S1. Supporting Information for

Chemical Reactivity of the Imidazole: a Semblance of Pyridine and Pyrrole?

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Contents:

S2. Complete Reference for Gaussian 03 Program

GAUSSIAN03.- Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J.R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S.S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.;Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H.P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.;Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma,K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A.D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J.B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.;Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M.A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.;Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision C.02; Gaussian, Inc.:Wallingford, CT, 2004.

S3. Geometries and Energies of the pyridine molecule

Molecular formula: C_5H_5N

Charge = 0 Multiplicity = 1

Zero-point correction= 0.088567 (Hartree/Particle)

Thermal correction to Energy= 0.092844

Thermal correction to Enthalpy= 0.093788

Thermal correction to Gibbs Free Energy= 0.061173

Sum of electronic and zero-point Energies= -248.272028

Sum of electronic and thermal Energies= -248.267752

Sum of electronic and thermal Enthalpies= -248.266808

Sum of electronic and thermal Free Energies= -248.299422

C,-1.1699055784,0.0000163232,-0.6708850879

C,-1.1647401941,-0.0002726654,0.7204985346

C,0.058573618,-0.0002406224,1.3788818797

C,1.2216414869,0.0000370114,0.6191402262

C,1.1087933224,0.0002392765,-0.767681928

H,-2.1074059162,-0.0000407707,-1.2147090949

H,-2.0967626592,-0.0005014674,1.2680651956

H,0.1 04467416,-0.0004313468,2.4595162536

H,2.1967465745,0.0000827717,1.0856860886

H,1.9968108826,0.000489618,-1.3890349099

N,-0.0600046039,0.0002464651,-1.4127493257

S4. Geometries and Energies of the pyrrole molecule

Molecular formula: C_4H_5N

Charge = 0 Multiplicity = 1

Zero-point correction= 0.082262 (Hartree/Particle)

Thermal correction to Energy= 0.086251

Thermal correction to Enthalpy= 0.087195

Thermal correction to Gibbs Free Energy= 0.055862

Sum of electronic and zero-point Energies= -210.155760

Sum of electronic and thermal Energies= -210.151772

Sum of electronic and thermal Enthalpies= -210.150828

Sum of electronic and thermal Free Energies= -210.182160

C,-0.975059207,0.0000287041,-0.6476625338

C,-0.9692937265,0.0001104554,0.7267559416

C,0.3897956356,-0.0000728748,1.1470682547

C,1.170453027,-0.0000007916,0.0158572181

N,0.3308580419,-0.0000464243,-1.0698413115

H,0.6272147912,-0.0001996385,-2.0281395237

H,-1.7892902658,0.0000666996,-1.3498797021

H,-1.840406735, 1,0.0002067635,1.3585757551

H,0.7521514504,-0.0001197464,2.1603461041

H,2.2389500917,-0.0000220662,-0.104126737

S5. Geometries and Energies of the imidazole molecule

Molecular formula: $C_3H_4N_2$

Charge = 0 Multiplicity = 1

Zero-point correction= 0.070928 (Hartree/Particle)

Thermal correction to Energy= 0.074704

Thermal correction to Enthalpy= 0.075649

Thermal correction to Gibbs Free Energy= 0.044656

Sum of electronic and zero-point Energies= -226.219309

Sum of electronic and thermal Energies= -226.215533

Sum of electronic and thermal Enthalpies= -226.214589

Sum of electronic and thermal Free Energies= -226.245581

C,-0.9374687737,-0.0003733317,-0.7012311126

C,-0.9447557222,0.0002144728,0.6665033309

H,2.1971290221,-0.0000437465,-0.1083710485

H,-1.7827434679,-0.0005909882,-1.367125687

H,-1.7412124638,0.0003188218,1.3875678403

N,0.3828319376,-0.0002989162,1.0342773854

C,1.1202909109,-0.000076899,-0.1130883582

N,0.3540539785,0.000622144,-1.1768990646

H,0.7402270062,-0.0005321343,1.9731774891

S6. Geometries and Energies of the benzene molecule

Molecular formula: C_6H_6

Charge = 0 Multiplicity = 1

Zero-point correction= 0.100307 (Hartree/Particle)

Thermal correction to Energy= 0.104701

Thermal correction to Enthalpy= 0.105645

Thermal correction to Gibbs Free Energy= 0.072849

Sum of electronic and zero-point Energies= -232.220358

Sum of electronic and thermal Energies= -232.215964

Sum of electronic and thermal Enthalpies= -232.215020

Sum of electronic and thermal Free Energies= -232.247815

C,-1.2055692679,0.0005499356,-0.6961852667

C,-1.2054564768,0.0009961918,0.6958552873

C,-0.0000476109,0.0004519594,1.3919339313

C,1.2055996566,-0.0005481757,0.696326592

C,1.2054865544,-0.0009983928,-0.695803072

C,-0.0000128593,-0.000445759,-1.3919341769

H,-2.1422933228,0.0009688066,-1.2369097779

H,-2.142181668,0.001754716,1.2366255186

H,-0.0001181427,0.0007776687,2.4735384728

H,2.1422527839,-0.0009810707,1.2369794195

H,2.1421437097,-0.0017695147,-1.2366910375

H,0.0001966637,-0.0007851621,-2.4735387694

Table S7. Condensed Fukui function and condensed softness values for pyridine molecule

Atom	f^-_k	s^-_k
C-2	0.003	0.000
C-3	0.116	0.021
C-4	0.094	0.017
C-5	0.116	0.021
C-6	0.003	0.000
H-6	0.105	0.019
H-5	0.096	0.017
H-4	0.086	0.016
H-3	0.096	0.017
H-2	0.105	0.019
N-1	0.175	0.032

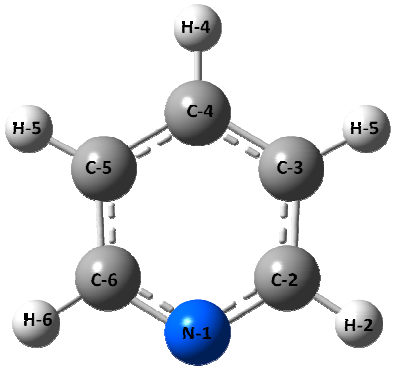

Table S8. Condensed Fukui function and condensed softness values for pyrrole molecule

Atom	f^-_k	s^-_k
C-5	0.186	0.040
C-4	0.058	0.012
C-3	0.058	0.012
C-2	0.186	0.040
N-1	0.000	0.000
H-1	0.073	0.016
H-2	0.110	0.023
H-3	0.109	0.023
H-4	0.109	0.023
H-5	0.110	0.023

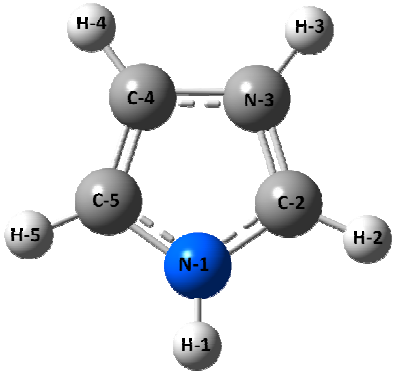

Table S9. Condensed Fukui function and condensed softness values for imidazole molecule

Atom	f^-_k	s^-_k
C-4	0.088	0.017
C-5	0.192	0.038
H-2	0.108	0.022
H-4	0.119	0.024
H-5	0.114	0.023
N-1	0.040	0.008
C-2	0.177	0.036
N-3	0.077	0.015
H-1	0.079	0.016