Supporting Information

Newly Identified C–H···O Hydrogen Bond in Histidine

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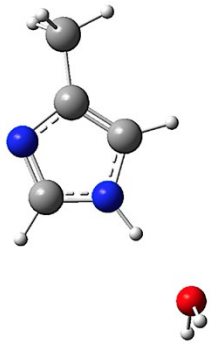
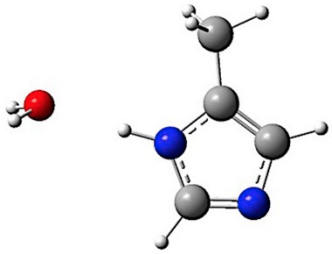
A. Optimized Geometries and Geometric Parameters for N–H···O and N–methylacetamide Complexes.

tau-5-methylimidazole /N3–H···water



pi-5-methylimidazole /N1–H···water



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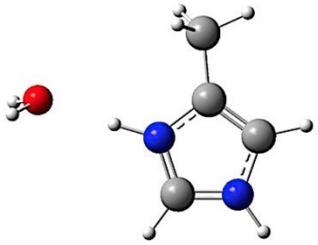

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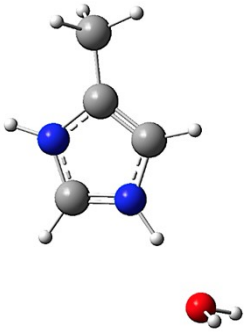
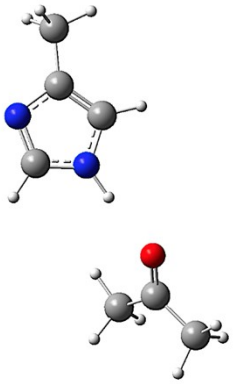
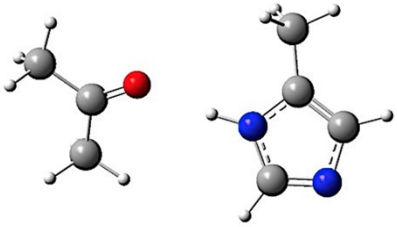


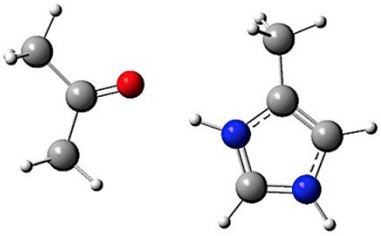
tau-5-methylimidazole /N3–H···acetone



pi-5-methylimidazole /N1–H···acetone



5-methylimidazolium /N1–H···acetone



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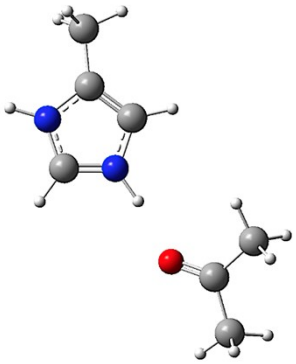

Figure S1. BHandHLYP/6-31+G(d,p) optimized geometries of the water and acetone complexes. Atoms are displayed with covalent radii scaled to 50%. Atom coloring scheme: carbon (grey), hydrogen (white), nitrogen (blue), oxygen (red). Visual images captured from GaussView 5.0 software. Note that the imidazolium species carry a +1 charge.

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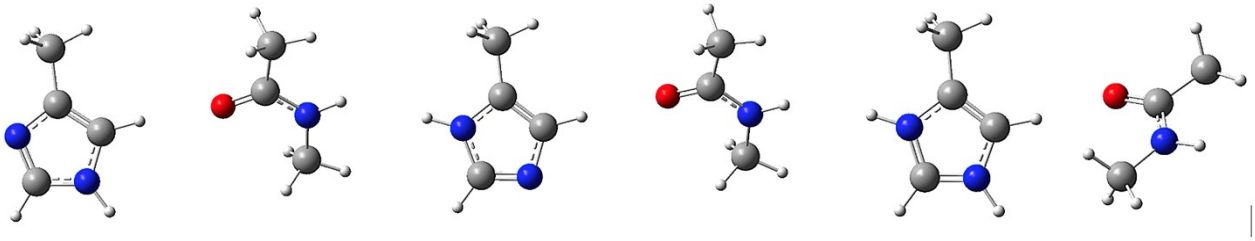
tau-5-methylimidazole /C4(δ)–H···amide

pi-5-methylimidazole /C4(δ)–H···amide

5-methylimidazolium /C4(δ)–H···amide



tau-5-methylimidazole /C2(ε)–H···amide

pi-5-methylimidazole /C2(ε)–H···amide

5-methylimidazolium /C2(ε)–H···amide

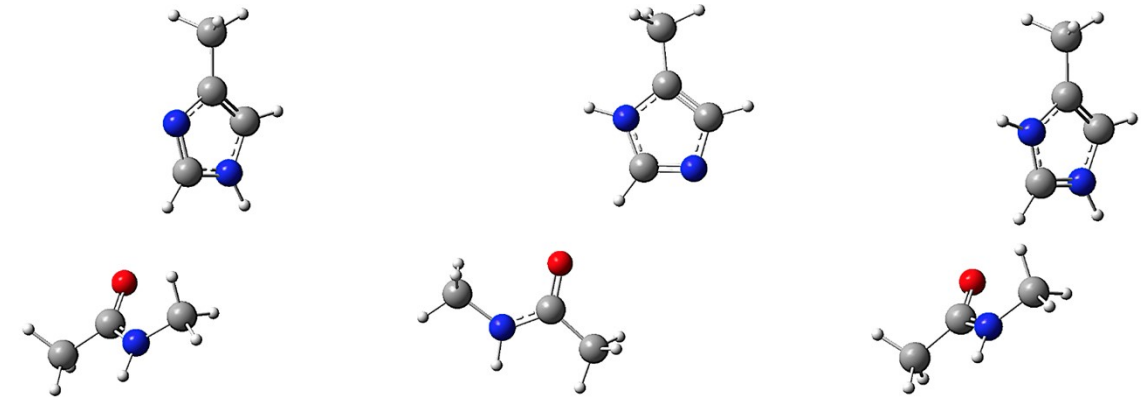


Figure S2. BHandHLYP/6-31+G(d,p) optimized geometries of the N-methylacetamide ("amide") complexes. Atoms are displayed with covalent radii scaled to 50%. Atom coloring scheme: carbon (grey), hydrogen (white), nitrogen (blue), oxygen (red). Visual images captured from GaussView 5.0 software. Note that the imidazolium species carry a +1 charge.

Table S1. Geometric data for complexes optimized at the BHandHLYP/6-31+G(d,p) level with C-PCM solvation (water). Complexes can be seen in Figures S1 and S2.

Complex Name	***H-bond length (Å)***	***O - - - C or O - - - N distance (Å)***	***C-H···O or N–H···O angle (degrees)***
tau-5-methylimidazole/C4-H···water	2.30	3.37	176
tau-5-methylimidazole/C2-H···water	2.26	3.34	179
pi-5-methylimidazole/C4-H···water	2.39	3.47	178
pi-5-methylimidazole/C2-H···water	2.27	3.34	179
5-methylimidazolium/C4-H···water	2.14	3.22	176
5-methylimidazolium/C2-H···water	2.03	3.11	179
tau-5-methylimidazole/C4-H···acetone	2.34	3.41	178
tau-5-methylimidazole/C2-H···acetone	2.30	3.38	177
pi-5-methylimidazole/C4-H···acetone	2.46	3.54	179
pi-5-methylimidazole/C2-H···acetone	2.30	3.38	176
5-methylimidazolium/C4-H···acetone	2.17	3.24	170
5-methylimidazolium/C2-H···acetone	2.04	3.12	175
tau-5-methylimidazole/C4-H···amide	2.27	3.34	175
tau-5-methylimidazole/C2-H···amide	2.23	3.31	174
pi-5-methylimidazole/C4-H···amide	2.40	3.48	178
pi-5-methylimidazole/C2-H···amide	2.24	3.31	174
5-methylimidazolium/C4-H···amide	2.10	3.17	174
5-methylimidazolium/C2-H···amide	1.97	3.04	172
tau-5-methylimidazole/N3-H···water	1.89	2.90	178
pi-5-methylimidazole/N1-H···water	1.89	2.90	179
5-methylimidazolium/N1-H···water	1.76	2.78	179
5-methylimidazolium/N3-H···water	1.75	2.78	179
tau-5-methylimidazole/N3-H···acetone	1.90	2.91	176
pi-5-methylimidazole/N1-H···acetone	1.90	2.91	174
5-methylimidazolium/N1-H···acetone	1.76	2.78	170
5-methylimidazolium/N3-H···acetone	1.75	2.77	173

B. Additional Data Analysis Details.

i. Calculation of total NPA charge transferred from water (or acetone) to the respective 5-methylimidazole isomer:

To calculate the total NPA charge transfer from electron pair donor to electron pair acceptor for the water complexes, the NPA atomic charges for all the atoms of water in respective complexes were summed up and noted to be positive for all complexes. The sum of the NPA charges on the atoms in isolated water (sum = 0) were then subtracted from this number. As would be expected, the sum of the atomic charges for the isolated water were almost always 0.000. Occasionally, the sum of the charges in a molecule that should have no net charge will be ±0.001 e. For charge transfer calculations in the acetone complexes, the same procedure as above was followed, but instead using summations of the NPA charges on acetone atoms. Again, the sum of the atomic charges of acetone in the acetone complexes were found to be positive, indicating a transfer of electron density from acetone to 5-methylimidazole.

ii. Calculation of Bond Critical Points using AIM-UC software:

In the AIM-UC v1.6.4 software, the "Find 3D Critical Points" under the "Process" tab was used to visually display the bond critical points in the complexes using the density cube files (see page S12). The default settings of the program for the bond critical point search were as follows:

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Min. Density: 0.001
Nuclear Density: 0.4
Min Atom Radius: 0.16
Convergence: 1*10^-6
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These default settings were not changed. In this way, BCP data was gathered for all of the complexes, as seen in Table 9.

iii. Experimental Control for BCP Analysis:

To give confidence that the bond critical points calculated for the complexes weren't simply artifacts, the following control study was conducted. The BHandHLYP/6-31+G(d,p) optimized pi-C4 complexes for both water and acetone were selected for the study. In each respective complex, the H-bond length was increased by 1.000 Å and a single point energy calculation at the MP2/aug-cc-pVTZ level was performed. Only the intermolecular distance was altered to increase the H-bond length; no intramolecular changes in either the water (or acetone) and 5-methylimidazole were made. From there, new density cube files were generated and examined in AIM-UC for bond critical points. It was observed, that upon increasing the H-bond length in the water complex by 1.000 Å, a BCP was still detected (ϱ = 0.001053 au, $\nabla^2\varrho$ = 0.004769). However, the electron density at the BCP of 0.001053 au falls well below the expected value (~0.024-0.139 au) for an H-bonding interaction reported by Koch and Popelier (1995). Upon increasing the H-bond length by 2.000 Å in the water complex, no BCP was detected using the AIM-UC default settings listed above. For the pi-C4 acetone complex it was observed that, upon increasing the H-bond length by 1.000 Å, no BCP was detected using the AIM-UC default settings listed above.

C. Additional Data Tables and Graphs.

i. New IR bands upon complex formation:

The new calculated IR bands in Table S2 were determined by visual inspection of the vibrational modes in GaussView 5.0. Only bands with relatively large displacement vectors on the water moiety were included in Table S2.

Table S2. New calculated IR bands (cm^{-1}) upon complex formation.

Complex Name	BHandHLYP/6-31+G(d)	BHandHLYP/6-31+G(d,p)	M06-2X/6-31+G(d,p)	MP2/6-31+G(d)	MP2/aug-cc-pVTZ
tau-5-methylimidazole/C4–H···water	134.9, 92.6, 84.5, 53.6, 35.9, 28.1	140.8, 136.3, 92.6, 75.3, 65.1, 50.3, 36.3	225.7, 202.6, 131.6, 108.5, 37.8, 37.0	157.1, 100.9, 97.9, 95.9, 56.4, 53.5, 30.4	116.3, 86.4, 72.7, 48.8, 41.6, 18.6
tau-5-methylimidazole/C2–H···water	158.8, 95.8, 89.7, 63.4, 45.6, 35.6	119.1, 95.1, 75.9, 41.3, 33.9, 25.6	184.9, 131.4, 107.4, 79.8, 39.1, 13.5	158.9, 101.5, 100.6, 94.0, 57.1, 52.5, 38.0	128.6, 122.1, 86.8, 72.6, 48.9, 41.1, 29.5
pi-5-methylimidazole/C4–H···water	103.6, 71.7, 69.7, 55.9, 43.4, 18.8	139.6, 136.5, 77.1, 74.0, 64.7, 51.2, 19.0	207.8, 184.3, 160.3, 85.8, 57.6, 51.1	127.9, 107.6, 104.5, 88.1, 56.0, 51.9, 28.1	93.5, 77.2, 74.0, 47.8, 34.0, 27.7
pi-5-methylimidazole/C2–H···water	145.7, 94.9, 80.1, 63.8, 45.6, 40.8	119.9, 96.1, 87.5, 70.7, 40.6, 39.5	222.2, 182.9, 127.7, 108.2, 33.0, 22.8	157.3, 102.9, 97.4, 66.2, 53.6, 44.2	125.9, 122.5, 87.6, 73.2, 46.3, 40.7, 33.23
5-methylimidazolium/C4–H···water	167.1, 118.6, 95.1, 66.3, 45.1, 22.4	151.8, 114.8, 97.6, 67.7, 57.6, 41.6	236.9, 206.9, 158.1, 124.0, 61.0, 10.0	143.6, 124.2, 103.4, 73.7, 63.1, 48.2, 42.6	142.5, 131.9, 110.1, 58.5, 50.3, 39.0, 27.2
5-methylimidazolium/C2–H···water	156.4, 141.2, 90.5, 61.1, 53.8	136.4, 132.1, 130.1, 85.5, 57.5, 51.8	211.5, 177.1, 140.2, 59.1, 48.0	241.8, 202.0, 139.7, 126.0, 104.4, 65.6, 50.2, 21.2	176.0, 123.5, 119.7, 105.6, 52.4, 44.4, 8.91
tau-5-methylimidazole/C4–H···acetone	51.2, 48.1, 24.9, 23.4, 20.4, 18.3	54.4, 50.7, 43.3, 26.7, 22.7, 21.8, 8.11	72.7, 65.0, 42.0, 37.2, 19.3	*	*
tau-5-methylimidazole/C2–H···acetone	55.5, 45.6, 31.1, 20.3, 15.5, 13.8	58.6, 57.5, 43.4, 29.7, 19.7, 16.1, 10.5	62.3, 32.9, 28.0, 20.6, 18.3, 6.08	*	*
pi-5-methylimidazole/C4–H···acetone	50.1, 45.0, 29.2, 27.2, 22.3, 15.1	51.5, 46.8, 29.8, 28.2, 24.4, 16.0	61.5, 47.8, 44.7, 31.6, 22.0, 11.5	*	*
pi-5-methylimidazole/C2–H···acetone	64.4, 51.7, 40.2, 31.1, 27.2, 20.6, 16.3	67.4, 53.9, 42.4, 30.7, 22.6, 21.6, 15.6	83.5, 71.7, 49.8, 45.6, 43.5, 29.3, 13.0	*	*
5-methylimidazolium/C4–H···acetone	74.6, 70.2, 50.9, 37.9, 25.6, 24.2, 8.93	77.3, 70.4, 53.9, 33.9, 30.9, 19.2, 11.3	99.5, 91.0, 78.6, 61.8, 33.4, 25.5, 7.67	*	*
5-methylimidazolium/C2–H···acetone	98.8, 70.3, 68.8, 49.0, 29.4, 26.8, 19.4	99.0, 74.4, 66.6, 55.6, 35.1, 33.4, 23.7	101.7, 93.1, 71.7, 55.0, 39.0, 32.9, 17.4	*	*

**Unable to geometrically optimize*

ii. Presentation of a wide variety of correlations and linear regression parameters:

It is of interest to examine whether various parameters of complex formation are correlated. For example, an IUPAC criterion for H-bonding is that the interaction energy of complex formation shows good correlation with the extent of charge transfer between donor and acceptor. Linear regression parameters were calculated in Microsoft Excel for the various properties at all levels of theory, as shown in Table S3A for water complexes and Table S3B for acetone complexes.

Table S3A. Linear regression parameters for 5-methylimidazole···water complexes for selected properties. ΔE* is assumed to equal E (complex) - Σ E (separated species). ΔE_{MP2} *is the change in MP2 energy upon complex formation. Change in NPA charge of hydrogen refers to H atom participating in the H-bond. Change in calculated isotropic shielding on hydrogen atom participating in H-bond is represented by Δσ, in units of ppm. The C–H refers to the C–H group of the methylimidazole ring that participates in the H-bond.

Level of Theory	y-axis	x-axis	Slope (m)	Intercept (b)	Coefficient of determination (r^2)
BHandHLYP/6-31+G(d)	$\Delta E_{BHandHLYP}$ (kcal/mol)	O···H hydrogen bond length (Å)	7.5222	-18.176	0.9742
	$\Delta E_{BHandHLYP}$ (kcal /mol)	C–H···O angle (degrees)	0.1774	-33.031	0.0479
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔC–H Bond length (Å)	-405.89	-0.1482	0.9931
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔO–H Bond length of water (Å)	-5558.5	0.3583	0.8016
	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	0.0024	0.017	0.7199
	$\Delta E_{BHandHLYP}$ (kcal/mol)	Total charge transfer (e) between species	-196.26	0.5514	0.9624
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	*	*	*
BHandHLYP/6-31+G(d,p)	$\Delta E_{BHandHLYP}$ (kcal/mol)	O···H hydrogen bond length (Å)	7.3075	-17.787	0.9722
	$\Delta E_{BHandHLYP}$ (kcal/mol)	C–H···O angle (degrees)	-0.0553	8.3727	0.0066
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔC–H Bond length (Å)	-409.89	-0.2071	0.9931
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔO–H Bond length of water (Å)	-9197.9	1.8039	0.9921
	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	-0.0054	0.0315	0.4466
	$\Delta E_{BHandHLYP}$ (kcal/mol)	Total charge transfer (e) between species	-209.33	0.1435	0.934
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	-211.45*	1.1566*	0.9536*
M06-2X/6-31+G(d,p)	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	O···H hydrogen bond length (Å)	8.0468	-19.526	0.961
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	C–H···O angle (degrees)	-0.0718	10.76	0.3465
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	ΔC–H Bond length (Å)	-378.77	-0.4148	0.9955
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	ΔO–H Bond length of water (Å)	-8423	0.6187	0.631

	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	0.002	0.0167	0.4576
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	Total charge transfer (e) between species	-199.53	0.2187	0.9819
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	*	*	*
MP2/6-31+G(d)	ΔE_{MP2} (kcal/mol)	O···H hydrogen bond length (Å)	8.614	-21.052	0.980
	ΔE_{MP2} (kcal/mol)	C–H···O angle (degrees)	2.7033	-485.62	0.6375
	ΔE_{MP2} (kcal/mol)	ΔC–H Bond length (Å)	-412.3	1.1508	0.9849
	ΔE_{MP2} (kcal/mol)	ΔO–H Bond length of water (Å)	-5308.5	3.5501	0.2251
	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	-0.0152	-0.0077	0.9775
	ΔE_{MP2} (kcal/mol)	Total charge transfer (e) between species	-163.47	-0.0431	0.9793
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	*	*	*
MP2/aug-cc-pVTZ	ΔE_{MP2} (kcal/mol)	O···H hydrogen bond length (Å)	5.4868	-14.058	0.9452
	ΔE_{MP2} (kcal/mol)	C–H···O angle (degrees)	2.265	-406.85	0.6338
	ΔE_{MP2} (kcal/mol)	ΔC–H Bond length (Å)	-340.23	0.8315	0.9903
	ΔE_{MP2} (kcal/mol)	ΔO–H Bond length of water (Å)	-10229	1.8579	0.7392
	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	-0.0084	-0.0004	0.9419
	ΔE_{MP2} (kcal/mol)	Total charge transfer (e) between species	-175.2	-0.0408	0.9591
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	*	*	*
* Bond critical point analysis only calculated at the MP2/aug-cc-pVTZ level on BHandHLYP/6-31+G(d,p) geometries.					

Table S3B. Linear regression parameters for 5-methylimidazole···acetone complexes for selected properties.

Level of Theory	y-axis	x-axis	Slope (m)	Intercept (b)	Coefficient of determination (r^2)
BHandHLYP/6-31+G(d)	$\Delta E_{BHandHLYP}$ (kcal/mol)	O···H hydrogen bond length (Å)	5.5395	-13.786	0.9309
	$\Delta E_{BHandHLYP}$ (kcal/mol)	C–H···O angle (degrees)	0.120	-22.01	0.2426
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔC–H Bond length (Å)	-351.84	-0.3739	0.9864
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔC=O Bond length of acetone (Å)	-1186.4	-0.1659	0.9991
	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	0.0009	0.0121	0.2006
	$\Delta E_{BHandHLYP}$ (kcal/mol)	Total charge transfer (e) between species	-139.1	-0.0398	0.9714
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	*	*	*
BHandHLYP/6-31+G(d,p)	$\Delta E_{BHandHLYP}$ (kcal/mol)	O···H hydrogen bond length (Å)	5.9342	-14.705	0.9394
	$\Delta E_{BHandHLYP}$ (kcal/mol)	C–H···O angle (degrees)	0.1697	-31.088	0.3609
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔC–H Bond length (Å)	-347.23	-0.3587	0.9862
	$\Delta E_{BHandHLYP}$ (kcal/mol)	ΔC=O Bond length of acetone (Å)	-1229	-0.2232	0.9927
	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	0.0005	0.0119	0.1285
	$\Delta E_{BHandHLYP}$ (kcal/mol)	Total charge transfer (e) between species	-141.82	-0.0173	0.9963
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	-190.66*	-0.0101*	0.9706*
M06-2X/6-31+G(d,p)	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	O···H hydrogen bond length (Å)	3.5084	-9.9743	0.4862
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	C–H···O angle (degrees)	-0.0061	-0.9404	0.0231
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	ΔC–H Bond length (Å)	-232.97	1.3092	0.6106
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	ΔC=O Bond length of acetone (Å)	-1004.1	0.6147	0.7883
	Change in NPA charge (Δe) of hydrogen	Δσ (ppm)	-0.026	-0.043	0.166
	$\Delta E_{M06\text{-}2X}$ (kcal/mol)	Total charge transfer (e) between species	-72.073	-1.1608	0.2837
	ΔE_{MP2} (kcal/mol)	electron density (au) at bond critical point	*	*	*
* Bond critical point analysis only calculated at the MP2/aug-cc-pVTZ level on BHandHLYP/6-31+G(d,p) geometries.					

iii. The effect of solvent dielectric on ΔE_{MP2} of complex formation:

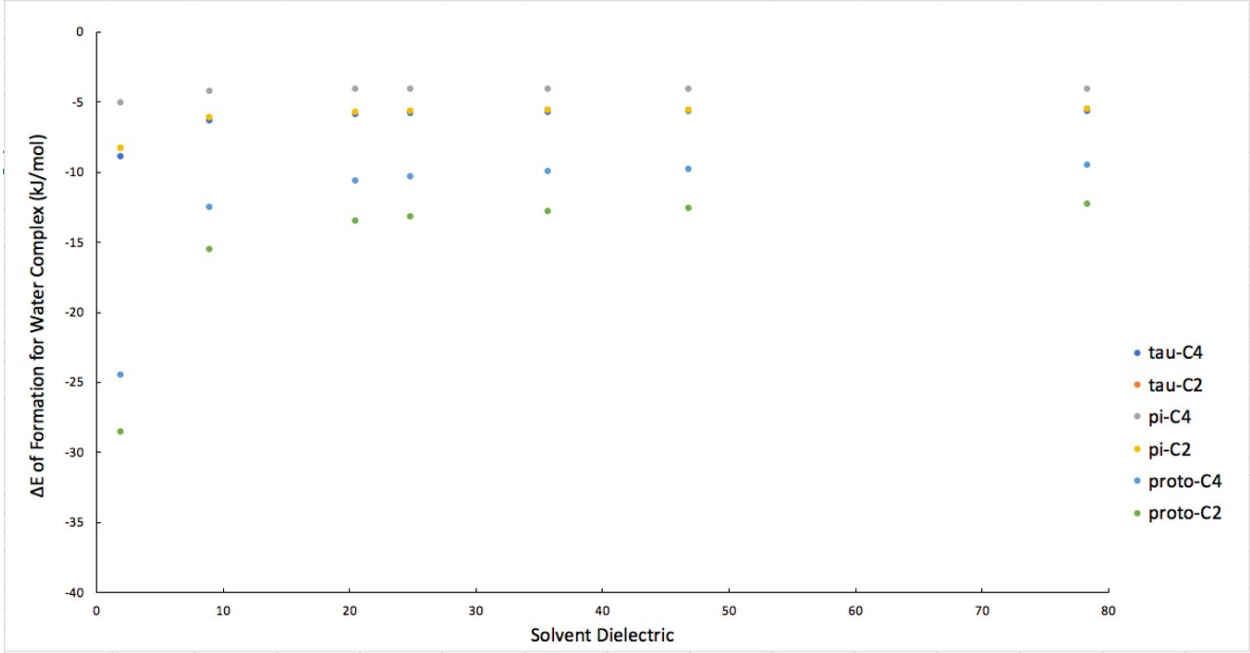


Figure S3. *ΔE_{MP2} vs. solvent dielectric for water complexes. Single point calculations performed at the MP2/aug-cc-pVTZ level on BHandHLYP/6-31+G(d,p) geometries. The C-PCM solvation model was used for testing different dielectrics. As solvent dielectric increases, ΔE_{MP2} becomes more positive and $\frac{d\Delta EMP2}{d\varepsilon}$ decreases.*

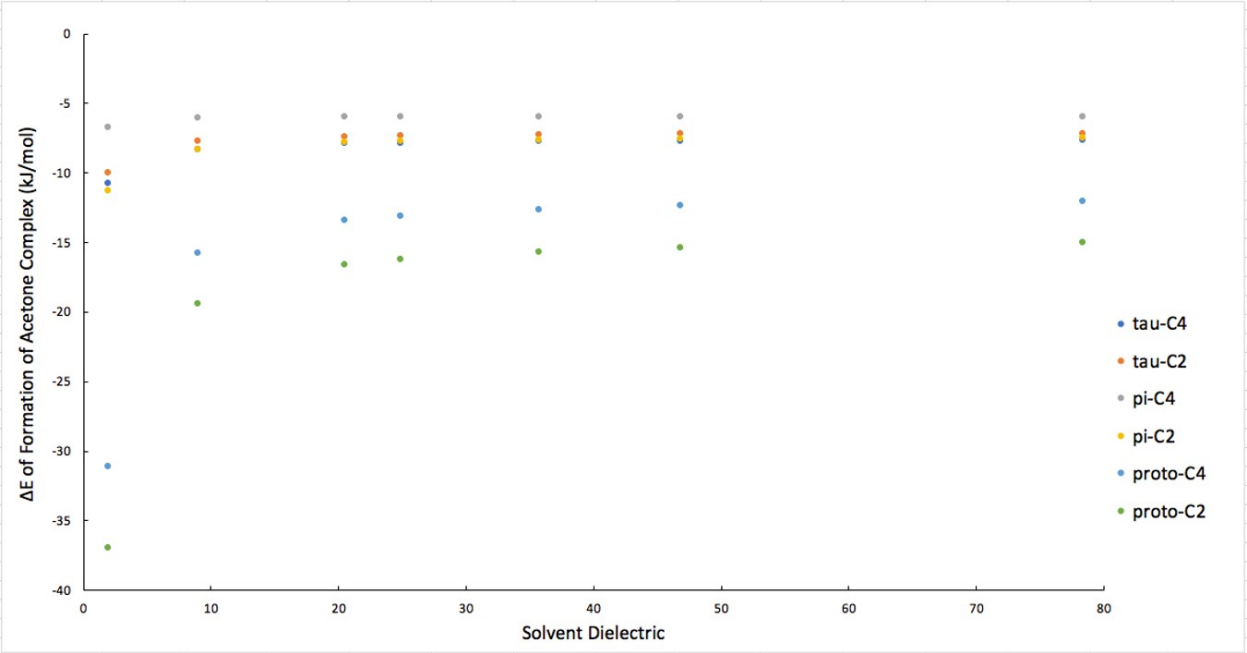


Figure S4. *ΔE_{MP2} vs. solvent dielectric for acetone complexes. Single point calculations performed at the MP2/aug-cc-pVTZ level on BHandHLYP/6-31+G(d,p) geometries. The C-PCM solvation model was used for testing different dielectrics. As solvent dielectric increases, ΔE_{MP2} becomes more positive and $\frac{d\Delta EMP2}{d\varepsilon}$ decreases.*

D. Electrostatic Potential Surfaces for H-bonding Complexes.

Shown below are the electrostatic potential surfaces for water, acetone, benzene, and a selection of the species analyzed in this study. Water, acetone, and benzene surfaces were generated as an experimental control; the fact that these surfaces show the expected color patterns gives reassurance that the surfaces of interest to this work are at least qualitatively reasonable. The cube files were generated using the G09 cubegen utility. The structures below were geometrically optimized at the BHandHLYP/6-31+G(d,p) level. Single point energy calculations were then performed on these optimized geometries at the MP2/aug-cc-pVTZ level. From the checkpoint files (.chk) generated during energy calculations, formcheck files (.fchk) were created using the G09 formcheck utility using the following line in a terminal window:

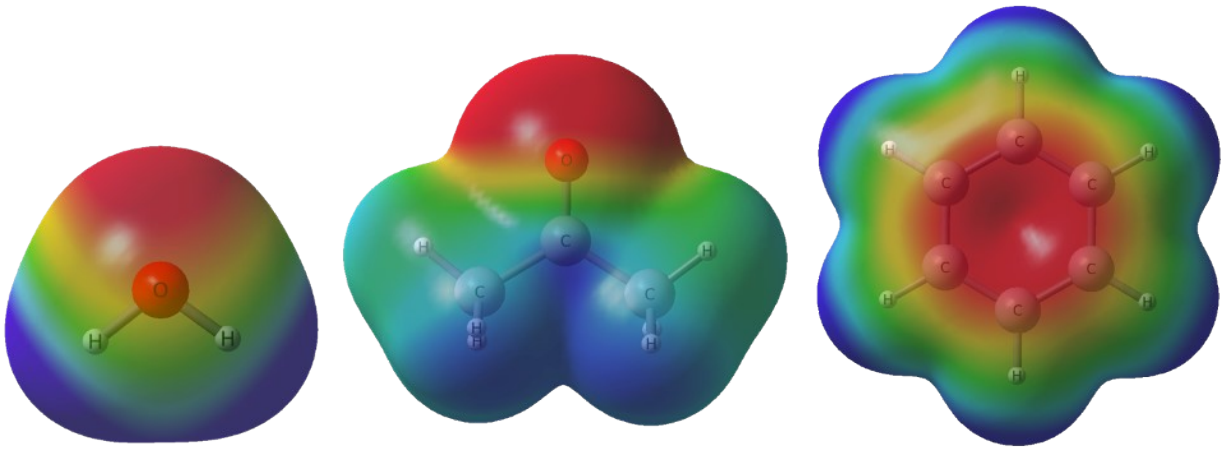
```
formchk filename.chk filename.fchk
```

Next, density and potential cube (.cube) files were generated in the G09 cubegen utility using the following respective lines in a terminal window:

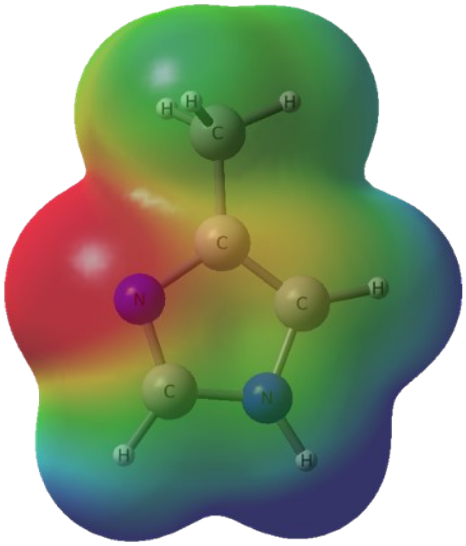
```
cubegen 0 density filename.fchk filename_density.cube 80
cubegen 0 potential filename.fchk filename_potential.cube 80
```

The electrostatic potential was mapped onto the 0.002 au electron density isosurface in GaussView 5.0. The range of electrostatic potentials on the 0.002 au surface is represented by the following color bar. In terms of electrostatic potential, the left side of the bar (dark red) is most negative, and the right side (dark blue) is most positive.

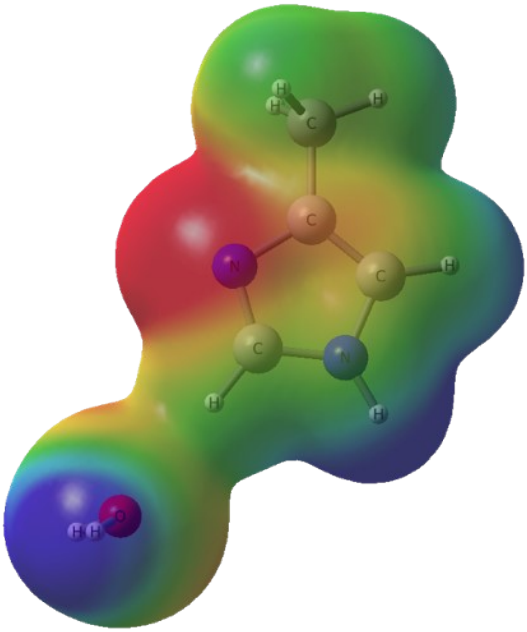
For neutral species, the range of electrostatic potentials is ± 38 kcal/mol (except benzene, for which the range is ±19 kcal/mol) and so the green in the middle of the color scale nicely represents an electrostatic potential of zero. For species of +1 charge, it was found that all potentials on the 0.002 au surface are positive, and so the color scale ranges from +56 kcal/mol at the red end to $+1.4*10^2$ kcal/mol at the blue end. The electrostatic potential ranges selected are not arbitrary; these respective ranges for the neutral and +1 species give the most visually satisfying range of colors.



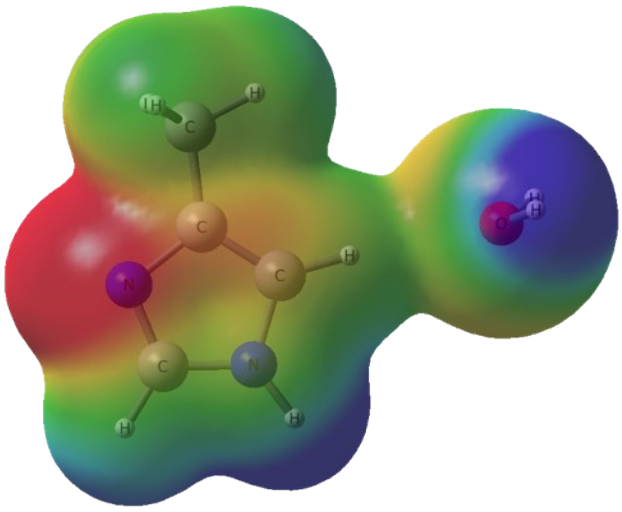
Water Acetone Benzene



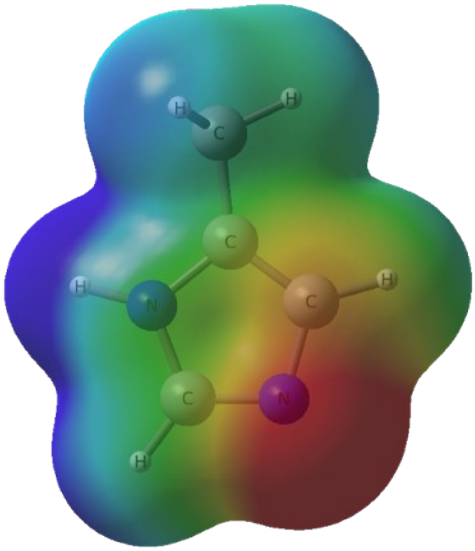
tau-5-methylimidazole



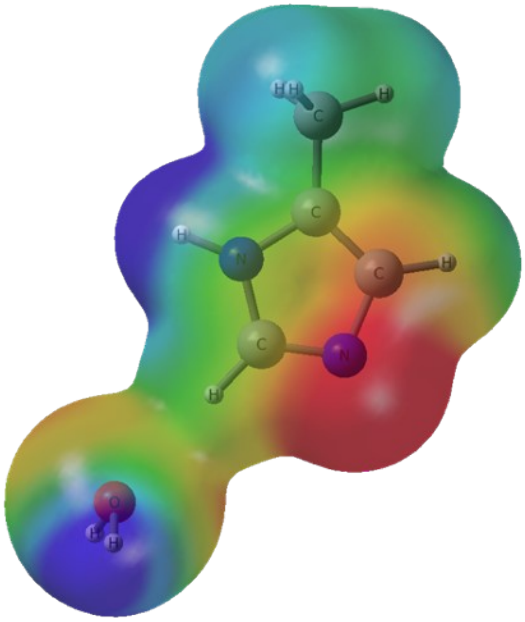
tau-5-methylimidazole/C2-H···water



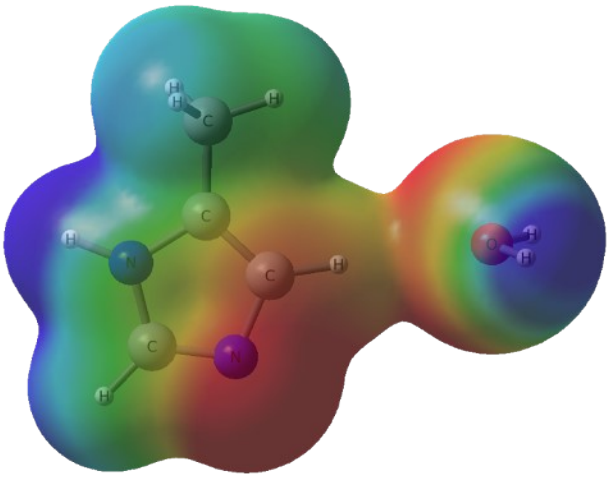
tau-5-methylimidazole/C4-H···water



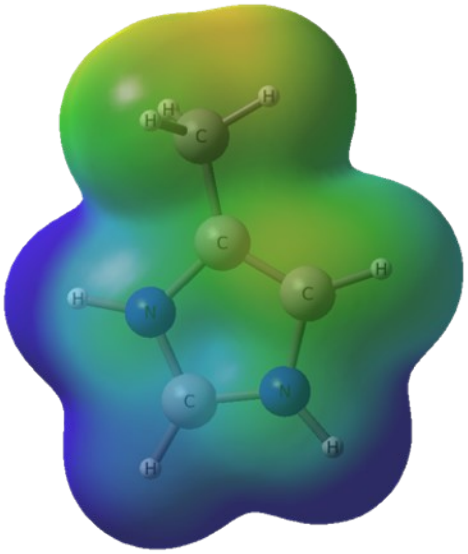
pi-5-methylimidazole



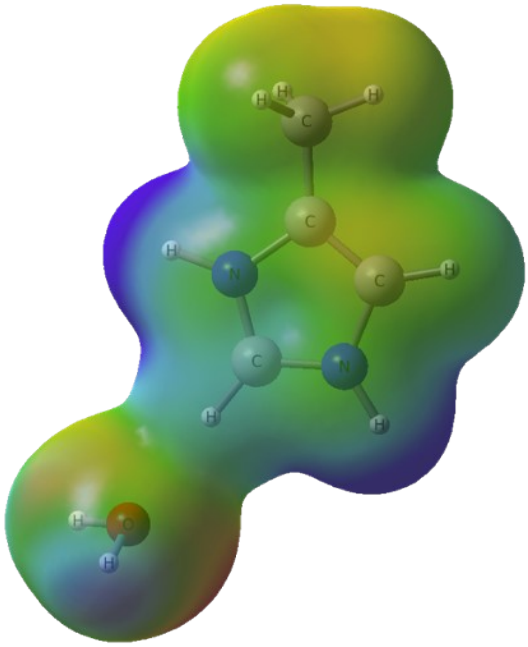
pi-5-methylimidazole/C2-H···water



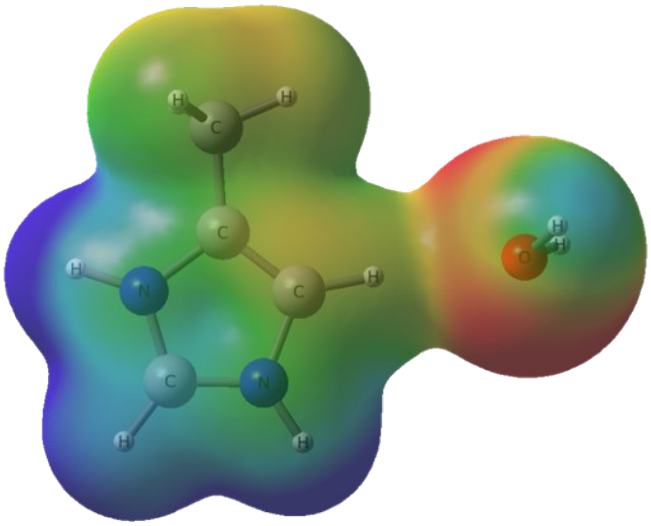
pi-5-methylimidazole/C4-H···water



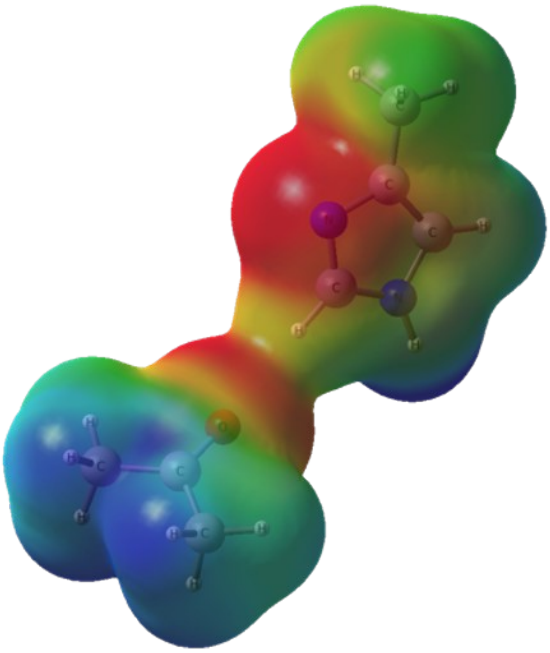
5-methylimidazolium



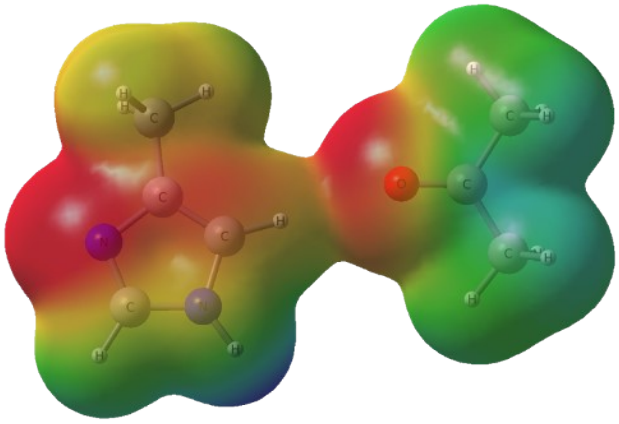
5-methylimidazolium/C2-H···water



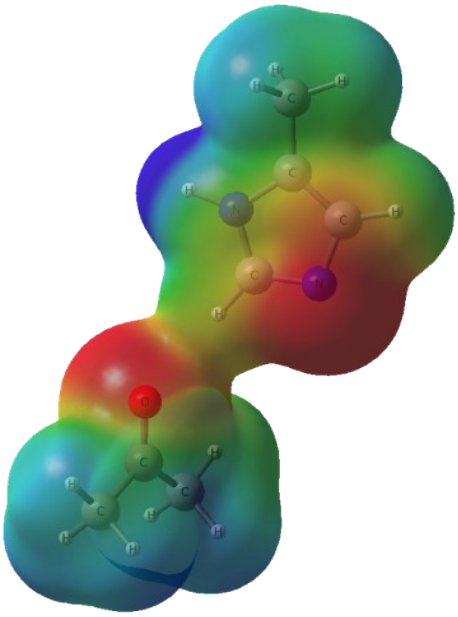
5-methylimidazolium/C4-H···water



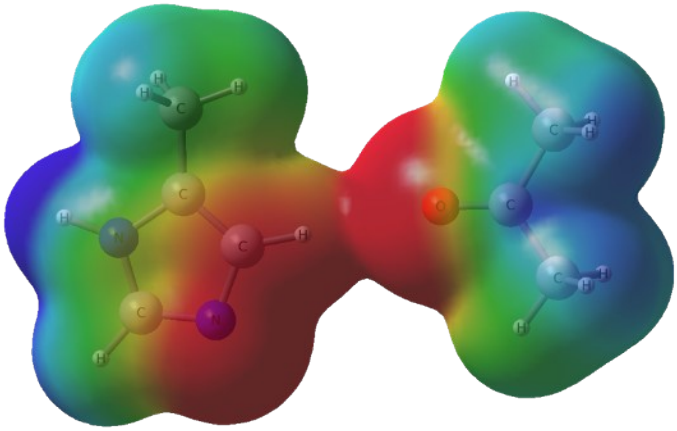
tau-5-methylimidazole/C2-H···acetone



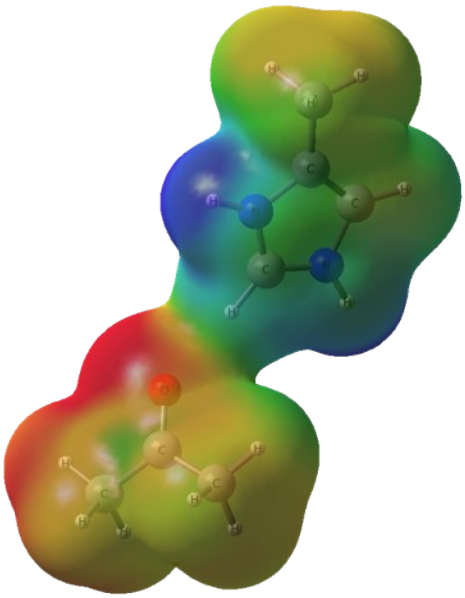
tau-5-methylimidazole/C4-H···acetone



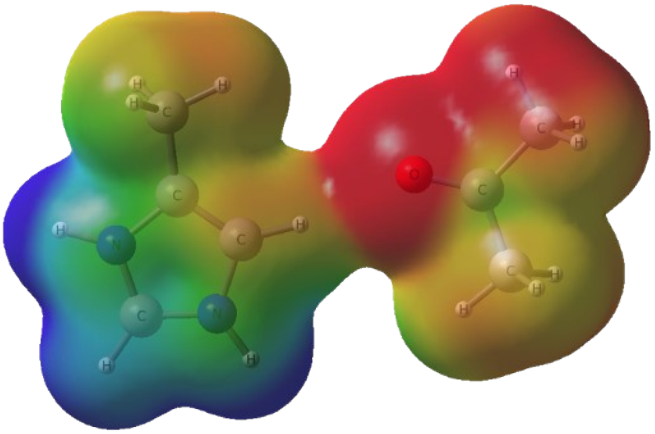
pi-5-methylimidazole/C2-H···acetone



pi-5-methylimidazole/C4-H···acetone



5-methylimidazolium/C2-H···acetone



5-methylimidazolium/C4-H···acetone

Table S4. Electrostatic potential (kcal/mol) on the 0.002 au isodensity surface for the three forms of 5-methylimidazole. For identification of the respective sites, see Figure S5.

	N1 site	*C2 site*	*N3 site*	*C4 site*
tau-5-methylimidazole	-62	35	80	38
pi-5-methylimidazole	80	35	-65	15
5-methylimidazolium	173	149	172	122

It was found, for the water complexes, that a plot of $\Delta E_{complex}$ calculated at the MP2/aug-cc-pVTZ level (Table 8a) vs. electrostatic potential at the respective acceptor position (either the C2 or C4 site) shown in Table S4 yields a line of best fit: y = -0.0134x – 0.812 with a coefficient of determination of 0.982. Hence, a strong linear correlation between the electrostatic potential of the Lewis acidic acceptor site and the strength of the hydrogen bond is observed.

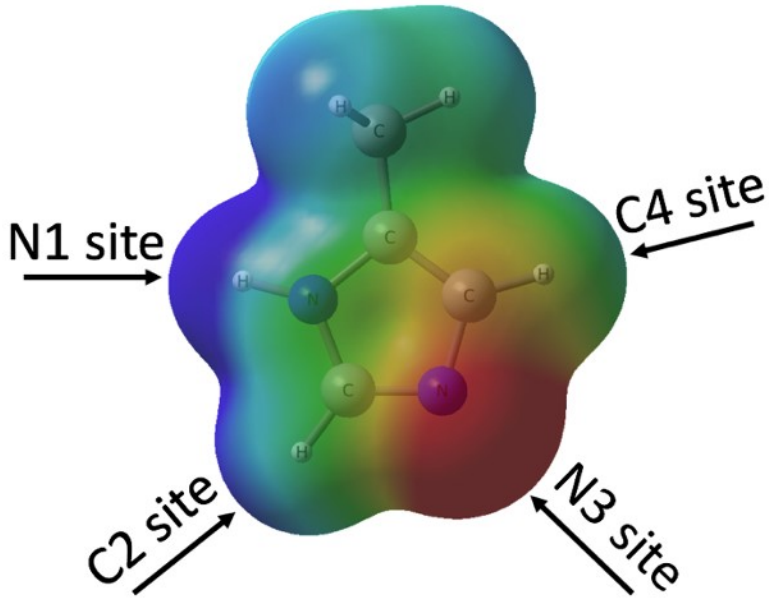


Figure S5. *Visual presentation of the sites referred to in Table S4. The tip of each arrow indicates the approximate site on the 0.002 au isodensity surface where the electrostatic potential was recorded and entered into Table S4. Pi-5-methylimidazole was arbitrarily selected as an example; the sites are labeled the same for each of the three forms of 5-methylimidazole.*

E. Addressing Basis Set Superposition Error.

It is shown below in Table S5a that geometries from 6-31+G(d,p) and 6-311+G(d,p) are remarkably similar, and therefore calculations based on double-zeta basis set equilibrium geometries are quite reasonable. Coordinates for both 6-31+G(d,p) and 6-311+G(d,p) optimized geometries are given in the section below.

Table S5a. Geometric data for the complexes. H-bond length (Å), O - - - C distance (Å), C-H···O angle (degrees).

Complex Name	*BHandHLYP/6-31+G(d)*	*BHandHLYP/6-31+G(d,p)*	*BHandHLYP/6-311+G(d,p)*	*MP2/aug-cc-pVTZ*
tau-5-methylimidazole/C4-H···water	2.30, 3.37, 179	2.30, 3.37, 176	2.31, 3.38, 176	2.30, 3.37, 172
tau-5-methylimidazole/C2-H···water	2.26, 3.34, 178	2.26, 3.34, 179	2.28, 3.35, 179	2.29, 3.37, 178
pi-5-methylimidazole/C4-H···water	2.39, 3.46, 178	2.39, 3.47, 178	2.41, 3.48, 178	2.43, 3.46, 160
pi-5-methylimidazole/C2-H···water	2.26, 3.34, 179	2.27, 3.34, 179	2.28, 3.35, 179	2.29, 3.37, 179
5-methylimidazolium/C4-H···water	2.14, 3.21, 176	2.14, 3.22, 176	2.15, 3.22, 176	2.14, 3.22, 175
5-methylimidazolium/C2-H···water	2.03, 3.10, 179	2.03, 3.11, 179	2.03, 3.11, 178	2.06, 3.14, 178
tau-5-methylimidazole/C4-H···acetone	2.35, 3.41, 173	2.34, 3.41, 178	2.32, 3.39, 178	*
tau-5-methylimidazole/C2-H···acetone	2.31, 3.38, 174	2.30, 3.38, 177	2.30, 3.37, 176	*
pi-5-methylimidazole/C4-H···acetone	2.48, 3.56, 179	2.46, 3.54, 179	2.44, 3.51, 177	*
pi-5-methylimidazole/C2-H···acetone	2.31, 3.38, 175	2.30, 3.38, 176	2.30, 3.37, 175	*
5-methylimidazolium/C4-H···acetone	2.18, 3.24, 169	2.17, 3.24, 170	2.17, 3.23, 173	*
5-methylimidazolium/C2-H···acetone	2.05, 3.12, 173	2.04, 3.12, 175	2.04, 3.11, 177	*

Table S5b. ΔC-H bond length (in pm) upon complex formation, ΔH-O_{water} (or ΔC=$O_{acetone}$) bond length (in pm) upon complex formation.

tau-5-methylimidazole/C4-H···water	0.214, 0.019	0.202, 0.031	0.208, 0.035	0.166, 0.033
tau-5-methylimidazole/C2-H···water	0.206, 0.022	0.200, 0.031	0.194, 0.038	0.152, 0.029
pi-5-methylimidazole/C4-H···water	0.076, 0.030	0.097, 0.026	0.101, 0.028	0.048, 0.035
pi-5-methylimidazole/C2-H···water	0.196, 0.021	0.195, 0.031	0.190, 0.036	0.150, 0.030
5-methylimidazolium/C4-H···water	0.441, 0.041	0.429, 0.040	0.423, 0.045	0.381, 0.038
5-methylimidazolium/C2-H···water	0.734, 0.059	0.713, 0.054	0.701, 0.061	0.644, 0.045
tau-5-methylimidazole/C4-H···acetone	0.105, 0.043	0.131, 0.040	0.142, 0.052	*
tau-5-methylimidazole/C2-H···acetone	0.081, 0.051	0.094, 0.052	0.126, 0.070	*
pi-5-methylimidazole/C4-H···acetone	0.036, 0.018	0.047, 0.019	0.053, 0.027	*
pi-5-methylimidazole/C2-H···acetone	0.110, 0.053	0.129, 0.055	0.129, 0.069	*
5-methylimidazolium/C4-H···acetone	0.331, 0.123	0.388, 0.107	0.385, 0.125	*
5-methylimidazolium/C2-H···acetone	0.665, 0.211	0.704, 0.215	0.710, 0.242	*

F. Other Potential C–H···O Hydrogen Bonds Found in XRD Structures.

Table S6. Potential C–H···O Hydrogen Bonds Found in XRD Structures.[1]

PDB ID	Protein Description	Residue	H-Bond Donor	H-Bond Acceptor	O - - - C distance (Å)
117E	Inorganic pyrophosphatase	His87 Chain A	Cδ	oxygen of water	3.1
117E	Inorganic pyrophosphatase	His87 Chain A	Cε	oxygen of water	3.3
117E	Inorganic pyrophosphatase	His87 Chain B	Cδ	oxygen of water	3.4
117E	Inorganic pyrophosphatase	His87 Chain B	Cε	oxygen of water	3.5
117E	Inorganic pyrophosphatase	His223 Chain A	Cδ	oxygen of water	3.5
117E	Inorganic pyrophosphatase	His223 Chain B	Cδ	oxygen of water	3.6
101M	Sperm whale myoglobin	His64	Cδ	oxygen of water	3.2
101M	Sperm whale myoglobin	His64	Cε	oxygen of water	3.0
101M	Sperm whale myoglobin	His81	Cδ	oxygen of water	3.0
101M	Sperm whale myoglobin	His116	Cδ	oxygen of water	2.8
101M	Sperm whale myoglobin	His116	Cε	oxygen of water	2.9
11AS	Asparagine synthetase	His209	Cε	oxygen of water	3.4
11BA	Bovine seminal ribonuclease	His12	Cε	oxygen of C=O group of uridylyl-2'-5'-phospho-adenosine	3.3
11BA	Bovine seminal ribonuclease	His12	Cδ	oxygen of water	3.1
12CA	Human carbonic anhydrase	His64	Cδ	oxygen of water	3.0
13PK	Phosphoglycerate kinase	His171	Cε	oxygen of water	2.9
13PK	Phosphoglycerate kinase	His393	Cε	oxygen of water	3.5
13PK	Phosphoglycerate kinase	His171 Chain B	Cε	oxygen of water	2.9
13PK	Phosphoglycerate kinase	His171 Chain B	Cε	oxygen of water	3.1

[1] apparent/assigned tautomeric state of histidines is τ-tautomer

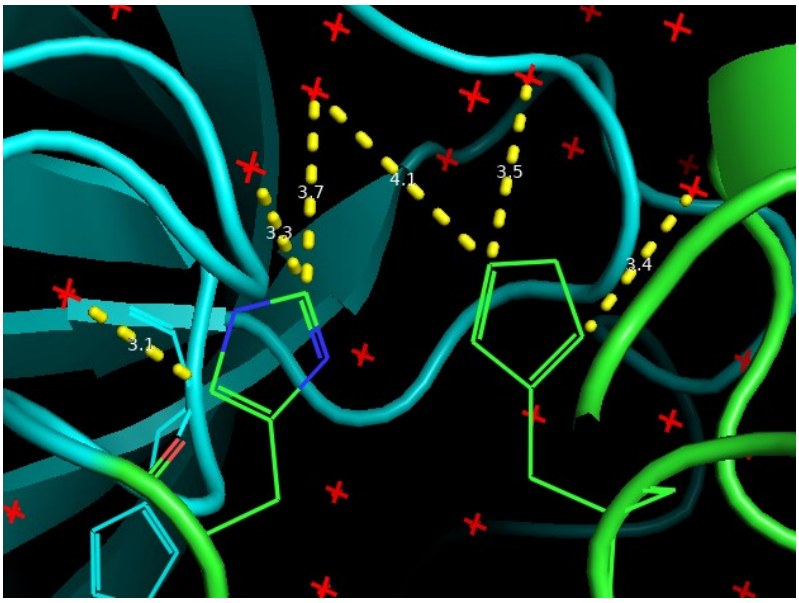


Figure S6. PDB ID 117E. Inorganic pyrophosphatase. His 87 Chain A, and His87 Chain B.

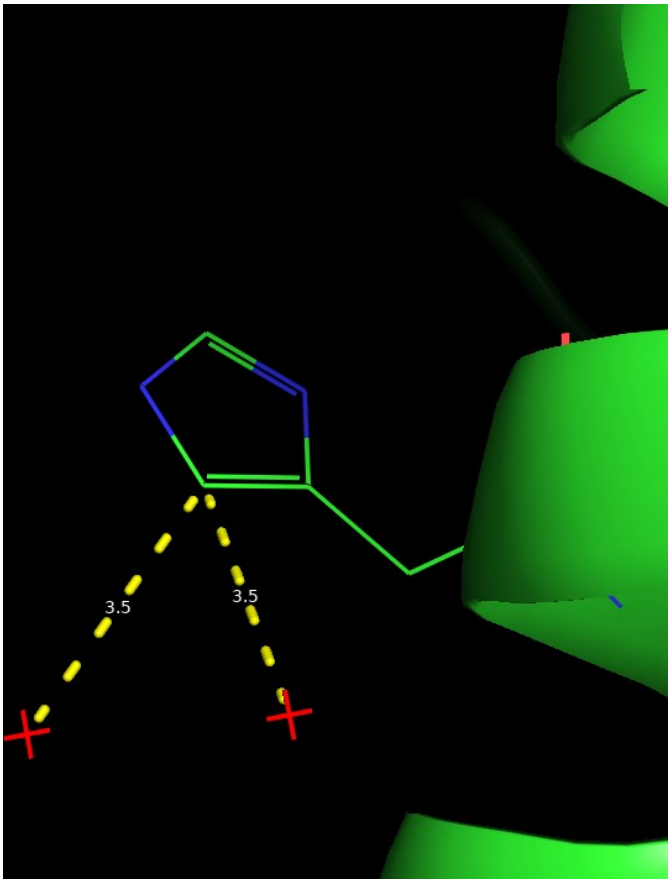


Figure S7. PDB ID 117E. Inorganic pyrophosphatase. His223 Chain A.

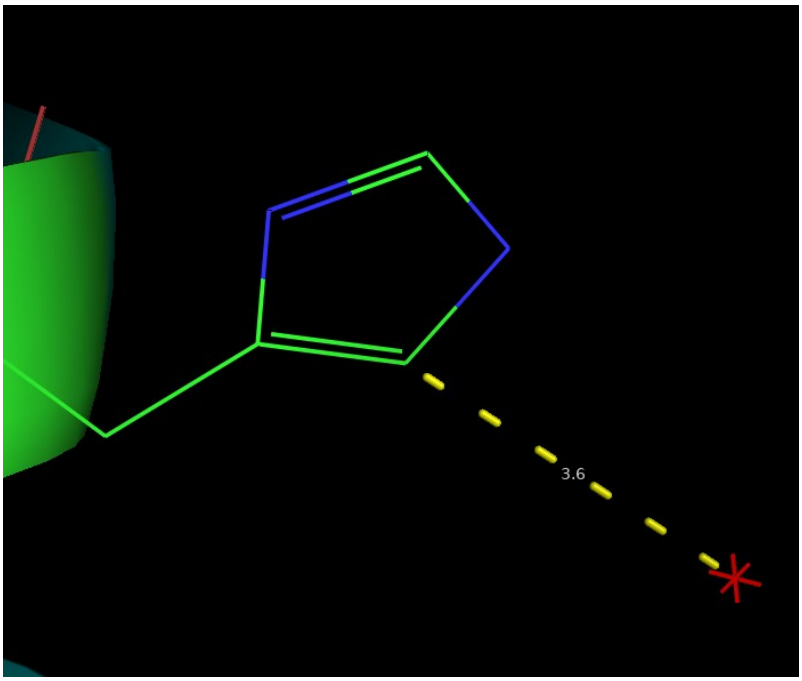


Figure S8. PDB ID 117E. Inorganic pyrophosphatase. His 223 Chain B.

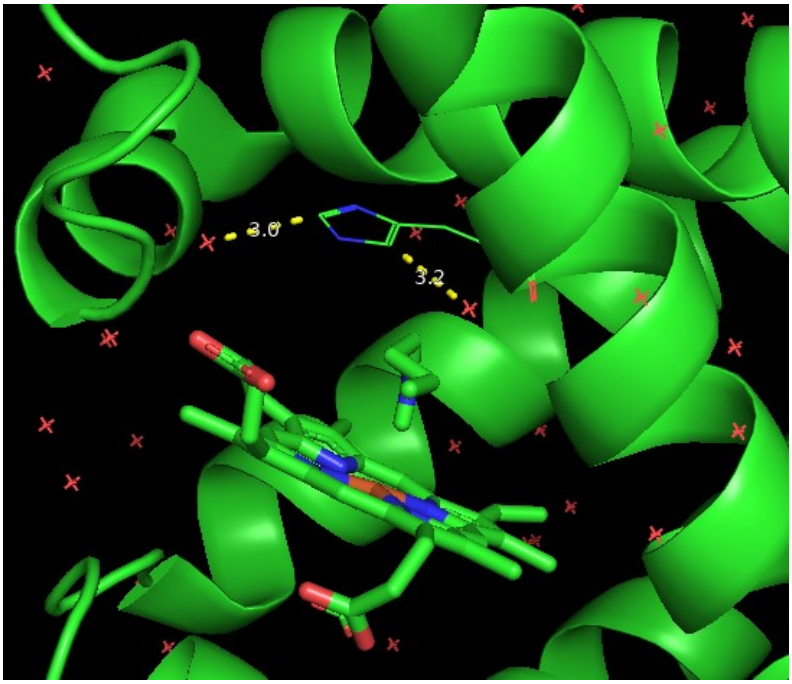


Figure S9. PDB ID 101M. Sperm whale myoglobin. His64.

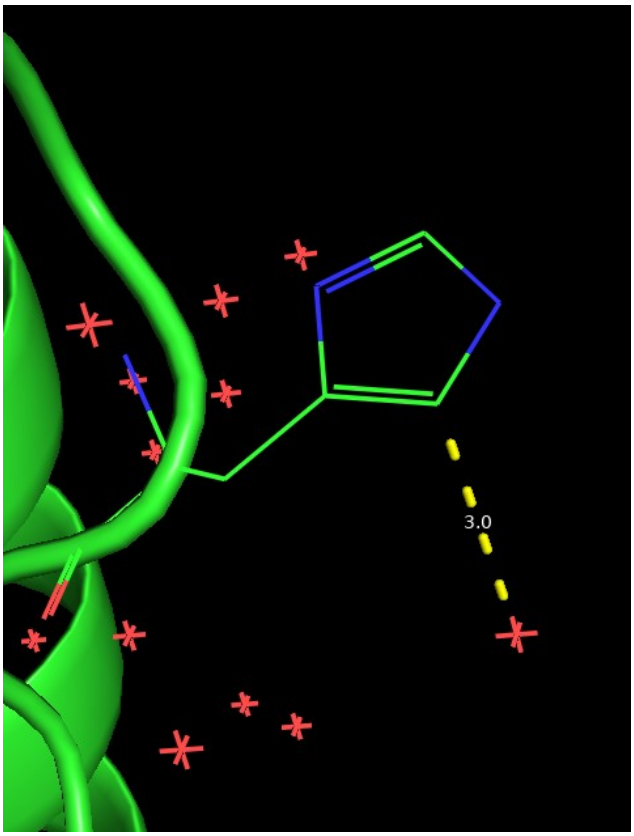


Figure S10. PDB ID 101M. Sperm whale myoglobin. His81.

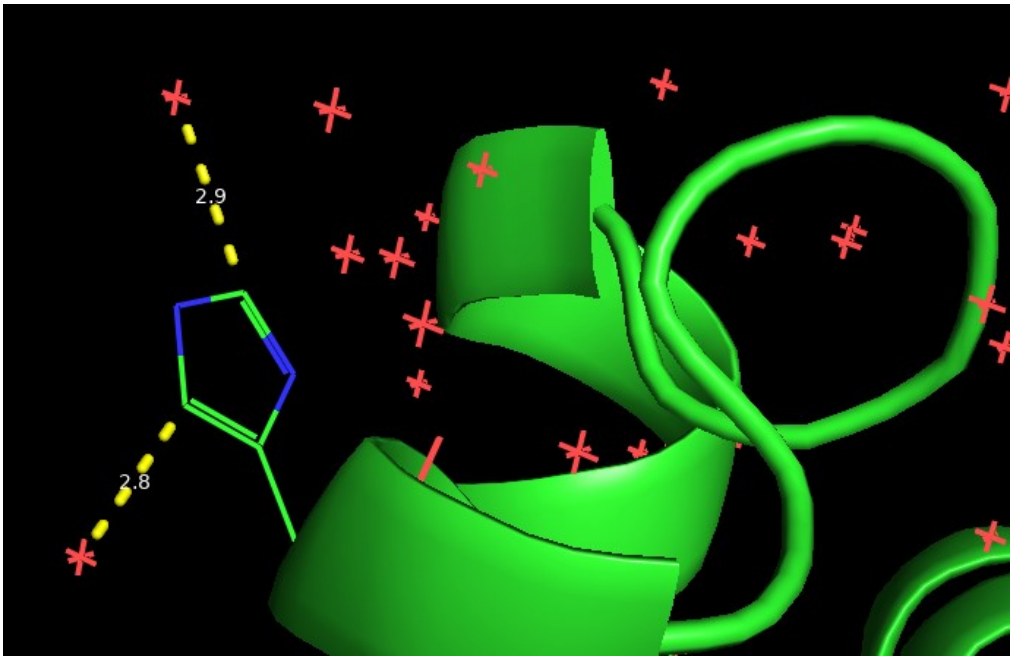


Figure S11. PDB ID 101M. Sperm whale myoglobin. His116.

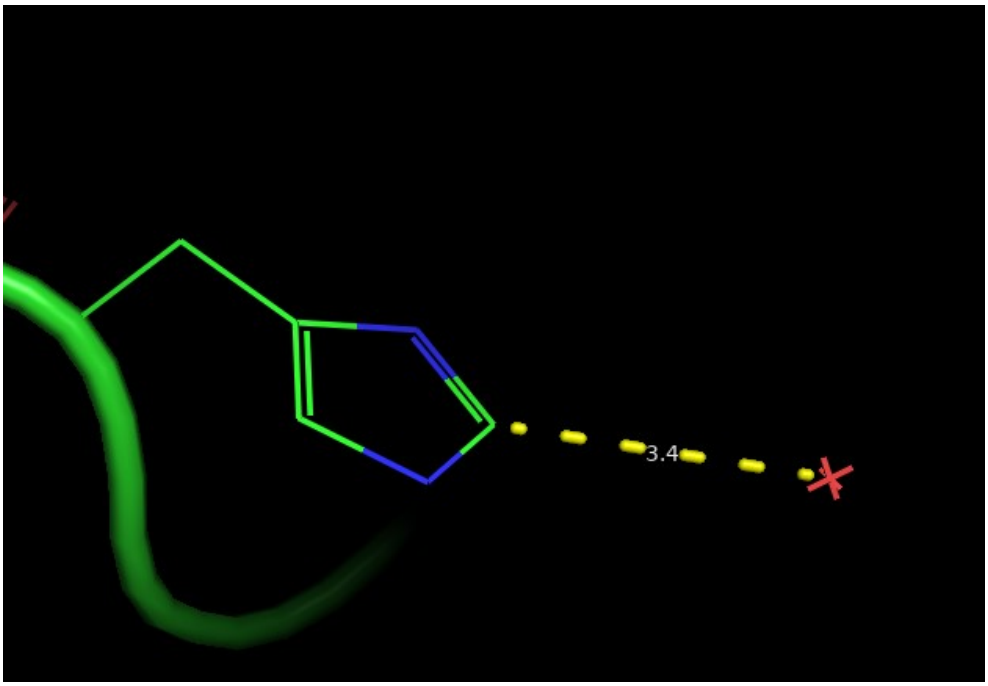


Figure S12. PDB ID 11AS. Asparagine synthetase. His209.

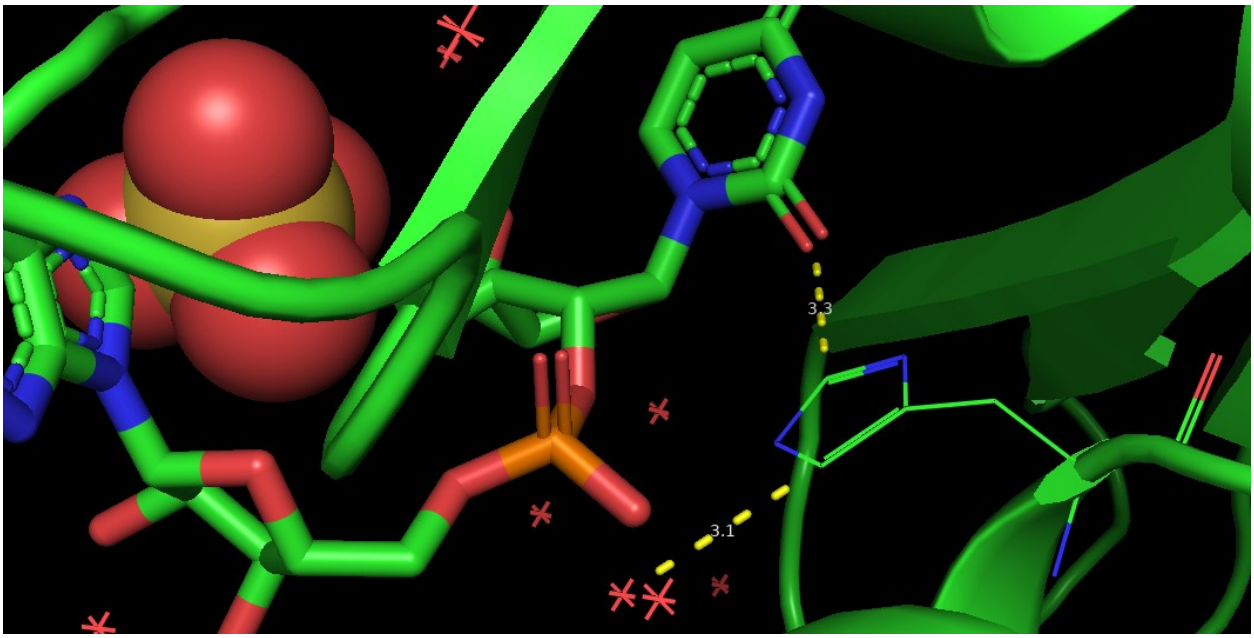


Figure S13. PDB ID 11BA. Bovine seminal ribonuclease. His12.

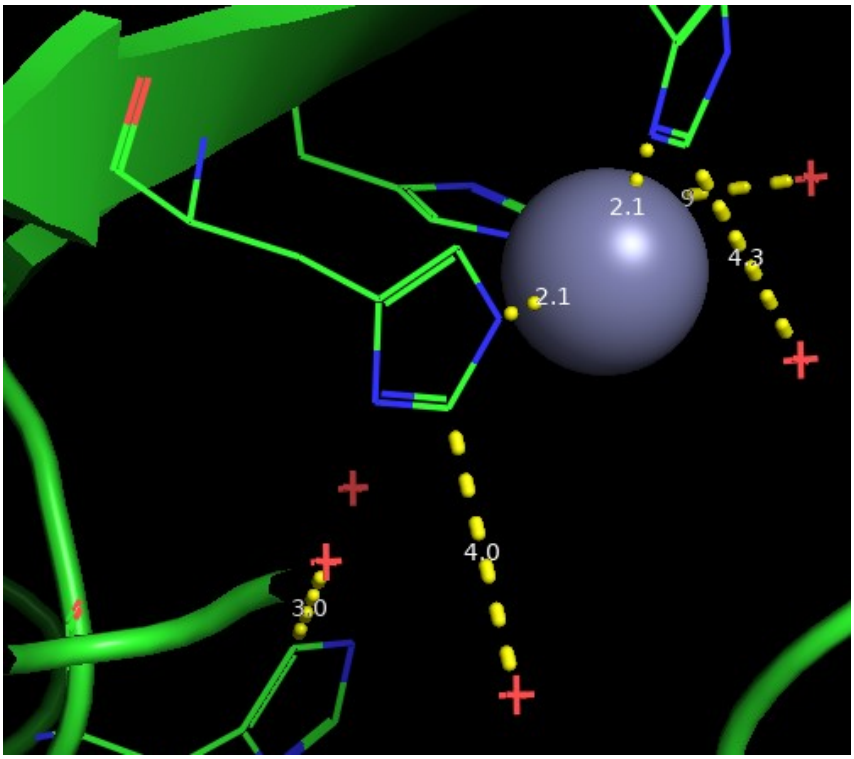


Figure S14. PDB ID 12CA. Human carbonic anhydrase. His64.

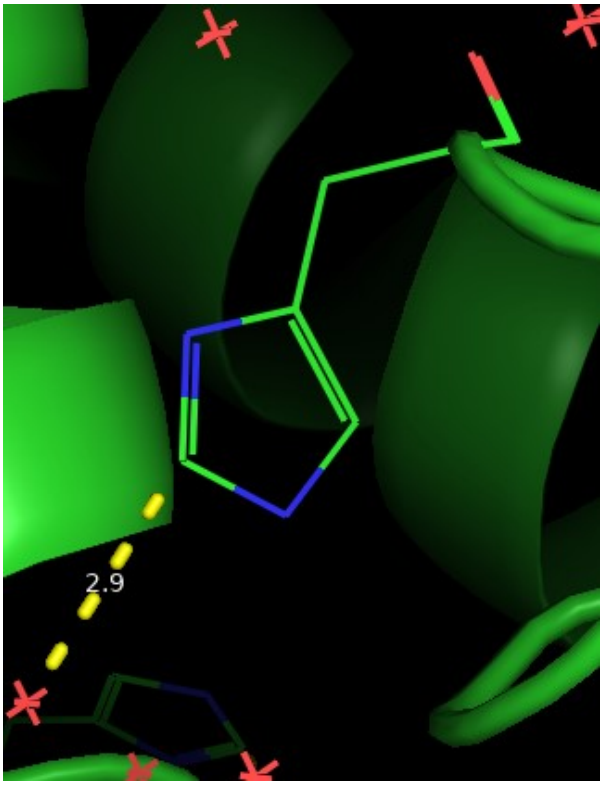


Figure S15. PDB ID 13PK. Phosphoglycerate kinase. His171.

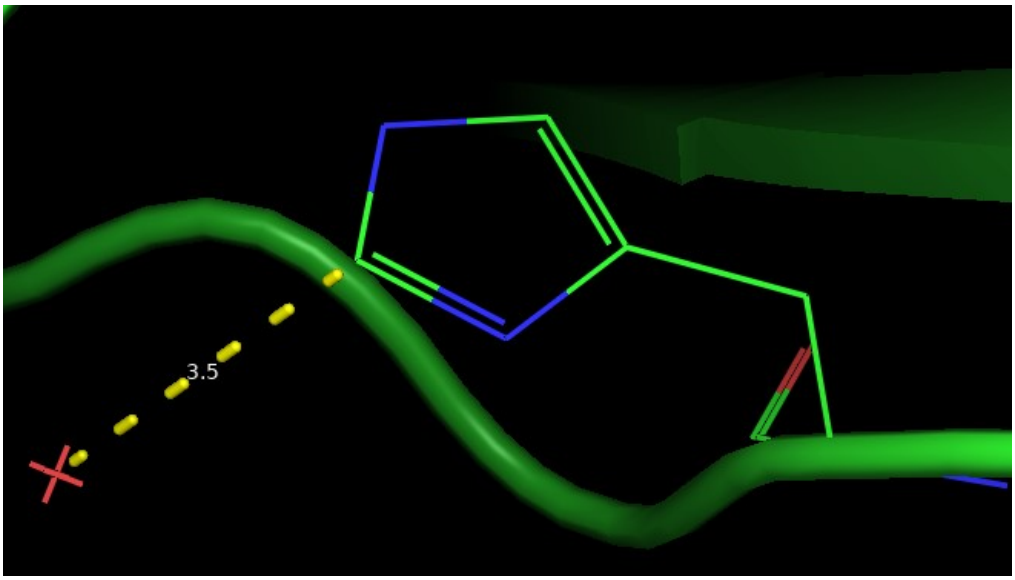


Figure S16. PDB ID 13PK. Phosphoglycerate kinase. His393.

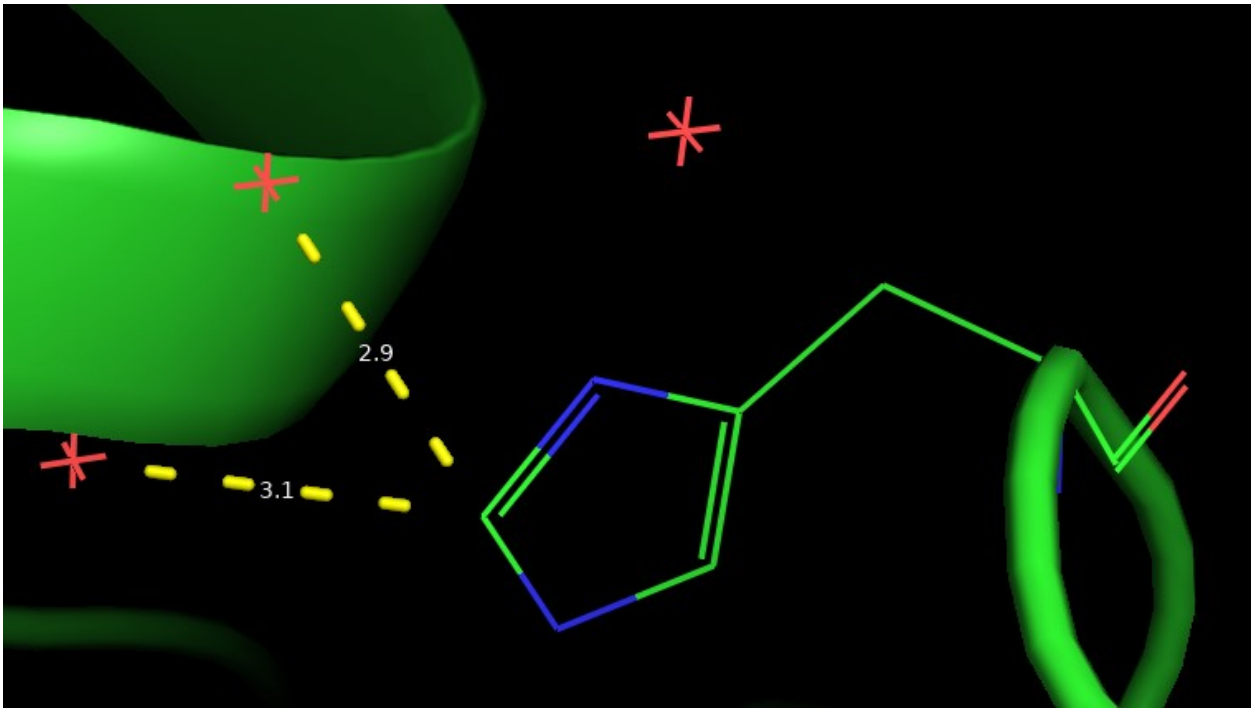


Figure S17. PDB ID 13PK. Phosphoglycerate kinase. His171 Chain B.

G. Atomic Coordinates for Geometrically Optimized Complexes.

Atomic coordinates are listed in three columns corresponding to x, y, and z respectively. The atomic label is listed to the left. The term "proto" in the file naming scheme represents the presence of the imidazolium ion.

Atomic Coordinates (x y z) for Optimized Geometries of 5-methylimidazole···water Complexes:

BHandHLYP/6-31+G(d) Level:

Water

O	0.00000000	0.00000000	0.11651700
H	0.00000000	-0.76176200	-0.46606700
H	0.00000000	0.76176200	-0.46606700

Tau-5-methylimidazole

N	0.09284700	-1.13791300	-0.00010200
N	1.44980300	0.58647200	0.00007600
C	-0.65541600	0.01672900	-0.00012400
C	0.17675500	1.09690200	0.00005500
C	1.34384800	-0.75488600	-0.00000800
H	-0.01589600	2.15124200	-0.00061800
H	2.30339900	1.11196300	0.00012500
H	2.20085900	-1.40120000	0.00022200
C	-2.14521700	-0.01380000	0.00008400
H	-2.52714300	-0.53199500	0.87764800
H	-2.55230500	0.99326800	-0.00035500
H	-2.52728800	-0.53286200	-0.87688500

Tau-C4 Complex

N	1.97147000	0.14893100	-0.00272000
N	0.50229200	-1.48021500	0.00066000
C	0.48293000	2.16251600	0.00340700
C	0.70529100	0.68877500	0.00166900
C	-0.22023400	-0.31341100	0.00383100
C	1.80660000	-1.14890700	-0.00320400
H	0.92616000	2.62867900	-0.87470300
H	-0.57869100	2.39291200	0.00666100
H	-1.29412400	-0.30382600	0.00698500
H	0.12963000	-2.41064000	0.00110800
O	-3.58964500	-0.29367100	-0.01182300
H	-3.96342300	0.22598500	-0.72615300
H	-3.98674000	0.05765400	0.78752100
H	2.58922700	-1.88366600	-0.00622500
H	0.93126500	2.62741400	0.87959500

Tau-C2 Complex

N	0.26475200	-0.83533600	-0.00047400
N	-0.05852800	1.33349700	0.00458200
C	2.76638600	-0.96867800	-0.00482300
C	1.48725700	-0.20400300	-0.00120500
C	1.30043200	1.14641500	0.00191600
C	-0.63530900	0.11668900	0.00300800

H	2.84040700	-1.60680400	-0.88345900
H	3.61930200	-0.29589000	-0.00478500
H	1.99062700	1.96651100	0.00242700
H	-0.53815800	2.21357000	0.00730200
H	-1.70193500	-0.02087800	0.00456900
O	-3.93725800	-0.37106700	0.01308600
H	-4.23399700	-0.98454000	0.68813400
H	-4.27752600	-0.72269400	-0.81195000
H	2.84317800	-1.61040600	0.87094900

Proto-5-methylimidazole

N	-0.11717200	-1.04821900	0.00016600
N	-1.45018000	0.61095200	-0.00003300
C	2.16353900	0.01554600	-0.00003100
C	0.68077700	0.07872500	-0.00000700
C	-0.17495000	1.12826200	0.00001500
C	-1.39430200	-0.70584200	-0.00015300
H	2.53018600	-0.50530600	-0.88055100
H	2.57140600	1.01966100	-0.00005400
H	0.01013000	2.18227200	0.00001800
H	-2.30228100	1.14426400	0.00041200
H	-2.22976100	-1.37583800	-0.00013100
H	0.21110700	-1.99895200	0.00001400
H	2.53029300	-0.50536800	0.88042100

Proto-C4 Complex

N	-1.85722900	0.02282700	0.00022900
N	-0.34741400	-1.47576100	-0.00159500
C	-0.55862000	2.17834000	0.00266400
C	-0.65155200	0.69662000	0.00099200
C	0.30480900	-0.26300200	-0.00013200
C	-1.65163800	-1.28330900	-0.00131900
H	-1.03688500	2.59853200	0.88357800
H	0.48308700	2.47802800	0.00284900
H	1.37706600	-0.19281700	-0.00011600
O	3.51431300	-0.20236400	-0.00760900
H	3.98072500	0.07284700	0.78435300
H	3.97085500	0.23018400	-0.73212200
H	-2.76662900	0.45136900	0.00072700
H	-2.40632100	-2.04315000	-0.00221600
H	0.09524700	-2.37793000	-0.00268100
H	-1.03714200	2.60049900	-0.87717200

Proto-C2 Complex

N	0.25704900	-0.76397200	0.00239000
N	-0.13397800	1.32529200	0.01483500
C	2.77032800	-0.90538400	-0.01630100
C	1.49349500	-0.14860500	-0.00402900
C	1.23500800	1.17997400	0.00387600
C	-0.71094000	0.13874900	0.01372800
H	2.84065900	-1.53574800	-0.89889100
H	3.60518500	-0.21414400	-0.02120500
H	1.89581600	2.02175900	0.00261800
H	-0.63090800	2.19858800	0.02266300
H	-1.77065700	-0.06033500	0.01987100
O	-3.76954300	-0.38866500	0.03359800
H	-4.09958500	-1.18804000	0.44940700
H	-4.22663400	-0.33321300	-0.80829500

H	0.09886400	-1.75687800	-0.00096500
H	2.85476700	-1.54031500	0.86179500

Pi-5-Methylimidazole

N	-0.18169600	-1.03078100	0.00026800
N	-1.52239500	0.70825600	-0.00002800
C	2.12416900	-0.02470000	-0.00002700
C	0.64005300	0.06781600	-0.00004900
C	-0.21402800	1.13119400	0.00002000
C	-1.46089600	-0.59589500	-0.00010800
H	2.49279300	-0.55046300	-0.87869400
H	2.55362700	0.97199100	-0.00035500
H	0.04009900	2.17465300	0.00010000
H	-2.29719700	-1.26875900	-0.00000800
H	0.11071900	-1.99029300	-0.00068300
H	2.49280400	-0.54993700	0.87893900

Pi-C4 Complex

N	1.90864700	0.02488700	-0.00942700
N	0.40785900	-1.57705500	0.01221400
C	0.54745900	2.13878900	-0.00141000
C	0.69153300	0.65859300	0.00173800
C	-0.22313700	-0.35359600	0.01507900
C	1.68521500	-1.30757100	-0.00258600
H	0.99925100	2.58407200	-0.88584500
H	-0.50462200	2.40513700	0.00791000
H	-1.29468000	-0.27178600	0.02646900
O	-3.67799400	-0.15350800	0.00220700
H	-4.16704600	-0.33714900	-0.80237700
H	-4.33865100	-0.13802000	0.69758700
H	2.80771800	0.46905300	-0.02030200
H	2.48385800	-2.02482700	-0.00895400
H	1.01616400	2.58947800	0.87142000

Pi-C2 Complex

N	0.29504700	-0.74777700	-0.00364800
N	-0.13304000	1.40414800	0.00463800
C	2.80822900	-0.87209100	-0.00221600
C	1.51984600	-0.12951700	0.00004500
C	1.22709600	1.20239600	0.00490300
C	-0.66124500	0.20830800	-0.00086600
H	2.90576700	-1.50330800	-0.88353000
H	3.63645900	-0.17059700	0.00117900
H	1.91892500	2.02401500	0.00898800
H	-1.71149400	-0.02262300	-0.00276500
O	-3.93023200	-0.47441100	-0.01344400
H	-4.44085800	-0.04387400	-0.70189900
H	-4.40147100	-0.28936400	0.80128200
H	0.13208300	-1.73742500	-0.00769900
H	2.90483100	-1.51069800	0.87385900

BHandHLYP/6-31+G(d,p) Level:

Water

O	0.00000000	0.00000000	0.11545900
H	0.00000000	-0.76082500	-0.46183800
H	0.00000000	0.76082500	-0.46183800

Tau-5-methylimidazole

N	0.09264500	-1.13781200	-0.00002000
N	1.44957500	0.58668300	0.00011200
C	-0.65543900	0.01648200	0.00007900
C	0.17653400	1.09690900	-0.00002100
C	1.34388100	-0.75464800	-0.00005600
H	-0.01805900	2.15028200	-0.00009100
H	2.30221300	1.11128400	-0.00037700
H	2.20060600	-1.40066000	0.00003600
C	-2.14476900	-0.01386800	-0.00000400
H	-2.52538000	-0.53153900	0.87745900
H	-2.55095400	0.99267500	-0.00118400
H	-2.52521200	-0.53338300	-0.87648000

Tau-C4 Complex

N	1.98494700	0.05485500	-0.01058600
N	0.41028400	-1.47270400	0.00929400
C	0.63280300	2.16265600	-0.00019000
C	0.75792100	0.67793000	0.00138200
C	-0.23227900	-0.26026600	0.01386400
C	1.73380800	-1.22933700	-0.00545200
H	1.09940800	2.59492300	-0.88255700
H	-0.41084400	2.46095600	0.00957900
H	-1.30232300	-0.17848900	0.02443100
H	-0.02353400	-2.37478200	0.01532000
O	-3.59720200	-0.16297600	0.00182300
H	-4.10172100	-0.04932400	-0.80145300
H	-4.18552200	0.08574200	0.71226800
H	2.46525400	-2.01447400	-0.01185500
H	1.11676700	2.59830100	0.87110200

Tau-C2 Complex

N	0.27947900	-0.84307700	-0.00853900
N	-0.06333200	1.32289000	0.00450400
C	2.78161600	-0.95353700	-0.00231600
C	1.49595000	-0.20092500	-0.00098700
C	1.29716900	1.14780400	0.00718400
C	-0.62912600	0.10101600	-0.00492800
H	2.86434400	-1.58585200	-0.88342800
H	3.62713500	-0.27288000	0.00506200
H	1.98114100	1.97226600	0.01435700
H	-0.55042700	2.19735500	0.00926400
H	-1.69404200	-0.04576900	-0.00864000
O	-3.93172100	-0.39488900	0.01009700
H	-4.36946200	-0.86180500	0.71936700
H	-4.45050300	-0.57090500	-0.77258900
H	2.85890200	-1.59813600	0.87034300

Proto-5-methylimidazole

N	-0.11724900	-1.04843200	0.00027200
N	-1.44972700	0.61154400	-0.00035200
C	2.16304400	0.01552400	0.00003200
C	0.68067600	0.07760700	-0.00041300
C	-0.17419300	1.12786400	0.00027900
C	-1.39434400	-0.70486100	0.00012400
H	2.52923200	-0.50680600	-0.87893600
H	2.56857000	1.01970600	-0.00153800

H	0.01368400	2.18079600	-0.00047700
H	-2.30096300	1.14412700	0.00100000
H	-2.22979300	-1.37434300	-0.00014900
H	0.20891800	-1.99868900	-0.00092400
H	2.52809000	-0.50337700	0.88145600

Proto-C4 Complex

N	-1.86139700	0.01813700	-0.00191000
N	-0.34611800	-1.47519600	0.00387500
C	-0.56994200	2.17711100	-0.00336200
C	-0.65839400	0.69578300	-0.00089100
C	0.30153600	-0.26017400	0.00280500
C	-1.65071700	-1.28711800	0.00098000
H	-1.05008800	2.59697000	0.87582800
H	0.47042500	2.47849100	-0.00323000
H	1.37268200	-0.18409100	0.00446800
O	3.52115300	-0.17558700	0.00688300
H	4.04302300	0.18089600	0.72343400
H	4.03685600	-0.03353900	-0.78480900
H	-2.77156900	0.44235300	-0.00441900
H	-2.40237900	-2.04948700	0.00089300
H	0.09855000	-2.37510300	0.00635400
H	-1.04901900	2.59401000	-0.88453000

Proto-C2 Complex

N	0.26179000	-0.76591700	-0.00359400
N	-0.13262300	1.32290700	0.01444200
C	2.77444000	-0.90240600	-0.01366800
C	1.49672200	-0.14843200	-0.00337100
C	1.23651300	1.17972700	0.00804300
C	-0.70722400	0.13555700	0.00720500
H	2.84803800	-1.52871900	-0.89802500
H	3.60660000	-0.20916300	-0.01306700
H	1.89710000	2.02097200	0.01207300
H	-0.63093600	2.19408000	0.02338200
H	-1.76609800	-0.06515300	0.00876900
O	-3.77078000	-0.39789700	0.02738000
H	-4.15686400	-1.13886000	0.49115600
H	-4.29890700	-0.27826600	-0.75996500
H	0.10465600	-1.75781000	-0.01083300
H	2.85578000	-1.53951600	0.86228000

Pi-5-Methylimidazole

N	-0.18149000	-1.03091000	0.00028600
N	-1.52181400	0.70848800	-0.00003500
C	2.12340600	-0.02497400	-0.00002200
C	0.63981400	0.06742000	-0.00004900
C	-0.21337300	1.13149100	0.00001200
C	-1.46084000	-0.59565800	-0.00009900
H	2.49071400	-0.55056300	-0.87843100
H	2.55142900	0.97141500	-0.00042100
H	0.04295800	2.17381900	0.00009700
H	-2.29690400	-1.26816300	0.00002400
H	0.11015700	-1.98931100	-0.00083600
H	2.49072500	-0.54991900	0.87875700

Pi-C4 Complex

N	1.90980700	0.03092500	-0.01116400
N	0.41603200	-1.57763700	0.01311200
C	0.53912500	2.13763300	-0.00035200
C	0.69015600	0.65865200	0.00235100
C	-0.22061300	-0.35702200	0.01730500
C	1.69218700	-1.30276100	-0.00411300
H	0.98768400	2.58384600	-0.88505000
H	-0.51365100	2.39765200	0.01032600
H	-1.29197600	-0.27798500	0.03032700
O	-3.68315200	-0.15925500	-0.00165200
H	-4.19080500	-0.32007900	-0.79476400
H	-4.31836100	-0.15261200	0.71184500
H	2.80583600	0.47828700	-0.02388800
H	2.49371700	-2.01614800	-0.01211900
H	1.00676600	2.58904600	0.87174900

Pi-C2 Complex

N	0.29330400	-0.74369000	-0.00952300
N	-0.11966300	1.41132800	0.00140000
C	2.80451600	-0.88512300	0.00268600
C	1.52177300	-0.13378900	0.00055100
C	1.23917600	1.20026800	0.00714900
C	-0.65631000	0.21940000	-0.00861200
H	2.90083400	-1.51401200	-0.87947200
H	3.63625300	-0.18925600	0.01197700
H	1.93802100	2.01512500	0.01572300
H	-1.70773500	-0.00405200	-0.01472500
O	-3.93454100	-0.44487800	-0.00272800
H	-4.51737800	-0.20032900	-0.71911200
H	-4.45862300	-0.36984100	0.79250300
H	0.12353800	-1.73089800	-0.01626400
H	2.89100000	-1.52571000	0.87741100

Tau-N3 Complex

N	1.17886200	1.18585300	0.00482000
N	-0.73030900	0.09354500	-0.00418800
C	2.83133300	-0.69633400	0.00089900
C	1.43979300	-0.16377500	-0.00032300
C	0.26131000	-0.85203800	-0.00596000
C	-0.12763900	1.29457100	0.00235900
H	3.37845300	-0.36312200	0.88000200
H	2.82843100	-1.78189200	-0.00254800
H	0.05002900	-1.90253400	-0.01085300
H	-1.72781300	-0.07700000	-0.00632300
O	-3.57444800	-0.46288600	-0.00521400
H	-4.08197300	-0.31709900	0.79136800
H	-4.12388700	-0.16367800	-0.72770300
H	-0.67863500	2.21565200	0.00514000
H	3.38233000	-0.35756300	-0.87364500

Pi-N1 Complex

N	0.21809000	-0.37464700	0.00035300
N	-1.81930800	-1.20671500	0.00052100
C	-0.14620100	2.11210000	-0.00086800
C	-0.62605000	0.70445200	-0.00016100
C	-1.88054300	0.16627600	-0.00011700
C	-0.54252500	-1.48959800	0.00061800
H	0.45900000	2.32788700	-0.87844900

H	-0.99388800	2.78874900	-0.00258000
H	-2.81735300	0.69072000	-0.00027300
H	-0.11746900	-2.47510400	0.00105800
O	3.11984800	-0.25795800	-0.00229700
H	3.60366400	-0.59542000	-0.75428800
H	3.60070800	-0.54554300	0.77199800
H	1.23016500	-0.34715100	0.00017200
H	0.45682500	2.32967400	0.87778100

Proto-N1 Complex

N	0.25491400	-0.36754900	0.00018600
N	-1.76325100	-1.06298500	-0.00003100
C	0.01715200	2.13438300	-0.00000900
C	-0.54055300	0.75881200	-0.00000100
C	-1.81952800	0.31147500	-0.00012800
C	-0.50095400	-1.44966000	0.00017800
H	0.63148400	2.30391400	-0.87950400
H	-0.79035600	2.85640500	-0.00041300
H	-2.74768600	0.84319600	-0.00028600
H	-2.55046600	-1.68551800	-0.00012000
H	-0.15412500	-2.46256000	0.00028900
O	3.03935900	-0.36251500	-0.00016700
H	3.50510100	-0.69642300	0.76526900
H	3.50305800	-0.69968800	-0.76541900
H	1.27893600	-0.37970600	0.00031600
H	0.63084000	2.30418700	0.87988500

Proto-N3 Complex

N	-1.09925700	1.10638400	-0.00104400
N	0.77620400	0.08674900	0.00052700
C	-2.79243200	-0.75453700	0.00042000
C	-1.40105600	-0.23947300	0.00033800
C	-0.20506400	-0.87616700	0.00136300
C	0.21471400	1.27673500	-0.00093200
H	-3.33207400	-0.41822800	-0.88022200
H	-2.77898400	-1.83762300	0.00150600
H	0.02497200	-1.92100000	0.00253600
O	3.52234600	-0.33826800	-0.00276400
H	3.92408200	-0.76901800	-0.75596200
H	3.93716500	-0.71137000	0.77374400
H	-1.76717300	1.85608800	-0.00204900
H	0.72465600	2.21813100	-0.00183500
H	1.78564500	-0.08565400	0.00085500
H	-3.33265800	-0.41645900	0.88002600

BHandHLYP/6-311+G(d,p) Level:

Water

O	0.00000000	0.00000000	0.11583400
H	0.00000000	-0.75610900	-0.46333600
H	0.00000000	0.75610900	-0.46333600

Tau-5-methylimidazole

N	0.09482800	-1.13606100	0.00004100
N	1.44737500	0.58682200	-0.00002900
C	-0.65455900	0.01647400	-0.00004000
C	0.17417700	1.09512100	-0.00003300
C	1.34250300	-0.75325500	0.00005900

H	-0.02112800	2.14691500	0.00026700
H	2.29845700	1.11188200	-0.00002800
H	2.19947900	-1.39734100	-0.00019300
C	-2.14227100	-0.01492400	-0.00003000
H	-2.52124800	-0.53368600	0.87622700
H	-2.54872100	0.99029400	0.00000600
H	-2.52136400	-0.53388800	-0.87610600

Tau-C4 Complex

N	1.98367600	0.06599300	0.00412700
N	0.42481300	-1.47206700	-0.00519000
C	0.61476000	2.16101400	0.00292000
C	0.75239700	0.67886500	0.00052200
C	-0.22742300	-0.26544300	-0.00527200
C	1.74476400	-1.21704000	0.00060700
H	1.08991500	2.59947400	-0.87046800
H	-0.43031400	2.45027600	-0.00067300
H	-1.29683700	-0.19338000	-0.00909100
H	-0.00118600	-2.37670000	-0.00842900
O	-3.60585000	-0.18948700	-0.00683000
H	-4.13490500	0.17163500	-0.71216900
H	-4.11130600	-0.03799400	0.78650500
H	2.48205500	-1.99535800	0.00201400
H	1.08296700	2.59608300	0.88173800

Tau-C2 Complex

N	-0.29411300	-0.85158300	0.00746400
N	0.07637600	1.30580400	-0.01437600
C	-2.79604800	-0.92855000	0.01296800
C	-1.50158100	-0.19423700	0.00339400
C	-1.28565200	1.14842400	-0.01004600
C	0.62481100	0.07762000	-0.00344200
H	-2.88197100	-1.55694500	0.89526000
H	-3.63148200	-0.23727400	0.00804600
H	-1.95754800	1.98092300	-0.01674600
H	0.57401400	2.17302100	-0.02403300
H	1.68692100	-0.08153100	-0.00376900
O	3.94152800	-0.39186700	-0.02638300
H	4.33657300	-1.12481000	-0.48968100
H	4.50171600	-0.24394700	0.73000500
H	-2.88545200	-1.57360100	-0.85687500

Proto-5-methylimidazole

N	-0.11899200	-1.04773600	-0.00007600
N	-1.44739800	0.61148900	-0.00006000
C	2.16014100	0.01451600	0.00017600
C	0.67980900	0.07770100	-0.00011200
C	-0.17146100	1.12628600	-0.00016100
C	-1.39316300	-0.70270300	0.00014300
H	2.52446400	-0.50659000	-0.87903600
H	2.56663400	1.01713700	0.00015800
H	0.01684900	2.17766700	-0.00050500
H	-2.29709600	1.14457200	0.00098500
H	-2.22850800	-1.37024800	0.00031300
H	0.20636300	-1.99720100	-0.00092000
H	2.52407100	-0.50640800	0.87968200

Proto-C4 Complex

N	-1.86098600	0.01982400	0.00254000
N	-0.35014500	-1.47378900	-0.00290000
C	-0.56519100	2.17455800	0.00041100
C	-0.65683000	0.69525400	-0.00046600
C	0.29908500	-0.25975600	-0.00396000
C	-1.65202600	-1.28349700	0.00101900
H	-1.04118600	2.59201600	0.88173700
H	0.47464300	2.47386500	-0.00300400
H	1.36887100	-0.18586800	-0.00689400
O	3.51884100	-0.17289700	-0.00178100
H	4.03663600	0.01723000	0.77522500
H	4.06599800	0.08289000	-0.73879200
H	-2.76951800	0.44517700	0.00540500
H	-2.40394100	-2.04378200	0.00272000
H	0.09279400	-2.37340800	-0.00478600
H	-1.04734400	2.59345800	-0.87687100

Proto-C2 Complex

N	0.26405900	-0.76757100	-0.00545300
N	-0.13486800	1.31745500	0.01425500
C	2.77573600	-0.89550600	-0.01263500
C	1.49712000	-0.14663600	-0.00304700
C	1.23443700	1.17742900	0.00941500
C	-0.70511200	0.13061400	0.00507200
H	2.85109400	-1.52043800	-0.89658500
H	3.60513100	-0.20065300	-0.01045000
H	1.89189400	2.01922900	0.01514400
H	-0.63457600	2.18662600	0.02354500
H	-1.76218100	-0.07201700	0.00543300
O	-3.76584800	-0.40126800	0.02229200
H	-4.18474400	-1.09860700	0.51884600
H	-4.32405700	-0.25687000	-0.73654100
H	0.10988200	-1.75886300	-0.01407700
H	2.85691000	-1.53286400	0.86189700

Pi-5-Methylimidazole

N	-0.18305500	-1.02989000	0.00014800
N	-1.51859000	0.70793800	-0.00005500
C	2.12080200	-0.02616400	0.00005100
C	0.63882800	0.06704300	-0.00007700
C	-0.21060600	1.12991900	-0.00004300
C	-1.46055100	-0.59258200	0.00006800
H	2.48650600	-0.55214500	-0.87748400
H	2.54961600	0.96865300	-0.00032900
H	0.04715300	2.17054600	0.00000000
H	-2.29645000	-1.26372700	0.00024700
H	0.10743500	-1.98751900	-0.00112600
H	2.48641300	-0.55144000	0.87804500

Pi-C4 Complex

N	-1.90885500	0.06299800	-0.01012500
N	-0.45714100	-1.57845200	0.00550500
C	-0.48704100	2.13330300	0.00902600
C	-0.67479200	0.66013800	0.00534800
C	0.20921700	-0.37465000	0.01484000
C	-1.72287900	-1.27439200	-0.00931600
H	-0.94351700	2.59105000	0.88242300
H	0.57068700	2.36705800	0.02052200

H	1.28086900	-0.32071200	0.02706700
O	3.68998300	-0.25072200	-0.01236900
H	4.27466600	-0.17648800	0.73618000
H	4.17106100	0.12921200	-0.74166500
H	-2.79282500	0.53164200	-0.01985200
H	-2.54096100	-1.96716500	-0.01992100
H	-0.92490000	2.59295800	-0.87285700

Pi-C2 Complex

N	0.29538300	-0.74403400	-0.00786600
N	-0.11853800	1.40685900	0.00177000
C	2.80488900	-0.88174100	0.00174900
C	1.52244700	-0.13294800	0.00040400
C	1.23993600	1.19773500	0.00621600
C	-0.65349400	0.21823100	-0.00670500
H	2.89961100	-1.51076800	-0.87919700
H	3.63519200	-0.18590000	0.00953100
H	1.93747700	2.01198400	0.01343300
H	-1.70365000	-0.00624000	-0.01166500
O	-3.94074100	-0.44567400	-0.00360300
H	-4.51535100	-0.18723000	-0.71835500
H	-4.46668500	-0.35247600	0.78538600
H	0.12698200	-1.73039400	-0.01371900
H	2.89176400	-1.52101800	0.87609600

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

Water

O	0.00000000	0.00000000	0.11703100
H	0.00000000	-0.76586700	-0.46812500
H	0.00000000	0.76586700	-0.46812500

Tau-5-methylimidazole

N	0.08826100	-1.14484800	0.00054200
N	1.45548600	0.58915500	0.00038500
C	-0.65806400	0.01605400	0.00026900
C	0.17998300	1.10372600	-0.00003700
C	1.34863900	-0.76084700	-0.00056700
H	-0.01402800	2.16491300	0.00107800
H	2.31609600	1.11759300	-0.00201000
H	2.21279500	-1.40956800	-0.00033000
C	-2.15318200	-0.01194800	-0.00021900
H	-2.53378100	-0.54024800	0.87904500
H	-2.55850300	1.00233100	0.00679400
H	-2.53306600	-0.52708000	-0.88773500

Tau-C4 Complex

N	1.95209800	0.29085800	-0.00287400
N	0.64222100	-1.48645100	0.00189300
C	0.26054600	2.14933700	0.00080700
C	0.63372200	0.70090500	0.00095800
C	-0.19542800	-0.39423100	0.00401500
C	1.91589700	-1.02645800	-0.00221000
H	0.64840900	2.65438100	-0.88918400
H	-0.82564800	2.26601200	0.01423500
H	-1.27309000	-0.48399500	0.00708700
H	0.36155700	-2.45660000	0.00315500

O	-3.50589300	-0.34054800	-0.00094600
H	-4.06847400	-0.21789800	-0.77417100
H	-4.08672600	-0.21864100	0.75881000
H	2.77128800	-1.68681200	-0.00428500
H	0.67116500	2.65976200	0.87736100

Tau-C2 Complex

N	0.29996400	-0.86855000	0.00574600
N	-0.09833300	1.30154600	0.00888900
C	2.81219300	-0.91368800	-0.01048300
C	1.50261500	-0.19134700	-0.00199400
C	1.27027700	1.16157000	-0.00021000
C	-0.63868400	0.05881000	0.01208900
H	2.89933900	-1.55412500	-0.89346600
H	3.64391000	-0.20568200	-0.01775900
H	1.93707500	2.00965500	-0.00434300
H	-0.61062000	2.17172700	0.01239600
H	-1.70855200	-0.11104300	0.01842300
O	-3.91908700	-0.38468800	0.00551300
H	-4.41155500	-0.86090200	0.68390900
H	-4.39923100	-0.54379100	-0.81524500
H	2.91251100	-1.55137900	0.87312600

Proto-5-methylimidazole

N	-0.11404300	-1.05248200	-0.00002200
N	-1.45524000	0.61373300	-0.00008300
C	2.17170200	0.01665600	-0.00001100
C	0.68429700	0.07818200	0.00012600
C	-0.17825400	1.13479800	-0.00003100
C	-1.40052600	-0.71188900	0.00004300
H	2.53663300	-0.50619500	-0.88730500
H	2.57579300	1.02888500	0.00034000
H	0.00926200	2.19563400	0.00013500
H	-2.31486900	1.14986700	0.00008200
H	-2.24157000	-1.38647500	0.00014800
H	0.21956300	-2.01002500	-0.00018300
H	2.53685800	-0.50693300	0.88674600

Proto-C4 Complex

N	-1.85996500	0.08432500	0.00162600
N	-0.41240500	-1.48861700	-0.00336900
C	-0.46271500	2.18421100	0.00322500
C	-0.62230000	0.70370000	0.00152500
C	0.29729200	-0.30444000	0.00055700
C	-1.71574500	-1.23874800	-0.00132500
H	-0.94550000	2.62615000	0.87828300
H	0.59838200	2.43309100	0.02849000
H	1.37923300	-0.27906200	-0.00042800
O	3.50020500	-0.22906400	-0.00239100
H	4.06977500	-0.08892000	0.76270900
H	3.99871900	0.10557500	-0.75667400
H	-2.75499300	0.55992100	0.00006400
H	-2.50907700	-1.96922400	-0.00236800
H	-0.00794300	-2.41716100	-0.00743600
H	-0.90284000	2.62384200	-0.89521000

Proto-C2 Complex

N	0.26298700	-0.76875100	-0.00216300
N	-0.13278200	1.33006000	0.01468800
C	2.78243700	-0.90880500	-0.01452400
C	1.50134500	-0.15010300	-0.00377700
C	1.23992600	1.18783700	0.00700900
C	-0.71425500	0.13603800	0.00899800
H	2.85093500	-1.53937900	-0.90429800
H	3.61876000	-0.20990800	-0.01685700
H	1.90516400	2.03518600	0.00960300
H	-0.63499200	2.20940400	0.02411100
H	-1.78140400	-0.06581700	0.01159000
O	-3.78071600	-0.39681500	0.03077100
H	-4.14877400	-1.17287400	0.46911700
H	-4.30044500	-0.28468000	-0.77367900
H	0.10669000	-1.77007300	-0.00912900
H	2.86163800	-1.54630100	0.86946100

Pi-5-Methylimidazole

N	-0.17797200	-1.03543800	0.00009600
N	-1.53080500	0.71145300	-0.00004100
C	2.13267900	-0.02314000	-0.00002700
C	0.64349200	0.06850400	0.00005400
C	-0.21866300	1.13744000	-0.00000100
C	-1.46637600	-0.60205500	-0.00003300
H	2.49994800	-0.55020900	-0.88558600
H	2.55906100	0.98153400	0.00059700
H	0.03996300	2.18732400	0.00006400
H	-2.30547300	-1.28287000	0.00007100
H	0.12117500	-2.00107100	-0.00035400
H	2.49996600	-0.55131300	0.88486200

Pi-C4 Complex

N	1.83766000	0.37665700	-0.00528400
N	0.82538200	-1.58742800	-0.00116500
C	-0.06016600	2.04036100	0.01346500
C	0.48986700	0.65329900	0.00627200
C	-0.11794100	-0.57849200	0.00867900
C	1.98888300	-0.97449100	-0.00932600
H	0.25393100	2.60099000	-0.87204000
H	-1.15081400	1.99595500	0.02001500
H	-1.18160800	-0.77896200	0.01754700
O	-3.50238400	-0.44180900	0.00959100
H	-3.95020800	-0.17356800	-0.80101200
H	-4.20819900	-0.68423100	0.61985700
H	2.58535800	1.05670200	-0.01000900
H	2.96071900	-1.44724900	-0.01859900
H	0.26473900	2.59617100	0.89813000

Pi-C2 Complex

N	0.28263500	-0.74199600	-0.00521000
N	-0.12094400	1.42862800	0.00336800
C	2.80100700	-0.89975000	-0.00062000
C	1.51844900	-0.13706700	0.00003400
C	1.24098800	1.20756400	0.00523000
C	-0.66826900	0.23096200	-0.00297200
H	2.88857300	-1.53320300	-0.88842400
H	3.64008000	-0.20188700	0.00439400
H	1.95158700	2.02265100	0.01042200

H	-1.72841600	0.00842300	-0.00562200
O	-3.91398000	-0.46535500	-0.00670000
H	-4.47544300	-0.15878600	-0.72796500
H	-4.44201500	-0.35227400	0.79188600
H	0.10788300	-1.73747400	-0.00995100
H	2.88470500	-1.54128300	0.88172500

MP2/6-31+G(d) Level:

Water

O	0.00000000	0.00000000	0.11901200
H	0.00000000	-0.76995200	-0.47604700
H	0.00000000	0.76995200	-0.47604700

Tau-5-methylimidazole

N	-0.08212400	-1.15233300	0.00000000
N	-1.45831600	0.59194200	-0.00009200
C	2.15808000	-0.01012500	0.00004500
C	0.66356400	0.01424400	-0.00003700
C	-0.18285900	1.10864300	0.00005100
C	-1.35854600	-0.76490000	-0.00003200
H	2.54247500	-0.52860200	-0.88441500
H	2.55661800	1.00870000	-0.00001300
H	0.00585400	2.17357900	-0.00051800
H	-2.32251100	1.12577000	0.00087700
H	-2.22325300	-1.41537800	-0.00003600
H	2.54246100	-0.52850200	0.88458400

Tau-C4 Complex

N	1.99408500	0.10171700	-0.01483000
N	0.44374400	-1.48905200	-0.00391300
C	0.56781600	2.17233600	0.00101200
C	0.73905900	0.68717100	-0.00338900
C	-0.23836000	-0.29267100	0.00363500
C	1.77623100	-1.21463500	-0.01482400
H	1.02636500	2.62458000	-0.88462100
H	-0.49470700	2.43324500	0.00685900
H	-1.32021400	-0.24690300	0.01299600
H	0.02623500	-2.41499700	-0.00156200
O	-3.56451000	-0.18976500	0.05857700
H	-4.20445000	-0.20184200	-0.67587800
H	-4.11536000	-0.11741900	0.85879300
H	2.53424800	-1.98691000	-0.02246400
H	1.03501800	2.62058400	0.88417700

Tau-C2 Complex

N	0.29890400	-0.87012300	0.01116000
N	-0.08157800	1.31690800	-0.00185100
C	2.81359100	-0.93108500	-0.00154100
C	1.51010800	-0.19937500	0.00038600
C	1.28613500	1.16571800	-0.00779100
C	-0.64320200	0.07658900	0.00943800
H	2.90166800	-1.57561900	-0.88237900
H	3.64871700	-0.22433900	-0.01018800
H	1.95861700	2.01279800	-0.01701600
H	-0.58627000	2.19832500	-0.00557800
H	-1.71439800	-0.08407500	0.01567400
O	-3.92696500	-0.43315400	-0.00059700

H	-4.56207100	-0.45654100	0.73764400
H	-4.46218600	-0.63938100	-0.78788200
H	2.91056700	-1.56451600	0.88638400

Proto-5-methylimidazole

N	-0.10903700	-1.05352200	-0.00018000
N	-1.45751200	0.61656800	0.00011000
C	2.17628300	0.01901900	0.00023200
C	0.68845300	0.07489100	-0.00047300
C	-0.18452900	1.13938900	0.00000300
C	-1.40690800	-0.71996800	0.00018300
H	2.54689600	-0.50078100	-0.88750600
H	2.57468000	1.03528500	0.00096600
H	0.00007900	2.20311800	-0.00072000
H	-2.32160300	1.15506900	0.00029500
H	-2.24744400	-1.39708700	0.00016000
H	0.22763400	-2.01526900	-0.00029200
H	2.54580700	-0.50164100	0.88791800

Proto-C4 Complex

N	1.86638500	0.03161600	0.00271500
N	0.34928800	-1.48518900	-0.00346900
C	0.55706500	2.18888900	0.00063900
C	0.65885800	0.70305200	-0.00054300
C	-0.30976800	-0.27597900	-0.00457800
C	1.67353200	-1.29480500	0.00093600
H	1.03725000	2.61428300	-0.88499500
H	-0.49598800	2.47689100	-0.00254500
H	-1.39071300	-0.20897700	-0.00755800
O	-3.51064200	-0.11718600	-0.00035400
H	-4.12811600	-0.12466900	-0.75400400
H	-4.08166800	-0.19777100	0.78491000
H	2.78498600	0.47128500	0.00599000
H	2.43695500	-2.05784000	0.00287600
H	-0.09680500	-2.40007200	-0.00559700
H	1.03140700	2.61242900	0.89029900

Proto-C2 Complex

N	0.26967900	-0.77026700	0.00013200
N	-0.12295200	1.33662300	-0.00003800
C	2.79006700	-0.91602000	0.00003300
C	1.50846400	-0.15782700	0.00000400
C	1.24617100	1.19316600	-0.00012300
C	-0.71751100	0.13738900	0.00007300
H	2.86764700	-1.55024600	-0.88742600
H	3.62549900	-0.21334000	-0.00025300
H	1.91368400	2.04173400	-0.00020700
H	-0.62521700	2.22179400	-0.00026800
H	-1.78437400	-0.06219600	0.00021100
O	-3.80600800	-0.38430700	-0.00019500
H	-4.25984100	-0.76855800	0.77139300
H	-4.25791300	-0.77339200	-0.77049000
H	0.11046900	-1.77628000	0.00023000
H	2.86787700	-1.54980000	0.88779200

Pi-5-Methylimidazole

N	-0.17343300	-1.03735100	-0.00033800

N	-1.53956700	0.71682600	-0.00010700
C	2.13809500	-0.02085600	-0.00016800
C	0.64885000	0.06889500	0.00042700
C	-0.22375900	1.14273700	0.00012300
C	-1.46969100	-0.61427300	0.00003500
H	2.50790200	-0.54786900	-0.88577800
H	2.56068100	0.98714100	-0.00192000
H	0.02911200	2.19613600	0.00025400
H	-2.30810200	-1.29831100	-0.00048000
H	0.13135000	-2.00718800	0.00200900
H	2.50909200	-0.54524500	0.88652700

Pi-C4 Complex

N	1.90738400	0.05975700	0.00607000
N	0.42636600	-1.59787200	-0.00455300
C	0.49369500	2.15062400	-0.00354600
C	0.67104200	0.66910500	-0.00308200
C	-0.23221500	-0.37961100	-0.00944100
C	1.72358000	-1.29138500	0.00516300
H	0.95252000	2.61050400	-0.88508200
H	-0.57365200	2.38606800	-0.01300100
H	-1.31416500	-0.32115600	-0.01693600
O	-3.64341800	-0.19932000	0.00021300
H	-4.27828700	-0.22538300	-0.73816800
H	-4.20128200	-0.13141600	0.79584100
H	2.54690400	-1.99361500	0.01134600
H	0.93654400	2.60914400	0.88683300
H	2.80590600	0.53481900	0.01228000

Pi-C2 Complex

N	0.28890200	-0.74387600	0.00875100
N	-0.11370100	1.44076200	-0.00147200
C	2.80938900	-0.90907700	-0.00197800
C	1.52909700	-0.14289200	-0.00030100
C	1.25035500	1.21239200	-0.00638300
C	-0.66959700	0.22760200	0.00770700
H	2.89232700	-1.55099600	-0.88519000
H	3.64945800	-0.20982200	-0.00886500
H	1.96097600	2.03021200	-0.01414300
H	-1.73021400	0.00785200	0.01348200
O	-3.93420400	-0.40689700	0.00079400
H	-4.48093100	-0.54050100	-0.79422000
H	-4.57291700	-0.40034200	0.73624500
H	0.11335000	-1.74512700	0.01444900
H	2.89970500	-1.54244700	0.88666200

MP2/aug-cc-pVTZ Level:

Water

O	0.00000000	0.00000000	0.11908400
H	0.00000000	0.75692900	-0.47633500
H	0.00000000	-0.75692900	-0.47633500

Tau-5-methylimidazole

N	-0.08397000	-1.14826700	0.00007600
N	-1.45285200	0.59098400	0.00003800
C	2.15153000	-0.00978500	-0.00002800

C	0.66145800	0.01199200	-0.00002300
C	-0.18163300	1.10378200	-0.00004200
C	-1.35452300	-0.76069500	-0.00006200
H	2.53324500	-0.52684000	-0.88027000
H	2.54860800	1.00379300	-0.00016500
H	0.00934300	2.16247000	-0.00026600
H	-2.31023100	1.12127200	0.00057100
H	-2.21744600	-1.40487500	-0.00009100
H	2.53324500	-0.52660100	0.88035500

Tau-C4 Complex

N	1.96968800	0.27472200	0.00864100
N	0.62919100	-1.48702100	-0.00454100
C	0.30225300	2.14977300	-0.00520200
C	0.65875000	0.70258500	-0.00293000
C	-0.18902300	-0.38665100	-0.01120200
C	1.91333400	-1.05260500	0.00731900
H	0.71303200	2.65173800	-0.88133600
H	-0.77919600	2.27522000	-0.01528000
H	-1.26370500	-0.46319600	-0.02029300
H	0.33191800	-2.45040400	-0.00749700
O	-3.55698800	-0.29859700	0.00026600
H	-4.19846600	-0.33325400	-0.71765400
H	-4.10169600	-0.20793400	0.78966800
H	2.75351500	-1.72632800	0.01439800
H	0.69646900	2.65041600	0.87925900

Tau-C2 Complex

N	-0.30120100	-0.86374000	-0.01537000
N	0.06353000	1.31826200	0.00069900
C	-2.80973200	-0.93771700	0.00391500
C	-1.51215000	-0.20469200	-0.00008200
C	-1.29742400	1.15809300	0.00992400
C	0.62974200	0.08570100	-0.01447200
H	-2.89099000	-1.58199000	0.87943200
H	-3.64360300	-0.23792900	0.01645800
H	-1.97415100	1.99445300	0.02242200
H	0.55976700	2.19580800	0.00437400
H	1.69755600	-0.06456200	-0.02357100
O	3.95920200	-0.42977700	0.00333100
H	4.59521700	-0.45698800	-0.71970000
H	4.48855700	-0.63351700	0.78196600
H	-2.90488700	-1.56701500	-0.88104000

Proto-5-methylimidazole

N	-0.10882700	-1.05025700	-0.00004000
N	-1.45257600	0.61453900	-0.00014700
C	2.16836300	0.01979300	0.00014700
C	0.68580600	0.07364700	-0.00005600
C	-0.18395100	1.13498700	0.00009500
C	-1.40060700	-0.71617000	-0.00002100
H	2.53452400	-0.49977100	-0.88354300
H	2.56531700	1.03097700	0.00043300
H	0.00234900	2.19263000	-0.00001000
H	-2.31127500	1.14758700	-0.00017200
H	-2.23727200	-1.38950600	-0.00007400
H	0.22434000	-2.00530000	-0.00007800
H	2.53416800	-0.50013300	0.88377000

Proto-C4 Complex

N	1.85512000	0.13722200	0.00808600
N	0.46992700	-1.49208700	-0.00784000
C	0.37965600	2.17386400	-0.00124700
C	0.60242200	0.70693700	-0.00209900
C	-0.28142400	-0.34372900	-0.01228300
C	1.76805000	-1.19439700	0.00455200
H	0.82704900	2.63255900	-0.88144400
H	-0.68814800	2.37446300	-0.00776200
H	-1.35905900	-0.35525800	-0.02148300
O	-3.49321800	-0.19971400	0.00340500
H	-4.11203800	-0.24782200	-0.73345800
H	-4.04784100	-0.32734200	0.78076600
H	2.73038700	0.64354600	0.01717100
H	2.58646000	-1.88981700	0.01068700
H	0.10552100	-2.43446100	-0.01293100
H	0.81585500	2.62984900	0.88594700

Proto-C2 Complex

N	0.27150000	-0.76970400	0.00481700
N	-0.12173100	1.33036700	-0.00422300
C	2.78444900	-0.90914000	0.00272600
C	1.50483800	-0.15823700	0.00091100
C	1.24249900	1.18821500	-0.00494500
C	-0.71075400	0.13481800	0.00170400
H	2.85949300	-1.54436400	-0.87824300
H	3.61416300	-0.20784400	-0.00112800
H	1.90831100	2.03090100	-0.00951700
H	-0.62300400	2.20758300	-0.00760500
H	-1.77265500	-0.06423300	0.00386100
O	-3.80343700	-0.38107800	-0.01126700
H	-4.28212100	-0.63182200	0.78643000
H	-4.22592500	-0.89478100	-0.70837200
H	0.11321200	-1.76840000	0.00938400
H	2.86144700	-1.53698900	0.88880000

Pi-5-Methylimidazole

N	-0.17365800	-1.03390700	-0.00020300
N	-1.53346800	0.71464700	-0.00008700
C	2.13043700	-0.02083400	-0.00004600
C	0.64598300	0.06717500	0.00007400
C	-0.22249100	1.13907700	-0.00018500
C	-1.46447800	-0.61087300	0.00039500
H	2.49751900	-0.54627400	-0.88156700
H	2.55178500	0.98194000	-0.00124300
H	0.03535100	2.18557300	-0.00041300
H	-2.29785600	-1.29284200	0.00048200
H	0.12845600	-1.99655200	0.00085100
H	2.49792000	-0.54430500	0.88248800

Pi-C4 Complex

N	1.84406300	0.39013100	0.00937100
N	0.85339100	-1.59152500	-0.00614600
C	-0.06758200	2.02876100	-0.00710800
C	0.49696100	0.65287200	-0.00450300
C	-0.09728400	-0.59282300	-0.01365500

C	2.01928600	-0.95732100	0.00778800
H	0.25323300	2.58984200	-0.88495700
H	-1.15389400	1.97114100	-0.01756000
H	-1.15478800	-0.80311300	-0.02523500
O	-3.55589700	-0.43836500	0.00081000
H	-4.20500100	-0.49684200	-0.70869400
H	-4.09478600	-0.38368800	0.79750400
H	2.99422100	-1.41472200	0.01707000
H	0.23647000	2.58621100	0.87897100
H	2.58126200	1.07891500	0.01871300

Pi-C2 Complex

N	-0.29486800	-0.74027200	-0.01170700
N	0.09815400	1.43860900	0.00027900
C	-2.80655500	-0.91206500	0.00421800
C	-1.53177400	-0.14622800	0.00072100
C	-1.25982400	1.20654600	0.00813300
C	0.65512800	0.23251200	-0.01173600
H	-2.88362000	-1.55294300	0.88263200
H	-3.64469100	-0.21873700	0.01405000
H	-1.97484700	2.01316000	0.01854400
H	1.71132000	0.01519000	-0.02005800
O	3.96553500	-0.40578500	0.00100000
H	4.50886200	-0.52249000	0.78789000
H	4.60586600	-0.38554100	-0.71845700
H	-0.11692300	-1.73345300	-0.01952000
H	-2.89510100	-1.54186200	-0.88110300

Atomic Coordinates (x y z) for Optimized Geometries of 5-methylimidazole···acetone Complexes:

BHandHLYP/6-31+G(d) Level:

Acetone

O	0.00000000	0.00000000	1.39043100
C	0.00000000	0.00000000	0.17776300
C	0.00000000	1.28062500	-0.60790600
H	0.12435500	2.13176400	0.05154800
H	0.79111800	1.26999200	-1.35424300
H	-0.94262000	1.37452100	-1.14488100
C	0.00000000	-1.28062500	-0.60790600
H	-0.79111800	-1.26999200	-1.35424300
H	0.94262000	-1.37452100	-1.14488100
H	-0.12435500	-2.13176400	0.05154800

Tau-5-methylimidazole

N	0.09284700	-1.13791300	-0.00010200
N	1.44980300	0.58647200	0.00007600
C	-0.65541600	0.01672900	-0.00012400
C	0.17675500	1.09690200	0.00005500
C	1.34384800	-0.75488600	-0.00000800
H	-0.01589600	2.15124200	-0.00061800
H	2.30339900	1.11196300	0.00012500
H	2.20085900	-1.40120000	0.00022200
C	-2.14521700	-0.01380000	0.00008400
H	-2.52714300	-0.53199500	0.87764800
H	-2.55230500	0.99326800	-0.00035500
H	-2.52728800	-0.53286200	-0.87688500

Tau-C4 Complex

N	3.61220100	0.00149300	-0.03925300
N	1.99173800	-1.47720000	-0.07324500
C	2.32715600	2.14466600	0.13287200
C	2.40576900	0.65915900	0.04109900
C	1.38807800	-0.24872500	0.02092500
C	3.32143500	-1.27239300	-0.10589600
H	2.78958700	2.61737700	-0.73168500
H	1.29328500	2.47419700	0.18345900
H	0.32175700	-0.13817000	0.06274900
H	1.52953000	-2.36577100	-0.11067200
O	-2.02382800	-0.19950000	0.12324200
H	4.02798800	-2.07732300	-0.17808000
H	2.84192700	2.51212800	1.01874000
C	-3.22108300	-0.03606700	0.01608300
C	-4.18440900	-1.18184600	0.14027000
H	-4.85768100	-1.00706400	0.97740500
H	-4.80065500	-1.25058100	-0.75381100
H	-3.65103500	-2.11323200	0.29082200
C	-3.80803000	1.32127800	-0.24715500
H	-4.34621900	1.31164800	-1.19314700
H	-4.53049200	1.57287700	0.52650400
H	-3.02843100	2.07343200	-0.27991800

Tau-C2 Complex

N	-1.96488200	-0.81428900	0.15135500
N	-1.73263100	1.32125200	-0.29148700
C	-4.45764500	-1.03292300	0.26829900
C	-3.21217600	-0.23904400	0.07002700
C	-3.08191200	1.08998200	-0.20490200
C	-1.10681500	0.14985900	-0.07048400
H	-4.48149600	-1.48623900	1.25753900
H	-5.33760400	-0.40440500	0.16479400
H	-3.80572300	1.86842800	-0.34289900
H	-1.28953200	2.19955900	-0.48349800
H	-0.03677900	0.05605700	-0.08257300
O	2.27471600	0.11464500	-0.09918500
H	-4.53068600	-1.83802900	-0.46049100
C	3.46657500	-0.08768900	0.00250000
C	4.06978200	-1.41842200	-0.34545300
H	4.76669200	-1.29885500	-1.17310000
H	4.64036700	-1.80379300	0.49688700
H	3.29708300	-2.12656800	-0.62127100
C	4.40653600	0.98135900	0.48155100
H	4.88264000	0.66212300	1.40690000
H	5.20001400	1.13692600	-0.24628800
H	3.87381200	1.91017200	0.64917800

Proto-5-methylimidazole

N	3.38829200	0.03127500	0.00531000
N	1.88535300	-1.47424600	0.03104000
C	2.08147800	2.18064000	-0.03959800
C	2.17959300	0.69978500	-0.01148300
C	1.22772200	-0.26416900	0.00507300
C	3.18884900	-1.27591100	0.03069600
H	2.58064500	2.58798900	-0.91486900
H	1.03915400	2.47606300	-0.06980700

H	0.15633300	-0.19766500	0.00226800
O	-1.95161900	0.36117400	-0.02628700
H	4.29587700	0.46340800	0.00023900
H	3.94796300	-2.03096100	0.04912500
H	1.44587400	-2.37757900	0.04936100
H	2.53634500	2.61846700	0.84520500
C	-3.11206300	0.00547400	-0.00641200
C	-4.23446100	0.99847300	0.07733600
H	-4.94477600	0.83403800	-0.73025400
H	-4.77614100	0.85714800	1.01127200
H	-3.85154800	2.01118600	0.03152400
C	-3.48810900	-1.44691400	-0.06567900
H	-2.60298400	-2.07174900	-0.03884400
H	-4.14489000	-1.70119300	0.76353600
H	-4.04246000	-1.64201700	-0.98251400

Proto-C4 Complex

N	-0.11717200	-1.04821900	0.00016600
N	-1.45018000	0.61095200	-0.00003300
C	2.16353900	0.01554600	-0.00003100
C	0.68077700	0.07872500	-0.00000700
C	-0.17495000	1.12826200	0.00001500
C	-1.39430200	-0.70584200	-0.00015300
H	2.53018600	-0.50530600	-0.88055100
H	2.57140600	1.01966100	-0.00005400
H	0.01013000	2.18227200	0.00001800
H	-2.30228100	1.14426400	0.00041200
H	-2.22976100	-1.37583800	-0.00013100
H	0.21110700	-1.99895200	0.00001400
H	2.53029300	-0.50536800	0.88042100

Proto-C2 Complex

N	-1.69132600	-0.71216900	-0.02191600
N	-1.58958800	1.39082800	-0.31434500
C	-4.14779800	-1.15486200	0.30633200
C	-2.99249000	-0.25637800	0.05940300
C	-2.91805000	1.08203500	-0.12769500
C	-0.86037200	0.29316600	-0.24759200
H	-4.04101100	-1.67464900	1.25483000
H	-5.06266200	-0.57425600	0.33490000
H	-3.68360700	1.82972800	-0.14421100
H	-1.21929400	2.31045000	-0.47797300
H	0.20968300	0.22285000	-0.35354100
O	2.20505800	-0.10698100	-0.68635700
H	-1.40152600	-1.67008200	0.07320400
H	-4.23787100	-1.89908200	-0.48055600
C	3.22456000	-0.09670400	-0.02589500
C	4.52900500	-0.56748200	-0.59870500
H	5.30628700	0.17537000	-0.43538200
H	4.84149400	-1.47388000	-0.08254100
H	4.42827200	-0.77305700	-1.65793700
C	3.23518600	0.38438200	1.39562200
H	3.69852000	-0.35720000	2.04237100
H	3.83855900	1.28797400	1.46517900
H	2.22883900	0.59613200	1.73752100

Pi-5-Methylimidazole

N	-0.18169600	-1.03078100	0.00026800

N	-1.52239500	0.70825600	-0.00002800
C	2.12416900	-0.02470000	-0.00002700
C	0.64005300	0.06781600	-0.00004900
C	-0.21402800	1.13119400	0.00002000
C	-1.46089600	-0.59589500	-0.00010800
H	2.49279300	-0.55046300	-0.87869400
H	2.55362700	0.97199100	-0.00035500
H	0.04009900	2.17465300	0.00010000
H	-2.29719700	-1.26875900	-0.00000800
H	0.11071900	-1.99029300	-0.00068300
H	2.49280400	-0.54993700	0.87893900

Pi-C4 Complex

N	-3.57835400	-0.01121400	-0.01265500
N	-2.03895100	-1.57640900	-0.01929000
C	-2.26805900	2.13496600	0.03118500
C	-2.37729000	0.65195100	0.00924300
C	-1.43895800	-0.33823600	0.00477100
C	-3.32249300	-1.33776700	-0.02910600
H	-2.74520300	2.55947500	0.91248700
H	-1.22250400	2.42570200	0.04296500
H	-0.37022000	-0.22961600	0.01753000
O	2.09491800	0.05120200	0.04511000
H	-4.48797300	0.41108900	-0.01574300
H	-4.10329800	-2.07417400	-0.04784800
H	-2.73230700	2.58427900	-0.84467900
C	3.30467300	-0.02689100	0.00765300
C	4.16934300	1.19956700	-0.06514200
H	4.71337000	1.20590600	-1.00817000
H	3.56503800	2.09620500	0.00933700
H	4.91177600	1.18650200	0.72981900
C	4.00716400	-1.35470200	0.03129800
H	4.60642000	-1.43381300	0.93671400
H	3.28886500	-2.16582700	0.00131500
H	4.69153800	-1.43530600	-0.81040700

Pi-C2 Complex

N	-2.01234300	-0.72394400	-0.31106100
N	-1.46164700	1.23100000	0.52006800
C	-4.52763700	-0.72840300	-0.25028000
C	-3.19924600	-0.10344700	-0.01324300
C	-2.83073000	1.10515800	0.49986000
C	-1.00390100	0.11158500	0.02480400
H	-4.63998400	-1.65551000	0.30859600
H	-5.31414500	-0.04982200	0.06418700
H	-3.47418800	1.88857100	0.85466900
H	0.03035900	-0.14513800	-0.11268000
O	2.28411500	-0.64826200	-0.23468600
H	-1.90666600	-1.63826800	-0.70950800
H	-4.68129200	-0.95645400	-1.30333900
C	3.39069200	-0.17292800	-0.08837500
C	3.81118200	1.07440200	-0.81192200
H	4.66621000	0.85952300	-1.45014900
H	2.99574300	1.45898600	-1.41333900
H	4.13043100	1.83071100	-0.09779700
C	4.40148700	-0.80447800	0.82556600
H	5.31268300	-1.03152600	0.27604300
H	4.67211900	-0.10449600	1.61393100
H	4.00265300	-1.71119600	1.26536200

BHandHLYP/6-31+G(d,p) Level:

Acetone

O	0.00000000	0.00000000	1.38985700
C	0.00000000	0.00000000	0.17692900
C	0.00000000	1.28028100	-0.60755900
H	0.12028800	2.12997600	0.05314900
H	0.79308900	1.26996800	-1.35074800
H	-0.94055500	1.37069500	-1.14726400
C	0.00000000	-1.28028100	-0.60755900
H	-0.79308900	-1.26996800	-1.35074800
H	0.94055500	-1.37069500	-1.14726400
H	-0.12028800	-2.12997600	0.05314900

Tau-5-Methylimidazole

N	0.09271300	-1.13774400	-0.00002200
N	1.44961300	0.58671000	0.00021400
C	-0.65546500	0.01646200	-0.00001200
C	0.17651900	1.09679600	0.00006600
C	1.34389000	-0.75462400	-0.00018700
H	-0.01820400	2.15014300	-0.00087500
H	2.30224600	1.11133800	-0.00021000
H	2.20063400	-1.40061900	0.00017800
C	-2.14481800	-0.01387800	0.00003100
H	-2.52535300	-0.53277100	0.87684400
H	-2.55085000	0.99271300	0.00047000
H	-2.52550700	-0.53209700	-0.87714400

Tau-C4 Complex

N	3.59960900	0.01697000	0.02191100
N	1.98453400	-1.46358600	-0.09428100
C	2.30482900	2.15825400	0.12383200
C	2.39019100	0.67322600	0.03823200
C	1.37557500	-0.23564100	-0.03359800
C	3.31395300	-1.25751100	-0.05784000
H	2.80971400	2.62927800	-0.71660400
H	1.26974300	2.48500700	0.12156900
H	0.30905600	-0.12332600	-0.04657700
H	1.52671900	-2.35176600	-0.15395700
O	-2.00933100	0.19295500	-0.09098900
H	4.02377500	-2.06154100	-0.09180800
H	2.77352700	2.52632100	1.03376000
C	-3.20422700	-0.00297300	-0.01351900
C	-4.19301700	1.11876300	-0.14583300
H	-4.84635000	0.93285000	-0.99527900
H	-4.82536100	1.16263700	0.73765200
H	-3.67997300	2.06316800	-0.27892000
C	-3.76005800	-1.37783000	0.21961400
H	-4.32329600	-1.39189100	1.14998300
H	-4.45426000	-1.63827000	-0.57569600
H	-2.96112100	-2.10752300	0.26504800

Tau-C2 Complex

N	-1.92639800	-0.77498400	0.24154400
N	-1.77415800	1.29072400	-0.47979900

C	-4.40738100	-1.05607600	0.43438900
C	-3.19345600	-0.25559000	0.11060300
C	-3.11316600	1.02951200	-0.33757400
C	-1.10510500	0.17893000	-0.12066100
H	-4.39719200	-1.37996800	1.47263000
H	-5.30860500	-0.47344500	0.27142000
H	-3.86613900	1.75814100	-0.56056900
H	-1.36532800	2.14876200	-0.79391100
H	-0.03307400	0.11795800	-0.14038600
O	2.27134300	0.08964000	-0.17102100
H	-4.46487200	-1.94814400	-0.18523800
C	3.45993900	-0.07655700	0.00807900
C	4.20694100	-1.18828000	-0.66957500
H	5.06788800	-0.79197200	-1.20202600
H	4.58715200	-1.87896000	0.08006600
H	3.55835200	-1.71814400	-1.35615000
C	4.24871100	0.82134900	0.91623900
H	4.78300400	0.23131900	1.65658200
H	4.99725700	1.35624400	0.33561500
H	3.59580800	1.53117900	1.40891400

Proto-5-Methylimidazole

N	-0.11724900	-1.04843200	0.00027200
N	-1.44972700	0.61154400	-0.00035200
C	2.16304400	0.01552400	0.00003200
C	0.68067600	0.07760700	-0.00041300
C	-0.17419300	1.12786400	0.00027900
C	-1.39434400	-0.70486100	0.00012400
H	2.52923200	-0.50680600	-0.87893600
H	2.56857000	1.01970600	-0.00153800
H	0.01368400	2.18079600	-0.00047700
H	-2.30096300	1.14412700	0.00100000
H	-2.22979300	-1.37434300	-0.00014900
H	0.20891800	-1.99868900	-0.00092400
H	2.52808900	-0.50337700	0.88145700

Proto-C4 Complex

N	3.37366300	-0.00803000	-0.00330500
N	1.82063300	-1.46214200	0.02974900
C	2.13589100	2.18251900	-0.04346200
C	2.18819800	0.69983900	-0.01384400
C	1.20442100	-0.23125600	0.00715800
C	3.12959000	-1.30711400	0.02313900
H	2.62299900	2.57124600	-0.93308400
H	1.10314900	2.50880600	-0.04711600
H	0.13645800	-0.12294200	0.00706100
O	-1.96066500	0.45128400	0.05340300
H	4.29446200	0.39271100	-0.01322400
H	3.86130000	-2.08855100	0.03711300
H	1.35407400	-2.35073400	0.04845000
H	2.62798200	2.60679800	0.82695100
C	-3.09515300	0.02150800	0.00849300
C	-3.37345900	-1.45052800	-0.07709700
H	-4.07550400	-1.74746900	0.69773000
H	-3.84290500	-1.67224200	-1.03330600
H	-2.45565300	-2.01782000	0.01579100
C	-4.28071500	0.94066300	0.03496500
H	-3.96083000	1.97447100	-0.00523400
H	-4.94506700	0.72286300	-0.79719900

H	-4.84785400	0.77001900	0.94762900

Proto-C2 Complex

N	-1.80927700	-0.77382700	0.15694100
N	-1.43903800	1.20810000	-0.51713200
C	-4.31186500	-0.86309700	0.40945800
C	-3.04650300	-0.16661900	0.07045700
C	-2.80151300	1.09328700	-0.35887000
C	-0.85358400	0.06901000	-0.20123100
H	-4.31291200	-1.18200600	1.44776300
H	-5.14910700	-0.19357800	0.25469700
H	-3.46906400	1.90399100	-0.56201200
H	-0.95152500	2.02922200	-0.82603700
H	0.20427900	-0.13459500	-0.22904900
O	2.19622200	-0.53334700	-0.46309900
H	-1.64260600	-1.72089200	0.44670100
H	-4.45134500	-1.74000700	-0.21608800
C	3.24240000	-0.14299800	0.01601200
C	4.56375300	-0.61663900	-0.51104600
H	5.08868500	0.22137000	-0.96502900
H	5.18715000	-0.97936300	0.30195200
H	4.42109100	-1.39681400	-1.24827400
C	3.26868900	0.83077600	1.15628400
H	3.68592200	0.34192300	2.03421600
H	3.91897800	1.66912600	0.92058900
H	2.27061900	1.18617300	1.38032500

Pi-5-Methylimidazole

N	-0.18149000	-1.03091000	0.00028600
N	-1.52181400	0.70848800	-0.00003500
C	2.12340600	-0.02497400	-0.00002200
C	0.63981400	0.06742000	-0.00004900
C	-0.21337300	1.13149100	0.00001200
C	-1.46084000	-0.59565800	-0.00009900
H	2.49071400	-0.55056300	-0.87843100
H	2.55142900	0.97141500	-0.00042100
H	0.04295800	2.17381900	0.00009700
H	-2.29690400	-1.26816300	0.00002400
H	0.11015700	-1.98931100	-0.00083600
H	2.49072500	-0.54991900	0.87875700

Pi-C4 Complex

N	-3.56961400	-0.00868500	-0.01457700
N	-2.03250700	-1.57617300	-0.02049200
C	-2.25602700	2.13425900	0.03401000
C	-2.36774600	0.65196600	0.01001300
C	-1.43020100	-0.33900200	0.00597100
C	-3.31569300	-1.33586000	-0.03216100
H	-2.73358900	2.55713700	0.91495900
H	-1.21049600	2.42184600	0.04756500
H	-0.36198600	-0.23008400	0.02056800
O	2.08387800	0.05733300	0.05066800
H	-4.47748600	0.41430300	-0.01894600
H	-4.09736700	-2.07067900	-0.05303800
H	-2.71823300	2.58418400	-0.84170600
C	3.29334800	-0.02678000	0.00852200
C	4.16237700	1.19500500	-0.07195800
H	4.70948800	1.18966700	-1.01230500

H	3.56082900	2.09321400	-0.00690600
H	4.90108200	1.18396900	0.72555300
C	3.98841200	-1.35745100	0.03389500
H	4.59894000	-1.43120500	0.93125500
H	3.26517100	-2.16346500	0.01923800
H	4.66064600	-1.44635800	-0.81584700

Pi-C2 Complex

N	-2.00251400	-0.72355500	-0.30731600
N	-1.45843800	1.23649100	0.51619400
C	-4.51689300	-0.73478900	-0.24796800
C	-3.19088000	-0.10533400	-0.01277200
C	-2.82726200	1.10664900	0.49573300
C	-0.99659600	0.11658500	0.02586000
H	-4.62555100	-1.65953100	0.31411800
H	-5.30409700	-0.05721400	0.06400500
H	-3.47475100	1.88786500	0.84625700
H	0.03826600	-0.13770800	-0.10990900
O	2.27884100	-0.66025100	-0.23017500
H	-1.89376100	-1.63802700	-0.70135500
H	-4.66844100	-0.96631400	-1.29981900
C	3.38175100	-0.17454900	-0.08796600
C	3.78657200	1.07672300	-0.81172400
H	4.64226000	0.87015400	-1.45054900
H	2.96558900	1.45157000	-1.41024100
H	4.09941000	1.83440900	-0.09732700
C	4.40107900	-0.79788400	0.82061000
H	5.31061700	-1.01575800	0.26610300
H	4.66875500	-0.09518100	1.60653500
H	4.01100800	-1.70722700	1.26079600

Tau-N3 Complex

N	-2.70293900	1.06445300	-0.42715200
N	-0.78010600	0.01368500	-0.23571800
C	-4.30176600	-0.65670200	0.44127700
C	-2.93097400	-0.18649700	0.09503400
C	-1.74373800	-0.84817500	0.21829600
C	-1.40697300	1.14205600	-0.60933500
H	-4.95052000	-0.65186200	-0.43180000
H	-4.27433500	-1.66800700	0.83497600
H	-1.50945100	-1.82946700	0.57943100
H	0.21566500	-0.16202600	-0.28269100
H	-0.88081400	1.98912800	-1.00635900
O	2.05596000	-0.58277900	-0.47229900
H	-4.75941500	-0.01496800	1.19090400
C	3.06840100	-0.12396800	0.02131800
C	3.02178500	1.01521600	0.99418400
H	3.61303300	0.78419000	1.87610000
H	3.46897800	1.89310900	0.53214300
H	2.00094000	1.23855900	1.27800400
C	4.41658400	-0.67900600	-0.32376400
H	5.09956900	0.12255600	-0.59172500
H	4.83218700	-1.17206000	0.55279800
H	4.33787700	-1.39142400	-1.13535000

Pi-N1 Complex

N	-1.12476500	-0.23789300	-0.07917700

N	-2.99435900	-1.39791200	-0.12511300
C	-1.89496000	2.13645100	0.21242400
C	-2.13519600	0.67636300	0.06381500
C	-3.28206200	-0.06325700	0.03250900
C	-1.68952600	-1.45887500	-0.18776500
H	-1.37210600	2.54548300	-0.64909400
H	-2.84205500	2.65622900	0.30868800
H	-4.29193100	0.29181900	0.11447400
H	-1.10758100	-2.35237000	-0.31007800
O	1.68492400	0.51881700	-0.19773400
H	-0.13271000	-0.03770300	-0.10020300
H	-1.29894600	2.35579000	1.09537800
C	2.77691500	0.01516600	-0.01747600
C	2.92348900	-1.41249300	0.41457500
H	3.32903100	-1.43685700	1.42403200
H	1.96785300	-1.92128400	0.39772300
H	3.63342900	-1.92935400	-0.22542800
C	4.03506900	0.80328200	-0.22027700
H	4.68902000	0.70103700	0.64151400
H	4.57187500	0.40043400	-1.07682200
H	3.80623100	1.84706000	-0.39511900

Proto-N1 Complex

N	1.05076300	-0.24801300	0.01408700
N	2.93208600	-1.25666600	0.00499200
C	1.68663100	2.18390700	-0.01836400
C	2.01631400	0.73668900	-0.00625400
C	3.20722900	0.09079100	-0.01187200
C	1.62436900	-1.43688700	0.02045300
H	1.11711400	2.45982800	0.86429300
H	2.59994900	2.76624900	-0.03406600
H	4.20836700	0.46717000	-0.02628000
H	3.61102900	-1.99575100	0.00546700
H	1.12087900	-2.38166100	0.03501900
O	-1.63140100	0.47850100	0.02990400
H	0.03934800	-0.08675700	0.02241300
H	1.09911400	2.44086800	-0.89493800
C	-2.74466100	-0.01497200	0.00441500
C	-3.96581600	0.85001600	0.00799900
H	-4.66384500	0.52662900	-0.75907200
H	-4.47099900	0.73875000	0.96557900
H	-3.69778100	1.88849800	-0.13958900
C	-2.94846100	-1.49754300	-0.03482400
H	-3.71490200	-1.79534000	0.67479900
H	-3.30633200	-1.77264100	-1.02535200
H	-2.02429500	-2.02310100	0.16963800

Proto-N3 Complex

N	-2.71804700	1.02979400	-0.25262600
N	-0.70392300	0.37717800	0.02330900
C	-4.08286300	-1.03785400	0.18765700
C	-2.79601100	-0.30732700	0.07723900
C	-1.51391800	-0.71036300	0.24997500
C	-1.45123200	1.41709800	-0.27863300
H	-4.62066700	-1.02284900	-0.75592000
H	-3.89349400	-2.06938100	0.45858200
H	-1.11711300	-1.66878300	0.51199700
O	2.05128100	0.61731800	0.24487600

H	-3.49748000	1.63269700	-0.44607800
H	-1.10139100	2.40347900	-0.50446200
H	0.31917700	0.39129400	0.07973200
H	-4.71831300	-0.59337600	0.94824700
C	3.03596200	-0.06541300	0.02499400
C	2.92473300	-1.45740000	-0.51425500
H	3.60402900	-1.59354000	-1.35100300
H	3.22914500	-2.15827000	0.26055400
H	1.90925900	-1.67718400	-0.81859300
C	4.40981300	0.46386500	0.29199200
H	4.35834000	1.41844500	0.80000800
H	4.97939200	-0.24771400	0.88357300
H	4.93374900	0.58220000	-0.65423200

BHandHLYP/6-311+G(d) Level:

Acetone

O	0.00000000	0.00000000	1.38632300
C	0.00000000	0.00000000	0.18009600
C	0.00000000	1.27777400	-0.60692300
H	0.14053400	2.12753500	0.04781100
H	0.77708200	1.25632300	-1.36491100
H	-0.94993200	1.37428100	-1.12693900
C	0.00000000	-1.27777400	-0.60692300
H	-0.77708200	-1.25632300	-1.36491100
H	0.94993200	-1.37428100	-1.12693900
H	-0.14053400	-2.12753500	0.04781100

Tau-C4 Complex

N	-3.57258700	-0.02605200	-0.08143200
N	-1.91667900	-1.45800800	-0.14092300
C	-2.35033900	2.13575700	0.22571300
C	-2.38748400	0.65677800	0.06231700
C	-1.34839300	-0.22114500	0.02706800
C	-3.24851900	-1.28469100	-0.19973100
H	-2.90227900	2.44536900	1.10904300
H	-1.32913000	2.48641700	0.32549300
H	-0.28881000	-0.08422900	0.10449700
H	-1.43230600	-2.33030900	-0.20707200
O	2.00487200	0.26940800	0.21854600
H	-3.93054500	-2.10175300	-0.32856900
H	-2.79733600	2.63497700	-0.62973200
C	3.17315600	0.02444600	0.04146400
C	3.74634100	-1.33018600	0.33718300
H	4.27017100	-1.71294600	-0.53376500
H	4.47812600	-1.24434400	1.13628700
H	2.96490600	-2.01769500	0.63219000
C	4.12286800	1.06015500	-0.48425500
H	4.97733300	1.15499500	0.17928500
H	4.50464300	0.74081200	-1.45052200
H	3.62533200	2.01517600	-0.58757300

Tau-C2 Complex

N	-2.02750600	-0.82332200	0.36561800
N	-1.50312600	1.12168200	-0.49168400
C	-4.52788900	-0.74951800	0.27934500
C	-3.18444200	-0.15461200	0.04242700

C	-2.87267000	1.05667100	-0.49168400
C	-1.04504900	-0.02938100	0.03191700
H	-4.67758300	-0.96832300	1.33309300
H	-5.31161000	-0.07131500	-0.03946500
H	-3.48314900	1.85402000	-0.86059900
H	-0.94413700	1.88313200	-0.81966500
H	0.00239300	-0.23397000	0.14576300
O	2.26492100	-0.61294800	0.22523200
H	-4.64397100	-1.68155800	-0.26701700
C	3.38250700	-0.17780200	0.08982700
C	4.36174900	-0.80738700	-0.85618100
H	4.77946200	-0.05602000	-1.51967700
H	5.18888200	-1.22579700	-0.28828400
H	3.88522000	-1.58924600	-1.43234800
C	3.85850700	1.01935500	0.85842200
H	4.80204400	0.80121300	1.34952800
H	4.04162100	1.83747600	0.16630700
H	3.11960200	1.32149300	1.58853400

Proto-C4 Complex

N	3.37071300	-0.02412400	0.05429900
N	1.80606600	-1.44993800	-0.13088600
C	2.15716800	2.17707400	0.14475600
C	2.19453400	0.69908500	0.04222000
C	1.20460000	-0.21301000	-0.07544100
C	3.11234900	-1.31425400	-0.05118800
H	2.69893100	2.63654000	-0.67559100
H	1.13048800	2.51703800	0.11206400
H	0.14059600	-0.09188600	-0.12367800
O	-1.96546300	0.40418800	-0.22902700
H	4.29402900	0.36103900	0.13096100
H	3.83339500	-2.10367600	-0.06856800
H	1.33075700	-2.32863000	-0.21809000
H	2.60195400	2.51249700	1.07598400
C	-3.09191200	0.01690400	-0.03121600
C	-4.26445700	0.94923000	-0.09918200
H	-5.03825400	0.53682500	-0.73945000
H	-4.69406200	1.05199400	0.89419900
H	-3.95752900	1.92083600	-0.46252600
C	-3.38444800	-1.41748800	0.29420100
H	-2.46622700	-1.97044800	0.44073600
H	-4.00691000	-1.48340200	1.18133500
H	-3.94792400	-1.85904100	-0.52393700

Proto-C2 Complex

N	-1.81475000	-0.77991300	0.16173400
N	-1.43407800	1.19632400	-0.51391300
C	-4.31649300	-0.85326700	0.41274700
C	-3.04828400	-0.16576400	0.07401500
C	-2.79707500	1.08889900	-0.35592700
C	-0.85628700	0.05636500	-0.19664200
H	-4.31694700	-1.17487200	1.44913900
H	-5.14864800	-0.17837500	0.26149700
H	-3.45893900	1.90198000	-0.56030300
H	-0.94289700	2.01387200	-0.82312700
H	0.19930200	-0.15278700	-0.22191900
O	2.18639900	-0.58163700	-0.38146300
H	-1.65381200	-1.72632900	0.45320800
H	-4.46202700	-1.72692800	-0.21420900

C	3.23966100	-0.14574400	0.02038200
C	4.54585900	-0.73860100	-0.41284900
H	5.21678300	0.04095500	-0.76057500
H	5.02205400	-1.21019500	0.44315500
H	4.39086900	-1.47352700	-1.19126000
C	3.30046600	1.01076500	0.97200100
H	3.94108100	0.77128300	1.81513800
H	3.74635700	1.86275300	0.46487900
H	2.31035400	1.27447500	1.31897200

Pi-C4 Complex

N	-3.51687400	0.01095700	-0.10723600
N	-2.02264300	-1.58746700	0.01395000
C	-2.16209400	2.12207000	0.02792300
C	-2.30598000	0.64409800	0.00474200
C	-1.39560700	-0.36476800	0.07850900
C	-3.29199100	-1.32043400	-0.09682100
H	-2.69424700	2.56118200	0.86737300
H	-1.11530700	2.38609100	0.11765200
H	-0.33079000	-0.27951600	0.17526600
O	2.09191100	-0.18150400	0.44637000
H	-4.41101100	0.45358800	-0.18269000
H	-4.08583800	-2.03692100	-0.17251000
H	-2.54772600	2.57397000	-0.88188300
C	3.23279500	-0.05375300	0.07529900
C	3.82905500	1.29868100	-0.18349000
H	4.04825300	1.39498800	-1.24394200
H	3.14385600	2.08019700	0.11674300
H	4.77085600	1.40331200	0.34680200
C	4.12450600	-1.23941900	-0.14932000
H	4.93262800	-1.22075400	0.57759600
H	3.56600900	-2.16019300	-0.04602400
H	4.58054700	-1.18718800	-1.13339800

Pi-C2 Complex

N	-2.01339500	-0.72234900	-0.31370100
N	-1.46701100	1.22516800	0.52734800
C	-4.52608600	-0.72561100	-0.26028500
C	-3.19993600	-0.10336800	-0.01670300
C	-2.83556300	1.10007600	0.50252200
C	-1.00743800	0.11191600	0.02966900
H	-4.63917300	-1.65250400	0.29532500
H	-5.31138200	-0.04788500	0.05216200
H	-3.48111300	1.87890000	0.85788200
H	0.02614500	-0.14347400	-0.10604000
O	2.27472400	-0.60591400	-0.23590600
H	-1.90653100	-1.63242600	-0.71566900
H	-4.67309300	-0.95038000	-1.31314100
C	3.38947500	-0.16762300	-0.08793800
C	3.85047400	1.06659900	-0.80551400
H	4.67236900	0.81240000	-1.46965500
H	3.04040900	1.49874100	-1.37763000
H	4.23093000	1.79227400	-0.09255800
C	4.37973700	-0.83029000	0.82350500
H	5.29856300	-1.04378200	0.28522900
H	4.63549100	-0.15076700	1.63234900
H	3.96845000	-1.74371900	1.23193000

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

Acetone

O	0.00000000	0.00000000	1.39809500
C	0.00000000	0.00000000	0.17893700
C	0.00000000	1.28431200	-0.61170600
H	0.16809100	2.13703100	0.04618100
H	0.76335600	1.25061500	-1.39424500
H	-0.96879500	1.39279100	-1.11089500
C	0.00000000	-1.28431200	-0.61170600
H	-0.76335600	-1.25061500	-1.39424500
H	0.96879500	-1.39279100	-1.11089500
H	-0.16809100	-2.13703100	0.04618100

Tau-5-Methylimidazole

N	0.08826100	-1.14484800	0.00054200
N	1.45548600	0.58915500	0.00038500
C	-0.65806400	0.01605400	0.00026900
C	0.17998300	1.10372600	-0.00003700
C	1.34863900	-0.76084700	-0.00056700
H	-0.01402800	2.16491300	0.00107800
H	2.31609600	1.11759300	-0.00201000
H	2.21279500	-1.40956800	-0.00033000
C	-2.15318200	-0.01194800	-0.00021900
H	-2.53378100	-0.54024800	0.87904500
H	-2.55850300	1.00233100	0.00679400
H	-2.53306600	-0.52708000	-0.88773500

Tau-C4 Complex

N	-2.82580500	0.86662100	0.15872300
N	-2.50156700	-1.31514900	0.04482400
C	-0.56877500	1.73384800	-0.53234200
C	-1.52859400	0.62341500	-0.24595800
C	-1.31144600	-0.73057900	-0.32155700
C	-3.37684300	-0.31932000	0.32251000
H	-0.35400000	2.31317200	0.37182300
H	0.37363100	1.33279800	-0.91363800
H	-0.42984000	-1.29592200	-0.58544800
H	-2.69318600	-2.30538700	0.09557800
O	1.97712600	-0.95435800	-0.78045600
H	-4.39339700	-0.51218800	0.63470400
H	-0.97850200	2.42115400	-1.27845100
C	2.61040500	-0.30457300	0.03510100
C	1.98162200	0.18446700	1.31575600
H	2.46495800	-0.31186700	2.16388100
H	2.15135900	1.25932900	1.43247000
H	0.91201700	-0.03091600	1.32164900
C	4.05756900	0.05207900	-0.19178300
H	4.14311500	1.13696800	-0.31479700
H	4.65585800	-0.22032000	0.68251100
H	4.43895100	-0.44828900	-1.08182900

Tau-C2 Complex

N	-2.02394600	-0.80911600	0.34286700
N	-1.63344800	1.18275200	-0.52357500
C	-4.53609600	-0.85501700	0.37223000

C	-3.22897900	-0.19101900	0.07684200
C	-3.00133100	1.05040100	-0.46318600
C	-1.08968900	0.04402900	-0.02960500
H	-4.63604800	-1.06396300	1.44176900
H	-5.36998600	-0.21783300	0.06934200
H	-3.67194000	1.82553300	-0.80000900
H	-1.12392900	1.98199700	-0.87215100
H	-0.02017400	-0.10658000	0.03614400
O	2.24191700	-0.23241400	0.16548300
H	-4.62011400	-1.80679200	-0.16085700
C	3.45357100	-0.12585200	0.07078900
C	4.26290700	-1.05604800	-0.79635900
H	4.92921400	-0.48219400	-1.44697600
H	4.89639000	-1.67915400	-0.15635700
H	3.60730000	-1.69127200	-1.39177600
C	4.21263600	0.94322100	0.81460300
H	5.06418000	0.50521900	1.34311100
H	4.61661300	1.66027100	0.09205900
H	3.55679400	1.46033600	1.51491100

Proto-5-Methylimidazole

N	-0.11404300	-1.05248200	-0.00002200
N	-1.45524000	0.61373300	-0.00008300
C	2.17170200	0.01665600	-0.00001100
C	0.68429700	0.07818200	0.00012600
C	-0.17825400	1.13479800	-0.00003100
C	-1.40052600	-0.71188900	0.00004300
H	2.53663300	-0.50619500	-0.88730500
H	2.57579300	1.02888500	0.00034000
H	0.00926200	2.19563400	0.00013500
H	-2.31486900	1.14986700	0.00008200
H	-2.24157000	-1.38647500	0.00014800
H	0.21956300	-2.01002500	-0.00018300
H	2.53685800	-0.50693300	0.88674600

Proto-C4 Complex

N	3.05249700	0.62980700	-0.19420200
N	2.50032800	-1.41028700	0.13284300
C	0.84904600	1.86320000	-0.10821900
C	1.67715200	0.62781700	-0.03858600
C	1.33271200	-0.67596000	0.16966000
C	3.53331200	-0.60655700	-0.08760600
H	0.91863800	2.32166800	-1.09793000
H	-0.19014600	1.59802600	0.09034700
H	0.36271900	-1.11785200	0.33644400
O	-1.71983100	-0.29330900	0.56132600
H	3.62392300	1.44937500	-0.36443900
H	4.56817000	-0.89941000	-0.16382400
H	2.57203400	-2.41320800	0.25473300
H	1.17881800	2.59277100	0.63566600
C	-2.84528900	-0.18272100	0.10130600
C	-3.56021600	1.14343900	0.08370300
H	-3.98538800	1.33514200	-0.90548100
H	-4.39543900	1.10354300	0.79107200
H	-2.88176600	1.94782800	0.36856100
C	-3.58157000	-1.36471500	-0.47330500
H	-3.04138100	-2.28844200	-0.26641000
H	-4.59501600	-1.41642900	-0.06544000
H	-3.67717300	-1.23019700	-1.55611300

Proto-C2 Complex

N	-1.85924700	-0.83760500	0.13262000
N	-1.33257500	1.16416500	-0.39553700
C	-4.37543900	-0.77473100	0.30542600
C	-3.05222900	-0.14042000	0.05352200
C	-2.70754900	1.13487300	-0.28334200
C	-0.82953100	-0.03845900	-0.14078700
H	-4.42075100	-1.18854600	1.31565500
H	-5.16195800	-0.02772400	0.19838900
H	-3.31734800	2.00701500	-0.45194000
H	-0.77620600	1.97625700	-0.63381900
H	0.22104200	-0.31210600	-0.15245200
O	2.21821900	-0.78631800	-0.28268100
H	-1.76943800	-1.81957800	0.36606800
H	-4.55969000	-1.58078300	-0.40890200
C	3.22575200	-0.16495600	0.01911100
C	4.59881300	-0.73642300	-0.21608800
H	5.21945200	-0.01525100	-0.75569700
H	5.08071700	-0.91486700	0.75081800
H	4.53382400	-1.67126900	-0.77225500
C	3.15424800	1.20459900	0.64215700
H	3.77393600	1.24020700	1.54270000
H	3.56491400	1.93712100	-0.06036500
H	2.12412200	1.46724800	0.88368000

Pi-5-Methylimidazole

N	-0.17797200	-1.03543800	0.00009600
N	-1.53080500	0.71145300	-0.00004100
C	2.13267900	-0.02314000	-0.00002700
C	0.64349200	0.06850400	0.00005400
C	-0.21866300	1.13744000	-0.00000100
C	-1.46637600	-0.60205500	-0.00003300
H	2.49994800	-0.55020900	-0.88558600
H	2.55906100	0.98153400	0.00059700
H	0.03996300	2.18732400	0.00006400
H	-2.30547300	-1.28287000	0.00007100
H	0.12117500	-2.00107100	-0.00035400
H	2.49996600	-0.55131300	0.88486200

Pi-C4 Complex

N	-1.72258300	0.26251700	-0.08549100
N	-0.96603200	-1.81344000	-0.11855700
C	0.37263900	1.66994200	0.03767900
C	-0.35128300	0.36701200	-0.02937700
C	0.09438600	-0.93198900	-0.05140500
C	-2.04243100	-1.05787700	-0.13752400
H	0.10246200	2.23203600	0.93691400
H	1.44674200	1.47422200	0.05721100
H	1.12261300	-1.26447900	-0.02380200
O	3.38478300	-0.15636300	-0.04358400
H	-2.37974300	1.03043300	-0.08838000
H	-3.06525300	-1.40318100	-0.18698400
H	0.14803800	2.29622600	-0.83124200
C	4.53702800	0.24276200	-0.06584900
C	4.86941800	1.67687000	-0.39289800
H	5.37650200	1.71124200	-1.36311500
H	3.96200700	2.27954800	-0.43491400
H	5.56354400	2.08560600	0.34683900

C	5.69760300	-0.67274100	0.23097300
H	6.15299600	-0.37202600	1.18055200
H	5.36041900	-1.70696000	0.29917700
H	6.46672300	-0.57302700	-0.54025800

Pi-C2 Complex

N	-1.97102500	-0.94489200	-0.06328200
N	-1.02960700	1.05259800	-0.06127100
C	-4.43866700	-0.46133800	0.14799800
C	-3.00829400	-0.04782200	0.05063700
C	-2.39890700	1.18266700	0.04930800
C	-0.80781000	-0.24363200	-0.12669200
H	-4.61709200	-1.07887000	1.03342200
H	-5.06992200	0.42623700	0.21821700
H	-2.87634400	2.15006800	0.12396300
H	0.16146400	-0.71922900	-0.21962300
O	2.42053700	-1.13264600	-0.24560000
H	-2.05608300	-1.95158900	-0.09570800
H	-4.74979500	-1.03323200	-0.73121600
C	3.14700200	-0.17498200	-0.03433900
C	2.63657700	1.24067500	-0.12517800
H	3.07787700	1.71365900	-1.00955900
H	1.54831300	1.26099700	-0.20554200
H	2.96360300	1.81947600	0.74344100
C	4.60044100	-0.35238600	0.32344400
H	5.22610400	0.28043000	-0.31257600
H	4.75555100	-0.02251700	1.35613600
H	4.89439800	-1.39730300	0.22464900

Atomic Coordinates (x y z) for Optimized Geometries of 5-methylimidazole···N-methylacetamide Complexes:

N-methylacetamide

O	-0.38895500	1.37581100	-0.00001400
C	-0.47686200	0.15051300	-0.00008100
C	-1.81461100	-0.53812900	0.00000800
H	-2.37061600	-0.22003000	-0.87631000
H	-1.73950600	-1.61947100	-0.00092100
H	-2.36952800	-0.22157200	0.87760300
N	0.60666100	-0.63614200	0.00010200
H	0.48383200	-1.62829400	-0.00044400
C	1.95121400	-0.10338400	0.00000800
H	2.12791500	0.50453400	0.88207400
H	2.64842900	-0.93113000	-0.00255600
H	2.12604400	0.50847200	-0.87966300

Tau-C4 Complex

N	3.92330500	-0.11582700	0.01874600
N	2.21774400	-1.44456400	-0.35376000
C	2.76805800	2.04780200	0.52140800
C	2.75775600	0.60126200	0.16446400
C	1.68703900	-0.21261000	-0.06423200
C	3.55745100	-1.33334500	-0.29086300
H	3.30359700	2.63206000	-0.22358500
H	1.75619200	2.43466100	0.58972100
H	0.62916300	-0.03313700	-0.04881400
H	1.70530000	-2.27646800	-0.57138300

O	-1.63615900	0.13930800	-0.04197200
H	4.21472200	-2.16082800	-0.47735100
H	3.25794600	2.21226100	1.47856900
C	-2.82008300	0.45757600	-0.13123300
C	-3.22776000	1.84969300	-0.52906300
H	-4.30236700	1.98335700	-0.57701300
H	-2.81426000	2.55223400	0.18776000
H	-2.79768400	2.07496800	-1.49984100
N	-3.80572900	-0.41164400	0.12047200
H	-4.75356900	-0.10612900	0.03238300
C	-3.55187300	-1.78037800	0.51316500
H	-4.50186000	-2.27328700	0.67348400
H	-3.00436000	-2.31110600	-0.25979500
H	-2.97431100	-1.81880200	1.43156200

Tau-C2 Complex

N	2.20624900	-0.16475100	-0.82985900
N	1.95896400	-0.05851900	1.34641000
C	4.69343800	0.01584200	-1.06055100
C	3.44589100	-0.03456400	-0.24784900
C	3.30656700	0.03265800	1.10669200
C	1.34210800	-0.17546100	0.15507300
H	4.67808100	0.85699700	-1.74995400
H	5.56571800	0.11827400	-0.42267200
H	4.02389900	0.13402600	1.89586000
H	1.51119800	-0.04261500	2.24151700
H	0.27483100	-0.26522300	0.06331000
O	-1.92830500	-0.63448500	0.01350500
H	4.81178800	-0.88893900	-1.65251000
C	-3.13719100	-0.43252200	-0.08296200
C	-4.11700200	-1.57218200	-0.13967600
H	-5.14705700	-1.24692800	-0.22913500
H	-3.86856900	-2.20341000	-0.98703100
H	-4.00968400	-2.16878100	0.76078000
N	-3.64276700	0.80472900	-0.14060900
H	-4.63258200	0.91976000	-0.22298100
C	-2.80775000	1.98502100	-0.09520300
H	-3.44554200	2.85865900	-0.12871300
H	-2.22281600	2.00888600	0.81892100
H	-2.12629900	2.01221500	-0.94016300

Proto-C4 Complex

N	-3.55750500	-0.03160000	0.02901400
N	-1.94996600	-1.27617300	-0.59827800
C	-2.42351900	2.10793900	0.70881500
C	-2.40912400	0.71816200	0.18926600
C	-1.38950100	-0.07899500	-0.21180300
C	-3.25841900	-1.22841200	-0.44625400
H	-2.83585400	2.14364800	1.71315000
H	-1.41210900	2.49423000	0.73905800
H	-0.33020100	0.09907300	-0.25424100
O	1.69214000	0.64053000	-0.43452700
H	-4.49128700	0.27416200	0.23733300
H	-3.95266100	-2.01299000	-0.66653100
H	-1.44786000	-2.07301300	-0.94539100
H	-3.02066300	2.75500600	0.07275700
C	2.86228200	0.34937900	-0.18941700
C	3.99081700	1.26098300	-0.58372100
H	4.96663400	0.87468200	-0.31289200

H	3.95472400	1.41605400	-1.65735900
H	3.84422800	2.22394600	-0.10462400
N	3.18922500	-0.78525000	0.43689200
H	4.15415500	-0.97831800	0.61421000
C	2.19746400	-1.74544300	0.86937100
H	1.62793100	-2.12118000	0.02469700
H	2.70573700	-2.57275600	1.34708000
H	1.50781300	-1.29729800	1.57803800

Proto-C2 Complex

N	1.94962900	0.12501900	-0.70151500
N	1.81620100	-0.71395400	1.24636700
C	4.41646000	0.49481000	-1.03034400
C	3.24668700	0.04866800	-0.23404200
C	3.15263400	-0.48581700	1.00570800
C	1.10145000	-0.33927300	0.20254500
H	4.33818500	1.54969800	-1.27701100
H	5.32491600	0.34148900	-0.46082200
H	3.90951100	-0.71941900	1.72453400
H	1.43002000	-1.10921100	2.08410300
H	0.02852600	-0.40193100	0.10087900
O	-1.88238700	-0.76392100	-0.20053700
H	1.67280900	0.47955100	-1.59919100
H	4.49186100	-0.06689100	-1.95701900
C	-3.03471500	-0.32793300	-0.20087200
C	-4.19309200	-1.20069300	-0.59308700
H	-5.14482000	-0.68307300	-0.56611500
H	-4.02077300	-1.57858600	-1.59577300
H	-4.23150500	-2.05149500	0.07995300
N	-3.31117000	0.93115000	0.14570600
H	-4.26288300	1.23787100	0.12794100
C	-2.28575700	1.87086300	0.54428600
H	-1.56980700	2.02549700	-0.25717700
H	-2.75826700	2.81510500	0.78060400
H	-1.75330000	1.51350600	1.42031900

Pi-C4 Complex

N	-3.87997700	-0.12610100	0.02142400
N	-2.22926100	-1.52691900	0.38573200
C	-2.73070400	2.04096900	-0.52886300
C	-2.73077700	0.60063400	-0.16063200
C	-1.72090500	-0.28719900	0.06997400
C	-3.52694500	-1.38947900	0.34603400
H	-3.23418400	2.64571400	0.22200400
H	-1.70966200	2.39556700	-0.61686800
H	-0.66343600	-0.10321400	0.02734700
O	1.71211400	0.24496400	-0.02086400
H	-4.81744600	0.21484800	-0.06943200
H	-4.25138500	-2.15695900	0.53989400
H	-3.22988000	2.21066300	-1.48019600
C	2.91485400	0.45424000	0.11878600
C	3.43042200	1.80249600	0.54249400
H	3.11158600	2.54210200	-0.18532300
H	2.98373800	2.06258500	1.49694200
H	4.50992100	1.83771700	0.63430500
N	3.82830700	-0.50007400	-0.09754600
H	4.79556400	-0.28030000	0.02754800
C	3.46850700	-1.83837200	-0.51147400
H	4.37430900	-2.42217000	-0.61072200
H	2.82240800	-2.31028700	0.22231400

H	2.95137100	-1.82405200	-1.46607600

Pi-C2 Complex

N	2.23119600	0.69806000	-0.07377800
N	2.14168000	-1.47845500	0.18812900
C	4.69325900	1.20603800	-0.14123200
C	3.53645300	0.27939500	-0.02688600
C	3.45445600	-1.07200900	0.13575400
C	1.43410100	-0.38665600	0.05870200
H	4.68948800	1.94984400	0.65233400
H	5.61934300	0.64584700	-0.07243700
H	4.26629900	-1.76964500	0.21752500
H	0.36106500	-0.31866500	0.05316700
O	-1.84375200	0.07418900	0.04273100
H	1.91757300	1.64255700	-0.18636900
H	4.68937300	1.73524200	-1.09146500
C	-2.98569600	-0.37342400	-0.04037600
C	-3.23817400	-1.84945400	-0.18185800
H	-2.72048500	-2.20850800	-1.06566300
H	-2.81699600	-2.35923700	0.67904100
H	-4.29036600	-2.09763000	-0.26111000
N	-4.06002200	0.42334400	-0.00858600
H	-4.96873300	0.01212500	-0.07775000
C	-3.95679700	1.85975600	0.12689300
H	-4.95515800	2.27736500	0.12661200
H	-3.46222600	2.12728500	1.05561000
H	-3.39475400	2.28738300	-0.69767100