Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Local Structure and Hydrogen Bond Characteristics of Imidazole Molecules for Proton Conduction in Acid and Base Proton-Conducting Composite Materials

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Table S1. Cartesian coordinates of (A) PVPA/Im.

		angstrom	
Atom	x	y	z
C	-3.053211	0.597111	-0.038650
C	-2.746722	2.060598	0.257173
H	-3.498754	0.476397	-1.026154
H	-3.756069	0.186948	0.686323
H	-3.660341	2.652626	0.242049
H	-2.287986	2.171637	1.238173
P	-1.591156	-0.446842	0.021711
O	-0.889625	-0.519758	1.328719
O	-0.714502	0.046022	-1.187272
H	0.285566	0.057443	-1.017510
O	-2.176427	-1.887302	-0.416238
H	-1.851415	-2.577473	0.170027
H	-2.064545	2.473766	-0.483419
N	1.865689	0.096340	-0.543575
C	2.084753	-0.071011	0.736342
N	3.403265	0.016874	1.003249
C	4.060010	0.254851	-0.179415
C	3.089793	0.300883	-1.127238
H	1.310870	-0.254749	1.465945
H	3.823537	-0.075843	1.909996
H	5.126609	0.365999	-0.235361
H	3.193874	0.467101	-2.184389

Table S2. Cartesian coordinates of (B) AA/Im.

		angstrom	
Atom	x	y	z
C	1.192971	0.586806	-1.297746
C	2.404412	-1.358417	-0.507685
C	2.153879	-0.712501	0.864504
C	2.475552	0.779036	0.891603
C	1.949864	1.531310	-0.346436
H	1.052412	1.117546	-2.240848
H	1.097813	-0.838946	1.100144
H	2.013719	1.217065	1.778428
H	2.832877	1.832951	-0.909652
H	3.469764	-1.545453	-0.630940
O	1.773812	-2.588113	-0.624168
O	2.016875	-0.506338	-1.585588
O	2.858091	-1.395957	1.870071
H	3.741972	-1.012293	1.904405
O	3.894170	0.877406	0.997113
H	4.136330	1.768754	1.257297
O	1.256542	2.711418	-0.016349
H	0.308894	2.529439	-0.005908
C	-0.214442	0.183257	-0.863167
O	-0.980209	1.227853	-0.616556
O	-0.596496	-0.962634	-0.778868
H	0.825936	-2.405034	-0.694672
H	-1.936499	0.939185	-0.347159
N	-3.381360	0.427571	0.058642
C	-3.602144	-0.862158	0.090610
N	-4.874742	-1.112481	0.450912
C	-5.500255	0.091611	0.660299
C	-4.558904	1.036407	0.412224
H	-2.869633	-1.616596	-0.139684

H	-5.287391	-2.022750	0.548362
H	-6.529307	0.163232	0.958437
H	-4.652046	2.106098	0.464431

Table S3. Cartesian coordinates of (C) PVPA(3)/Im.

		angstrom	
Atom	x	y	z
C	2.712430	2.707129	-1.269514
H	2.615786	3.786538	-1.423040
H	2.192223	2.204494	-2.092578
C	2.147928	2.298601	0.091601
C	2.478567	0.846449	0.529523
H	2.604235	2.942885	0.857041
P	0.400773	2.764247	0.278474
H	3.488781	0.894623	0.953051
H	1.824832	0.534072	1.349535
O	-0.217027	2.385468	1.607477
O	-0.456881	2.248077	-0.985044
O	0.497250	4.372275	0.034904
H	-1.013565	1.453415	-0.742784
H	-0.331023	4.819191	0.252935
C	2.480040	-0.224988	-0.576029
C	1.132351	-0.775615	-1.082748
H	2.979232	0.198512	-1.458235
P	3.618946	-1.580886	-0.169619
H	0.508598	0.073623	-1.375079
H	1.354046	-1.301545	-2.018484
C	0.337168	-1.772069	-0.202801
O	3.615144	-2.791176	-1.055465
O	3.305319	-1.881270	1.405557
O	5.088979	-0.846063	-0.126902
C	-0.169904	-2.943322	-1.052571
H	0.977967	-2.173098	0.591642
P	-1.067269	-1.059582	0.726825
H	3.594709	-2.767306	1.660960
H	5.711709	-1.348101	-0.668962

H	0.686807	-3.464517	-1.495942
H	-0.749673	-3.647377	-0.448665
H	-0.813650	-2.582635	-1.866223
O	-2.060874	-2.087679	1.186004
O	-1.725953	0.057158	-0.282366
O	-0.406664	-0.201387	1.917260
H	-2.754489	-0.020814	-0.347776
H	-0.449311	0.792814	1.846330
H	3.777867	2.449756	-1.323878
N	-4.318805	-0.191754	-0.411362
C	-5.284248	0.464959	-1.014714
N	-6.484763	-0.089748	-0.729291
C	-6.264876	-1.163703	0.107079
C	-4.913044	-1.213989	0.295214
H	-5.165109	1.330801	-1.655146
H	-7.378498	0.230430	-1.069637
H	-7.071714	-1.779022	0.483291
H	-4.304343	-1.896841	0.879352

Table S4. Cartesian coordinates of (D) PVPA(3)/2Im.

		angstrom	
Atom	x	y	z
C	3.648132	2.898676	-1.492821
H	3.424681	3.964736	-1.603348
H	3.038360	2.352789	-2.221566
C	3.370767	2.433431	-0.063278
C	3.898055	1.013353	0.279179
H	3.895383	3.112326	0.623941
P	1.644638	2.730651	0.433661
H	4.950929	1.148042	0.552681
H	3.402249	0.628033	1.175957
O	1.336554	2.334260	1.863669
O	0.637268	2.118148	-0.644550
O	1.546710	4.347812	0.194754
H	0.223475	1.220450	-0.323153
H	0.794612	4.717956	0.673962
C	3.829327	-0.037094	-0.843518
C	2.472992	-0.704315	-1.137178
H	4.143977	0.440047	-1.781473
P	5.130188	-1.292952	-0.648819
H	1.738842	0.086729	-1.315503
H	2.586557	-1.218631	-2.098517
C	1.920152	-1.746011	-0.133684
O	5.034890	-2.529021	-1.492921
O	5.257282	-1.642015	0.951503
O	6.464894	-0.374698	-0.892414
C	1.445994	-2.998797	-0.878170
H	2.700330	-2.043401	0.577680
P	0.570186	-1.132104	0.956952
H	5.070211	-2.578457	1.097519
H	7.261472	-0.917970	-0.948789

H	2.287702	-3.437030	-1.428127
H	1.036393	-3.737524	-0.183002
H	0.658992	-2.742459	-1.600748
O	-0.247570	-2.275755	1.518530
O	-0.290501	-0.079575	0.127185
O	1.345519	-0.308531	2.122864
H	-1.696275	-0.398934	0.242527
H	1.237292	0.677261	2.095832
H	4.706248	2.744298	-1.740805
N	-2.754199	-0.697224	0.365409
C	-3.823535	-0.079593	-0.111107
N	-4.918403	-0.748615	0.261150
C	-4.523010	-1.838258	1.007107
C	-3.160063	-1.802709	1.070985
H	-3.817267	0.823274	-0.707558
H	-5.897731	-0.480787	0.022263
H	-5.236320	-2.537249	1.422848
H	-2.412689	-2.436160	1.540132
N	-7.570834	-0.014131	-0.411079
C	-8.398711	0.748990	0.268727
N	-9.583147	0.871050	-0.375933
C	-9.506562	0.140525	-1.539091
C	-8.251914	-0.400911	-1.543335
H	-8.189525	1.228293	1.218228
H	-10.378153	1.404307	-0.056562
H	-10.328854	0.073415	-2.239829
H	-7.800099	-1.043551	-2.290187

Table S5. Cartesian coordinates of (E) AA/2Im.

		angstrom	
Atom	x	y	z
C	2.546471	0.433570	-1.175635
C	1.776280	-1.748494	-0.499030
C	1.368970	-0.977374	0.768553
C	2.513198	-0.134636	1.311568
C	3.161252	0.741201	0.208353
H	3.209717	0.848305	-1.944392
H	0.539093	-0.311513	0.513973
H	2.131481	0.537096	2.092701
H	4.211377	0.423866	0.145133
H	2.361872	-2.631932	-0.220309
O	0.643510	-2.213477	-1.192810
O	2.582273	-0.970650	-1.361987
O	0.854662	-1.868252	1.742035
H	1.614323	-2.236121	2.214300
O	3.428763	-1.071681	1.884945
H	4.112725	-0.596478	2.367068
O	3.144705	2.110424	0.535571
H	2.406169	2.512064	0.035414
C	1.161579	1.065726	-1.420640
O	1.067634	2.303901	-1.124869
O	0.223199	0.370610	-1.854096
H	0.326744	-1.411250	-1.666930
H	-0.416152	2.630474	-0.781956
N	-1.388077	2.573348	-0.315410
C	-2.053242	1.427151	-0.285205
N	-3.089291	1.548050	0.543823
C	-3.089497	2.821776	1.067308
C	-2.014993	3.464237	0.525269
H	-1.764445	0.546955	-0.845476

H	-3.653369	0.716460	0.798484
H	-3.837033	3.160703	1.772005
H	-1.651038	4.472129	0.675134
N	-3.615850	-1.191028	0.758141
C	-2.371236	-1.601762	0.942933
N	-1.960333	-2.407131	-0.058456
C	-2.999308	-2.524381	-0.946087
C	-4.019905	-1.774468	-0.423170
H	-1.722376	-1.340712	1.771605
H	-0.988799	-2.685106	-0.226176
H	-2.924173	-3.114968	-1.850180
H	-5.016648	-1.624920	-0.822690

Table S6. Cartesian coordinates of (F) Im3.

		angstrom	
Atom	x	y	z
N	5.736278	-0.924026	-0.663109
C	4.524854	-0.464147	-1.042961
N	3.790333	-0.161894	-0.005226
C	4.560856	-0.438656	1.096281
C	5.772471	-0.912802	0.707709
H	6.474384	-1.220824	-1.275707
H	4.231476	-0.370503	-2.074541
H	4.196254	-0.280422	2.095576
H	6.632625	-1.234622	1.264325
N	1.041438	0.843893	-0.000151
C	0.636765	2.150949	0.008577
C	-0.723650	2.119850	0.002775
N	-1.158293	0.820174	-0.009298
C	-0.071567	0.086419	-0.010577
H	2.008188	0.500707	-0.000212
H	1.334905	2.967397	0.019165
H	-1.412255	2.946375	0.007385
H	-0.043989	-0.990018	-0.017738
N	-3.906090	-0.196524	-0.010110
C	-4.682809	-0.462113	-1.103684
C	-5.860361	-0.943818	-0.613815
N	-5.824159	-0.980057	0.754224
C	-4.639637	-0.525349	1.075939
H	-2.949655	0.174720	-0.012209
H	-4.338243	-0.288158	-2.106641
H	-6.728053	-1.264317	-1.164362
H	-4.263713	-0.413290	2.079186

Table S7. Cartesian coordinates of (G) Im4(H^+).

		angstrom	
Atom	x	y	z
N	-7.871879	1.049651	0.793750
C	-6.814057	0.223800	0.889865
N	-5.886806	0.553469	0.024178
C	-6.373075	1.641894	-0.660018
C	-7.605669	1.962455	-0.193281
H	-8.708878	1.001663	1.348375
H	-6.765460	-0.590076	1.592541
H	-5.810167	2.121712	-1.440453
H	-8.299055	2.735557	-0.466706
C	-2.292926	-0.307161	0.104565
H	-2.162995	0.469456	0.836751
N	-3.445407	-0.643688	-0.458633
C	-3.211473	-1.670948	-1.335884
C	-1.885024	-1.941104	-1.281844
N	-1.330095	-1.076147	-0.375205
H	-4.382055	-0.191829	-0.260884
H	-3.997181	-2.116636	-1.916498
H	-1.297236	-2.670236	-1.807406
H	-0.278725	-1.027959	-0.088577
N	1.243620	-0.988429	0.362454
C	2.251760	-0.329346	-0.171500
N	3.391588	-0.567118	0.488409
C	3.101959	-1.430281	1.508292
C	1.770370	-1.685418	1.421683
H	2.191995	0.320978	-1.027183
H	4.324900	-0.167678	0.266120
H	3.851588	-1.780726	2.193141
H	1.164895	-2.319026	2.045063
N	5.948958	0.541988	-0.068970

C	6.419042	1.717927	0.463169
C	7.690655	1.938698	0.043392
N	7.999038	0.872891	-0.761242
C	6.923693	0.061200	-0.798425
H	5.816994	2.327832	1.112726
H	8.385385	2.733916	0.238969
H	8.870580	0.720103	-1.237314
H	6.900762	-0.855663	-1.361934