Supporting Information

1. Complete Ref. 42:

(42) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03, Revision B.05, Gaussian, Inc., Pittsburgh PA, 2003.

2. Geometries and energies of results from electronic stucture calculations under B3LYP/6-31+g** theory level. Geometries are given in Cartesian coordinates. The figure number from the paper is given to reference each structure.

Figure 3 -1: The neutral form for one-proton transfer model

C	2.14971	-0.55007	0.61166
C	3.13956	0.43958	0.87121
C	2.77822	1.80786	0.74578
C	1.49508	2.16389	0.38024
C	0.49363	1.19027	0.11714
C	0.86918	-0.17723	0.24654

O	4.37717	0.15436	1.22273
H	4.63679	-0.88402	1.314
C	-0.81136	1.64441	-0.25633
C	-1.96073	0.96017	-0.56609
C	-3.2155	1.63883	-0.92939
N	-2.15644	-0.43101	-0.59626
N	-4.09838	0.56454	-1.15759
C	-3.39595	-0.62088	-0.93993
O	-3.52285	2.83004	-1.03648
C	-5.4802	0.73295	-1.54717
H	-5.6597	1.80879	-1.61628
H	-6.16437	0.30447	-0.80508
C	-4.04036	-1.95857	-1.09678
H	-4.89165	-2.08024	-0.41478
H	-5.68399	0.27432	-2.5221
H	-3.29888	-2.72787	-0.87535
H	2.42352	-1.59961	0.70689
H	3.53819	2.55757	0.94524
H	1.2369	3.21757	0.28926
H	-4.41452	-2.11042	-2.11735
H	0.12378	-0.93987	0.05139
H	-0.93301	2.72647	-0.30955
C	4.69952	-3.27061	1.37407
H	5.38073	-4.13253	1.58052
O	3.52626	-3.52259	1.04939
O	5.26508	-2.13094	1.5124

Figure3 -2: The transition state for one-proton transfer model

C	0	2.1028	-0.58532	0.59668
C	0	3.11968	0.38993	0.86493
C	0	2.75297	1.76806	0.73826
C	0	1.47504	2.13294	0.37454
C	0	0.46022	1.16911	0.10744
C	0	0.82784	-0.20415	0.23352

O	0	4.33191	0.08317	1.20995
H	0	4.75648	-1.09056	1.35863
C	0	-0.83587	1.63216	-0.26275
C	0	-1.99714	0.96012	-0.57557
C	0	-3.24046	1.652	-0.93493
N	0	-2.20679	-0.42905	-0.61004
N	0	-4.13692	0.58723	-1.16694
C	0	-3.44887	-0.60632	-0.95398
O	0	-3.5394	2.84795	-1.03919
C	0	-5.51583	0.77427	-1.55541
H	0	-5.68094	1.85285	-1.62032
H	0	-6.20633	0.35203	-0.81515
C	0	-4.10764	-1.93687	-1.11493
H	0	-4.95994	-2.05379	-0.43287
H	0	-5.72665	0.32212	-2.53222
H	0	-3.37367	-2.7144	-0.89637
H	0	2.36694	-1.63556	0.6868
H	0	3.51767	2.51308	0.93938
H	0	1.22387	3.18909	0.28612
H	0	-4.48418	-2.08336	-2.13573
H	0	0.07463	-0.95878	0.03525
H	0	-0.94881	2.71548	-0.31303
C	0	4.87805	-3.22234	1.42534
H	0	5.60686	-4.02873	1.65838
O	0	3.73323	-3.51485	1.0802
O	0	5.40118	-2.0448	1.56917

Figure3 -3: The anionic form for one-proton transfer model

C	2.08422	-0.58859	0.59384
C	3.11125	0.38305	0.85817
C	2.74306	1.76432	0.72467
C	1.46661	2.1303	0.36081
C	0.44668	1.16857	0.09823
C	0.811	-0.20637	0.23055

O	4.31456	0.06777	1.20041
H	4.82269	-1.17242	1.36891
C	-0.84632	1.63312	-0.27242
C	-2.01224	0.96402	-0.58207
C	-3.25148	1.65893	-0.94301
N	-2.22717	-0.42446	-0.6105
N	-4.15313	0.59654	-1.17019
C	-3.47039	-0.59887	-0.95291
O	-3.54725	2.8561	-1.05247
C	-5.53109	0.78845	-1.55856
H	-5.691	1.86767	-1.62709
H	-6.22353	0.37206	-0.81664
C	-4.13455	-1.92758	-1.10776
H	-4.98675	-2.03909	-0.4245
H	-5.7449	0.33399	-2.53378
H	-3.4032	-2.70693	-0.88652
H	2.34474	-1.63901	0.69005
H	3.50962	2.5088	0.92156
H	1.21777	3.18681	0.26778
H	-4.51263	-2.07761	-2.1276
H	0.05439	-0.95892	0.03665
H	-0.95592	2.71662	-0.32739
C	4.94978	-3.23222	1.45064
H	5.69527	-4.02269	1.67486
O	3.80141	-3.52929	1.1393
O	5.47332	-2.04416	1.5687

Figure6 -1: The neutral form for two-proton transfer model

C	-1.69042	0.30147	0.05338
C	-2.73609	-0.05953	-0.83551
C	-2.47234	-1.02712	-1.83399
C	-1.22043	-1.60709	-1.93043
C	-0.16454	-1.26138	-1.04765
C	-0.44157	-0.28563	-0.05308

O	-3.95188	0.46859	-0.77319
H	-4.06903	1.14018	0.01451
C	1.10604	-1.91054	-1.21373
C	2.2822	-1.77817	-0.52587
C	3.49433	-2.54843	-0.86695
N	2.55763	-0.93627	0.56524
N	4.43283	-2.09	0.07689
C	3.80194	-1.1426	0.88249
O	3.72612	-3.39461	-1.73262
C	5.79986	-2.55928	0.14192
H	5.91888	-3.29704	-0.65524
H	6.51365	-1.74315	-0.01839
C	4.52174	-0.4521	1.9931
H	4.89063	-1.16633	2.7399
H	6.01659	-3.03657	1.10453
H	3.83219	0.24082	2.47744
O	-4.22597	2.02773	1.18767
H	-1.89557	1.0481	0.81421
H	-4.8027	1.64941	1.86195
H	-4.52025	3.10207	1.09811
H	-3.27435	-1.29704	-2.51403
C	-4.11306	5.22445	1.55825
H	-1.03472	-2.35005	-2.70352
H	5.38749	0.11097	1.62263
H	0.35015	-0.00091	0.63022
H	1.16086	-2.6367	-2.02458
O	-4.92003	4.36416	1.04029
O	-4.28558	6.44273	1.67647
H	-3.15438	4.78711	1.93679

Figure6 -2: The transition state for two-proton transfer model

C	-1.67901	0.3198	0.124
C	-2.74541	-0.00148	-0.75951
C	-2.50062	-0.93571	-1.79725

C	-1.25494	-1.51892	-1.93485
C	-0.18162	-1.21287	-1.05708
C	-0.43693	-0.27092	-0.02356
O	-3.95097	0.53058	-0.65625
H	-4.06004	1.19328	0.1721
C	1.07902	-1.86553	-1.26533
C	2.26741	-1.77201	-0.58975
C	3.46469	-2.5418	-0.97639
N	2.56677	-0.97591	0.52917
N	4.42126	-2.13073	-0.028
C	3.81247	-1.20835	0.82214
O	3.67633	-3.35708	-1.87649
C	5.78191	-2.62081	0.00235
H	5.87996	-3.33186	-0.82152
H	6.50556	-1.80974	-0.13896
C	4.55372	-0.56992	1.94988
H	4.92127	-1.31653	2.66516
H	6.0042	-3.13446	0.94485
H	3.87801	0.11214	2.46809
O	-4.20021	2.03175	1.30429
H	-1.86689	1.04036	0.91392
H	-4.74126	1.6197	1.98838
H	-4.54253	3.1652	1.22521
H	-3.31488	-1.17576	-2.47407
C	-4.05042	5.1906	1.61185
H	-1.08625	-2.23418	-2.73756
H	5.42272	-0.00365	1.59199
H	0.36753	-0.01648	0.65695
H	1.11558	-2.56073	-2.10399
O	-4.92352	4.33737	1.18125
O	-4.19544	6.41012	1.7144
H	-3.07717	4.73472	1.91329

Figure6 -3: The anionic form for two-proton transfer model

C	-1.42694	0.39385	0.20346
C	-2.55578	0.09624	-0.64275
C	-2.33332	-0.88267	-1.67276
C	-1.11184	-1.49957	-1.82258
C	-0.00046	-1.2082	-0.97636
C	-0.20986	-0.23099	0.0432
O	-3.70265	0.65891	-0.50193
H	-4.00144	1.56656	0.61889
C	1.22588	-1.89652	-1.19473
C	2.44278	-1.8327	-0.54888
C	3.59499	-2.64624	-0.94938
N	2.79557	-1.02736	0.54795
N	4.59193	-2.25426	-0.02948
C	4.03995	-1.297	0.81865
O	3.7646	-3.48657	-1.84159
C	5.93297	-2.79233	-0.02808
H	5.98089	-3.51896	-0.84319
H	6.68323	-2.0116	-0.20265
C	4.82985	-0.66603	1.918
H	5.18445	-1.41011	2.64326
H	6.16525	-3.30005	0.91592
H	4.19069	0.05146	2.43549
O	-4.26266	2.17112	1.4311
H	-1.56358	1.13928	0.98269
H	-4.56401	1.57236	2.12412
H	-5.16139	3.4341	1.26721
H	-3.16838	-1.11891	-2.32649
C	-4.89505	5.3468	1.18686
H	-0.97938	-2.23911	-2.61136
H	5.71282	-0.13897	1.53369
H	0.61988	0.01395	0.69744
H	1.22279	-2.6106	-2.01866
O	-5.70163	4.29822	1.23876
O	-5.27416	6.50254	1.17233

H		-3.82132	5.08053	1.15715

Figure8 -1: The neutral form for three-proton transfer model

C	0	1.75244	1.34992	-0.59264
C	0	2.16792	2.65869	-0.90688
C	0	1.20058	3.67321	-1.03869
C	0	-0.14293	3.38185	-0.83767
C	0	-0.57769	2.07976	-0.4932
C	0	0.41159	1.07144	-0.38389
O	0	3.46554	2.98101	-1.09112
H	0	4.0601	2.21407	-0.86728
C	0	-1.98503	1.83739	-0.2605
C	0	-2.59966	0.68765	0.14156
C	0	-4.05984	0.56326	0.37341
N	0	-1.98328	-0.53851	0.42508
N	0	-4.19417	-0.76755	0.79396
C	0	-2.92032	-1.35516	0.80176
O	0	-4.98532	1.36755	0.25468
C	0	-5.45669	-1.37366	1.15729
H	0	-6.23089	-0.61814	1.00339
H	0	-5.46402	-1.68447	2.20817
C	0	-2.69763	-2.77191	1.20848
H	0	-3.07506	-2.95184	2.22334
H	0	-5.6753	-2.24531	0.53056
H	0	-1.6257	-3.00112	1.18286
O	0	5.11577	0.96403	-0.37667
H	0	2.48244	0.55101	-0.51676
H	0	4.73621	0.02948	-0.43004
H	0	5.44779	1.0579	0.52382
H	0	1.52704	4.67781	-1.29022
H	0	1.07627	-2.30725	-0.1522
H	0	-0.8799	4.17638	-0.93649
H	0	-3.22928	-3.46046	0.53831
H	0	0.10929	0.06438	-0.12637

H	0	-2.65441	2.68375	-0.41004
O	0	2.69834	-2.81642	0.94723
C	0	1.4439	-2.91769	0.71155
O	0	0.60522	-3.60427	1.32078
O	0	4.08711	-1.41986	-0.59176
C	0	4.62107	-2.27446	-1.5825
H	0	3.48254	-1.97892	0.07174
H	0	5.25939	-1.68493	-2.25201
H	0	3.82666	-2.73895	-2.18531
H	0	5.22957	-3.07902	-1.14236

Figure8 -2: The transition state for three-proton transfer model

C	0	1.37904	1.19611	-0.52163
C	0	1.85127	2.50408	-0.81876
C	0	0.90128	3.54984	-0.94203
C	0	-0.44775	3.29625	-0.78034
C	0	-0.93535	1.99592	-0.48548
C	0	0.02544	0.95601	-0.36119
O	0	3.12994	2.79366	-0.98758
H	0	3.80032	1.96463	-0.88112
C	0	-2.35078	1.81527	-0.33258
C	0	-3.09334	0.69875	-0.05202
C	0	-4.5634	0.72899	0.06648
N	0	-2.63507	-0.61137	0.16694
N	0	-4.88144	-0.61097	0.35875
C	0	-3.68981	-1.33524	0.40021
O	0	-5.38965	1.63762	-0.04365
C	0	-6.23111	-1.08761	0.56693
H	0	-6.89209	-0.22517	0.45149
H	0	-6.36071	-1.50411	1.57253
C	0	-3.66883	-2.79963	0.68907
H	0	-4.09483	-3.02197	1.6755
H	0	-6.50744	-1.84979	-0.17085

H	0	-2.63371	-3.14358	0.66734
O	0	4.73717	0.92396	-0.78375
H	0	2.09302	0.38366	-0.41957
H	0	4.38742	-0.22736	-0.66548
H	0	5.45062	1.10801	-0.16202
H	0	1.26515	4.54762	-1.16796
H	0	3.1974	-2.59651	1.98065
H	0	-1.16066	4.11255	-0.88051
H	0	-4.24668	-3.36538	-0.05261
H	0	-0.31989	-0.04605	-0.13446
H	0	-2.95573	2.71323	-0.45783
O	0	5.04643	-2.78403	1.15866
C	0	4.19391	-3.06336	2.11785
O	0	4.43275	-3.76664	3.0883
O	0	4.0012	-1.36382	-0.57346
C	0	3.91065	-1.9842	-1.83696
H	0	4.60276	-2.15727	0.40702
H	0	4.84875	-1.8979	-2.40991
H	0	3.10565	-1.53731	-2.44041
H	0	3.68614	-3.05388	-1.7171

Figure8 -3: The anionic form for three-proton transfer model

C	0	0.84151	1.14551	0.18182
C	0	1.50542	2.23968	-0.48516
C	0	0.65357	3.13246	-1.22685
C	0	-0.70834	2.94278	-1.28459
C	0	-1.35809	1.85964	-0.61993
C	0	-0.52292	0.9669	0.11675
O	0	2.77372	2.42465	-0.43362
H	0	3.74026	1.54123	0.3295
C	0	-2.77171	1.73588	-0.72892
C	0	-3.65552	0.81484	-0.2073
C	0	-5.0991	0.87479	-0.4566
N	0	-3.36577	-0.29232	0.60893

N	0	-5.58779	-0.24365	0.25326
C	0	-4.50253	-0.87781	0.85348
O	0	-5.81114	1.65327	-1.10279
C	0	-6.98468	-0.61005	0.30229
H	0	-7.52384	0.12587	-0.29973
H	0	-7.37473	-0.58634	1.3271
C	0	-4.66793	-2.10562	1.68747
H	0	-5.32131	-1.92587	2.55118
H	0	-7.15625	-1.60859	-0.11752
H	0	-3.68534	-2.414	2.04879
O	0	4.43145	0.95846	0.82745
H	0	1.45656	0.44986	0.7476
H	0	4.65073	-0.54295	0.25714
H	0	4.25793	1.07234	1.76845
H	0	1.12917	3.96378	-1.74001
H	0	5.68304	-3.67808	1.51775
H	0	-1.32153	3.63913	-1.8554
H	0	-5.10727	-2.93146	1.11281
H	0	-0.98981	0.13353	0.63067
H	0	-3.26473	2.49887	-1.33186
O	0	6.92451	-2.83344	0.13717
C	0	6.69322	-3.7467	1.07111
O	0	7.49822	-4.58758	1.41773
O	0	4.74896	-1.45463	-0.15155
C	0	4.09383	-1.46769	-1.41873
H	0	6.1089	-2.24602	0.01122
H	0	4.57397	-0.77991	-2.12644
H	0	3.03946	-1.18807	-1.31433
H	0	4.15375	-2.48502	-1.81641

3. The energy (in Hartrees) of the different forms for the proton transfer models, the number is parentheses are the imagery frequencies for the transition states.

	One-Proton Model	Two-Proton Model	Three-Proton Model

Neutral form	-913.789806564	-990.235178013	-1105.98541308
Transition state	-913.7889686 (298.5256i)	-990.235173710 (264.7301i)	-1105.9819494 (512.9416i)
Anionic form	-913.789030423	-990.239625711	-1105.98875045