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

Modern *ab initio* Valence Bond Theory Calculations Reveal Charge Shift Bonding in Protic Ionic Liquids

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Electronic Supplementary Information

Co-ordinates of the geometries optimized at B3LYP-D3/6-31+G* level of theory

AANA

H 1.249535 1.897940 -4.525922

O 1.249535 1.897940 -3.488253

N 1.256364 1.889704 -6.162052

N 1.859627 0.735283 -3.100050

O 1.946112 0.569184 -1.902634

O 2.254780 -0.016609 -3.990216

H 1.722114 1.008339 -6.377822

H 1.791551 2.642848 -6.592067

H 0.334584 1.874058 -6.596333

EANA

H 0.082061 0.015750 -1.014469

O 0.082061 0.015750 0.049860

N 0.050135 -0.000262 -2.567099

C -2.058358 -1.286937 -2.640745

C -0.587522 -1.251773 -3.044816

H -2.522054 -2.222030 -2.973600

H -2.168699 -1.216903 -1.552982

H -0.487866 -1.355475 -4.134453

H -0.041155 -2.078070 -2.579402

H 1.030629 0.029901 -2.847133

H -0.406839 0.815514 -2.976261

H -2.615977 -0.457737 -3.095883

N 1.017415 -0.893625 0.440669

O 1.620988 -1.496976 -0.449263

O 1.163059 -1.020908 1.638957

PANA

C 0.115080 0.217265 1.323634

C -0.577948 -0.669371 0.289733

N 0.417340 -1.440514 -0.493736

H 0.829083 0.874274 0.810861

H -1.296628 -1.336939 0.787273

H -1.133766 -0.054468 -0.425691

H -0.050723 -2.034542 -1.178265

H 0.959452 -2.053096 0.116666

H 1.290739 -0.473076 -1.332322

H 0.702363 -0.413279 2.008047

N 1.095984 0.724752 -2.866223

O -0.075266 0.340942 -2.899561

O 1.625036 1.522665 -3.612804

O 1.891598 0.207504 -1.890387

C -0.885608 1.054902 2.126244

H -0.370990 1.682468 2.862219

H -1.596101 0.417551 2.668000

H -1.462555 1.716468 1.468222

BANA

C 0.113717 -0.104880 0.818295

C -0.568276 -0.991568 -0.222039

N 0.436625 -1.756321 -0.999991

H 0.831428 0.555822 0.313563

H -1.287234 -1.664182 0.267863

H -1.121423 -0.378126 -0.940628

H -0.023652 -2.353044 -1.687486

H 0.979062 -2.365431 -0.386433

H 1.306650 -0.782671 -1.830632

H 0.697634 -0.733681 1.508764

N 1.112324 0.414728 -3.365562

O -0.055289 0.020637 -3.407382

O 1.639333 1.217838 -4.108149

O 1.905542 -0.095886 -2.384658

C -0.886352 0.735598 1.621437

H -1.607927 0.070267 2.117351

H -1.467548 1.361905 0.929962

C -0.203915 1.623371 2.667225

H -0.937380 2.214935 3.227448

H 0.498303 2.321129 2.194032

H 0.361654 1.020317 3.389243

[EAmm][NO_3]

N 0.107816 0.039952 -2.678398

C -1.943326 -1.342071 -2.459053

C -0.565284 -1.237037 -3.094179

H -2.419251 -2.272308 -2.785802

H -1.875131 -1.357869 -1.365828

H -0.616990 -1.229531 -4.184970

H 0.091315 -2.046225 -2.771643

H 1.045814 0.116100 -3.080541

H -0.418181 0.858891 -2.996705

H -2.586248 -0.506452 -2.760074

H 0.199845 0.100734 -1.634500

O 0.251715 0.194722 0.119851

N 0.789728 -0.891014 0.523062

O 1.176864 -1.732351 -0.327791

O 0.919191 -1.099325 1.749951

[PAmm][NO_3]

N 0.357610 -1.544897 -0.491340

C 0.127100 0.270671 1.194574

C -0.611943 -0.725600 0.308869

H 0.738088 0.930691 0.565995

H -1.213579 -1.422093 0.898094

H -1.254926 -0.219046 -0.413307

H -0.127600 -2.205231 -1.104474

H 0.968382 -2.098576 0.116087

H 0.813611 -0.270950 1.859212

C -0.855433 1.102352 2.026467

H -0.316497 1.816221 2.658876

H -1.461140 0.461642 2.679460

H -1.536918 1.670056 1.380799

H 0.964814 -0.935699 -1.093702

O 1.997198 0.131387 -2.025825

N 1.216471 0.871705 -2.714271

O -0.025368 0.691292 -2.630792

O 1.697219 1.759581 -3.452811

[BAmm][NO_3]

N 0.354829 -1.869140 -1.008916

C 0.109855 -0.103596 0.726548

C -0.621639 -1.067515 -0.199128

C -0.872365 0.716931 1.572877

H -1.500456 0.034451 2.162445

H -1.548884 1.270233 0.906648

C -0.157055 1.696613 2.508949

H -0.876772 2.271905 3.103420

H 0.455468 2.407541 1.939705

H 0.505191 1.164076 3.203776

H 0.736186 0.571896 0.128727

H -1.236584 -1.777362 0.359514

H -1.249871 -0.535906 -0.916027

H -0.125204 -2.509967 -1.646381

H 0.955486 -2.441797 -0.409110

H 0.782566 -0.668309 1.387678

H 0.972588 -1.245663 -1.586313

O 2.022439 -0.158700 -2.466602

N 1.255242 0.612887 -3.136334

O 0.011444 0.435557 -3.077630

O 1.750811 1.526625 -3.831623