-1.086124	3.456245	1504.0550	1506.0727	1517.9523	1532.3629
	H	3.648509	-1.756197	3.212493	1572.4834	1620.5750	1641.9022	1689.4243
	H	4.715498	-1.227978	4.509102	1857.4038	3066.6786	3068.7394	3087.8353
	C	4.838504	1.408412	3.498079	3092.0182	3120.6974	3125.6667	3141.7451
	H	5.631775	1.378751	2.751946	3142.2966	3147.7311	3149.8788	3151.9465
	H	4.256912	2.310945	3.315607	3155.6508	3256.1599	3315.0136	
	C	5.674046	-1.355118	2.571210				
	H	6.535729	-0.752635	2.858321				
	H	5.960986	-2.401870	2.648209				
	H	5.434895	-1.145303	1.528031				
	C	5.416157	1.416961	4.901963				
	H	6.082013	0.570658	5.067388				
	H	5.989804	2.328113	5.061540				
	H	4.621941	1.380524	5.647954				

2HPM-DEA	C	-0.107538	0.190807	0.235445	28.5592	34.1915	51.2019	88.2154
	N	0.027496	-0.346364	1.436749	96.6962	114.5549	150.6304	195.5437
	C	0.952293	0.733988	-0.476972	204.9109	257.7152	299.1728	323.2511
	C	2.182894	0.682699	0.150848	425.2826	459.3121	509.3484	546.5127
	C	1.260181	-0.344068	1.949900	547.9497	606.1141	655.5027	773.4630
	N	2.355562	0.151957	1.355261	809.0204	814.4576	848.5627	854.4379
	O	1.393110	-0.877525	3.145289	887.4562	909.9756	924.6009	1013.7140
	H	-1.110495	0.187068	-0.177677	1026.5506	1030.1805	1040.7502	1068.0568
	H	0.824759	1.167921	-1.455848	1087.2491	1105.9866	1116.5501	1129.6103
	H	3.070650	1.082442	-0.326923	1168.1746	1196.5110	1216.0336	1227.5741
	H	4.331706	-0.558640	2.942999	1301.2118	1307.5299	1331.4124	1381.1510
	N	3.939839	-0.574310	3.879009	1398.6291	1407.7851	1412.1637	1417.6711
	H	2.363736	-0.834212	3.441893	1463.4720	1489.3781	1492.1555	1499.4018
	C	4.642413	-1.555015	4.708685	1503.3108	1505.2550	1510.2800	1517.4770
	H	4.628178	-2.499059	4.164043	1530.6120	1547.2915	1650.6547	1674.0245
	H	4.057131	-1.713567	5.615072	2799.2774	3031.4831	3060.3819	3064.4696
	C	3.908557	0.799625	4.393903	3079.3838	3098.4382	3108.7889	3132.7720
	H	4.913625	1.226173	4.477617	3136.3065	3139.0605	3144.6642	3174.4961
	H	3.368847	1.389165	3.651706	3176.3264	3251.4640	3527.6529	
	C	6.075199	-1.185620	5.072487				
	H	6.112331	-0.305215	5.713898				
	H	6.553289	-2.005840	5.606917				
	H	6.661847	-0.976894	4.176417				
	C	3.196901	0.878253	5.733625				
	H	3.762417	0.380895	6.521937				
	H	3.067005	1.918598	6.027296				
	H	2.212986	0.412909	5.668819				
2PM-FA	C	0.017443	0.000350	0.019337	47.6510	74.4803	109.8103	169.6074
	N	0.017218	-0.000017	1.323360	186.9460	230.0910	230.9288	410.8391
	C	1.173338	0.000138	-0.792685	525.5804	534.0397	602.9231	644.2195
	C	2.359518	-0.000345	-0.130458	727.5153	800.7491	834.4431	896.3162
	C	1.217369	-0.000681	1.978992	972.4824	1006.7992	1035.9274	1038.0691
	N	2.371511	-0.000703	1.212067	1055.4005	1061.3984	1125.8226	1138.5644
	O	1.306453	-0.000735	3.206580	1207.0184	1262.8743	1319.2484	1401.9352
	H	-0.960427	0.000690	-0.453138	1425.1707	1476.6964	1490.9779	1517.5327
	H	1.118986	0.000395	-1.868010	1624.3100	1704.2348	1721.7615	1792.0435
	H	3.325277	-0.000492	-0.616094	2797.6769	3093.7241	3163.5944	3169.1225
	H	3.259699	-0.001071	1.739130	3226.9705	3268.1647		
	C	4.511543	-0.002674	4.033325				
	H	5.386820	-0.003551	4.691398				
	O	4.628837	-0.002412	2.822789				
	O	3.396389	-0.002325	4.697541				
	H	2.586226	-0.001641	4.081288				

ATS _{FA}	C	2.776756	-0.356765	0.000002	-543.6929	46.2227	92.9383	153.2549
	N	1.814478	-1.250915	-0.000010	195.1269	248.9760	362.0009	383.2518
	C	2.566310	1.028415	0.000016	421.2537	539.6144	580.4658	655.0170
	C	1.259957	1.428677	0.000012	781.8458	809.0016	843.9157	851.7382
	C	0.547000	-0.803463	-0.000009	916.1514	1023.3917	1035.4923	1067.1921
	N	0.272273	0.526558	0.000000	1091.0078	1102.2431	1151.8804	1247.7948
	O	-0.410463	-1.642662	-0.000017	1250.2661	1290.6503	1307.8764	1400.8576
	H	3.787518	-0.750808	0.000002	1417.1098	1437.5913	1484.8195	1552.4953
	H	3.380754	1.733327	0.000024	1625.6919	1632.3536	1703.6324	1748.3352
	H	0.949159	2.464997	0.000018	1788.2452	1839.2388	3091.0073	3171.3283
	H	-0.823660	0.885531	-0.000015	3223.8262	3242.6156		
	C	-2.945666	0.408370	0.000009				
	H	-4.005530	0.692892	0.000031				
	O	-2.106369	1.339982	-0.000040				
	O	-2.693308	-0.817762	0.000036				
	H	-1.440523	-1.223311	0.000004				
2HPM-FA	C	0.017027	0.000111	0.010807	48.8815	71.2445	128.0818	173.5587
	N	0.012505	-0.000026	1.331809	196.7674	220.2234	234.2401	426.1532
	C	1.181853	0.000041	-0.749064	519.8728	545.1099	610.7738	664.8512
	C	2.359514	-0.000034	-0.035789	734.7062	818.7863	848.5554	888.8987
	C	1.202164	-0.000228	1.931860	912.4984	1028.1229	1029.3494	1037.5394
	N	2.382888	-0.000147	1.296490	1063.3721	1105.3485	1122.6524	1126.5899
	O	1.188699	-0.000028	3.244045	1231.7473	1290.0919	1305.1198	1408.9024
	H	-0.955987	0.000135	-0.467648	1411.9574	1428.8995	1494.9697	1521.5902
	H	1.165426	0.000081	-1.826788	1566.8043	1641.6493	1687.9038	1789.4802
	H	3.325123	-0.000036	-0.527897	2778.3716	3099.9906	3184.1223	3191.2720
	H	3.869353	-0.000180	2.015881	3258.6590	3303.6168		
	C	4.679926	-0.000593	3.737299				
	H	5.648908	-0.001062	4.246318				
	O	4.796410	-0.000489	2.438135				
	O	3.633940	-0.000470	4.350599				
	H	2.101893	0.000081	3.623639				

2PM-AA	C	-3.342257	-0.305002	0.000146	40.5524	64.5200	81.4045	106.0578
	N	-2.404363	-1.210723	0.000067	111.4736	161.8316	168.1697	177.8178
	C	-3.124404	1.090858	0.000081	411.2370	462.8417	525.6568	534.4575
	C	-1.823668	1.484487	-0.000059	601.5554	614.2791	642.8694	644.0779
	C	-1.098131	-0.802008	-0.000107	796.7210	834.5847	894.2735	931.0137
	N	-0.849498	0.561967	-0.000146	978.9668	1006.7595	1033.6535	1036.8856
	O	-0.151494	-1.586905	-0.000125	1037.5178	1057.4570	1060.1285	1079.7937
	H	-4.361436	-0.680510	0.000253	1137.2869	1204.8851	1262.9623	1359.2341
	H	-3.936204	1.798126	0.000147	1399.1646	1413.3565	1471.6052	1477.4586
	H	-1.503255	2.517000	-0.000109	1481.9485	1506.6060	1520.2380	1624.6232
	H	0.149709	0.832373	-0.000232	1705.1247	1731.8268	1783.7801	2903.7318
	C	2.685179	0.184015	0.000027	3087.4587	3123.2464	3153.9572	3162.9002
	O	1.854301	1.079514	-0.000045	3200.1677	3226.9250	3270.0371	
	O	2.388176	-1.089725	0.000048				
	H	1.389699	-1.245704	-0.000021				
	C	4.161167	0.449439	0.000107				
	H	4.607766	-0.015743	0.877405				
	H	4.607774	-0.015434	-0.877355				
	H	4.347783	1.517369	0.000280				
ATs _{AA}	C	3.249052	-0.202469	0.007168	-776.6614	42.5644	69.9030	90.3945
	N	2.354208	-1.163659	0.007219	127.6481	155.4816	192.7487	247.6492
	C	2.939734	1.163976	0.001738	350.2603	422.2300	500.2949	540.6947
	C	1.607180	1.468558	-0.003317	582.0031	620.3310	648.0068	713.2607
	C	1.055584	-0.808111	0.001759	778.9111	795.6030	845.8693	915.8838
	N	0.686008	0.500015	-0.003070	967.6598	1013.4135	1021.9356	1042.8011
	O	0.159549	-1.708791	0.001330	1057.2472	1079.1233	1081.9995	1141.7633
	H	4.285873	-0.522138	0.011696	1242.7005	1275.4286	1291.5725	1323.4899
	H	3.701267	1.925772	0.001700	1378.2413	1414.2680	1461.5389	1470.3356
	H	1.224987	2.480968	-0.007576	1482.0106	1507.5663	1555.3442	1576.1825
	H	-0.451858	0.775166	-0.007167	1630.0366	1674.3714	1701.2833	1781.3807
	C	-2.528959	0.139923	-0.015073	1791.8156	3077.7332	3152.6098	3187.5424
	O	-1.736596	1.120111	-0.012644	3190.3197	3201.2325	3230.1985	
	O	-2.166071	-1.066299	-0.018472				
	H	-0.922094	-1.357423	-0.007610				
	C	-4.004702	0.423143	0.018179				
	H	-4.554517	-0.382693	-0.458332				
	H	-4.310599	0.476058	1.063707				
	H	-4.216971	1.379519	-0.449900				

2HPM-AA	C	0.024275	0.000000	0.013966	40.3721	49.4379	59.9537	113.5357
	N	0.017938	-0.000141	1.335011	116.8580	160.7692	168.8150	199.0047
	C	1.189794	0.000125	-0.744373	425.7953	458.5167	522.8154	545.8621
	C	2.366873	0.000143	-0.029013	610.6045	610.6818	648.1251	664.8509
	C	1.207583	-0.000148	1.936489	821.0229	849.3062	904.6421	912.7598
	N	2.389419	0.000014	1.302484	931.1928	1025.5505	1028.6994	1035.6358
	O	1.195082	-0.000221	3.247778	1036.9030	1053.2871	1080.9678	1105.8951
	H	-0.948207	-0.000032	-0.465764	1125.9695	1231.2198	1292.6773	1356.5954
	H	1.174826	0.000213	-1.822157	1412.8839	1417.8827	1426.0827	1470.7497
	H	3.332792	0.000253	-0.520784	1481.2629	1493.6664	1530.3772	1561.2868
	H	3.891941	0.000058	2.046793	1642.7638	1686.2661	1789.1115	2884.1317
	C	4.692535	-0.000275	3.776739	3088.7058	3155.2413	3182.5722	3187.7868
	O	4.811819	0.000023	2.467788	3202.5586	3237.2826	3256.8614	
	O	3.617249	-0.000329	4.349298				
	H	2.112499	-0.000201	3.625051				
	C	6.004484	0.000077	4.499716				
	H	6.575435	0.878918	4.204338				
	H	5.837183	-0.001272	5.570771				
	H	6.577210	-0.876869	4.202224				
2PM-MFA	C	-1.572422	-0.792092	-0.000104	36.1382	49.8862	93.7140	95.3277
	N	-1.200030	0.541586	-0.000006	103.7462	117.9159	169.9583	179.4628
	C	-2.086327	1.550261	0.000037	314.8248	411.0753	502.1854	525.4850
	C	-3.416923	1.275769	0.000012	536.6767	580.4429	606.3513	644.2867
	C	-3.760868	-0.094174	0.000023	688.9707	796.4925	834.4738	897.6570
	N	-2.908264	-1.081096	-0.000027	934.1044	971.3526	1007.1179	1035.1070
	O	-0.702400	-1.664301	0.000024	1038.3878	1049.7061	1061.1992	1073.5652
	O	1.839022	-1.434614	0.000054	1137.5068	1170.5823	1208.4066	1262.6487
	C	2.257571	-0.200406	-0.000016	1277.7055	1329.6848	1401.4734	1431.2316
	O	1.556457	0.791051	-0.000023	1477.2015	1486.0270	1515.9265	1521.8123
	C	3.768093	-0.133856	-0.000005	1623.5987	1704.9652	1729.3356	1810.7085
	F	4.199828	1.160294	-0.000015	2740.3778	3084.0529	3132.0092	3164.7514
	H	4.143323	-0.645544	-0.887219	3166.9777	3226.3251	3271.9476	
	H	4.143306	-0.645486	0.887254				
	H	-4.809687	-0.375862	-0.000029				
	H	-4.160996	2.053986	0.000015				
	H	-1.672387	2.548861	0.000071				
	H	-0.183233	0.722167	0.000034				
	H	0.819913	-1.494287	0.000103				

AT _S _{MFA}	N	-1.024885	-0.454155	-0.000038	-405.509	42.8679	46.7809	95.4433
	C	-1.826497	-1.525376	0.000214	121.1726	135.6377	185.4002	197.0785
	C	-3.184678	-1.375512	0.000279	295.663	393.2755	419.3137	539.4381
	C	-3.650245	-0.054568	0.000034	548.8006	580.4013	594.1679	656.2966
	N	-2.870920	1.003676	-0.000197	709.1038	819.953	842.5104	867.4404
	C	-1.544131	0.799161	-0.000201	917.0923	957.8019	1021.6097	1040.7835
	O	-0.760027	1.805699	-0.000379	1050.6841	1075.4792	1107.2322	1157.4972
	O	1.642367	1.398168	0.000542	1164.093	1224.5904	1249.523	1277.8461
	C	2.115195	0.234654	0.000199	1290.3914	1299.559	1377.3146	1415.1465
	C	3.628276	0.167114	0.000356	1481.2568	1484.0302	1524.1706	1547.6361
	H	3.997295	0.682111	0.887820	1613.447	1633.0045	1703.6069	1780.7034
	O	1.457864	-0.829622	-0.000396	1790.2161	1895.719	3086.0816	3134.7981
	F	4.088124	-1.121509	-0.000443	3178.3005	3219.653	3264.0522	
	H	3.997662	0.683341	-0.886241				
	H	-4.716594	0.144269	0.000025				
	H	-3.852988	-2.220267	0.000480				
	H	-1.326828	-2.484978	0.000343				
	H	0.117253	-0.607105	-0.000213				
	H	0.312574	1.582759	-0.000009				
2HPM-MFA	N	-2.866353	-1.168391	0.000139	30.9503	46.6679	89.2341	106.9579
	C	-1.584122	-0.805886	-0.000152	107.1135	122.3583	161.6527	199.4891
	N	-1.145384	0.461471	-0.000204	312.6599	425.2873	494.3937	527.986
	C	-2.064387	1.426720	-0.000049	544.9817	576.4075	610.9606	665.7719
	C	-3.413773	1.154868	0.000182	693.6181	819.5469	848.0613	882.4825
	C	-3.756984	-0.193139	0.000309	912.6326	934.7938	1028.064	1029.9168
	O	-0.707080	-1.781128	-0.000198	1037.9528	1048.9041	1077.4568	1105.3971
	O	1.387398	1.256503	-0.000278	1127.1672	1175.754	1231.3439	1279.8642
	C	2.191225	0.222113	-0.000128	1289.6789	1322.6842	1411.9621	1417.3604
	C	3.641299	0.646172	0.000155	1446.8742	1485.543	1493.5176	1534.8061
	F	4.466006	-0.438205	0.000358	1574.2007	1642.0019	1688.4981	1820.6733
	O	1.837817	-0.936177	-0.000127	2724.7424	3084.1203	3131.6941	3184.4746
	H	3.830672	1.252063	-0.887187	3190.9638	3258.8339	3301.138	
	H	3.830317	1.252126	0.887531				
	H	-4.797114	-0.499392	0.000472				
	H	-4.155124	1.937255	0.000282				
	H	-1.686324	2.442416	-0.000133				
	H	0.418195	0.934057	-0.000447				
	H	0.222841	-1.444912	-0.000364				

2PM-TFA	C	-4.399657	-0.249616	-0.000121	19.6831	35.4572	58.7820	90.0853
	N	-3.475826	-1.170830	-0.000091	90.1756	106.2201	170.0232	171.4668
	C	-4.156455	1.141681	-0.000073	266.7991	292.2220	410.0230	418.0110
	C	-2.850445	1.513226	0.000053	447.2256	523.9741	529.2124	537.4008
	C	-2.167713	-0.785183	0.000004	599.5850	621.6130	645.5189	730.9842
	N	-1.892276	0.570288	0.000095	799.5327	812.3232	833.1732	854.0128
	O	-1.237713	-1.596888	0.000090	901.8332	953.6052	1007.7578	1029.1932
	H	-5.424343	-0.608547	-0.000239	1038.2365	1062.4203	1121.2731	1138.6121
	H	-4.955355	1.863506	-0.000124	1214.8343	1240.6305	1242.8498	1258.6870
	H	-2.510395	2.539100	0.000115	1286.9944	1398.1143	1434.1014	1475.6929
	H	-0.896841	0.827832	0.000187	1505.8240	1549.4407	1621.8015	1701.1069
	C	1.595289	-0.002361	0.000304	1717.6366	1828.5718	2485.8470	3169.3688
	O	0.882626	0.977129	0.000166	3231.5797	3254.1779	3271.8974	
	O	1.244961	-1.241104	0.000149				
	H	0.212976	-1.355985	0.000119				
	C	3.132599	0.153080	-0.000056				
	F	3.655238	-0.426009	1.079459				
	F	3.654846	-0.426612	-1.079446				
	F	3.479914	1.430380	-0.000458				
^{AT} S _{TFA}	C	4.293137	-0.102766	0.023982	-26.2868	12.4243	30.9197	57.1147
	N	3.442154	-1.102460	0.015222	107.8464	117.3363	194.8791	222.7028
	C	3.923872	1.250786	0.014163	269.7758	301.1601	416.5649	430.8952
	C	2.583637	1.500450	-0.006610	461.7291	499.5043	529.4364	537.1616
	C	2.132005	-0.810517	-0.004252	585.3922	612.7453	658.2673	749.2697
	N	1.711127	0.481962	-0.015680	816.1055	823.9638	838.5787	874.0794
	O	1.279774	-1.753815	-0.012238	910.7364	991.3665	1019.7211	1043.4435
	H	5.342544	-0.376495	0.039809	1080.7044	1133.4458	1191.6699	1195.3604
	H	4.651787	2.044544	0.022168	1219.9714	1244.8362	1251.1290	1275.6685
	H	2.149430	2.490613	-0.016786	1279.6231	1296.4835	1419.8320	1482.6692
	H	0.643002	0.695065	-0.034271	1526.8054	1545.7684	1622.2413	1657.2263
	C	-1.494516	-0.051043	-0.049482	1708.2036	1778.9114	1887.4795	2306.2231
	O	-0.819773	0.989390	-0.059891	3184.1943	3227.0379	3269.7489	
	O	-1.095606	-1.234685	-0.037096				
	H	0.212861	-1.474840	-0.024497				
	C	-3.029816	0.136372	0.002534				
	F	-3.404050	0.310691	1.275408				
	F	-3.410235	1.208098	-0.686559				
	F	-3.678789	-0.916814	-0.476786				

2HPM-TFA	C	-4.354180	-0.055549	0.000245	24.8857	35.6386	53.5427	96.3936
	N	-3.581999	1.016174	0.000146	96.8854	124.4305	137.5901	201.9518
	C	-3.857308	-1.355228	0.000138	266.9137	288.9686	416.3397	425.2114
	C	-2.486863	-1.470775	-0.000088	445.2487	518.0021	528.5192	543.4522
	C	-2.268179	0.805011	-0.000057	605.0137	615.6141	669.1725	735.2893
	N	-1.686699	-0.402935	-0.000188	806.1036	826.8383	830.8997	848.8271
	O	-1.510026	1.877516	-0.000177	857.3992	911.9567	1028.5159	1033.8694
	H	-5.422511	0.128719	0.000410	1038.7564	1106.4024	1130.7834	1135.1603
	H	-4.503463	-2.217797	0.000221	1232.1754	1237.2869	1238.7397	1285.4773
	H	-1.991742	-2.434528	-0.000201	1293.9452	1406.5141	1410.4434	1451.7232
	H	-0.147641	-0.699240	-0.000490	1492.2419	1536.8620	1604.6786	1641.5703
	C	1.563306	0.155582	-0.000130	1692.5449	1830.9938	2432.8403	3184.2985
	O	0.865646	-0.933920	-0.000390	3195.7923	3257.0945	3412.0919	
	O	1.149888	1.290679	-0.000037				
	H	-0.551978	1.654420	-0.000302				
	C	3.079596	-0.134517	0.000084				
	F	3.411087	-0.841784	-1.079248				
	F	3.777712	0.987391	0.000194				
	F	3.410748	-0.841783	1.079535				
2PZ	C	0.003456	0.000125	0.004800	169.0014	408.2974	446.6121	507.6590
	C	0.006395	-0.000065	2.793963	563.6216	619.9854	726.6570	778.5391
	N	1.166971	-0.000377	2.036940	828.5227	844.0340	959.3757	974.5126
	O	0.027532	0.000372	4.007038	997.6360	1063.6918	1155.9887	1233.1096
	H	-0.027298	0.000158	-1.072822	1279.6613	1366.1236	1421.2193	1506.0020
	H	2.030249	-0.000651	2.561189	1599.6449	1695.3165	1802.5049	3189.7743
	C	-1.199823	0.000590	1.956926	3236.8823	3256.5667	3612.7753	
	H	-2.145186	0.001285	2.487609				
	C	1.174355	-0.000347	0.674437				
	H	2.138554	-0.000670	0.189074				
	N	-1.197771	0.000608	0.670203				
^B TS	C	0.003688	0.000256	0.007365	-1866.5029	193.1379	433.8004	490.5189
	C	0.004221	0.000652	2.700910	507.4136	630.3340	672.3218	767.6717
	N	1.163366	-0.000087	2.016809	851.8778	918.6916	946.5494	991.9318
	O	0.313203	0.000767	3.939765	1019.4835	1097.0921	1135.5119	1188.0187
	H	-0.024915	0.000098	-1.071771	1253.1567	1327.0057	1383.3014	1500.3889
	H	1.503672	0.000059	3.247282	1570.0118	1598.4994	1684.4152	2138.1682
	C	-1.207865	0.001188	1.967355	3218.1494	3226.9734	3243.3071	
	H	-2.164957	0.001824	2.470249				
	C	1.203167	-0.000275	0.684858				
	H	2.165391	-0.000854	0.194021				
	N	-1.175017	0.000984	0.656112				

2HPZ	C	0.000428	-0.000355	0.006481	215.6612	417.5520	440.2394	479.3781
	C	0.002796	0.000968	2.654005	569.1695	587.1267	647.5208	789.3675
	N	1.178496	0.000519	2.066678	880.1143	887.7526	962.9112	1010.6176
	O	-0.053428	0.001055	3.996406	1032.2509	1102.2500	1154.8043	1226.3572
	H	0.008331	-0.000650	-1.074691	1243.5408	1349.8056	1357.7502	1492.8066
	H	0.853902	0.001021	4.325592	1529.1734	1638.3450	1672.1920	3200.7797
	C	-1.197979	0.000549	1.929980	3207.8350	3221.5089	3825.8878	
	H	-2.148150	0.000585	2.447987				
	C	1.175247	-0.000197	0.731648				
	H	2.139248	-0.000279	0.239643				
	N	-1.190136	-0.000023	0.613737				
2PZ-AM	C	-0.004658	0.000991	0.005005	60.4657	119.7380	142.2499	175.7840
	C	0.036353	-0.001476	2.783321	177.7145	290.9039	418.7371	452.7045
	N	1.187653	-0.001842	2.024730	461.2534	543.2126	571.0988	628.1522
	O	0.061264	-0.002663	4.006340	770.1511	835.4779	855.8851	959.5095
	H	-0.045444	0.001980	-1.072564	962.7043	1003.0126	1007.8898	1069.8370
	H	2.066583	-0.002934	2.561616	1119.0751	1180.3563	1247.9883	1283.9524
	C	-1.179514	0.000257	1.970436	1370.1952	1449.9450	1527.0660	1600.4701
	H	-2.118419	0.000650	2.512346	1649.5100	1673.5712	1690.7972	1774.3373
	C	1.173900	-0.000646	0.667758	3187.5696	3220.5874	3230.7914	3250.2188
	H	2.133288	-0.001047	0.171899	3459.6708	3587.0911	3628.5899	
	N	-1.195505	0.001449	0.680847				
	N	3.089099	-0.004049	4.201075				
	H	2.175857	-0.003676	4.652673				
	H	3.595200	0.810628	4.524909				
	H	3.594286	-0.819475	4.524451				
BTS _{AM}	C	0.008028	0.000371	0.012922	-729.6636	78.2447	191.5678	323.6605
	C	0.016965	-0.000968	2.745156	375.7912	389.9474	410.8747	456.4447
	N	1.195293	-0.001302	2.064371	568.5676	569.1596	609.1065	666.0984
	O	-0.011026	-0.001572	4.008604	789.9268	818.9688	853.1710	884.9010
	H	0.000151	0.000902	-1.066932	962.7160	986.7677	1025.0365	1094.7756
	H	2.235387	-0.002302	3.086632	1191.7857	1258.1909	1298.6207	1353.0824
	C	-1.185954	0.000102	1.949161	1385.1328	1512.2414	1541.0405	1553.3947
	H	-2.133322	0.000382	2.475594	1568.8981	1602.9746	1665.2580	1677.3051
	C	1.176139	-0.000633	0.720549	1896.4955	2618.3057	3187.8618	3189.8155
	H	2.135876	-0.000929	0.218437	3230.0247	3548.8062	3637.5432	
	N	-1.187938	0.000737	0.648878				
	N	2.539955	-0.002979	4.213402				
	H	1.502808	-0.002543	4.505287				
	H	3.029109	0.828375	4.520345				
	H	3.028163	-0.835169	4.519585				

2HPZ-AM	C	0.016254	0.000057	0.020814	55.8180	105.8312	114.6523	209.6309
	C	0.003405	-0.000189	2.685765	211.1282	275.3825	391.9546	442.9491
	N	1.185275	-0.000548	2.092414	500.4480	562.6109	597.9825	651.3243
	O	-0.085698	-0.000423	4.009588	790.1075	874.1542	891.6487	965.5220
	H	0.031380	0.000191	-1.060172	998.4789	1004.7876	1029.7019	1098.3346
	H	2.814583	-0.000756	3.918918	1104.3040	1182.1182	1233.2984	1306.3677
	C	-1.191121	0.000243	1.935739	1365.8613	1424.1133	1522.7418	1530.4198
	H	-2.143150	0.000459	2.451274	1626.0664	1648.8848	1664.9830	1677.8123
	C	1.181516	-0.000430	0.754830	3093.7634	3191.4910	3202.1406	3219.5950
	H	2.147231	-0.000670	0.264859	3488.3827	3610.0140	3636.0729	
	N	-1.180537	0.000385	0.623030				
	N	2.501359	-0.001047	4.885088				
	H	0.825795	-0.000776	4.418592				
	H	2.881051	0.816962	5.344310				
	H	2.881014	-0.819345	5.343824				
2PZ-MA	C	0.080860	-0.071603	0.077213	47.2892	79.3360	97.1144	114.1279
	C	0.208644	-0.117291	2.851644	174.7589	184.6029	197.9465	420.3358
	N	1.317397	0.102045	2.062831	450.6898	461.2526	544.9967	571.1089
	O	0.275442	-0.136109	4.073204	628.3631	771.5913	835.7271	856.4070
	H	0.006785	-0.057641	-0.998521	912.7110	962.9809	970.4482	991.6471
	H	2.199902	0.254017	2.584823	1002.6007	1054.0532	1069.8683	1076.3026
	C	-1.012950	-0.320178	2.073538	1181.2181	1195.8566	1248.0955	1285.3793
	H	-1.919643	-0.498568	2.640466	1351.0683	1371.9022	1450.3351	1459.8201
	C	1.260733	0.126954	0.707731	1506.3295	1526.9284	1534.0210	1602.8030
	H	2.188318	0.309404	0.185279	1630.8094	1689.1160	1774.0011	3049.1716
	N	-1.069207	-0.298463	0.784966	3093.2401	3115.0526	3144.6487	3189.3051
	N	3.263311	0.240517	4.114723	3227.5687	3250.5619	3508.9709	3603.5211
	H	2.489317	0.595674	4.667751				
	H	4.095320	0.756417	4.368900				
	C	3.425714	-1.190521	4.388794				
	H	2.488713	-1.692814	4.152189				
	H	4.207438	-1.597825	3.749568				
	H	3.675136	-1.415259	5.427914				

BTS _{MA}	C	0.028462	-0.041530	0.035836	-463.8509	51.0851	75.8059	124.1057
	C	0.078014	-0.025892	2.772277	165.8953	203.4700	320.4564	415.2557
	N	1.244348	0.051825	2.070380	439.8239	527.4228	566.2793	604.0993
	O	0.069132	-0.021998	4.030499	660.9878	786.0191	795.8843	849.6605
	H	0.004982	-0.047527	-1.043779	883.7942	960.1890	974.1698	984.6552
	H	2.301921	0.149482	3.084624	1018.5034	1062.5038	1072.3064	1096.6731
	C	-1.134455	-0.114216	1.989332	1192.4690	1258.6860	1291.4659	1326.9991
	H	-2.071896	-0.177036	2.530048	1343.2879	1383.6693	1467.4439	1504.5178
	C	1.203011	0.044214	0.726657	1514.7647	1517.6043	1548.1129	1571.3569
	H	2.152245	0.109437	0.208327	1611.2772	1624.3869	1680.4164	1929.7244
	N	-1.156348	-0.122259	0.690117	3019.4656	3090.9630	3170.2346	3173.7862
	N	2.675906	0.093560	4.178398	3183.8629	3186.5901	3229.0060	3574.2360
	H	1.711608	0.207905	4.571442				
	H	3.303998	0.835283	4.462404				
	C	3.184975	-1.255387	4.471535				
	H	2.437201	-1.965433	4.125925				
	H	4.116696	-1.425870	3.939073				
	H	3.341790	-1.392193	5.538231				
2HPZ-MA	C	0.108585	-0.176497	0.116887	45.01	67.68	95.73	112.41
	C	0.030556	0.044818	2.774720	182.23	217.25	234.15	418.17
	N	1.225073	-0.019725	2.212083	442.68	505.41	563.1	599.47
	O	-0.088332	0.156615	4.088903	651.13	790.22	874.5	888.95
	H	0.149865	-0.266943	-0.959914	894.26	964.16	984.43	1004.24
	H	2.797857	0.469691	4.131229	1028.97	1070.52	1087.82	1103.92
	C	-1.147341	0.000535	1.993351	1182.35	1195.31	1234.47	1309.81
	H	-2.111362	0.058083	2.484021	1343.6	1366.98	1438.19	1457.47
	C	1.255277	-0.131267	0.878505	1508.17	1524.39	1530.3	1537.13
	H	2.233135	-0.185521	0.415339	1624.87	1638.23	1676.09	2916.84
	N	-1.103294	-0.108539	0.687456	3057.05	3124.63	3152.22	3188.5
	N	2.426558	0.156067	5.021623	3199.84	3217.82	3522.57	3609.12
	H	0.824372	0.165174	4.523092				
	H	2.745451	0.789305	5.743422				
	C	2.846697	-1.222430	5.287463				
	H	2.472399	-1.857045	4.485882				
	H	3.929399	-1.347349	5.352619				
	H	2.401458	-1.560763	6.220986				

2PZ-DMA	C	0.049989	-0.402861	0.095888	40.0164	46.7577	76.4223	108.2459
	C	0.031506	0.108054	2.713262	123.2414	182.4328	189.5465	224.5817
	N	1.214950	-0.036950	2.137817	296.8680	406.4188	420.4174	460.3209
	O	-0.053776	0.361653	4.010103	545.4471	570.3301	628.5681	771.7616
	H	0.067312	-0.610148	-0.965033	835.0999	856.1579	899.6014	961.3802
	H	2.862827	0.677106	4.023508	963.2181	973.4620	1002.0332	1037.2577
	C	-1.161038	-0.004381	1.966697	1057.7716	1070.1717	1106.5670	1180.8966
	H	-2.114032	0.119396	2.465442	1191.2857	1213.8287	1248.8748	1271.0424
	C	1.213200	-0.292705	0.824993	1284.9764	1371.9272	1439.4167	1451.9293
	H	2.179509	-0.411726	0.350558	1469.1351	1474.2859	1492.8866	1507.2780
	N	-1.147765	-0.256255	0.678488	1519.2425	1524.0519	1532.2463	1603.4688
	N	2.463292	0.363916	4.901515	1688.4114	1772.3214	3007.9049	3015.7894
	H	0.876222	0.418852	4.412373	3046.1706	3092.5358	3096.6714	3141.1699
	C	2.956325	1.167655	6.012462	3141.3926	3189.1694	3228.7843	3250.0781
	H	4.029311	1.031610	6.186021	3515.6689			
	H	2.760103	2.220730	5.821981				
	H	2.427081	0.880801	6.920884				
	C	2.742725	-1.059216	5.064691				
	H	2.391810	-1.592359	4.182871				
	H	3.808668	-1.265047	5.208105				
	H	2.201615	-1.430112	5.935186				
BTS _{DMA}	C	0.001310	0.017801	0.007966	-402.1787	22.0370	51.6667	102.9031
	C	0.036140	0.066393	2.748298	170.4108	195.4429	203.6705	221.5310
	N	1.203973	-0.047410	2.050314	253.9647	398.8422	439.0376	458.9897
	O	0.025836	0.091653	4.001539	549.2759	565.2873	624.5600	657.7683
	H	-0.017466	-0.000925	-1.071530	787.6408	848.6089	877.3168	944.1736
	H	2.236445	-0.122477	3.040791	961.2678	984.0919	1006.1758	1035.6548
	C	-1.171354	0.156040	1.953329	1056.8229	1081.8099	1091.7750	1173.3787
	H	-2.110624	0.247404	2.487022	1193.1109	1254.6591	1260.8940	1294.3050
	C	1.170484	-0.070495	0.706049	1340.5795	1381.9373	1442.7438	1475.9906
	H	2.121318	-0.162743	0.194634	1485.7944	1498.2857	1507.3509	1516.2669
	N	-1.186113	0.133269	0.655086	1518.3371	1525.7326	1549.3437	1602.4460
	N	2.690127	-0.105239	4.125272	1616.8326	1680.0748	1866.1906	3071.9937
	H	1.761712	-0.163983	4.581771	3072.5880	3144.0233	3147.7419	3165.5303
	C	3.281021	1.209653	4.391966	3166.8810	3181.8903	3184.1032	3206.8590
	H	4.173966	1.335684	3.782485	3227.6570			
	H	2.550132	1.970998	4.128712				
	H	3.546380	1.307784	5.443882				
	C	3.554884	-1.242852	4.440426				
	H	3.030158	-2.164369	4.200787				
	H	4.463172	-1.181897	3.843683				
	H	3.822796	-1.242965	5.496516				

2HPZ-DMA	C	0.049989	-0.402861	0.095888	39.6299	42.8902	69.9468	102.7612
	C	0.031506	0.108054	2.713262	130.4623	206.8422	217.7545	222.1056
	N	1.214950	-0.036950	2.137817	303.7222	407.0830	442.4275	490.0941
	O	-0.053776	0.361653	4.010103	563.6022	596.7476	650.7999	790.4365
	H	0.067312	-0.610148	-0.965033	872.8748	874.8824	895.6062	955.3486
	H	2.862827	0.677106	4.023508	964.2582	1004.9347	1028.3282	1039.4380
	C	-1.161038	-0.004381	1.966697	1079.9944	1104.2584	1116.3512	1183.0064
	H	-2.114032	0.119396	2.465442	1196.1313	1217.9573	1234.7683	1269.8822
	C	1.213200	-0.292705	0.824993	1312.5559	1367.7104	1440.5220	1444.5792
	H	2.179509	-0.411726	0.350558	1469.1695	1473.0438	1495.0835	1508.9740
	N	-1.147765	-0.256255	0.678488	1518.1712	1521.9232	1530.6327	1545.2658
	N	2.463292	0.363916	4.901515	1629.0375	1677.1326	2814.4504	3025.2127
	H	0.876222	0.418852	4.412373	3029.1658	3104.3068	3106.8848	3147.4526
	C	2.956325	1.167655	6.012462	3148.2872	3190.2191	3202.1020	3218.8937
	H	4.029311	1.031610	6.186021	3535.1123			
	H	2.760103	2.220730	5.821981				
	H	2.427081	0.880801	6.920884				
	C	2.742725	-1.059216	5.064691				
	H	2.391810	-1.592359	4.182871				
	H	3.808668	-1.265047	5.208105				
	H	2.201615	-1.430112	5.935186				

2PZ-DEA	C	0.019912	0.507657	0.103487	31.7710	38.3494	44.0793	85.9960
	C	0.071150	-0.138669	2.690921	101.7034	114.1359	124.6817	178.6566
	N	1.235687	0.103182	2.108533	187.8223	251.0942	296.1501	322.4103
	O	0.021360	-0.463956	3.972806	421.1351	459.9457	472.9298	509.9803
	H	0.009220	0.770350	-0.945206	546.5056	571.1817	628.8016	772.1636
	H	2.974394	-0.649820	3.995647	780.2770	808.0349	835.5852	847.4096
	C	-1.137224	-0.055305	1.965871	858.2211	917.0312	926.7700	962.0201
	H	-2.073920	-0.258685	2.469458	972.1571	1002.0063	1039.9037	1059.3664
	C	1.198645	0.425898	0.811311	1070.7662	1079.4439	1097.8862	1163.0014
	H	2.149182	0.624093	0.331355	1181.6611	1196.9668	1215.1200	1250.6707
	N	-1.158547	0.263453	0.692619	1285.4732	1310.5021	1331.4120	1371.4208
	N	2.521712	-0.408278	4.871454	1382.4799	1401.6476	1411.9603	1418.8957
	H	0.964303	-0.493963	4.359674	1455.4753	1486.9949	1490.4305	1497.5114
	C	2.729185	1.022329	5.122286	1501.9891	1506.6329	1512.2970	1529.3708
	H	2.409439	1.537487	4.215972	1533.9611	1604.4212	1688.2217	1771.5025
	H	2.046402	1.329098	5.915728	2996.9714	3024.1704	3059.8530	3062.7845
	C	2.955155	-1.317420	5.935527	3069.1099	3092.4207	3104.1781	3132.1058
	H	2.754232	-2.330865	5.587968	3134.6564	3136.4240	3142.3747	3188.6139
	H	4.033216	-1.247558	6.115821	3227.4099	3250.1625	3501.0771	
	C	2.198856	-1.063202	7.228204				
	H	2.431911	-1.836627	7.958100				
	H	2.465662	-0.102306	7.667893				
	H	1.123651	-1.069868	7.047281				
	C	4.156849	1.415080	5.476626				
	H	4.241997	2.498398	5.553455				
	H	4.468172	0.989867	6.430931				
	H	4.854029	1.074393	4.709477				

BTS _{DEA}	C	-0.017666	0.046598	0.007821	-347.8615	32.5160	39.7285	59.9915
	C	0.032275	-0.218987	2.737750	89.6800	100.8042	165.7607	195.1441
	N	1.173447	0.099495	2.057276	207.0937	256.2590	286.7848	312.9392
	O	0.032800	-0.346118	3.982258	369.8046	438.9789	486.3142	515.1369
	H	-0.042592	0.150349	-1.066714	564.5739	578.7908	655.1342	658.3810
	H	2.187454	0.231746	3.055429	786.9913	790.3203	808.3234	846.7077
	C	-1.156793	-0.397898	1.927563	867.3186	877.9855	928.7289	960.3022
	H	-2.075139	-0.651734	2.445158	982.3514	1003.3777	1031.2728	1046.0337
	C	1.132543	0.226884	0.719402	1081.1168	1091.1259	1101.0415	1166.7738
	H	2.062248	0.480997	0.223266	1191.3778	1202.0576	1241.3729	1261.0316
	N	-1.178738	-0.272167	0.635558	1311.1901	1316.9464	1342.4238	1380.3005
	N	2.679740	0.193180	4.124174	1396.5007	1409.4046	1422.9129	1427.3106
	H	1.792722	0.244404	4.643754	1490.0237	1494.0044	1499.1007	1503.8947
	C	3.574323	1.324875	4.417622	1505.9830	1514.2543	1515.5328	1530.8952
	H	3.005539	2.228947	4.203481	1547.7927	1607.4942	1617.1266	1680.0834
	H	3.817466	1.334360	5.480584	1838.3899	3065.9076	3068.9614	3083.5930
	C	3.221472	-1.168973	4.304639	3092.2964	3118.4025	3125.2315	3142.4736
	H	2.394862	-1.836691	4.063016	3147.2059	3149.1968	3152.9109	3176.6104
	H	4.002982	-1.323984	3.561873	3181.1041	3227.8663	3331.8546	
	C	3.735360	-1.427803	5.708061				
	H	4.028571	-2.471251	5.807598				
	H	4.605358	-0.814236	5.942157				
	H	2.958596	-1.223889	6.445556				
	C	4.835207	1.280988	3.574667				
	H	5.407439	2.195322	3.717788				
	H	5.474172	0.442074	3.847871				
	H	4.588458	1.195604	2.515970				

2HPZ-DEA	C	0.019912	0.507657	0.103487	28.1851	33.0258	37.1936	81.9549
	C	0.071150	-0.138669	2.690921	90.6797	111.6055	142.9829	205.0832
	N	1.235687	0.103182	2.108533	217.8955	254.5177	294.9027	321.4751
	O	0.021360	-0.463956	3.972806	441.7954	444.1815	508.5145	519.2170
	H	0.009220	0.770350	-0.945206	564.0197	597.8557	650.6266	777.2098
	H	2.974394	-0.649820	3.995647	790.8309	806.7013	847.5050	875.0654
	C	-1.137224	-0.055305	1.965871	886.1044	897.0012	926.1428	963.7175
	H	-2.073920	-0.258685	2.469458	1004.2673	1027.7065	1040.9317	1066.7703
	C	1.198645	0.425898	0.811311	1088.8485	1103.4287	1122.5777	1167.2223
	H	2.149182	0.624093	0.331355	1182.6545	1196.4672	1216.3654	1234.1705
	N	-1.158547	0.263453	0.692619	1308.3472	1311.7973	1331.4716	1366.2988
	N	2.521712	-0.408278	4.871454	1382.6611	1400.9795	1413.4372	1418.7452
	H	0.964303	-0.493963	4.359674	1446.9296	1488.8330	1490.2046	1497.0608
	C	2.729185	1.022329	5.122286	1503.7220	1504.4165	1514.0250	1528.6505
	H	2.409439	1.537487	4.215972	1531.1488	1548.1757	1628.0911	1676.6331
	H	2.046402	1.329098	5.915728	2729.9154	3029.1785	3059.3026	3065.8578
	C	2.955155	-1.317420	5.935527	3077.4758	3098.1612	3109.0884	3132.5230
	H	2.754232	-2.330865	5.587968	3137.6013	3138.3801	3145.2199	3189.1704
	H	4.033216	-1.247558	6.115821	3200.4398	3218.1051	3523.1879	
	C	2.198856	-1.063202	7.228204				
	H	2.431911	-1.836627	7.958100				
	H	2.465662	-0.102306	7.667893				
	H	1.123651	-1.069868	7.047281				
	C	4.156849	1.415080	5.476626				
	H	4.241997	2.498398	5.553455				
	H	4.468172	0.989867	6.430931				
	H	4.854029	1.074393	4.709477				
2PZ-FA	C	0.010751	-0.000015	0.021643	47.7364	74.7385	109.0152	183.5075
	C	0.014992	-0.000004	1.375473	196.7152	223.4886	226.9235	421.8295
	C	2.401751	0.000006	1.404004	495.8710	547.1136	577.9414	637.4900
	N	1.196383	-0.000003	2.042265	726.0425	772.5648	843.8077	874.6548
	O	3.474158	0.000046	2.021523	964.1864	969.4200	1011.0045	1014.7812
	H	-0.910838	-0.000037	-0.538470	1047.9438	1076.6512	1121.5122	1185.6250
	H	-0.880414	-0.000021	1.978298	1251.5523	1295.1644	1314.2390	1377.6361
	H	1.231516	-0.000012	3.074214	1424.3166	1452.7333	1489.9201	1524.9537
	C	2.718137	-0.000087	5.256101	1599.5816	1685.4703	1725.4168	1790.1632
	H	2.894497	-0.000125	6.336906	2839.0307	3094.4958	3187.3550	3197.8612
	O	1.593522	-0.000105	4.796003	3236.0706	3253.2031		
	O	3.826908	-0.000031	4.577950				
	H	3.658782	0.000002	3.576955				
	C	2.298768	0.000061	-0.044417				
	H	3.229447	0.000047	-0.599124				
	N	1.177108	0.000020	-0.686551				

BTS _{FA}	C	0.003431	-0.000205	0.004837	-689.5493	50.4014	91.9091	152.9822
	C	0.000907	0.000164	1.367844	217.0471	240.6949	333.4731	378.1405
	C	2.334749	0.000184	1.400566	435.7871	562.5145	588.7740	651.0242
	N	1.164356	0.000339	2.049601	752.6158	784.3974	803.2878	862.0365
	O	3.453249	0.000369	2.023483	898.8844	966.3419	996.8822	1059.5707
	H	-0.915976	-0.000352	-0.560500	1096.2626	1100.1074	1203.3803	1254.1230
	H	-0.901658	0.000316	1.961706	1271.7263	1294.7526	1321.9146	1385.4650
	H	1.163117	0.000564	3.214913	1408.0452	1435.2911	1498.2231	1532.5922
	C	2.305414	0.001769	5.066693	1590.9478	1609.7046	1671.9506	1718.8617
	H	2.363019	0.002272	6.162314	1778.8680	1820.0347	3066.8055	3206.2709
	O	1.158830	0.000814	4.558730	3228.1354	3244.7159		
	O	3.393691	0.002207	4.447454				
	H	3.390655	0.001167	3.140287				
	C	2.284147	-0.000225	-0.026850				
	H	3.221452	-0.000378	-0.568576				
	N	1.163705	-0.000410	-0.689080				
2HPZ-FA	C	0.006642	0.000027	0.019552	49.6310	67.8778	124.5761	173.0733
	C	0.010318	-0.000006	1.392758	214.1498	218.0085	232.8306	443.4915
	C	2.288122	-0.000035	1.414628	477.7515	560.7807	599.9634	655.7304
	N	1.153462	-0.000041	2.095109	732.6252	787.2446	866.5461	875.3359
	O	3.453044	-0.000019	2.034121	891.2369	967.5126	1002.9083	1040.6388
	H	-0.917044	0.000042	-0.540999	1056.7067	1104.8311	1119.9816	1186.6566
	H	-0.909301	-0.000015	1.963324	1236.8991	1298.6832	1304.8179	1373.1906
	H	1.045820	-0.000085	3.759652	1403.8386	1426.1338	1498.8327	1531.1668
	C	2.155371	-0.000491	5.307530	1553.8111	1625.8106	1685.6691	1786.8035
	H	2.122626	-0.000603	6.401483	2824.3274	3101.6037	3204.5215	3208.6902
	O	0.966123	-0.000286	4.772270	3228.5292	3268.5801		
	O	3.204163	-0.000342	4.698462				
	H	3.346852	0.000019	3.019038				
	C	2.275120	0.000000	0.002338				
	H	3.215386	0.000026	-0.533866				
	N	1.154413	0.000027	-0.675971				

2PZ-AA	C	0.013038	-0.000074	0.025992	39.6752	65.9705	81.6404	102.6890
	C	0.013983	-0.000092	1.380072	108.8338	160.3132	171.7802	196.2472
	C	2.400487	0.000068	1.415690	422.2253	455.8260	499.3546	547.8292
	N	1.192602	-0.000020	2.050438	577.9876	613.3949	632.4464	646.6056
	O	3.468901	0.000136	2.038166	772.8222	842.5422	873.9454	929.3523
	H	-0.906941	-0.000129	-0.536781	963.3422	971.4084	1010.7075	1017.9040
	H	-0.883550	-0.000161	1.979889	1036.3143	1045.2750	1076.0156	1079.6217
	H	1.228710	-0.000030	3.084687	1184.0030	1252.4549	1293.9356	1355.9800
	C	2.673626	-0.000027	5.298316	1376.0000	1405.9188	1457.8857	1471.6631
	O	1.565367	-0.000053	4.786861	1481.9056	1504.1316	1526.5227	1599.7578
	O	3.793417	0.000051	4.619019	1686.4179	1732.9473	1782.7244	2939.5996
	H	3.630197	0.000085	3.624155	3087.5076	3142.2682	3153.9588	3196.3050
	C	2.882331	-0.000028	6.783275	3200.6815	3236.7692	3253.8284	
	H	3.463614	-0.877345	7.062442				
	H	3.463279	0.877503	7.062475				
	H	1.925881	-0.000209	7.293597				
	N	1.181525	0.000012	-0.679137				
	C	2.301268	0.000077	-0.033609				
	H	3.233348	0.000158	-0.586068				
BTS-AA	C	0.006047	-0.010779	0.007495	-913.8051	30.0289	44.8233	70.6445
	C	0.002548	-0.014894	1.370759	123.2393	154.0674	215.7104	235.4226
	C	2.335272	0.009910	1.408471	349.6936	436.4433	480.7309	563.7336
	N	1.162955	-0.004397	2.056276	591.5032	618.4724	640.1211	712.7311
	O	3.448047	0.019974	2.036223	723.8481	784.8664	858.7628	899.7293
	H	-0.912670	-0.018930	-0.558964	964.2307	966.8833	994.4439	1023.7260
	H	-0.902679	-0.026373	1.960848	1054.9216	1078.0069	1095.7862	1197.4783
	H	1.168904	-0.008255	3.240936	1268.1972	1276.5450	1288.7603	1332.6472
	C	2.309781	-0.003191	5.086961	1373.4598	1386.8016	1437.0148	1468.8625
	O	1.167906	-0.013379	4.552822	1480.2024	1502.6601	1532.5567	1558.0214
	O	3.395112	0.003395	4.446765	1595.7265	1665.6866	1694.8787	1768.7119
	H	3.380566	0.012030	3.180943	1784.1834	3084.5733	3158.5017	3196.6513
	C	2.385040	0.033453	6.586952	3207.6204	3225.7552	3243.6536	
	H	3.316786	-0.405291	6.930019				
	H	2.361078	1.079094	6.896200				
	H	1.525739	-0.469797	7.019767				
	N	1.167346	0.003745	-0.685240				
	C	2.286104	0.013641	-0.020387				
	H	3.224267	0.025217	-0.560675				

2HPZ-AA	C	0.006642	0.000027	0.019552	49.6310	67.8778	124.5761	173.0733
	C	0.010318	-0.000006	1.392758	214.1498	218.0085	232.8306	443.4915
	C	2.288122	-0.000035	1.414628	477.7515	560.7807	599.9634	655.7304
	N	1.153462	-0.000041	2.095109	732.6252	787.2446	866.5461	875.3359
	O	3.453044	-0.000019	2.034121	891.2369	967.5126	1002.9083	1040.6388
	H	-0.917044	0.000042	-0.540999	1056.7067	1104.8311	1119.9816	1186.6566
	H	-0.909301	-0.000015	1.963324	1236.8991	1298.6832	1304.8179	1373.1906
	H	1.045820	-0.000085	3.759652	1403.8386	1426.1338	1498.8327	1531.1668
	C	2.155371	-0.000491	5.307530	1553.8111	1625.8106	1685.6691	1786.8035
	H	2.122626	-0.000603	6.401483	2824.3274	3101.6037	3204.5215	3208.6902
	O	0.966123	-0.000286	4.772270	3228.5292	3268.5801		
	O	3.204163	-0.000342	4.698462				
	H	3.346852	0.000019	3.019038				
	C	2.275120	0.000000	0.002338				
	H	3.215386	0.000026	-0.533866				
	N	1.154413	0.000027	-0.675971				
2PZ-MFA	N	-3.858502	0.058382	0.000022	35.5089	51.6986	92.7235	93.6445
	C	-3.438572	-1.239627	0.000007	102.4	118.1302	174.5342	197.7006
	C	-2.120156	-1.548019	-0.000013	312.3343	422.2837	483.7163	518.1015
	N	-1.199213	-0.551785	-0.000018	547.4335	579.0204	579.3775	638.3818
	C	-1.542611	0.767290	-0.000002	687.9739	771.8998	842.261	875.3481
	C	-2.974851	1.001819	0.000017	932.7585	964.6573	968.7641	1011.6025
	O	-0.694400	1.669905	-0.000007	1013.8772	1049.3104	1061.5079	1077.0506
	O	1.859568	1.438422	-0.000005	1171.2132	1184.0712	1252.0638	1277.6709
	C	2.273780	0.200747	-0.000022	1294.5514	1325.4326	1375.32	1425.0893
	C	3.784128	0.129934	0.000007	1456.8576	1486.0499	1519.4005	1523.7421
	F	4.211176	-1.165468	0.000033	1598.9276	1685.9329	1730.795	1812.2308
	O	1.568589	-0.786491	-0.000022	2784.1964	3083.8309	3131.723	3186.0635
	H	4.160958	0.640416	-0.887260	3199.9674	3237.8188	3254.9732	
	H	4.160929	0.640441	0.887271				
	H	-4.196197	-2.007123	0.000012				
	H	-1.739335	-2.558013	-0.000026				
	H	-0.187027	-0.755188	-0.000032				
	H	0.843625	1.499632	-0.000006				
	H	-3.299890	2.035311	0.000030				

BTS _{MFA}	C	-2.928491	0.922758	-0.000002	-532.324	43.5658	47.4976	96.168
	N	-3.733855	-0.100287	0.000007	117.8014	136.9159	171.6846	218.8542
	C	-3.200831	-1.342093	0.000012	287.6036	381.9738	436.3493	531.6657
	C	-1.850039	-1.526402	0.000006	562.3446	593.4401	593.5502	654.2422
	N	-1.020611	-0.463294	-0.000005	703.1277	785.3335	815.6887	864.7508
	C	-1.508671	0.781739	-0.000008	899.2788	957.0962	970.2731	999.9101
	O	-0.741347	1.809497	-0.000017	1050.6736	1079.2231	1099.4221	1159.4687
	O	1.657162	1.405305	0.000022	1207.4441	1227.9896	1273.2825	1277.9731
	C	2.122782	0.238255	0.000002	1298.0785	1315.8551	1375.3288	1389.2967
	O	1.460442	-0.822961	-0.000026	1481.6574	1498.437	1519.8169	1536.918
	C	3.635225	0.161311	0.000014	1586.5853	1627.0948	1687.0763	1752.8911
	F	4.085449	-1.129953	-0.000006	1779.8447	1847.4552	3085.7447	3134.4135
	H	4.007440	0.674738	0.887119	3207.832	3227.9916	3244.4013	
	H	4.007456	0.674771	-0.887065				
	H	-3.883493	-2.178096	0.000020				
	H	-1.380309	-2.499331	0.000008				
	H	0.131398	-0.624620	-0.000015				
	H	0.340748	1.595375	-0.000002				
	H	-3.340926	1.923677	-0.000006				
2HPZ-MFA	C	3.429471	-1.119507	0.000071	31.0456	47.3134	87.2285	104.7432
	C	2.091139	-1.426248	-0.000064	107.2044	120.7475	159.5427	218.952
	C	1.554642	0.788334	-0.000009	312.3986	442.5721	468.9421	511.5207
	N	1.148545	-0.471167	-0.000100	560.3695	576.3046	600.0537	656.7091
	O	0.689254	1.783465	-0.000060	692.7951	787.3	860.8799	873.68
	H	4.184072	-1.892793	0.000104	891.2293	933.8038	968.3521	1002.9955
	H	1.742963	-2.450943	-0.000143	1041.0141	1048.9093	1066.7643	1104.7545
	H	-0.431463	-0.949746	-0.000217	1175.3398	1186.9909	1237.0805	1279.5002
	C	-2.200994	-0.224871	-0.000249	1297.4047	1321.6825	1372.6709	1406.6352
	O	-1.400536	-1.262017	-0.000085	1443.4733	1485.442	1505.8162	1534.89
	O	-1.845684	0.932943	-0.000275	1563.4014	1627.5135	1685.788	1818.9922
	H	-0.246735	1.459790	-0.000321	2776.7291	3084.8591	3132.6975	3204.532
	C	-3.652098	-0.645487	0.000160	3209.276	3228.6493	3268.673	
	F	-4.473069	0.441867	0.000270				
	H	-3.843270	-1.250618	-0.887225				
	H	-3.842871	-1.250494	0.887724				
	C	2.933706	1.094268	0.000137				
	H	3.243489	2.131371	0.000203				
	N	3.847449	0.155820	0.000177				

2PZ-TFA	C	4.176915	1.106335	0.000016	19.7952	34.2568	61.1133	87.1161
	C	2.884910	1.509888	-0.00001	87.6618	106.6498	164.3045	199.3704
	C	2.142915	-0.758298	-0.000012	265.9393	290.0267	417.2585	421.2493
	N	1.894828	0.580438	-0.000027	443.2604	508.4623	528.5850	546.2778
	O	1.232856	-1.601596	-0.000027	577.9948	611.7900	640.5140	730.3735
	H	4.988286	1.816773	0.000030	770.8431	811.5303	843.4797	853.0887
	H	2.577204	2.544287	-0.000025	876.8948	961.1684	964.9399	1002.4952
	H	0.905066	0.858825	-0.000047	1012.3506	1077.0964	1108.5945	1184.3981
	C	-1.608784	-0.003406	0.000006	1240.8350	1241.1415	1250.5546	1288.2635
	O	-0.892642	0.972197	-0.000011	1296.6046	1377.6632	1423.7496	1454.4353
	O	-1.262429	-1.245290	0.000001	1517.6151	1548.6498	1598.7778	1683.8370
	H	-0.235046	-1.361625	-0.000013	1722.3877	1829.5271	2543.0211	3200.9305
	C	-3.145958	0.155185	0.000007	3240.4494	3257.0583	3270.3335	
	F	-3.669036	-0.423451	-1.079442				
	F	-3.669032	-0.423431	1.079468				
	F	-3.489812	1.432983	-0.000004				
	C	3.552791	-1.096341	0.000015				
	H	3.802098	-2.150559	0.000027				
	N	4.501499	-0.218334	0.000030				
BTs _{TFA}	C	3.868956	-1.269193	0.000056	-197.8311	18.8696	32.5544	61.8228
	C	2.523885	-1.495065	0.000049	107.2540	123.8123	210.6484	221.0657
	C	2.117904	0.799076	-0.000036	232.1396	271.8885	345.0901	436.9124
	N	1.664423	-0.455545	-0.000002	448.9039	490.7953	529.0749	561.2727
	O	1.321963	1.814641	-0.000072	576.7520	609.0949	647.4618	746.6851
	H	4.576264	-2.084501	0.000097	784.1146	822.9944	856.3555	866.5892
	H	2.081334	-2.480465	0.000079	889.9046	903.3413	970.3803	1003.3115
	H	0.527107	-0.665591	-0.000057	1097.0935	1132.3413	1137.8871	1217.6376
	C	-1.493060	0.107608	0.000004	1228.8962	1247.6702	1280.9908	1286.5636
	O	-0.800992	-0.936191	-0.000138	1304.3370	1313.6232	1387.8989	1494.3134
	O	-1.106546	1.283505	0.000167	1513.2036	1543.1150	1575.2210	1625.5442
	H	0.296857	1.573564	0.000024	1698.2000	1777.1645	1827.2211	2286.3176
	C	-3.020497	-0.141056	-0.000006	3212.0465	3230.1954	3246.2698	
	F	-3.711265	0.989255	-0.000137				
	F	-3.369795	-0.843763	-1.079152				
	F	-3.369815	-0.843524	1.079296				
	C	3.528293	0.986490	-0.000037				
	H	3.910318	1.999209	-0.000074				
	N	4.363819	-0.013416	0.000007				

2HPZ-TFA	C	-3.876633	-1.323799	-0.000023	25.4288	34.3042	56.0118	93.6350
	C	-2.512250	-1.472507	0.000095	95.6865	122.8950	136.6014	221.0159
	C	-2.240425	0.792585	0.000001	266.0529	287.5286	416.3570	439.8468
	N	-1.690431	-0.410369	0.000104	443.3075	481.1866	528.2739	560.2755
	O	-1.497366	1.884067	0.000038	598.9889	611.8447	658.5341	734.0690
	H	-4.535819	-2.179728	-0.000028	786.9125	801.8405	818.7532	856.0663
	H	-2.043419	-2.447669	0.000182	877.5140	890.0331	972.1666	1007.8513
	H	-0.131753	-0.715128	0.000243	1044.1151	1105.7788	1122.4805	1187.4007
	C	1.571645	0.152908	-0.000007	1235.8493	1237.3256	1240.5680	1292.4651
	O	0.878166	-0.939811	0.000084	1294.2978	1372.1206	1397.4403	1446.6381
	O	1.155361	1.286932	0.000195	1508.9915	1533.4402	1592.9117	1628.9202
	H	-0.534983	1.674989	0.000195	1688.1245	1831.7495	2515.6518	3207.1736
	C	3.089055	-0.133662	-0.000076	3207.8985	3229.1672	3388.2117	
	F	3.421406	-0.839718	-1.079396				
	F	3.782973	0.990894	-0.000260				
	F	3.421465	-0.839403	1.079460				
	C	-3.645178	0.934244	-0.000134				
	H	-4.075045	1.927580	-0.000223				
	N	-4.440734	-0.105934	-0.000144				
3PZ	C	-1.12658	1.15748	0.00005	174.38	376.55	459.49	527.3
	C	-1.73501	-0.13716	0.00002	568.06	615.37	748.1	765.84
	C	1.03776	0.06679	-0.00027	838.83	856.56	938.04	1016.49
	N	0.28145	-1.09947	-0.00004	1035.24	1037.06	1142.64	1205.25
	O	2.25132	0.01942	0.00011	1274.11	1401.53	1434.35	1464.09
	H	-1.75757	2.03619	0.00011	1617.64	1691.93	1802.82	3207.73
	H	-2.80806	-0.25922	0.00006	3231.76	3241.3	3607.98	
	H	0.79914	-1.96697	0.00008				
	N	-1.04239	-1.22817	0.00005				
	C	0.21545	1.26534	0.00000				
	H	0.73280	2.21342	0.00009				
cTS	C	1.26011	1.03267	0.00000	-1849.79	203.2	409.35	510.69
	C	1.69802	-0.30743	0.00000	514.73	613.04	696.47	763.18
	C	-0.93258	0.22204	0.00000	833.93	892.25	931.05	1022.86
	N	-0.39937	-1.01798	0.00000	1054.29	1060.39	1142.98	1149.8
	O	-2.19675	0.04097	0.00000	1236.94	1295.42	1405.23	1442.42
	H	2.00010	1.82129	0.00000	1548.09	1619.72	1690.17	2145.99
	H	2.74819	-0.55700	0.00000	3214.8	3239.33	3249.35	
	H	-1.68032	-1.21486	0.00000				
	N	0.86432	-1.32987	0.00000				
	C	-0.07445	1.33781	0.00000				
	H	-0.45523	2.34721	0.00000				

3HPZ	C	-1.21243	1.10529	-0.00000	220.63	397.84	420.53	498.52
	C	-1.74305	-0.18850	-0.00000	580.64	583.63	645.52	775.69
	C	0.87623	0.04425	0.00001	846.58	869.34	956.52	1025.06
	N	0.32499	-1.15260	0.00000	1041.39	1074.85	1127.73	1182.65
	O	2.21745	0.10058	-0.00000	1210.9	1286.25	1358.53	1474.21
	H	-1.86439	1.96714	-0.00000	1509.87	1650.47	1671.42	3212.17
	H	-2.80991	-0.36229	-0.00000	3225.9	3241.83	3807.21	
	H	2.53991	-0.81058	-0.00000				
	N	-0.99276	-1.27286	-0.00000				
	C	0.14780	1.23735	0.00000				
	H	0.65788	2.18898	-0.00000				
3PZ-AM	C	0.017626	-0.000349	-0.006457	58.9451	114.2419	136.2343	172.8577
	C	-0.004767	0.000012	1.420135	177.1282	273.4510	383.6033	434.3335
	C	2.434546	0.000024	0.110449	473.0810	553.8943	572.1679	619.3417
	N	2.235160	0.000359	1.479116	756.6526	847.7754	855.2546	933.7431
	O	3.563934	0.000109	-0.361292	983.4155	1024.2149	1033.2300	1040.0392
	H	-0.917203	-0.000631	-0.550898	1099.3200	1143.0562	1208.7337	1276.9101
	H	-0.932676	0.000018	1.973013	1409.3547	1436.2332	1507.1382	1620.5285
	H	3.083090	0.000604	2.058685	1649.5738	1672.2237	1688.4302	1777.4207
	N	1.077484	0.000357	2.130615	3208.1134	3229.3656	3238.1988	3286.0426
	C	1.201074	-0.000342	-0.651355	3469.0074	3594.5257	3632.0496	
	H	1.289144	-0.000606	-1.727907				
	N	5.038640	0.001250	2.299891				
	H	5.541207	0.817774	2.623800				
	H	5.063314	0.000032	1.282409				
	H	5.543392	-0.813050	2.625974				
cTS _{AM}	C	0.019182	0.000265	0.006646	-561.1706	77.4475	195.4770	344.4473
	C	0.023047	-0.000252	1.417495	385.8612	387.1640	419.5505	429.3626
	C	2.411566	-0.000300	0.127618	572.3863	590.7800	595.6640	662.2788
	N	2.295487	-0.000770	1.484787	772.7545	854.9834	865.1800	904.2515
	O	3.565163	-0.000367	-0.404465	928.2159	1023.6500	1038.0953	1059.7728
	H	-0.919683	0.000666	-0.531389	1142.9155	1220.1463	1252.0024	1397.4904
	H	-0.894747	-0.000262	1.988725	1405.9290	1436.7558	1540.6584	1548.3209
	H	3.705621	-0.001354	2.037951	1594.7551	1615.7602	1660.8746	1678.4234
	N	1.130085	-0.000747	2.114567	1968.0411	2453.1445	3181.5649	3196.0048
	C	1.208294	0.000244	-0.645890	3216.3693	3551.7700	3643.3448	
	H	1.293600	0.000621	-1.723085				
	N	4.819833	-0.001625	1.802059				
	H	5.307766	0.830152	2.109280				
	H	4.599529	-0.000726	0.730060				
	H	5.306864	-0.834470	2.107828				

3HPZ-AM	C	0.012443	0.000196	0.003068	59.5882	120.0618	122.0440	211.8931
	C	0.014646	0.000362	1.403649	215.2297	290.9346	398.8672	407.3896
	C	2.364305	-0.000266	0.180202	513.4031	564.6751	589.3697	646.4105
	N	2.299364	-0.000065	1.504669	775.4113	852.4915	872.1475	954.2970
	O	3.557070	-0.000510	-0.401646	1012.6990	1024.8812	1039.1743	1072.3203
	H	-0.919120	0.000313	-0.545569	1106.6027	1131.1730	1206.7099	1227.0811
	H	-0.905236	0.000608	1.971923	1362.3845	1403.2054	1496.5750	1525.0753
	H	4.532009	-0.001529	2.302041	1635.4004	1656.1367	1668.5503	1675.8187
	N	1.121933	0.000249	2.114848	3058.6364	3206.7196	3220.6040	3237.0069
	C	1.218610	-0.000116	-0.633790	3477.8964	3601.4041	3635.4093	
	H	1.327497	-0.000254	-1.708412				
	N	5.330395	-0.001010	1.672278				
	H	5.892968	0.816754	1.869580				
	H	4.279975	-0.000561	0.291034				
	H	5.892901	-0.819120	1.868339				
3PZ-MA	C	-0.003525	0.015478	0.002257	45.0640	77.7941	90.4744	111.7458
	C	-0.002904	0.010423	1.350225	172.9640	184.8293	195.3945	385.3908
	C	1.238953	-0.006386	2.052338	438.1675	474.2446	555.5383	572.2110
	N	2.380890	-0.016840	1.441668	619.3417	759.1892	848.4778	855.9188
	N	2.362427	-0.012644	0.113720	899.5976	935.8555	987.4000	1025.9395
	C	1.255954	0.004143	-0.715530	1030.6747	1038.3491	1040.5649	1079.0334
	O	1.386631	0.006010	-1.932597	1142.9744	1190.9366	1208.7694	1277.8413
	N	4.396027	-0.194506	-1.890928	1350.2357	1409.1969	1436.3889	1456.2686
	C	4.294448	-1.625346	-2.186612	1506.1318	1511.6235	1530.5677	1622.3714
	H	-0.928102	0.019095	1.910891	1631.8236	1685.7415	1777.6326	3045.1907
	H	1.280142	-0.010287	3.131707	3111.7816	3143.2719	3177.9433	3206.6352
	H	3.278654	-0.014576	-0.362156	3228.9888	3238.4533	3515.1815	3608.3974
	H	-0.907133	0.028566	-0.589459				
	H	5.320584	0.157358	-2.100408				
	H	3.725482	0.311892	-2.459707				
	H	4.956082	-2.181585	-1.524442				
	H	3.270202	-1.942640	-1.994939				
	H	4.539308	-1.884182	-3.219461				

CTS _{MA}	C	0.061210	-0.068955	0.028950	-296.8091	51.0587	103.7396	116.2725
	C	0.064837	-0.011037	1.438724	182.6144	210.8450	345.8761	401.3730
	C	2.456540	-0.003132	0.146401	447.4690	552.6901	570.6560	590.1747
	N	2.338419	0.047767	1.505436	657.5349	772.8523	856.8768	863.3215
	O	3.605991	0.005027	-0.384372	908.4930	928.3397	976.1012	1025.9751
	H	-0.877736	-0.115355	-0.507404	1036.2243	1058.9686	1070.0073	1128.2737
	H	-0.852835	-0.011542	2.010304	1149.5181	1215.0178	1247.2815	1320.5715
	H	3.769517	0.143336	2.064657	1399.7363	1410.1150	1432.1599	1491.2803
	N	1.171844	0.044211	2.133915	1510.7513	1519.8790	1541.7884	1587.5968
	C	1.249950	-0.065979	-0.623725	1611.9244	1641.2221	1686.6572	2104.7884
	H	1.334933	-0.108386	-1.700286	2784.3552	3083.6861	3164.7322	3170.7737
	N	4.873624	0.082304	1.861804	3184.8902	3198.0041	3213.9956	3565.2309
	H	5.413493	0.849139	2.243356				
	H	4.720787	0.158908	0.810351				
	C	5.395906	-1.245332	2.217817				
	H	5.387030	-1.376234	3.296541				
	H	4.741681	-1.984397	1.761028				
	H	6.405914	-1.378442	1.839047				
3HPZ-MA	C	0.161625	-0.173136	0.068910	47.0952	64.3259	97.3391	112.6686
	C	0.210377	-0.244854	1.466725	183.7111	222.3051	237.4974	399.6235
	C	2.505984	0.068602	0.179807	425.1505	517.4325	564.5882	590.3286
	N	2.485105	-0.006589	1.504976	645.9532	776.1107	850.9124	872.7695
	O	3.672858	0.223384	-0.428635	899.1628	950.9943	987.8920	1024.3839
	H	-0.782619	-0.244112	-0.452858	1038.0003	1071.6371	1073.6675	1102.4682
	H	-0.684932	-0.372207	2.059485	1131.0414	1196.8712	1205.5474	1227.3544
	H	4.835129	0.616572	2.236324	1344.6667	1365.9270	1412.7893	1455.6016
	N	1.334847	-0.163395	2.145940	1501.9324	1508.9794	1525.1347	1536.1912
	C	1.339176	-0.011670	-0.600296	1627.8023	1649.6319	1675.5978	2865.2588
	H	1.410815	0.055610	-1.675962	3057.2764	3123.7026	3151.3939	3207.2923
	N	5.472295	0.219882	1.553938	3221.0143	3235.8716	3515.5275	3607.1927
	H	6.347267	0.725540	1.597675				
	H	4.415065	0.281498	0.257550				
	C	5.663204	-1.207374	1.829946				
	H	6.115326	-1.408162	2.802837				
	H	4.688894	-1.691686	1.795430				
	H	6.291224	-1.643383	1.055459				

3PZ-DMA	C	0.038074	-0.161151	0.027280	36.9764	42.9166	69.8401	105.0963
	C	0.021736	0.064961	1.435789	119.7038	178.4354	191.7159	224.1311
	C	2.453925	-0.092952	0.124690	294.1052	385.3403	404.5558	471.8316
	N	2.261317	0.119027	1.477219	555.6083	572.0095	619.0173	759.2558
	O	3.583559	-0.144781	-0.344549	848.2560	855.7189	885.3486	935.8146
	H	-0.899028	-0.266309	-0.502981	963.3313	1025.1186	1027.2321	1036.2267
	H	-0.903808	0.134366	1.988350	1039.9385	1045.3146	1106.1537	1142.6682
	H	3.122459	0.232800	2.038723	1192.6561	1208.5334	1210.2309	1270.3806
	N	1.107228	0.199894	2.129260	1276.8332	1409.1374	1435.8741	1438.5876
	C	1.218442	-0.239628	-0.619163	1466.3166	1474.6464	1492.5359	1505.9228
	H	1.300949	-0.408358	-1.682898	1513.9030	1518.6962	1524.6928	1622.9251
	N	4.994843	0.163012	2.323551	1685.3910	1776.2897	3007.3280	3010.5155
	H	5.139987	0.488920	1.373412	3091.0201	3095.3520	3134.2128	3140.4682
	C	5.229986	-1.274881	2.352939	3140.7121	3207.6798	3229.4303	3239.2622
	H	4.929435	-1.670100	3.324251	3525.2697			
	H	4.631333	-1.750386	1.577285				
	H	6.282305	-1.536673	2.189997				
	C	5.845635	0.885553	3.255853				
	H	5.673841	1.956247	3.162417				
	H	5.593896	0.589620	4.274758				
	H	6.913136	0.685626	3.101254				
c ^{TS} _{DMA}	C	1.238910	0.016563	-0.649697	-167.2123	20.3631	54.7449	90.1220
	C	0.057910	0.037393	0.015450	197.8975	204.8691	208.1762	222.1867
	C	0.076422	0.037922	1.427346	328.1345	399.9970	411.0698	496.9242
	N	1.191123	0.019043	2.111536	569.7226	587.0032	650.7841	708.8289
	N	2.350589	-0.001410	1.470414	773.4932	858.5303	865.0214	931.1477
	C	2.457043	-0.004061	0.107809	946.5458	1024.8834	1037.9247	1056.3339
	O	3.598811	-0.024117	-0.430251	1062.6849	1077.6849	1134.1484	1151.7663
	N	4.890118	-0.044846	1.858792	1174.8632	1216.5980	1243.6259	1254.2213
	C	5.490859	-1.291270	2.338452	1403.8118	1407.3942	1438.3887	1442.9568
	H	-0.886927	0.053427	-0.512122	1485.4407	1500.3932	1500.5891	1515.3089
	H	-0.835139	0.054047	2.008226	1529.6975	1540.7392	1556.1474	1596.0134
	H	3.771955	-0.025488	2.015038	1630.8169	1681.7707	2039.6594	2946.3250
	H	1.310867	0.014680	-1.728000	3074.5329	3078.3324	3150.0537	3151.2694
	C	5.533891	1.180003	2.338160	3166.9196	3167.0380	3196.1785	3214.7895
	H	4.780443	-0.043256	0.812435	3230.1587			
	H	5.443562	-1.324317	3.425234				
	H	4.929239	-2.126565	1.926976				
	H	6.530105	-1.359592	2.020265				
	H	6.574927	1.211984	2.020089				
	H	5.001795	2.034282	1.926427				
	H	5.487662	1.214969	3.424925				

3HPZ-DMA	C	0.061055	-0.021082	-0.027027	40.8026	43.6833	75.8055	103.9057
	C	0.061705	0.238713	1.311974	134.8147	210.1590	222.5690	225.3695
	C	1.301150	0.387181	1.947037	306.2877	400.1054	408.2676	497.0811
	N	2.446701	0.286515	1.306745	565.3214	588.7107	645.4843	777.2959
	N	2.457203	0.034174	0.004949	852.3878	870.8839	893.4195	953.6627
	C	1.315122	-0.117280	-0.655633	958.6447	1025.9840	1037.7049	1039.6103
	O	1.363598	-0.366694	-1.955302	1072.3739	1087.2143	1123.8460	1131.8034
	N	3.956952	-0.353584	-2.568919	1198.3564	1205.6196	1219.2644	1228.8403
	C	4.595866	-1.171888	-3.590548	1269.6535	1367.3284	1417.3289	1439.7068
	H	-0.858058	0.328821	1.873098	1466.9672	1471.7911	1494.7402	1506.2151
	H	1.374682	0.593995	3.005818	1509.7065	1518.8293	1522.1871	1544.4984
	H	4.236760	-0.646440	-1.638417	1650.3339	1675.5614	2759.4646	3024.2409
	H	-0.838984	-0.152646	-0.609563	3029.1554	3102.5410	3105.1210	3146.6194
	C	4.251468	1.068281	-2.715944	3147.6301	3206.5318	3220.5658	3237.0298
	H	2.333753	-0.415154	-2.261303	3528.5276			
	H	5.682111	-1.033282	-3.620853				
	H	4.379676	-2.223016	-3.410700				
	H	4.192988	-0.902495	-4.566799				
	H	5.326752	1.274843	-2.728234				
	H	3.822147	1.426993	-3.651629				
	H	3.795672	1.609781	-1.888966				

3PZ-DEA	C	-3.76796	0.09847	0.19869	28.72	35.39	43.72	86.68
	C	-3.10626	1.32689	0.49541	99.47	112.19	123.58	176.4
	C	-1.61140	-0.83104	-0.38077	191.97	250.87	296.07	321.82
	N	-1.13033	0.42235	-0.05118	386.49	469.63	472.95	508.72
	O	-0.84979	-1.71264	-0.75771	556.58	572.33	619.19	760.29
	H	-4.84088	0.03219	0.32071	779.12	809.06	844.82	849.91
	H	-3.64941	2.19487	0.83952	856.14	904.2	924.61	936.3
	H	-0.10688	0.55057	-0.15446	1025.21	1031.53	1037.75	1039.95
	N	-1.82531	1.47247	0.36976	1050.98	1074.78	1095.87	1142.19
	C	-3.04739	-0.95786	-0.22858	1160.54	1197.27	1208.82	1217.05
	H	-3.48615	-1.91483	-0.47053	1277.28	1310.21	1331.76	1381.97
	N	1.66221	-0.01265	-0.41854	1400.74	1409.17	1411.9	1418.9
	H	1.33695	-0.70786	-1.08418	1435.76	1486.64	1490.46	1498.09
	C	1.91974	-0.69585	0.85157	1502.34	1506.11	1512.2	1516.98
	H	2.02723	0.05856	1.63312	1530.69	1623.34	1684.64	1775.71
	H	1.01814	-1.26644	1.07893	3015.07	3058.19	3063.18	3068.99
	C	2.78534	0.73856	-0.97618	3090.59	3094.74	3103.89	3131.38
	H	2.44999	1.15893	-1.92468	3134.62	3135.15	3141.62	3207.1
	H	3.64309	0.09331	-1.20058	3228.84	3238.9	3510.4	
	C	3.22584	1.86129	-0.05194				
	H	3.67270	1.47449	0.86402				
	H	3.96983	2.48625	-0.54372				
	H	2.37410	2.48465	0.22148				
	C	3.12688	-1.62633	0.85760				
	H	4.06065	-1.07926	0.72461				
	H	3.18812	-2.16095	1.80512				
	H	3.04610	-2.36335	0.05726				

C _{TS} _{DEA}	C	-0.014308	0.160583	0.021705	-85.8706	20.4020	42.9905	76.0611
	C	-0.014913	0.104604	1.432179	82.0478	108.8777	198.0914	201.2940
	C	2.379884	0.003020	0.140654	204.7553	258.1259	290.0205	321.8036
	N	2.255812	-0.045266	1.501542	401.1926	487.1919	502.9001	520.7785
	O	3.525944	-0.045835	-0.385166	570.3373	587.5578	648.6053	735.9022
	H	-0.950043	0.241711	-0.516168	773.9732	804.7623	812.2835	857.9453
	H	-0.932346	0.141425	2.002877	860.2964	871.6488	927.9695	929.2365
	H	3.699689	-0.180850	2.062601	1026.1373	1033.8016	1045.8368	1056.6800
	N	1.089164	0.005062	2.127730	1083.2923	1095.9733	1135.8446	1148.5938
	C	1.173801	0.110438	-0.629447	1180.7792	1195.1210	1212.6696	1244.0826
	H	1.260009	0.147880	-1.706143	1302.4202	1317.2292	1379.4951	1402.4246
	N	4.805409	-0.170634	1.922314	1406.7690	1416.1395	1424.9085	1425.8617
	H	4.730619	-0.202710	0.877517	1492.8428	1495.7539	1501.3236	1505.1820
	C	5.467362	-1.363890	2.476440	1512.2166	1517.6420	1518.8563	1550.9652
	H	5.278737	-1.393174	3.548692	1557.6478	1596.3919	1636.2713	1681.5686
	H	4.962684	-2.221144	2.032941	2129.2917	3019.9699	3067.0675	3068.5323
	C	5.308746	1.152458	2.339521	3090.1840	3096.0610	3121.6610	3127.4901
	H	4.678217	1.875859	1.822906	3143.3726	3148.8603	3150.1292	3151.3237
	H	6.327729	1.281812	1.976341	3196.4411	3214.4791	3227.3533	
	C	5.224721	1.341597	3.841772				
	H	5.913929	0.685118	4.372578				
	H	5.479510	2.367731	4.099174				
	H	4.212352	1.142693	4.194771				
	C	6.955421	-1.402258	2.182097				
	H	7.487977	-0.603479	2.697517				
	H	7.374156	-2.349919	2.515523				
	H	7.140603	-1.306242	1.112082				

3HPZ-DEA	C	0.072423	0.284401	0.003862	26.3969	34.7603	39.3024	82.8783
	C	0.087587	0.540246	1.380690	92.7103	113.3242	142.5486	205.0105
	C	2.383887	-0.133849	0.238200	223.1708	252.7125	295.8160	322.0516
	N	2.331042	0.121381	1.541007	399.9834	447.5871	512.1571	525.6946
	O	3.549015	-0.465339	-0.295127	565.0237	588.9247	645.0406	776.9358
	H	-0.846890	0.362238	-0.559888	780.9604	807.5053	850.1245	851.9778
	H	-0.809611	0.820256	1.915346	872.3713	901.5632	927.3985	952.2482
	H	4.617266	-0.600440	2.410077	1024.7368	1037.1703	1041.5863	1068.3449
	N	1.181136	0.458186	2.108764	1071.2571	1091.6641	1129.4475	1132.0871
	C	1.249854	-0.063089	-0.590560	1169.4444	1197.3370	1204.4714	1217.7573
	H	1.345419	-0.280647	-1.644276	1227.8580	1309.9107	1331.7124	1366.1907
	N	5.305339	-0.392552	1.692341	1383.1777	1400.7720	1414.2536	1418.7537
	H	4.269415	-0.487068	0.430872	1419.5141	1488.6120	1489.6898	1494.7022
	C	6.432711	-1.323218	1.777098	1502.1127	1504.4444	1509.3432	1515.4443
	H	6.952451	-1.245184	2.738032	1529.6691	1546.3719	1648.5604	1673.6016
	H	6.018519	-2.329956	1.719492	2676.6384	3029.9671	3059.8310	3064.7812
	C	5.638979	1.033587	1.779870	3075.8118	3096.7957	3108.8413	3132.9473
	H	4.687555	1.566046	1.765214	3136.8503	3137.4772	3143.5909	3206.6658
	H	6.174542	1.313991	0.871746	3220.7117	3236.7118	3514.7878	
	C	6.443641	1.432173	3.009434				
	H	7.439229	0.987788	3.003711				
	H	6.564107	2.514253	3.046497				
	H	5.934775	1.117221	3.921628				
	C	7.418566	-1.112188	0.640647				
	H	7.939617	-0.159325	0.732648				
	H	8.169117	-1.900919	0.641885				
	H	6.901278	-1.127388	-0.319116				
3PZ-FA	C	0.022656	-0.001087	0.001489	44.0474	67.9494	105.6916	176.8902
	C	0.021363	-0.000397	1.425895	198.8804	213.9797	220.2169	383.5228
	C	2.429269	0.001258	0.094616	499.1366	557.9854	582.8622	626.2919
	N	2.261737	0.001821	1.452758	718.8279	757.6086	856.4794	862.9885
	O	3.558139	0.002264	-0.410225	943.4176	972.5599	1029.2593	1033.4520
	H	-0.918606	-0.002305	-0.531027	1033.8828	1043.7942	1110.8664	1143.8221
	H	-0.898024	-0.001073	1.992703	1211.2089	1299.3066	1301.2921	1415.3786
	H	3.115000	0.003427	2.025369	1421.3508	1435.5141	1476.4353	1500.8705
	N	1.113499	0.001093	2.121927	1620.5093	1681.7048	1736.4297	1801.2555
	C	1.199682	-0.000217	-0.658019	2947.3104	3091.9811	3214.0953	3232.3849
	H	1.279451	-0.000613	-1.734904	3243.5738	3301.5005		
	C	5.829931	0.016194	2.019958				
	H	6.822838	0.021750	2.482617				
	O	5.898703	0.014891	0.717603				
	H	4.977651	0.009915	0.306167				
	O	4.815036	0.012694	2.682018				

CTS _{FA}	C	0.012313	0.000086	0.001229	-802.8065	46.7233	89.5112	159.1055
	C	0.008754	0.000033	1.413466	223.2145	243.2947	336.7062	388.9212
	C	2.385213	-0.000156	0.143233	397.6081	568.1510	570.5576	621.5571
	N	2.267018	-0.000196	1.475381	716.2632	770.2401	790.6456	856.2792
	O	3.545462	-0.000250	-0.413611	882.0072	957.2312	1032.8939	1058.7922
	H	-0.922129	0.000199	-0.542266	1099.4845	1100.7199	1143.6366	1223.5053
	H	-0.911027	0.000105	1.980231	1225.5855	1300.6446	1349.4483	1405.5511
	H	3.249437	-0.000325	2.183972	1413.1748	1433.0055	1440.4198	1555.1315
	N	1.106223	-0.000104	2.117080	1575.5685	1620.4048	1697.7077	1709.2688
	C	1.205154	-0.000008	-0.644351	1773.3897	1914.6282	3065.3829	3217.9299
	H	1.305942	0.000022	-1.719251	3231.6948	3244.8065		
	C	5.372157	-0.000511	2.291442				
	H	6.292553	-0.000618	2.888643				
	O	5.498437	-0.000451	1.049621				
	H	4.396883	-0.000339	0.270297				
	O	4.290331	-0.000461	2.932999				
3HPZ-FA	C	0.017089	0.000302	0.006467	52.1052	69.4971	130.2000	178.6583
	C	0.020281	-0.000134	1.411102	220.8286	229.4747	238.2939	400.2723
	C	2.372723	-0.000346	0.169271	485.2892	565.7011	590.0255	654.6213
	N	2.297067	-0.000749	1.492466	733.4796	773.5513	852.1219	873.8378
	O	3.554166	-0.000429	-0.414486	916.8413	962.5502	1028.0709	1051.5869
	H	-0.916446	0.000713	-0.538346	1072.0170	1075.1984	1135.5334	1137.1788
	H	-0.898077	-0.000080	1.981094	1213.6310	1252.1176	1318.9901	1373.2385
	H	3.551158	-0.001380	2.547657	1397.3867	1424.6759	1485.4120	1518.5857
	N	1.125269	-0.000636	2.116557	1548.2430	1641.4247	1683.8543	1774.7529
	C	1.217402	0.000203	-0.635704	2716.6879	3095.1394	3163.7711	3213.0076
	H	1.323013	0.000528	-1.710340	3226.1656	3243.2108		
	C	5.459439	-0.002287	2.518092				
	H	6.342914	-0.002449	3.164549				
	O	5.561968	-0.001411	1.306234				
	H	4.295525	-0.000612	0.251153				
	O	4.347602	-0.002019	3.189258				

3PZ-AA	C	0.027561	-0.000547	0.002057	37.8730	60.6343	83.6000	100.5090
	C	0.023574	-0.000394	1.426425	105.0842	152.2981	167.6881	199.3029
	C	2.434621	0.000642	0.099466	383.8594	456.2579	499.5730	557.9315
	N	2.264004	0.000695	1.458056	581.9671	611.1270	625.3160	638.8882
	O	3.564540	0.001117	-0.400578	757.9558	856.1436	862.2954	924.9821
	H	-0.912855	-0.001056	-0.532078	942.5268	982.1684	1015.8534	1032.7518
	H	-0.896934	-0.000777	1.991453	1033.1491	1034.2734	1043.2877	1079.0412
	H	3.119670	0.001212	2.029773	1143.6027	1210.4586	1297.9691	1347.6767
	N	1.114705	0.000214	2.124483	1402.4623	1414.8990	1435.5200	1471.3294
	C	1.205698	-0.000042	-0.655414	1482.2455	1496.2395	1502.3415	1621.1721
	H	1.286980	-0.000112	-1.732209	1683.0479	1743.3315	1796.5710	3044.3041
	C	5.841033	0.004469	2.069904	3087.0027	3153.2847	3200.1626	3212.5007
	O	5.913672	0.004520	0.757680	3231.8789	3242.0966	3267.6804	
	H	4.998826	0.003152	0.347465				
	O	4.794291	0.002960	2.690747				
	C	7.186798	0.006431	2.732725				
	H	7.746072	-0.870505	2.410595				
	H	7.743726	0.884717	2.410220				
	H	7.068983	0.006487	3.810422				
CTS-AA	C	0.016179	0.001497	0.001174	-931.1253	28.8805	41.1523	68.3624
	C	0.011272	-0.014698	1.413671	121.6168	158.5546	223.7836	236.6097
	C	2.391116	0.007924	0.144266	355.7463	397.4992	487.7682	570.9103
	N	2.269543	-0.007763	1.477850	576.6498	616.3421	626.7171	706.3415
	O	3.551409	0.018339	-0.403372	719.7591	771.1669	857.2625	883.2505
	H	-0.918147	0.004557	-0.542696	958.0593	964.5748	1032.4832	1040.7490
	H	-0.909252	-0.024311	1.979230	1059.6437	1078.7209	1090.4347	1142.7760
	H	3.262673	-0.013376	2.183161	1224.0187	1257.8693	1287.7902	1347.6585
	N	1.108344	-0.019115	2.117968	1378.8323	1412.6998	1414.3306	1467.9891
	C	1.209202	0.012892	-0.643575	1477.7668	1498.5399	1536.8799	1565.5536
	H	1.309907	0.025465	-1.718455	1595.0828	1675.8072	1696.3890	1772.5708
	C	5.394438	-0.006519	2.290125	1791.3241	3085.0249	3157.2638	3195.8334
	O	5.495056	0.004179	1.037016	3214.8512	3228.8243	3246.0562	
	H	4.425201	0.011376	0.300506				
	O	4.299219	-0.019991	2.918953				
	C	6.657390	0.024754	3.103968				
	H	7.505162	-0.291900	2.505276				
	H	6.818895	1.051548	3.433509				
	H	6.544036	-0.595563	3.988793				

3HPZ-AA	C	0.027561	-0.000547	0.002057	40.2038	47.9334	58.0626	111.6875
	C	0.023574	-0.000394	1.426425	122.5765	165.7313	174.6794	225.7851
	C	2.434621	0.000642	0.099466	399.5966	453.0388	497.8746	565.9645
	N	2.264004	0.000695	1.458056	590.2228	613.1030	646.6014	655.7950
	O	3.564540	0.001117	-0.400578	773.5752	851.6509	875.1030	932.3670
	H	-0.912855	-0.001056	-0.532078	933.8527	960.5311	1027.7874	1034.6370
	H	-0.896934	-0.000777	1.991453	1052.0941	1074.4125	1075.4014	1084.2217
	H	3.119670	0.001212	2.029773	1134.7459	1214.6693	1249.4553	1364.3809
	N	1.114705	0.000214	2.124483	1374.5516	1400.1625	1423.4388	1469.6639
	C	1.205698	-0.000042	-0.655414	1481.0045	1485.4908	1527.8892	1548.3651
	H	1.286980	-0.000112	-1.732209	1642.4247	1682.5275	1772.0265	2812.1704
	C	5.841033	0.004469	2.069904	3088.7763	3095.1540	3155.5180	3201.9128
	O	5.913672	0.004520	0.757680	3213.8968	3227.1466	3243.0299	
	H	4.998826	0.003152	0.347465				
	O	4.794291	0.002960	2.690747				
	C	7.186798	0.006431	2.732725				
	H	7.746072	-0.870505	2.410595				
	H	7.743726	0.884717	2.410220				
	H	7.068983	0.006487	3.810422				
3PZ-MFA	C	-2.982464	1.041736	0.000221	32.9663	47.1512	88.3065	90.4378
	C	-3.847515	0.006046	0.000235	100.1864	116.1098	171.1081	201.9932
	C	-3.341470	-1.325027	0.000042	306.2019	383.6621	488.4778	514.1233
	N	-2.072831	-1.586108	-0.000149	557.9617	577.2388	585.5011	626.5901
	N	-1.238662	-0.551849	-0.000166	684.8447	758.5144	857.6633	864.1738
	C	-1.566239	0.775960	0.000000	929.1456	948.7064	973.6458	1032.3829
	O	-0.691109	1.651193	-0.000009	1033.5954	1033.9931	1044.5109	1049.2886
	O	1.881431	1.441507	-0.000070	1143.9362	1171.3897	1212.4995	1277.6177
	C	2.291755	0.197929	-0.000452	1301.3574	1315.2938	1416.3229	1421.1582
	C	3.802455	0.127271	0.000054	1436.1433	1486.0577	1497.9962	1512.1149
	F	4.230467	-1.167786	0.000562	1620.5831	1681.2972	1739.7242	1826.9508
	O	1.582223	-0.782119	-0.000411	2897.7003	3083.0787	3130.726	3212.5201
	H	4.179348	0.637874	0.887270	3230.9493	3245.3193	3298.7473	
	H	4.179830	0.637359	-0.887244				
	H	-4.916667	0.168651	0.000390				
	H	-3.998165	-2.182508	0.000043				
	H	-0.237350	-0.782519	-0.000312				
	H	-3.291758	2.076280	0.000363				
	H	0.871517	1.492504	-0.000030				

C _{TS-MFA}	C	2.817168	1.163549	0.000000	-694.1517	27.7862	60.4124	84.4648
	C	3.733709	0.163727	-0.000013	116.4077	135.8395	171.6156	225.7666
	C	3.275692	-1.172368	-0.000017	290.5408	378.9798	396.8818	548.508
	N	2.008852	-1.479095	-0.000008	570.3584	576.5465	592.0301	615.957
	N	1.121637	-0.492893	0.000006	723.0449	736.2738	770.6628	856.8966
	C	1.445172	0.804058	0.000009	881.4885	959.3997	960.9727	1033.7614
	O	0.530736	1.710886	0.000020	1050.1817	1058.712	1107.1873	1144.6217
	O	-1.263300	-1.217510	0.000027	1162.1422	1201.8418	1226.7863	1279.6178
	C	-2.082466	-0.254939	0.000010	1305.0084	1336.5056	1379.8902	1413.9666
	C	-3.536610	-0.677636	0.000012	1436.0364	1482.0924	1523.4008	1553.3466
	F	-4.384846	0.394280	-0.000040	1575.6388	1630.5526	1698.6478	1719.6477
	O	-1.796574	0.955356	-0.000005	1778.3333	1990.6097	3087.1929	3135.6921
	H	-3.720167	-1.284935	0.887032	3216.9941	3230.6989	3246.4435	
	H	-3.720151	-1.285009	-0.886961				
	H	4.794390	0.372142	-0.000021				
	H	3.959992	-2.008412	-0.000028				
	H	-0.031596	-0.843332	0.000017				
	H	3.072657	2.212488	0.000003				
	H	-0.487816	1.344253	0.000010				
3HPZ-MFA	C	-2.929804	1.123240	0.000130	32.3659	50.1339	86.9144	105.3652
	C	-3.804466	0.080223	0.000201	113.003	125.4335	161.8414	226.8249
	C	-3.278590	-1.222372	0.000107	318.5327	398.9984	474.8796	513.6478
	N	-1.990463	-1.465474	-0.000038	565.68	579.2983	590.1031	655.7438
	N	-1.135862	-0.449719	-0.000107	693.4675	773.5864	851.9323	874.3997
	C	-1.557582	0.807019	-0.000034	908.0047	936.0969	962.6884	1029.1136
	O	-0.679392	1.788803	-0.000111	1049.3182	1052.9272	1076.0341	1101.1871
	O	1.380038	-1.264512	-0.000192	1135.7849	1172.7409	1214.735	1253.1261
	C	2.174497	-0.230174	-0.000309	1279.0143	1333.1346	1373.0971	1397.1185
	C	3.627550	-0.646000	0.000161	1447.8596	1483.0525	1486.2916	1531.4407
	H	3.819755	-1.250517	0.887584	1557.6325	1642.4777	1684.621	1804.7537
	O	1.822909	0.932135	-0.000239	2651.1646	3085.917	3134.008	3166.2734
	F	4.448081	0.443043	0.00036100	3214.1639	3227.2513	3244.0116	
	H	3.820239	-1.250562	-0.887117				
	H	-4.873712	0.238361	0.000325				
	H	-3.918519	-2.093395	0.000156				
	H	0.401022	-0.957201	-0.000270				
	H	-3.232072	2.159860	0.000189				
	H	0.256777	1.449392	-0.000295				

3PZ-TFA	C	0.032006	-0.000380	0.005847	19.3068	33.1325	56.5035	82.5901
	C	0.034398	-0.000424	1.429815	82.9126	105.7938	160.5086	202.9610
	C	2.436249	0.000513	0.092774	265.0551	286.5893	382.3480	415.7548
	N	2.274325	0.000416	1.448886	443.8167	507.8633	528.4549	558.3720
	O	3.564638	0.000958	-0.420903	584.7215	612.2154	627.6030	727.3911
	H	-0.910098	-0.000718	-0.524926	757.6078	809.3660	849.7511	857.3173
	H	-0.882896	-0.000789	1.999890	865.9619	946.6590	959.0252	1034.5466
	H	3.124435	0.000736	2.020407	1035.0070	1044.3724	1082.3016	1144.6119
	N	1.128277	-0.000030	2.122962	1211.9856	1237.3729	1238.5975	1288.0128
	C	1.207590	0.000082	-0.656992	1305.9216	1416.3492	1417.3304	1436.4729
	H	1.284693	0.000148	-1.733962	1491.3088	1541.8351	1620.9463	1680.4274
	C	5.848831	0.002359	1.913829	1733.3061	1843.2127	2673.1217	3215.2147
	O	5.875948	0.002455	0.620838	3234.2739	3244.8266	3356.5148	
	H	4.928346	0.001839	0.228210				
	O	4.882852	0.001678	2.637704				
	C	7.276617	0.003272	2.504132				
	F	7.943832	1.083115	2.098706				
	F	7.945251	-1.075661	2.098623				
	F	7.242746	0.003199	3.826575				
CTS _{TFA}	C	0.023377	-0.003147	0.002207	-612.1102	26.4853	40.4058	61.2404
	C	0.012613	-0.005774	1.412491	105.7631	125.2744	154.1800	229.2750
	C	2.388143	0.003837	0.163235	235.3569	275.4241	329.4183	396.1975
	N	2.272723	0.002178	1.489900	452.5497	521.0363	531.4172	543.0598
	O	3.557626	0.007514	-0.402410	569.0850	600.6291	624.2945	704.8889
	H	-0.907269	-0.005101	-0.547572	755.2590	771.1245	823.1886	856.4531
	H	-0.910076	-0.010066	1.974710	875.9112	882.6018	968.8861	1033.4717
	H	3.257543	0.006449	2.246892	1060.2078	1085.3789	1106.4921	1143.6021
	N	1.106586	-0.002885	2.123399	1224.3700	1234.8310	1255.1150	1284.2221
	C	1.221884	0.001805	-0.635638	1304.5368	1345.9999	1408.7736	1429.6590
	H	1.331259	0.004073	-1.709698	1516.9964	1538.4907	1561.0648	1642.3093
	C	5.329221	0.004460	2.400696	1697.3288	1753.4082	1800.9502	2578.8681
	O	5.517321	-0.004352	1.183568	3207.1914	3223.3490	3229.4676	
	H	4.350256	0.003066	0.259211				
	O	4.232181	0.010340	3.019545				
	C	6.567729	0.030321	3.327434				
	F	7.695637	-0.127499	2.649716				
	F	6.490267	-0.935817	4.241381				
	F	6.626218	1.201023	3.967263				

3HPZ-TFA	C	0.020480	-0.003273	0.008578	23.2651	35.2861	57.1029	95.8572
	C	0.024020	0.019881	1.413691	100.3777	128.2173	134.8234	227.6266
	C	2.375726	-0.010253	0.167845	267.1824	290.5795	399.4203	415.1186
	N	2.298526	0.012044	1.490220	442.7979	487.2282	528.7559	566.6498
	O	3.556249	-0.024838	-0.419263	589.1885	610.9443	658.2884	734.8794
	H	-0.913343	-0.008471	-0.535528	773.7754	810.4799	847.1764	857.7960
	H	-0.893576	0.032957	1.984466	866.4174	873.5001	962.2357	1031.8297
	H	3.474533	0.024882	2.505897	1053.8657	1078.0131	1136.2650	1159.9484
	N	1.128492	0.027098	2.117943	1214.0016	1240.2258	1241.7709	1256.8187
	C	1.219588	-0.018783	-0.635090	1290.7319	1367.9595	1392.4623	1457.9798
	H	1.324091	-0.036958	-1.709601	1480.0976	1531.6142	1585.0411	1642.1686
	C	5.391521	0.014414	2.552706	1686.5262	1814.3435	2355.8901	3217.4672
	O	5.567158	-0.008584	1.354133	3229.8239	3242.5695	3277.9511	
	H	4.296899	-0.018671	0.237744				
	O	4.269587	0.033163	3.185359				
	C	6.597370	0.023630	3.517854				
	F	6.567183	1.114956	4.280777				
	F	7.739790	0.007340	2.851714				
	F	6.555989	-1.043617	4.314068				
4PM	C	1.125975	1.132876	0.000025	176.0695	369.1358	464.5642	518.5465
	N	1.809399	-0.059923	0.000015	543.5728	666.6854	744.8450	787.0828
	C	-0.220492	1.250149	-0.000006	851.4250	872.5044	990.6486	1001.1722
	C	-1.051291	0.066239	-0.000574	1044.6872	1046.4505	1150.0181	1227.8857
	N	-0.276846	-1.106175	-0.000058	1262.6562	1403.8090	1458.9375	1481.3625
	H	1.751746	2.016229	0.000216	1609.5852	1692.2987	1818.3361	3194.1481
	H	-0.714879	2.209155	0.000254	3202.2517	3250.9945	3610.1687	
	H	-0.797049	-1.972358	0.000109				
	C	1.075500	-1.118115	0.000083				
	H	1.540543	-2.097221	0.000270				
	O	-2.260797	0.002499	0.000285				
pTS	C	1.261050	1.008516	0.000019	-1849.4509	195.0395	383.7467	499.6579
	N	1.776103	-0.239088	0.000124	517.9183	627.0804	704.9148	779.6643
	C	-0.078653	1.318194	-0.000105	856.0508	932.7415	1004.8619	1024.3761
	C	-0.942669	0.212605	-0.000077	1046.5409	1068.1911	1127.5707	1217.9978
	N	-0.404800	-1.034810	-0.000205	1253.4000	1350.0647	1432.8647	1463.3674
	H	1.992878	1.807318	0.000077	1563.4261	1616.5300	1703.0429	2144.1929
	H	-0.444731	2.331760	-0.000110	3194.1886	3214.5396	3262.4738	
	H	-1.672731	-1.210365	0.000147				
	C	0.908955	-1.227379	0.000016				
	H	1.272355	-2.246998	0.000048				
	O	-2.204874	0.045495	0.000162				

4HPM	C	-1.209832	1.077554	0.000019	214.2571	394.1444	429.7555	521.2826
	N	-1.820575	-0.113137	0.000030	564.9492	588.0433	693.1011	810.3794
	C	0.158390	1.221434	-0.000027	871.5485	895.9050	1009.9714	1020.1192
	C	0.887928	0.034503	0.000030	1048.7424	1091.5110	1177.1875	1204.9837
	N	0.312481	-1.154519	0.000019	1288.6041	1365.7464	1384.5392	1453.3211
	H	-1.854199	1.948443	0.000025	1533.3641	1656.3347	1680.1722	3191.9879
	H	0.649281	2.181654	-0.000059	3198.5915	3253.4078	3816.5102	
	H	2.549086	-0.823545	0.000015				
	C	-1.020033	-1.164331	-0.000117				
	H	-1.489790	-2.140596	0.000225				
	O	2.225446	0.086585	0.000001				
4PM-AM	C	2.247233	0.219420	-0.000072	63.4783	119.0179	140.8889	177.8078
	C	0.729676	-1.439184	0.000033	181.0387	292.0172	377.8242	448.9401
	C	-0.093646	0.830747	0.000049	479.0645	545.7744	551.9725	672.3096
	N	-0.284892	-0.553270	0.000045	788.2287	864.9793	874.0296	975.2901
	O	-1.049106	1.590523	0.000037	1003.6408	1017.2469	1045.7235	1054.4392
	H	3.298298	0.480076	-0.000034	1116.9126	1189.8444	1232.3677	1287.8373
	H	0.441208	-2.484011	0.000003	1405.2654	1464.9923	1520.8646	1611.4932
	H	-1.268080	-0.862052	-0.000002	1650.4815	1672.9316	1688.2301	1789.8750
	N	1.983556	-1.125408	-0.000008	3194.0912	3198.0929	3211.6928	3249.7492
	C	1.303190	1.189665	-0.000025	3461.8559	3588.4115	3628.9337	
	H	1.555632	2.238700	-0.000022				
	N	-3.174372	-0.578624	-0.000097				
	H	-3.749062	-0.755161	-0.814483				
	H	-2.926571	0.409367	-0.001034				
	H	-3.747343	-0.753880	0.815784				
^D TS _{AM}	C	2.175352	0.376539	0.000007	-645.9731	81.5765	192.8709	328.7362
	C	0.808124	-1.401598	-0.000005	380.7391	382.9796	407.3188	434.2864
	C	-0.199094	0.710865	-0.000004	565.8128	570.9267	586.6778	712.2478
	N	-0.302066	-0.661296	-0.0000080	808.3661	843.7123	880.7144	895.9635
	O	-1.239124	1.422429	-0.000009	1006.3617	1027.5121	1044.3898	1074.5431
	H	3.193114	0.749590	0.000012	1210.5658	1235.8343	1325.4338	1386.1397
	H	0.658598	-2.477016	-0.000009	1427.3981	1475.2116	1539.2044	1554.3482
	H	-1.748350	-0.954352	0.000000	1601.6181	1606.6165	1665.3487	1685.9588
	N	2.045932	-0.972204	0.000002	1917.9440	2612.9206	3164.1903	3183.3353
	C	1.124632	1.242948	0.000005	3242.7430	3549.0856	3637.7121	
	H	1.257347	2.314038	0.000009				
	N	-2.840084	-0.570678	0.000009				
	H	-3.367571	-0.802757	-0.832168				
	H	-2.493155	0.450533	0.000000				
	H	-3.367550	-0.802745	0.832202				

4HPM-AM	C	-2.249309	0.423484	0.000447	61.3769	116.4940	117.0609	209.0337
	C	-0.951162	-1.409186	-0.000319	216.4888	288.8815	397.5981	404.5290
	C	0.102505	0.596560	-0.000251	511.4660	572.0149	578.4906	696.0427
	N	0.196557	-0.731371	-0.000520	811.1067	876.8785	901.3353	1009.5707
	O	1.202169	1.328292	-0.000537	1017.7705	1031.2393	1048.3779	1090.8823
	H	-3.246095	0.848577	0.000829	1103.5809	1205.1445	1233.1750	1338.9470
	H	-0.862625	-2.489884	-0.000430	1385.2637	1437.1725	1487.5356	3486.9157
	H	2.567500	-1.217212	0.000021	3608.6069	3635.9632		
	N	-2.175086	-0.915477	0.000201				
	C	-1.143821	1.236262	0.000220				
	H	-1.207758	2.313173	0.000393				
	N	3.249376	-0.464074	0.000467				
	H	3.835319	-0.563121	0.819645				
	H	2.013328	0.740145	-0.000975				
	H	3.837775	-0.564277	-0.816802				
4PM-MA	C	-2.63693	0.14743	0.23085	42.5586	75.27	92.4677	110.94
	C	-1.08075	-1.43732	-0.11766	183.215	196.461	202.762	376.336
	C	-0.35487	0.86390	-0.13070	447.17	478.558	544.296	552.117
	N	-0.11455	-0.50770	-0.23846	672.009	788.193	864.826	871.415
	O	0.56022	1.66324	-0.25034	908.653	982.404	994.91	1001.93
	H	-3.68172	0.35892	0.42282	1040.62	1049.89	1057.59	1076.28
	H	-0.75865	-2.46704	-0.22519	1190.92	1195.06	1229.35	1289.86
	H	0.87174	-0.76482	-0.42926	1352.2	1402.03	1457.83	1461.61
	N	-2.32757	-1.18222	0.11140	1508.65	1524.42	1533.06	1612
	C	-1.74317	1.15911	0.12598	1630.41	1685.27	1789.63	3043.54
	H	-2.03075	2.19429	0.22646	3094.22	3114.89	3149.77	3182.71
	N	2.69863	-0.43135	-0.57790	3196.05	3225.56	3503.91	3602.13
	H	2.50802	0.46728	-1.01008				
	H	3.42982	-0.88716	-1.10760				
	C	3.11250	-0.21281	0.81147				
	H	2.31649	0.32479	1.32498				
	H	3.25525	-1.17340	1.30406				
	H	4.03177	0.36838	0.91152				

DTS _{MA}	C	-2.66558	0.26710	0.23714	51.0897	64.0583	105.868	114.712
	C	-1.23765	-1.41213	-0.19250	214.382	217.963	241.763	396.313
	C	-0.36567	0.67751	-0.08931	426.28	515.652	570.965	580.539
	N	-0.16429	-0.62643	-0.27461	695.839	810.69	874.457	898.352
	O	0.65756	1.50698	-0.15640	904.248	991.101	1006.9	1015.73
	H	-3.68128	0.58594	0.44101	1043.73	1075.53	1092.99	1117.26
	H	-1.06170	-2.47148	-0.34520	1197.64	1204.07	1235.52	1341.31
	H	2.28019	-0.77234	-1.06712	1348.88	1384.33	1443.82	1458.44
	N	-2.48261	-1.04854	0.05265	1506.12	1512.57	1528.35	1538.31
	C	-1.64534	1.18254	0.17800	1631.2	1653.68	1682.49	2873.19
	H	-1.79801	2.24019	0.32689	3058.41	3123.38	3151.96	3178.9
	N	2.79102	-0.05241	-0.56841	3182.04	3232.07	3523.3	3613.39
	H	1.50710	0.99681	-0.36434				
	H	3.62191	0.17648	-1.09784				
	C	3.12622	-0.52089	0.77981				
	H	2.19835	-0.75388	1.29961				
	H	3.76250	-1.40769	0.78997				
	H	3.62978	0.27698	1.32198				
4HPM-MA	C	-2.61896	0.16451	0.22778	-375.678	48.6207	86.2063	127.112
	C	-1.07301	-1.41578	-0.15043	189.356	206.543	329.921	394.705
	C	-0.32429	0.80382	-0.08229	441.173	536.602	561.437	579.419
	N	-0.06782	-0.54272	-0.23408	708.794	805.083	829.742	877.467
	O	0.61116	1.63636	-0.16234	891.34	973.869	1000.4	1019.64
	H	-3.66067	0.40129	0.41345	1040.79	1064.83	1069.79	1088.03
	H	-0.80418	-2.46014	-0.28230	1210.76	1230.1	1313.55	1331.24
	H	1.38957	-0.64378	-0.49537	1380.88	1424.15	1469.23	1473.87
	N	-2.33738	-1.15258	0.07078	1511.1	1517.24	1555.87	1589.06
	C	-1.68806	1.15557	0.16495	1620.62	1631.88	1691.91	1960.22
	H	-1.94215	2.19679	0.29346	3020.22	3082.04	3149.56	3162.7
	N	2.44140	-0.18547	-0.54546	3167.53	3180.11	3219.31	3576.96
	H	2.06846	0.79489	-0.56729				
	H	2.97027	-0.41901	-1.37685				
	C	3.17342	-0.42994	0.70708				
	H	2.51806	-0.14649	1.52740				
	H	3.42224	-1.48420	0.79355				
	H	4.08117	0.16611	0.75138				

4PM-DMA	C	3.077515	-0.059498	0.051154	40.1238	46.6616	76.0057	109.3301
	C	1.321295	-1.462640	0.084292	122.7956	182.9501	192.9039	224.0240
	C	0.866238	0.890496	-0.188640	297.1000	378.3065	406.5996	477.7719
	N	0.459955	-0.440603	-0.075456	545.7311	552.1489	671.3852	789.3285
	O	0.040086	1.778288	-0.332771	865.1953	872.5740	897.2266	964.1043
	H	4.154357	0.039248	0.109550	988.9879	1001.9321	1037.0596	1042.9029
	H	0.874322	-2.447645	0.156814	1053.5684	1063.8640	1107.0623	1189.8998
	H	-0.567736	-0.588795	-0.129836	1194.0306	1213.6120	1231.5519	1270.5886
	N	2.607032	-1.342385	0.153929	1291.6464	1403.3443	1439.7146	1462.6537
	C	2.298980	1.036152	-0.112081	1468.2748	1474.3123	1493.0857	1507.2520
	H	2.712275	2.029900	-0.189221	1519.1524	1523.2484	1529.9151	1614.1373
	N	-2.346290	-0.069154	-0.157645	1685.3025	1787.5301	3006.0418	3016.0267
	H	-2.078561	0.750848	-0.693651	3040.1189	3092.8433	3096.9348	3141.4473
	C	-3.516481	-0.707746	-0.742051	3142.0821	3190.6582	3196.8907	3249.8480
	H	-3.324016	-0.953474	-1.784706	3517.3579			
	H	-3.725487	-1.634488	-0.206764				
	H	-4.413241	-0.079208	-0.688799				
	C	-2.570025	0.348258	1.222030				
	H	-2.715739	-0.533469	1.847531				
	H	-1.696511	0.893875	1.575894				
	H	-3.450365	0.991759	1.331331				
DTS _{DMA}	C	-3.005736	0.029657	0.002908	-302.6480	34.5832	55.9091	104.2325
	C	-1.302113	-1.427637	0.069923	193.1564	199.4232	224.0300	233.2018
	C	-0.746368	0.848756	-0.082486	280.9196	395.3141	404.2882	489.6166
	N	-0.368423	-0.477367	-0.003570	559.0288	561.9408	615.0451	704.9616
	O	0.122816	1.744408	-0.151956	806.3969	879.4505	883.4428	945.8703
	H	-4.078826	0.184775	0.008732	1004.9430	1014.7927	1041.5176	1043.2987
	H	-0.933554	-2.448064	0.129141	1063.3106	1070.8932	1084.0114	1173.2607
	H	1.080592	-0.472797	-0.032919	1212.4322	1231.6287	1259.7408	1316.3987
	N	-2.601404	-1.263933	0.078829	1378.0351	1422.5481	1447.5590	1471.6606
	C	-2.158184	1.090709	-0.076923	1480.0035	1492.3376	1501.7613	1519.6231
	H	-2.512144	2.108756	-0.136836	1520.4204	1525.5145	1563.3945	1614.4828
	N	2.144610	0.001625	-0.050414	1623.7700	1689.0012	1875.9623	3068.6564
	H	1.786065	0.954527	-0.244739	3074.6935	3145.9313	3150.8557	3152.5895
	C	2.728692	-0.037835	1.293941	3163.0162	3168.6105	3172.8392	3216.8430
	H	2.000319	0.365018	1.994128	3222.8014			
	H	2.957091	-1.068644	1.558651				
	H	3.641323	0.555409	1.334281				
	C	3.012711	-0.509072	-1.112548				
	H	3.255024	-1.550813	-0.910153				
	H	2.488499	-0.440795	-2.062639				
	H	3.935591	0.067609	-1.164805				

4HPM-DMA	C	-3.114343	0.338167	0.073433	42.2077	42.7553	72.8652	106.1493
	C	-1.717955	-1.381172	-0.297566	132.9174	210.5369	218.4685	222.8044
	C	-0.776695	0.656410	0.023753	307.1760	396.9600	407.9225	500.1516
	N	-0.610549	-0.644294	-0.216232	571.6829	576.5002	695.0498	811.6440
	O	0.281271	1.436727	0.116591	875.2695	881.1241	905.9729	955.8319
	H	-4.132181	0.693636	0.183521	1008.1867	1016.2961	1040.2855	1045.8777
	H	-1.570103	-2.437563	-0.493135	1091.3135	1092.7708	1132.5094	1199.5285
	H	1.899480	-0.827356	-0.768448	1205.3696	1219.2471	1236.0088	1269.6953
	N	-2.966585	-0.972981	-0.167518	1344.5813	1387.6370	1440.4230	1444.0628
	C	-2.057029	1.205779	0.180080	1468.5451	1471.3850	1495.1563	1508.9209
	H	-2.181269	2.259809	0.373849	1516.5892	1520.8566	1524.9703	1539.4139
	N	2.386950	-0.159944	-0.180321	1652.1484	1682.5603	2746.0528	3026.5431
	H	1.130271	0.890985	-0.026212	3030.3066	3104.7492	3107.3176	3147.9488
	C	2.552699	-0.739295	1.149235	3148.2362	3180.9409	3187.7130	3248.2339
	H	1.580147	-1.059040	1.518999	3533.9652			
	H	3.236853	-1.594126	1.152510				
	H	2.950300	0.021079	1.821451				
	C	3.651220	0.240548	-0.784439				
	H	4.368795	-0.584889	-0.842205				
	H	3.475730	0.626717	-1.786357				
	H	4.095708	1.034851	-0.185182				

4PM-DEA	C	3.74237	0.12854	0.19931	31.3894	38.704	43.7749	86.9171
	C	1.91656	1.42759	0.37782	102.344	113.811	124.712	178.889
	C	1.60413	-0.83751	-0.38803	192.434	250.771	296.226	322.37
	N	1.12229	0.42712	-0.04524	378.683	471.432	478.547	510.146
	O	0.83691	-1.70984	-0.76544	546.557	552.969	671.553	780.229
	H	4.81678	0.06120	0.31728	790.267	808.25	847.824	867.124
	H	1.41462	2.36004	0.61066	873.524	915.712	926.382	989.486
	H	0.09200	0.54502	-0.14594	1001.82	1038.98	1043.41	1054.46
	N	3.19975	1.34550	0.51862	1062.18	1081.35	1098.31	1162.89
	C	3.03451	-0.94087	-0.23520	1192.89	1197.86	1215.36	1232.65
	H	3.50357	-1.88223	-0.47634	1292.97	1310.79	1331.98	1382.69
	N	-1.64512	-0.00262	-0.40109	1400.95	1404.63	1412.19	1419.44
	H	-1.30613	-0.69927	-1.05956	1463.99	1487.14	1490.45	1497.59
	C	-1.91717	-0.69006	0.86559	1502.08	1506.7	1512.54	1528.21
	H	-1.01146	-1.24645	1.11095	1532.9	1614.51	1685.06	1786.67
	H	-2.05276	0.06256	1.64452	2991.06	3023.51	3059.77	3062.92
	C	-2.77135	0.73029	-0.97969	3069.34	3092.44	3104.22	3132.08
	H	-2.42665	1.15549	-1.92264	3134.68	3136.32	3142.54	3188.63
	H	-3.61164	0.06853	-1.21886	3196.56	3249.15	3501.61	
	C	-3.25123	1.84418	-0.06489				
	H	-4.00008	2.45215	-0.57009				
	H	-3.70448	1.44960	0.84442				
	H	-2.41947	2.48859	0.22188				
	C	-3.10825	-1.63992	0.84623				
	H	-3.17807	-2.17754	1.79127				
	H	-4.04858	-1.10875	0.69662				
	H	-2.99882	-2.37374	0.04648				

DTS _{DEA}	C	-3.64850	0.02967	-0.07270	-179.78	30.8614	37.6016	75.5369
	C	-1.85316	1.19335	-0.74480	87.8174	103.046	169.42	196.6
	C	-1.44864	-0.87274	0.29833	206.72	255.906	291.393	316.169
	N	-0.98547	0.27828	-0.31107	395.87	432.186	501.609	510.814
	O	-0.63936	-1.72925	0.70722	561.007	568.927	701.869	705.763
	H	-4.72876	-0.02574	0.00092	790.844	805.417	806.791	866.463
	H	-1.41820	2.07189	-1.21436	878.577	885.151	925.652	1005.44
	H	0.46466	0.15392	-0.32108	1014.47	1040.71	1041.47	1048.33
	N	-3.15996	1.14896	-0.66672	1070.27	1079.61	1097.42	1177.99
	C	-2.87425	-0.97825	0.41128	1197.49	1209.55	1225.38	1248.78
	H	-3.29570	-1.85570	0.87809	1313.87	1345.23	1375.56	1394.6
	N	1.51056	-0.27447	-0.05694	1408.65	1417.07	1424.43	1439.02
	H	1.18804	-1.23004	0.14708	1474.35	1488.61	1494.57	1496.25
	C	2.48165	-0.22549	-1.16288	1504.31	1506.14	1518.03	1531.58
	H	2.02335	-0.75393	-1.99758	1561.76	1618.6	1630.26	1689.2
	H	2.59674	0.81507	-1.46351	1852.84	3067.55	3068.84	3088.51
	C	1.90153	0.35437	1.22266	3093.72	3121.74	3126.89	3143.24
	H	1.04555	0.20992	1.88145	3147.58	3148.48	3150.46	3152.55
	H	2.74668	-0.18320	1.65184	3178.53	3237.15	3334.91	
	C	2.21247	1.82824	1.04987				
	H	2.36323	2.28864	2.02413				
	H	3.11687	1.98862	0.46330				
	H	1.38336	2.33866	0.55866				
	C	3.82399	-0.83955	-0.80913				
	H	4.46168	-0.86916	-1.69068				
	H	4.34067	-0.26197	-0.04341				
	H	3.70030	-1.85992	-0.44540				

4HPM-DEA	C	3.81100	-0.33184	-0.23714	29.1057	40.0433	54.4303	85.6359
	C	2.44961	1.26109	0.57007	97.2703	119.576	167.605	216.832
	C	1.47602	-0.66203	-0.13421	221.011	283.539	302.477	336.021
	N	1.33379	0.55605	0.39035	399.135	449.588	513.093	527.469
	O	0.40879	-1.40607	-0.33830	575.378	579.304	695.22	785.773
	H	4.81896	-0.65135	-0.47563	810.417	813.523	853.481	881.243
	H	2.32104	2.24958	0.99793	896.301	908.614	928.791	1015.05
	H	-1.18892	0.58621	1.09950	1016.67	1041.56	1050.7	1071.91
	N	3.68670	0.89574	0.28860	1094.12	1096.59	1145.91	1175.56
	C	2.74252	-1.15966	-0.47212	1200.26	1205.68	1219.86	1235.34
	H	2.84884	-2.14643	-0.89549	1309.93	1334.15	1350	1384.62
	N	-1.68064	0.03954	0.39938	1387.22	1403.23	1417.6	1421.6
	H	-0.43201	-0.90443	-0.03696	1449.31	1489.97	1492.56	1498.89
	C	-2.86910	-0.58575	0.98566	1505.54	1508.26	1515.21	1525.84
	H	-2.53205	-1.16650	1.84457	1533.51	1540.93	1652.19	1683.6
	H	-3.57589	0.16163	1.36158	2663.47	3037.65	3059.05	3063.08
	C	-1.91511	0.89428	-0.77047	3073.53	3097.14	3107.17	3133.61
	H	-0.94689	1.32559	-1.02720	3136.27	3137.15	3147.09	3180.94
	H	-2.20707	0.25489	-1.60478	3193.83	3242.09	3507.19	
	C	-2.94578	1.99577	-0.56671				
	H	-2.98488	2.64122	-1.44346				
	H	-3.94525	1.59004	-0.40857				
	H	-2.68806	2.61189	0.29619				
	C	-3.56611	-1.50096	-0.00607				
	H	-4.36204	-2.05425	0.48978				
	H	-4.01476	-0.93914	-0.82531				
	H	-2.85845	-2.21526	-0.42801				
4PM-FA	C	2.916904	0.311787	0.000205	48.2504	75.8469	106.8522	183.0525
	C	1.484651	-1.421043	-0.000308	199.2765	220.4476	227.1867	376.3749
	C	0.558436	0.790571	-0.000023	509.8976	551.3186	559.7973	678.3759
	N	0.426888	-0.583861	-0.000287	724.2853	790.5327	876.8711	886.6103
	O	-0.438071	1.519110	0.000039	967.6736	1006.4583	1015.1538	1042.4989
	H	3.952998	0.625843	0.000388	1048.8516	1062.4112	1118.6489	1188.1914
	H	1.245241	-2.477430	-0.000538	1247.7611	1295.5381	1311.4441	1402.3958
	H	-0.538612	-0.948284	-0.000584	1424.4145	1465.3427	1483.1511	1517.9178
	C	-3.130934	-0.435808	0.000151	1616.2173	1680.6368	1736.9856	1794.4510
	H	-4.195473	-0.692384	0.000230	2875.6473	3095.6483	3198.0590	3202.3695
	O	-2.269789	-1.292344	0.000560	3206.1926	3253.2439		
	O	-2.936750	0.850275	-0.000414				
	H	-1.950573	1.081543	-0.000462				
	C	1.921279	1.232950	0.000218				
	H	2.112956	2.294435	0.000426				
	N	2.720016	-1.040538	-0.000054				

DTS _{FA}	C	2.830619	0.206700	-0.000055	-707.8581	52.5849	94.6252	152.6812
	C	1.272903	-1.409941	-0.000063	218.7672	243.2665	339.4671	385.3846
	C	0.529388	0.804980	0.000080	387.4762	569.7202	570.3598	663.1993
	N	0.267163	-0.519773	0.000036	756.8902	801.6280	802.4598	879.8838
	O	-0.422235	1.659051	0.000160	911.8488	1004.8432	1051.3286	1059.4914
	H	3.884114	0.457009	-0.000092	1100.1640	1100.3363	1205.7705	1250.3220
	H	0.972653	-2.450796	-0.000096	1279.7236	1325.6297	1327.2368	1406.8311
	H	-0.853528	-0.898385	0.000139	1410.8669	1435.7166	1470.7778	1544.1100
	C	-2.945875	-0.403660	-0.000060	1595.6556	1608.5281	1688.8574	1709.6133
	H	-4.001784	-0.700884	-0.000145	1780.6074	1841.3742	3068.9849	3201.3567
	O	-2.098174	-1.330429	0.000248	3207.0880	3257.0398		
	O	-2.703332	0.822807	-0.000281				
	H	-1.449543	1.241603	-0.000023				
	C	1.886469	1.192444	0.000041				
	H	2.135103	2.241782	0.000081				
	N	2.541678	-1.115212	-0.000114				
4HPM-FA	C	2.897471	0.095110	-0.000192	52.0019	70.4720	127.3639	177.1991
	C	1.229127	-1.407759	0.000100	216.9051	223.7968	233.6349	395.4389
	C	0.645095	0.798513	0.000089	490.9748	570.9879	574.1547	703.9440
	N	0.265616	-0.479517	0.000188	734.5730	807.4882	874.2365	902.2381
	O	-0.256769	1.753381	0.000218	915.4809	1008.2429	1030.3334	1048.1116
	H	3.963949	0.284495	-0.000344	1062.4079	1094.5003	1123.9938	1202.8194
	H	0.890743	-2.437756	0.000179	1244.6509	1310.0138	1331.4568	1391.2199
	H	-1.304165	-1.005257	0.000412	1416.4369	1433.7648	1464.1541	1536.7216
	C	-3.082647	-0.319662	-0.000241	1557.0457	1641.0056	1692.2414	1783.2839
	H	-4.134203	-0.622930	-0.000519	2777.5917	3101.0821	3190.5928	3193.9531
	O	-2.267770	-1.335519	0.000098	3210.9705	3255.4258		
	O	-2.755808	0.849524	-0.000135				
	H	-1.182643	1.392300	0.000400				
	C	2.004949	1.135293	-0.000104				
	H	2.308056	2.170340	-0.000174				
	N	2.525394	-1.196089	-0.000090				

4PM-AA	C	-3.40472	0.15488	0.00001	41.0371	66.9302	82.8716	103.65
	C	-1.84774	-1.46630	0.00000	110.239	158.902	171.948	199.826
	C	-1.08794	0.80773	0.00001	377.277	458.161	511.672	551.759
	N	-0.85549	-0.55422	-0.00000	560.518	613.185	641.671	678.283
	O	-0.14689	1.60531	0.00001	791.146	876.841	886.095	928.869
	H	-4.46118	0.39199	0.00002	975.44	1006.68	1016.06	1036.08
	H	-1.53157	-2.50235	-0.00002	1037.98	1049.73	1064.08	1079.69
	H	0.13752	-0.84356	-0.00001	1190.42	1247.85	1296.15	1355.03
	C	2.70016	-0.18049	-0.00009	1399.78	1409.79	1466.4	1471.86
	O	1.86344	-1.06846	-0.00003	1481.98	1502.35	1520.51	1616.44
	O	2.41010	1.09759	-0.00004	1681.34	1744.81	1787.12	2971.58
	H	1.41595	1.25455	-0.00002	3087.42	3153.68	3153.85	3199.51
	C	4.17465	-0.45234	0.00007	3200.61	3205.89	3254.48	
	H	4.62366	0.01055	-0.87722				
	H	4.62339	0.01016	0.87772				
	H	4.35580	-1.52119	-0.00011				
	N	-3.10891	-1.17904	0.00000				
	C	-2.48021	1.14745	0.00002				
	H	-2.75111	2.19156	0.00003				
DTS _{AA}	C	3.29241	0.04643	0.00763	-912.171	31.4991	46.1103	70.7644
	C	1.62053	-1.45153	-0.00268	125.816	151.867	217.416	236.797
	C	1.03891	0.81128	0.00088	356.821	387.721	487.031	569.274
	N	0.68165	-0.49264	-0.00372	573.069	619.673	655.479	706.837
	O	0.15027	1.72611	-0.00009	746.166	802.621	879.818	913.784
	H	4.36146	0.21921	0.01225	965.289	1006.02	1026.7	1049.99
	H	1.24710	-2.46864	-0.00680	1057.13	1078.4	1081.6	1203.51
	H	-0.48151	-0.78251	-0.00926	1267.47	1276.54	1329.63	1331.89
	C	-2.53075	-0.12950	-0.01472	1377.25	1409.35	1430.38	1468.42
	O	-1.73292	-1.10744	-0.01573	1470.07	1481.56	1532.95	1564.11
	O	-2.17368	1.07748	-0.01610	1609.16	1674.75	1690.89	1771.59
	H	-0.93369	1.37564	-0.00748	1784.09	3085.4	3158.67	3196.52
	C	-4.00251	-0.42741	0.01941	3197.45	3203.72	3257.51	
	H	-4.21225	-1.34376	-0.52453				
	H	-4.28830	-0.57831	1.06104				
	H	-4.56852	0.40868	-0.37865				
	N	2.90834	-1.25150	0.00281				
	C	2.42282	1.09794	0.00690				
	H	2.74790	2.12621	0.01068				

4HPM-AA	C	3.36660	-0.04524	0.00011	41.8482	49.1502	59.2087	112.609
	C	1.60726	-1.44024	-0.00004	117.767	165.318	170.889	219.272
	C	1.16201	0.79730	-0.00001	395.395	453.407	501.123	571.504
	N	0.70351	-0.45502	-0.00007	574.532	611.378	648.819	703.617
	O	0.31998	1.80407	-0.00003	808.162	876.241	903.428	932.262
	H	4.44288	0.07751	0.00018	932.448	1009.88	1027.58	1036.02
	H	1.20602	-2.44752	-0.00010	1047.45	1055.92	1080.96	1094.2
	H	-0.92306	-0.87278	-0.00017	1204.47	1243.81	1333.75	1359.79
	C	-2.65515	-0.06781	-0.00018	1393.52	1418.27	1433.41	1466.73
	O	-1.89897	-1.14019	-0.00015	1472	1480.99	1544.86	1552.14
	O	-2.20921	1.06768	-0.00014	1641.89	1690.75	1781.38	2874.74
	H	-0.62857	1.49550	-0.00014	3088.9	3137.95	3155.48	3189.4
	C	-4.12277	-0.36601	0.00026	3195.18	3202.83	3253.45	
	H	-4.36608	-0.96118	0.87899				
	H	-4.68919	0.55827	-0.00098				
	H	-4.36621	-0.96383	-0.87660				
	N	2.91508	-1.31074	0.00004				
	C	2.54060	1.04856	0.00009				
	H	2.90831	2.06251	0.00015				
4PM-MFA	C	2.114362	-1.533925	0.000022	35.2217	51.1481	92.5151	93.5185
	N	3.395538	-1.360101	0.000009	102.9376	117.0792	173.9813	201.3149
	C	3.810687	-0.058842	0.000004	311.5019	376.1532	491.7672	522.0504
	C	2.978913	1.013079	0.000004	551.9844	563.5141	578.9839	678.7842
	C	1.563169	0.798945	-0.000033	687.4685	791.2375	877.9725	888.1547
	N	1.208318	-0.534741	-0.000010	932.0973	967.844	1007.0255	1016.6191
	O	0.699133	1.682160	-0.000024	1048.2071	1049.4597	1054.1484	1064.1831
	O	-1.860424	1.444720	0.000015	1171.3859	1188.5498	1248.9427	1277.6115
	C	-2.272208	0.205293	0.000008	1296.3273	1323.893	1402.581	1427.0918
	O	-1.564305	-0.779282	-0.000008	1466.2177	1485.8404	1514.1486	1518.8942
	C	-3.782333	0.131749	0.000041	1615.5008	1680.5202	1743.3441	1815.924
	F	-4.206504	-1.164521	-0.000038	2823.628	3083.871	3131.7685	3196.7196
	H	-4.160244	0.641388	-0.887241	3200.9727	3207.1322	3254.9832	
	H	-4.160224	0.641303	0.887382				
	H	4.884163	0.082084	0.000024				
	H	1.705368	-2.536889	0.000008				
	H	0.196393	-0.736556	-0.000004				
	H	-0.846733	1.505946	0.000009				
	H	3.342044	2.028734	0.000019				

DTS _{MFA}	N	-3.139149	-1.459684	0.000120	-605.3591	45.2419	47.455	95.2952
	C	-3.672733	-0.216938	0.000053	120.6686	139.2406	161.4261	219.764
	C	-2.931270	0.929759	-0.000044	289.0602	386.8112	390.6875	532.4389
	C	-1.526983	0.803356	-0.000073	569.5751	571.6112	593.6653	667.0182
	N	-1.017910	-0.445795	-0.000019	703.7329	796.3903	802.4601	882.2918
	C	-1.837390	-1.510289	0.000076	911.5683	956.7399	1004.6263	1050.7502
	O	-0.753692	1.825190	-0.000153	1052.0991	1064.1973	1113.4361	1160.2286
	O	1.451122	-0.815317	-0.000289	1206.1524	1220.09	1278.1945	1285.105
	C	2.115979	0.247308	0.000014	1319.5084	1326.5984	1377.1186	1408.8194
	C	3.627765	0.164201	0.000075	1469.2513	1481.6847	1522.5897	1544.534
	F	4.073658	-1.128267	-0.000020	1594.1748	1622.5998	1694.9454	1734.1671
	O	1.650329	1.411700	0.000262	1779.3201	1908.9164	3085.6817	3134.2587
	H	4.001488	0.676746	-0.886929	3201.2904	3208.0801	3255.1407	
	H	4.001400	0.676496	0.887257				
	H	-4.754534	-0.170189	0.000083				
	H	-1.345640	-2.475510	0.000116				
	H	0.155981	-0.611775	-0.000136				
	H	0.316480	1.606499	0.000008				
	H	-3.372956	1.913524	-0.000090				
4HPM-MFA	C	3.792751	0.049840	0.000514	32.6654	48.1929	88.741	106.2359
	C	2.087989	-1.411416	-0.000176	109.2006	122.4856	162.6222	219.9493
	C	1.558254	0.809354	-0.000095	315.8225	394.1819	478.4313	515.9172
	N	1.147650	-0.459519	-0.000351	570.4877	574.1801	577.4088	693.3889
	O	0.681160	1.786200	-0.000293	705.102	807.2801	873.7148	902.3496
	H	4.863584	0.212603	0.000862	909.745	935.1218	1008.3463	1031.0427
	H	1.723913	-2.432665	-0.000399	1048.5928	1049.1057	1077.3276	1093.7052
	H	-0.415989	-0.943956	-0.000719	1175.2108	1203.2178	1244.5353	1279.5889
	C	-2.188632	-0.222512	-0.000351	1326.1529	1330.6386	1392.5841	1426.579
	O	-1.388262	-1.257113	-0.000359	1442.5852	1469.685	1485.5774	1547.6784
	O	-1.834885	0.937071	-0.000585	1564.9748	1641.8492	1692.5149	1814.1851
	H	-0.253856	1.450030	-0.000777	2722.6525	3084.9454	3132.7832	3190.3878
	C	-3.640113	-0.641977	0.000402	3195.181	3208.8284	3255.6716	
	H	-3.830631	-1.247034	0.887984				
	F	-4.460898	0.445581	0.000671				
	H	-3.831471	-1.247247	-0.886849				
	C	2.926238	1.111708	0.000363				
	H	3.254898	2.138924	0.000569				
	N	3.388723	-1.231927	0.000241				

4PM-TFA	C	4.46369	-0.10133	0.00001	20.2135	35.9467	61.0656	88.588
	C	2.88167	1.49610	-0.00001	89.3336	105.838	165.834	202.768
	C	2.16064	-0.78993	0.00000	265.957	288.956	374.761	417.427
	N	1.90371	0.56458	-0.00000	444.394	519.842	528.579	552.031
	O	1.23550	-1.61208	-0.00000	561.885	612.47	680.631	729.572
	H	5.52365	-0.32127	0.00001	790.308	811.122	852.496	878.475
	H	2.54765	2.52630	-0.00000	889.886	949.894	1007.91	1008.87
	H	0.91455	0.84297	-0.00000	1049.19	1066.12	1100.72	1185.38
	C	-1.60828	-0.00670	-0.00002	1240.55	1240.69	1251.82	1288.7
	O	-0.88999	0.96662	-0.00001	1295.06	1401.39	1426.98	1465.18
	O	-1.26384	-1.24999	-0.00001	1505.73	1547.89	1615.57	1678.33
	H	-0.23929	-1.36572	-0.00001	1735.19	1833.49	2589.86	3202.4
	C	-3.14513	0.15346	0.00000	3209.65	3257.01	3283.44	
	F	-3.66873	-0.42482	-1.07945				
	F	-3.66870	-0.42485	1.07945				
	F	-3.48752	1.43144	0.00003				
	C	3.55449	-1.10883	0.00000				
	H	3.84026	-2.14884	0.00000				
	N	4.14513	1.22650	0.00000				
DTS _{TF} A	C	4.30525	-0.13885	0.00743	-391.231	19.4241	40.5075	64.8251
	C	2.50270	-1.47777	-0.00542	108.817	127.808	161.828	222.787
	C	2.13769	0.82133	0.00079	230.038	275.548	333.135	382.156
	N	1.65592	-0.43392	-0.00519	453.521	504.755	531.077	560.99
	O	1.34028	1.83615	0.00002	566.046	601.002	647.759	745.938
	H	5.38545	-0.06380	0.01276	791.905	799.027	823.741	873.831
	H	2.03551	-2.45541	-0.01110	879.952	909.673	990.386	1046.36
	H	0.48233	-0.65150	-0.00877	1067.76	1123.11	1132.4	1206.86
	C	-1.48823	0.12079	-0.01872	1233.59	1254.41	1284.64	1293.62
	O	-0.78890	-0.92310	-0.01233	1314.16	1324.65	1408.57	1466.33
	O	-1.10525	1.29415	-0.02290	1508.01	1543.85	1579.76	1632.06
	H	0.32703	1.59379	-0.00934	1704.15	1766.59	1804.68	2450.24
	C	-3.01312	-0.14070	0.00003	3196.78	3201.09	3232.11	
	F	-3.35980	-0.68685	1.16860				
	F	-3.71101	0.97399	-0.15939				
	F	-3.35367	-0.99016	-0.96855				
	C	3.53296	0.98953	0.00795				
	H	3.94727	1.98511	0.01354				
	N	3.80267	-1.39244	0.00038				

4HPM-TFA	C	-4.37352	-0.20102	0.00027	24.7532	35.781	56.6163	96.6555
	C	-2.51327	-1.45904	-0.00008	97.322	124.407	138.098	221.262
	C	-2.24274	0.81069	-0.00007	266.451	289.584	393.983	416.548
	N	-1.68954	-0.40258	-0.00020	442.765	492.675	528.461	571.163
	O	-1.48385	1.88405	-0.00019	573.526	610.821	707.071	735.233
	H	-5.45584	-0.16277	0.00045	804.472	811.049	849.673	857.506
	H	-2.03239	-2.43057	-0.00019	886.705	900.933	1008.57	1034.38
	H	-0.14786	-0.71218	-0.00051	1050.98	1096.64	1134.05	1202.32
	C	1.56081	0.15287	-0.00020	1238.28	1240.66	1244.68	1293.97
	O	0.86722	-0.93717	-0.00045	1326.17	1390.82	1417.81	1444.52
	O	1.14573	1.28881	-0.00007	1473.25	1546.47	1597.54	1641.52
	H	-0.52153	1.66128	-0.00029	1696.83	1824.95	2438.41	3194.33
	C	3.07844	-0.13152	0.00009	3199.32	3253.35	3325.28	
	F	3.41199	-0.83688	-1.07932				
	F	3.77147	0.99374	0.00027				
	F	3.41153	-0.83692	1.07964				
	C	-3.63502	0.95384	0.00016				
	H	-4.07931	1.93653	0.00026				
	N	-3.82460	-1.42775	0.00015				
AM	N	0.006467	-0.009784	0.005099	1031.9665		1659.1115	1659.9964
	H	0.000252	-0.000311	1.017175	3508.4383		3632.9466	3634.1498
	H	0.975515	0.003616	-0.286754				
	H	-0.379954	-0.898518	-0.286708				
MA	H	0.023849	0.002755	-0.000408	287.2922		826.4789	971.6716
	N	-0.008716	0.005405	1.010303	1086.0227		1173.1903	1342.8810
	H	0.949399	0.000307	1.333685	1459.6169		1507.7354	1525.1405
	C	-0.728378	-1.163894	1.507335	1656.6178		3024.5596	3103.1852
	H	-1.757707	-1.126562	1.154046	3137.0858		3539.6213	3618.4431
	H	-0.301887	-2.127468	1.210132				
	H	-0.758734	-1.128916	2.595259				
DMA	H	0.017620	0.043205	0.014260	229.3521		275.9823	392.5263
	N	-0.011830	0.011961	1.024223	779.1815		962.4760	1036.6011
	C	1.338887	-0.009431	1.556058	1106.3987		1192.2384	1198.2393
	H	1.884045	-0.936822	1.329660	1270.8662		1439.9675	1469.6355
	H	1.906630	0.832462	1.163676	1477.3347		1492.7086	1504.0654
	H	1.295984	0.092638	2.641403	1519.0234		1521.9096	2982.9909
	C	-0.789678	-1.133987	1.459205	2983.2835		3085.2579	3087.4267
	H	-1.774644	-1.112700	0.996039	3135.8393		3136.1261	3565.2608
	H	-0.314592	-2.098487	1.229845				
	H	-0.927143	-1.081694	2.540236				

DEA	H	-0.022605	0.006168	0.003089	102.7300	153.1683	251.2062
	N	-0.003607	0.009541	1.014762	292.1938	314.9163	430.0360
	C	1.381339	0.000712	1.472475	495.9166	730.1447	794.9260
	H	1.890569	0.820085	0.964148	817.2807	871.8659	920.9996
	H	1.391747	0.250400	2.534975	1040.4298	1066.9784	1089.5015
	C	-0.841251	-1.074121	1.518131	1151.5162	1199.2899	1218.7069
	H	-1.828873	-0.947708	1.073392	1305.0697	1328.9319	1376.0857
	H	-0.482461	-2.067431	1.215481	1396.9934	1405.2902	1413.3148
	C	-0.965006	-1.030256	3.032529	1487.0333	1490.0997	1497.8831
	H	-1.702963	-1.755089	3.373843	1503.4203	1507.1399	1513.6056
	H	-0.019387	-1.269041	3.519948	1529.4366	2988.6927	3055.2144
	H	-1.273673	-0.036375	3.356048	3062.9104	3069.3915	3087.6460
	C	2.150094	-1.299402	1.246903	3098.5035	3126.3861	3132.1888
	H	3.193385	-1.182564	1.540435	3133.6732	3141.3960	3553.3144
	H	1.731892	-2.119816	1.830599			
	H	2.123711	-1.587666	0.194462			
FA	H	-0.007136	0.000002	0.021830	644.3905	672.6897	1075.4458
	C	-0.014296	-0.000008	1.897322	1161.3815	1317.3031	1414.5474
	H	0.692320	0.000003	2.733569	1868.8596	3100.7672	3793.5220
	O	0.647680	-0.000025	0.734794			
	O	-1.202647	0.000073	2.004655			
AA	H	0.012554	0.000192	0.044887	78.6931	427.9119	545.4364
	C	-0.024402	-0.000195	1.921641	597.5930	660.8554	885.3103
	O	0.662480	0.000143	0.760567	1010.7832	1075.7514	1227.6665
	O	-1.222539	-0.000333	1.956410	1350.0239	1422.6667	1475.6280
	C	0.892572	0.000067	3.106827	1480.6995	1873.5079	3089.4061
	H	1.533577	0.879285	3.068205	3155.9324	3203.7173	3810.0413
	H	0.306029	-0.001268	4.018425			
	H	1.535931	-0.877354	3.066970			
MFA	H	0.042354	-0.000149	0.040280	96.0258	259.6232	469.6082
	C	-0.062937	0.000016	1.917516	503.2949	641.2036	651.8831
	O	0.660683	0.000070	0.783540	889.7578	1047.0024	1160.4777
	O	-1.254209	-0.000242	1.954398	1194.2536	1280.0999	1331.5114
	C	0.864145	0.000377	3.111044	1456.0656	1487.6978	1907.2512
	F	0.145654	0.000345	4.267844	3084.9484	3132.8812	3811.2405
	H	1.497438	-0.887065	3.070873			
	H	1.497019	0.888109	3.070662			

TFA	C	-0.014921	0.000010	0.019563	38.4689	238.7123	245.8967
	O	0.031707	-0.000007	1.207336	394.4444	431.9798	511.9312
	O	1.018842	0.000005	-0.815881	591.7797	599.2783	680.5415
	H	1.834190	-0.000015	-0.294558	806.0860	823.3855	1177.6687
	C	-1.334195	0.000033	-0.780924	1240.7917	1242.2791	1307.0518
	F	-1.401453	1.079420	-1.557693	1455.8314	1923.2729	3800.2776
	F	-1.401485	-1.079348	-1.557698			
	F	-2.369490	0.000046	0.037666			

Table S15 Absolute energies of all species (in Hartree) calculated at the four different levels of theory

Species	B3LYP/ 6-311++G(d,p)	B97D/ 6-311++G(d,p)	M06-2X/ 6-311++G(d,p)	M06-2X/ aug-cc-pVTZ
2PM	-339.65610359	-339.42267918	-339.51637436	-339.55393025
TS	-339.59653393	-339.36695732	-339.45716555	-339.49611996
2HPM	-339.65812580	-339.42193980	-339.52233598	-339.55999116
2PM-TFA	-866.65158134	-866.13409898	-866.33805077	-866.43431156
TS	-866.64808532	-866.12916784	-866.33343970	-866.43091824
2HPM-TFA	-866.64538923	-866.13078980	-866.33831491	-866.43413245
2PM-MFA	-668.10554227	-667.68213659	-667.84177282	-667.91509582
TS	-668.09612625	-667.67447788	-667.84177282	-667.90888359
2HPM-MFA	-668.10195097	-667.67853261	-667.84174768	-667.91483358
2PM-FA	-529.51164759	-529.16670565	-529.29563081	-529.35473024
TS	-529.50128738	-529.15809070	-529.28740232	-529.34792992
2HPM-FA	-529.50867256	-529.16345843	-529.29654377	-529.35527093
2PM-AA	-568.84837682	-568.47267038	-568.61105192	-568.67408886
TS	-568.83646555	-568.46284545	-568.60169660	-568.66627114
2HPM-AA	-568.84580819	-568.46969078	-568.61231563	-568.67510110
2PM-AM	-396.25474789	-395.98754780	-396.08099674	-396.12447399
TS	-396.23330268	-395.96760974	-396.06048569	-396.10340452
2HPM-AM	-396.25574911	-395.98661553	-396.08573395	-396.12947806
2PM-MA	-435.56626152	-435.27006985	-435.37116536	-435.41840601
TS	-435.54979515	-435.25505549	-435.35531675	-435.40214427
2HPM-MA	-435.56791734	-435.26981338	-435.37653810	-435.42415581
2PM-DMA	-474.88187467	-474.55776531	-474.66586401	-474.71709761
TS	-474.86859709	-474.54628852	-474.65362721	-474.70433621
2HPM-DMA	-474.88389302	-474.55800976	-474.67169500	-474.72326860
2PM-DEA	-553.53249355	-553.15322031	-553.27645846	-553.33542847
TS	-553.52016733	-553.14322354	-553.26572446	-553.32406780
2HPM-DEA	-553.53471064	-553.15369528	-553.28251786	-553.34200888

Species	B3LYP/ 6-311++G(d,p)	B97D/ 6-311++G(d,p)	M06-2X/ 6-311++G(d,p)	M06-2X/ aug-cc-pVTZ
2PZ	-339.64781593	-339.41499056	-339.50721856	-339.54406460
TS	-339.58472641	-339.35605566	-339.44394810	-339.48244380
2HPZ	-339.64816191	-339.41274670	-339.51135719	-339.54849760
2PZ-TFA	-866.64203732	-866.12529975	-866.32748831	-866.42293087
TS	-866.63444509	-866.11932864	-866.32187185	-866.41844625
2HPZ-TFA	-866.63785975	-866.12126691	-866.32703768	-866.42232373
2PZ-MFA	-668.09608438	-667.67341137	-667.83134666	-667.90381903
TS	-668.08563770	-667.66498962	-667.82291792	-667.89677253
2HPZ-MFA	-668.09193192	-667.66930008	-667.83093150	-667.90343426
2PZ-FA	-529.50232790	-529.15811290	-529.28537647	-529.34358781
TS	-529.49101437	-529.14870555	-529.27625508	-529.33602255
2HPZ-FA	-529.49880430	-529.15428382	-529.28567117	-529.34382238
2PZ-AA	-568.83912946	-568.46414478	-568.60079905	-568.66302110
TS	-568.82637488	-568.45370426	-568.59079829	-568.65459497
2HPZ-AA	-568.83607651	-568.46065812	-568.60159253	-568.66378184
2PZ-AM	-396.24608254	-395.97963279	-396.07138638	-396.11412033
TS	-396.22491969	-395.95988667	-396.05107060	-396.09318792
2HPZ-AM	-396.24649887	-395.97816744	-396.07550593	-396.11870594
2PZ-MA	-435.55761383	-435.26217203	-435.36152449	-435.40804470
TS	-435.54147177	-435.24747944	-435.34605802	-435.39210852
2HPZ-MA	-435.55870740	-435.26144078	-435.36641513	-435.41343390
2PZ-DMA	-474.87320522	-474.54986428	-474.65624185	-474.70673130
TS	-474.86020343	-474.53868495	-474.64436208	-474.69425649
2HPZ-DMA	-474.87466792	-474.54960357	-474.66155623	-474.71253394
2PZ-DEA	-553.52383092	-553.14533875	-553.26678722	-553.32505086
TS	-553.51177514	-553.13565827	-553.25633661	-553.31401207
2HPZ-DEA	-553.52548159	-553.14530347	-553.27239466	-553.33107798

Species	B3LYP	B97D	M06-2X	M06-2X
	/6-311++G(d,p)	/6-311++G(d,p)	/6-311++G(d,p)	/aug-cc-pVTZ
3PZ	-339.63246036	-339.40097685	-339.49018437	-339.52687399
TS	-339.56450074	-339.33769370	-339.42199462	-339.46086038
3HPZ	-339.61864818	-339.38498342	-339.48020105	-339.51817621
3PZ-TFA	-866.62416129	-866.10837176	-866.30813657	-866.40330772
TS	-866.61093085	-866.09681532	-866.29775871	-866.39427421
3HPZ-TFA	-866.61277795	-866.09759448	-866.30026864	-866.39615688
3PZ-MFA	-668.07737614	-667.65573455	-667.81116094	-667.88341013
TS	-668.06219699	-667.64262080	-667.79840383	-667.87243866
3HPZ-MFA	-668.06644904	-667.64511583	-667.80379978	-667.87691285
3PZ-FA	-529.48385496	-529.14065338	-529.26539460	-529.32336718
TS	-529.46783499	-529.12643295	-529.25208271	-529.31190198
3HPZ-FA	-529.47292542	-529.12991486	-529.25805248	-529.31691571
3PZ-AA	-568.82039386	-568.44640702	-568.58066029	-568.64260192
TS	-568.80327556	-568.43161987	-568.56640751	-568.63038445
3HPZ-AA	-568.80988269	-568.43602203	-568.57372667	-568.63659294
3PZ-AM	-396.22822348	-395.96299189	-396.05189612	-396.09458366
TS	-396.20137840	-395.93770352	-396.02569256	-396.06818593
3HPZ-AM	-396.21825455	-395.95162348	-396.04562934	-396.08947435
3PZ-MA	-435.53977720	-435.24549728	-435.34196251	-435.38844988
TS	-435.51822634	-435.22525869	-435.32054465	-435.36718389
3HPZ-MA	-435.53040057	-435.23487361	-435.33641224	-435.38418310
3PZ-DMA	-474.85546113	-474.53324876	-474.63672938	-474.68722293
TS	-474.83747226	-474.51662806	-474.61899831	-474.66964792
3HPZ-DMA	-474.84637286	-474.52306361	-474.63154478	-474.68329422
3PZ-DEA	-553.50608658	-553.12872043	-553.24729612	-553.30550088
TS	-553.48952146	-553.11383563	-553.23109040	-553.28957254
3HPZ-DEA	-553.49713582	-553.11870215	-553.24230207	-553.30176289

Species	B3LYP/ 6-311++G(d,p)	B97D/ 6-311++G(d,p)	M06-2X/ 6-311++G(d,p)	M06-2X/ aug-cc-pVTZ
4PM	-339.66245694	-339.42878926	-339.52304729	-339.55995627
TS	-339.59983888	-339.37019641	-339.46038818	-339.49895493
4HPM	-339.65927184	-339.42322521	-339.52339790	-339.56060506
4PM-TFA	-866.65618081	-866.13846384	-866.34292219	-866.43840117
TS	-866.64727108	-866.13110779	-866.33608356	-866.43262196
4HPM-TFA	-866.64993278	-866.13266508	-866.34012652	-866.43551990
4PM-MFA	-668.11017712	-667.68652947	-667.84670665	-667.91927294
TS	-668.09842599	-667.67683827	-667.83721121	-667.91112355
4HPM-MFA	-668.10405008	-667.68054917	-667.84407173	-667.91669953
4PM-FA	-529.51651355	-529.17132754	-529.30078438	-529.35910461
TS	-529.50397499	-529.16082179	-529.29074686	-529.35050805
4HPM-FA	-529.51086820	-529.16568733	-529.29871281	-529.35701033
4PM-AA	-568.85334573	-568.47737007	-568.61635269	-568.67859047
TS	-568.83948976	-568.46590288	-568.60525562	-568.66914031
4HPM-AA	-568.84814689	-568.47207317	-568.61464465	-568.67698420
4PM-AM	-396.26056931	-395.99315578	-396.08717236	-396.12994332
TS	-396.23912747	-395.97305665	-396.06641475	-396.10857416
4HPM-AM	-396.25829668	-395.98933934	-396.08827854	-396.13149343
4PM-MA	-435.57210341	-435.27568884	-435.37722017	-435.42381200
TS	-435.55587164	-435.26078926	-435.36155237	-435.40762984
4HPM-MA	-435.57053055	-435.27265687	-435.37917736	-435.42627559
4PM-DMA	-474.88768989	-474.56339863	-474.67194565	-474.72254162
TS	-474.87471848	-474.55212569	-474.66001791	-474.70994712
4HPM-DMA	-474.88639340	-474.56084252	-474.67436070	-474.72539477
4PM-DEA	-553.53830020	-553.15883335	-553.28251700	-553.34085099
TS	-553.52634048	-553.14917269	-553.27224533	-553.32988312
4HPM-DEA	-553.53732288	-553.15656767	-553.28518942	-553.34398006

Table S16 Sum of electronic and thermal free energies of all species (in Hartree) calculated at M06-2X/ aug-cc-pVTZ levels of theory (at 298 K)

Species	Pair A	Pair B	Pair C	Pair D
Amide	-339.500221	-339.490347	-339.473061	-339.505768
TS	-339.447032	-339.433651	-339.412281	-339.449722
Imidic Acid	-339.50903	-339.494876	-339.465134	-339.506485
Amide-TFA	-866.353657	-866.342284	-866.322751	-866.357211
TS _{TFA}	-866.352402	-866.340614	-866.316923	-866.354746
Imidic Acid-TFA	-866.353123	-866.341490	-866.316159	-866.354388
Amide-MFA	-667.815663	-667.804410	-667.784130	-667.819451
TS _{MFA}	-667.813188	-667.801544	-667.777884	-667.815587
Imidic Acid-MFA	-667.815356	-667.804241	-667.778287	-667.817077
Amide-FA	-529.272387	-529.260943	-529.240898	-529.276066
TS _{FA}	-529.269508	-529.258044	-529.234283	-529.272042
Imidic Acid-FA	-529.272043	-529.261265	-529.234933	-529.274005
Amide-AA	-568.566356	-568.555368	-568.535022	-568.570414
TS _{AA}	-568.563445	-568.553027	-568.529192	-568.567127
Imidic Acid-AA	-568.567694	-568.556717	-568.53019	-568.569478
Amide-AM	-396.038117	-396.027893	-396.008634	-396.043243
TS _{AM}	-396.019114	-396.008788	-395.98417	-396.023528
Imidic Acid-AM	-396.04335	-396.032881	-396.003969	-396.044969
Amide-MA	-435.305409	-435.295047	-435.27569	-435.310686
TS _{MA}	-435.291222	-435.281079	-435.255776	-435.295752
Imidic Acid-MA	-435.311022	-435.300564	-435.271959	-435.312607
Amide-DMA	-474.578271	-474.567944	-474.548801	-474.58336
TS _{DMA}	-474.567219	-474.558021	-474.532724	-474.572121
Imidic Acid-DMA	-474.58427	-474.573792	-474.545043	-474.586137
Amide-DEA	-553.143103	-553.132747	-553.113444	-553.148134
TS _{DEA}	-553.133286	-553.123421	-553.097943	-553.13818
Imidic Acid-DEA	-553.149337	-553.139293	-553.110576	-553.150406