Histidine in Continuum Electrostatics Protonation State Calculations

Supporting Information

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Table S1: Hartree-Fock 6-31G(d) Mulliken charge distributions for the various charge states of methylimidazole. States are described according to the bound protons as (n^{δ},n^{ε}). Derived charges determined from Eqn. (5).

Atom Name	(1,1)	(1,0)	(0,1)	(0,0)	(0,0) derived	Δ	Δ^2
CB	-0.526	-0.517	-0.503	-0.493	-0.495	-0.002	0.000
HB3	0.229	0.178	0.181	0.123	0.131	0.008	0.000
HB2	0.229	0.178	0.181	0.123	0.131	0.008	0.000
HB1	0.235	0.193	0.160	0.115	0.118	0.003	0.000
CG	0.278	0.269	0.183	0.175	0.175	0.000	0.000
ND1	-0.722	-0.757	-0.545	-0.638	-0.579	0.059	0.003
HD1	0.462	0.394	0.000	0.000	-0.068	-0.068	0.005
CD2	-0.008	-0.096	-0.036	-0.120	-0.124	-0.004	0.000
HD2	0.306	0.194	0.214	0.081	0.102	0.021	0.000
CE1	0.409	0.268	0.276	0.160	0.136	-0.024	0.001
HE1	0.329	0.208	0.210	0.077	0.090	0.013	0.000
NE2	-0.686	-0.513	-0.719	-0.603	-0.547	0.056	0.003
HE2	0.467	0.000	0.397	0.000	-0.070	-0.070	0.005
Total Charge	1.000	0.000	0.000	-1.000	-1.000	RMSD >	0.037

Table S2: CHARMM charge distributions for the various charge states of methylimidazole

Atom Name	(1,1)	(1,0)	(0,1)	(0,0) derived
N	-0.47	-0.47	-0.47	-0.47
H	0.31	0.31	0.31	0.31
CA	0.07	0.07	0.07	0.07
HA	0.09	0.09	0.09	0.09
C	0.51	0.51	0.51	0.51
O	-0.51	-0.51	-0.51	-0.51
CB	-0.05	-0.09	-0.08	-0.12
HB3	0.09	0.09	0.09	0.09
HB2	0.09	0.09	0.09	0.09
CG	0.19	-0.05	0.22	-0.02
ND1	-0.51	-0.36	-0.70	-0.55
HD1	0.44	0.32	0.00	-0.12
CD2	0.19	0.22	-0.05	-0.02
HD2	0.13	0.10	0.09	0.06
CE1	0.32	0.25	0.25	0.18
HE1	0.18	0.13	0.13	0.08
NE2	-0.51	-0.70	-0.36	-0.55
HE2	0.44	0.00	0.32	-0.12
Total Charge	1.00	0.00	0.00	-1.00

Table S3: AMBER charge distributions for the various charge states of methylimidazole.

Atom Name	(1,1)	(1,0)	(0,1)	(0,0) derived
N	-0.35	-0.42	-0.42	-0.48
H	0.27	0.27	0.27	0.27
CA	-0.14	0.02	-0.06	0.10
HA	0.12	0.09	0.14	0.10
C	0.73	0.60	0.60	0.46
O	-0.59	-0.57	-0.57	-0.55
CB	-0.04	-0.05	-0.01	-0.01
HB3	0.08	0.04	0.04	0.00
HB2	0.08	0.04	0.04	0.00
CG	0.00	-0.03	0.19	0.16
ND1	-0.15	-0.38	-0.54	-0.77
HD1	0.39	0.36	0.00	-0.02
CD2	-0.11	0.13	-0.22	0.02
HD2	0.23	0.11	0.19	0.07
CE1	-0.02	0.21	0.16	0.39
HE1	0.27	0.14	0.14	0.01
NE2	-0.17	-0.57	-0.28	-0.68
HE2	0.39	0.00	0.33	-0.06
Total Charge	1.00	0.00	0.00	-1.00

Table S4: PARSE charge distributions for the various charge states of methylimidazole.

Atom Name	(1,1)	(1,0)	(0,1)	(0,0) derived
N	-0.40	-0.40	-0.40	-0.40
H	0.40	0.40	0.40	0.40
CA	0.00	0.00	0.00	0.00
HA	0.00	0.00	0.00	0.00
C	0.55	0.55	0.55	0.55
O	-0.55	-0.55	-0.55	-0.55
CB	0.13	0.13	0.13	0.13
HB3	0.00	0.00	0.00	0.00
HB2	0.00	0.00	0.00	0.00
CG	0.14	-0.13	0.16	-0.11
ND1	-0.35	-0.40	-0.56	-0.61
HD1	0.45	0.40	0.00	-0.05
CD2	0.14	0.16	-0.13	-0.11
HD2	0.13	0.13	0.13	0.13
CE1	0.14	0.16	0.16	0.17
HE1	0.13	0.13	0.13	0.13
NE2	-0.35	-0.56	-0.40	-0.61
HE2	0.45	0.00	0.40	-0.05
Total Charge	1.00	0.00	0.00	-1.00