

# Methylenebis(N-butyl)imidazolium Diiodide Acetonitrile Solvate

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## Supporting information

### S1. NMR and Elemental Analysis

NMR spectra were recorded on a Bruker Avance 300 MHz or a Bruker ARX 300 MHz instruments. To reference chemical shifts (ppm) residual solvent peaks were used. Elemental analyses C/H/N were acquired with a PerkinElmer 2400 CHNS/O analyzer.

<sup>1</sup>H NMR (CD<sub>3</sub>CN, δ ppm, 300 MHz): 9.83 (s, 2H; H2), 8.09 (m, 2H; H5), 7.49 (m, 2H; H4), 6.85 (s, 2H; N-CH<sub>2</sub>-N bridge), 4.21 (t, 4H, J<sub>H-H</sub> = 7.3; N-CH<sub>2</sub>-C), 1.87 (m, 4H; N-CH<sub>2</sub>-CH<sub>2</sub>-C), 1.36 (m, 4H; C-CH<sub>2</sub>-CH<sub>3</sub>), 0.95 (t, 6H, J<sub>H-H</sub> = 7.3; C-CH<sub>3</sub>). <sup>13</sup>C NMR (CD<sub>3</sub>CN, δ ppm, 300 MHz): 138.1 (C2), 124.0 (C4), 123.4 (C5), 58.5 (N-CH<sub>2</sub>-N bridge), 50.9 (N-CH<sub>2</sub>-C), 32.09 (N-CH<sub>2</sub>-CH<sub>2</sub>-C), 19.9 (C-CH<sub>2</sub>-CH<sub>3</sub>), 13.7 (C-CH<sub>3</sub>). Anal. Calcd. for C<sub>15</sub>H<sub>24</sub>N<sub>4</sub>I<sub>2</sub>: C, 34.88; H, 5.08; N, 10.85. Found: C, 34.90; H, 4.95; N, 10.92.

**Figure S1** <sup>1</sup>H NMR spectrum of [H<sub>2</sub>BisBuIm]<sub>2</sub> (CD<sub>3</sub>CN, δ ppm, 300 MHz) and assignment of NMR resonances.

**Figure S2** HSQC spectrum of [H<sub>2</sub>BisBuIm]<sub>2</sub> (CD<sub>3</sub>CN, δ ppm, 300 MHz). Butyl side arms N-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub> are indicated as N-CH<sub>2</sub><sub>a</sub>-CH<sub>2</sub><sub>b</sub>-CH<sub>2</sub><sub>c</sub>-CH<sub>3</sub>.

**Figure S3** HMBC spectrum of [H<sub>2</sub>BisBuIm]<sub>2</sub> (CD<sub>3</sub>CN, δ ppm, 300 MHz). Butyl side arms N-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub> are indicated as N-CH<sub>2</sub><sub>a</sub>-CH<sub>2</sub><sub>b</sub>-CH<sub>2</sub><sub>c</sub>-CH<sub>3</sub>.

**Figure S4** <sup>13</sup>C NMR spectrum of [H<sub>2</sub>BisBuIm]<sub>2</sub> (CD<sub>3</sub>CN, δ ppm, 300 MHz). Butyl side arms N-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub> are indicated as N-CH<sub>2</sub><sub>a</sub>-CH<sub>2</sub><sub>b</sub>-CH<sub>2</sub><sub>c</sub>-CH<sub>3</sub>.

### S2. X-Ray Diffraction Studies

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Data collection for  $[\text{H}_2\text{BisBuIm}]_2\cdot\text{CH}_3\text{CN}$  was recorded at 100 K on an APEX-II diffractometer equipped with an area detector and graphite monochromated Mo  $K\alpha$  radiation (0.71073 Å). Data reduction of the diffraction images was performed using the APEX2 software (Bruker, 2011). The structure of  $[\text{H}_2\text{BisBuIm}]_2\cdot\text{CH}_3\text{CN}$  was solved by direct methods and refined by full-matrix least-squares methods based on  $F^2$  using the SHELXL2014 program (Sheldrick, 2015). Heavy atoms were refined anisotropically. Hydrogen atoms were positioned geometrically in idealized positions and refined with isotropic displacement parameters according to the riding model. Distance and angle calculations were estimated using the SHELXL2014 program (Sheldrick, 2015).

### S3. DFT Calculations

Quantum chemical calculations were performed with the Gaussian09 (Gaussian, 2009) software using the M11L functional (Peverati *et al.*, 2009) and the polarizable continuum method (SMD) (Marenich *et al.*, 2009) with acetonitrile as solvent. The basis sets were 6-311++G(d,p) (C, N, H) and SDD (I) (Andrae *et al.*, 1990; Dolg *et al.*, 1993).

### S4. Hirshfeld surface analysis

Hirshfeld surface analysis were carried out with the CrystalExplorer (Version 3.1) program (Spackman & Jayatilaka, 2009; Wolff *et al.*, 2012).

**Table S1** DFT coordinates.

I	1.222458	-0.760002	2.657309
N	-1.308273	0.875518	-0.309566
C	-0.228352	1.653320	-0.229071
H	0.612506	1.650393	-0.907862
N	-0.361605	2.413606	0.846107
C	-1.544945	2.116170	1.472798
H	-1.848049	2.615491	2.377217
C	-2.142794	1.140644	0.747711
H	-3.074706	0.614779	0.879955
C	0.606497	3.395364	1.299051
H	1.559400	3.148620	0.815685
H	0.729836	3.252578	2.377836
C	0.185272	4.805578	0.964981
H	0.933427	5.477703	1.410361
H	-0.769913	5.036132	1.461524
C	0.079084	5.070633	-0.520121
H	1.017712	4.761069	-1.008924
H	-0.711771	4.439985	-0.955667
C	-0.212931	6.519096	-0.823372
H	-0.302684	6.699620	-1.900643
H	0.581899	7.174321	-0.443884

H	-1.153124	6.841184	-0.356486
N	-1.010263	-1.402366	-0.887182
C	0.243667	-1.819317	-1.078239
H	1.008465	-1.261965	-1.596573
N	0.364923	-3.002207	-0.496542
C	-0.830759	-3.351686	0.078008
H	-0.953159	-4.279958	0.608903
C	-1.700736	-2.343516	-0.166459
H	-2.737698	-2.212422	0.098445
C	1.572152	-3.809049	-0.443069
H	1.420402	-4.685728	-1.085776
H	1.666857	-4.164701	0.590661
C	2.791969	-3.030644	-0.848553
H	2.864179	-2.122410	-0.230257
H	2.703274	-2.693210	-1.892658
C	4.060132	-3.840252	-0.703066
H	3.996297	-4.745911	-1.326689
H	4.154566	-4.190340	0.336530
C	5.275685	-3.032739	-1.086299
H	6.199794	-3.613785	-0.989009
H	5.373479	-2.141292	-0.452687
H	5.210639	-2.685342	-2.126341
C	-1.521146	-0.128012	-1.316317
H	-1.008667	0.173058	-2.230955
H	-2.592955	-0.220995	-1.500156
I	3.564415	1.043801	-1.436893
I	-5.701406	-0.757993	-0.656457

**Table S2** Comparison between X-ray and DFT data (distances in Å, angles in degrees).

	X-ray		DFT	
N1–C2	1.330(3)	1.337(3)	1.333	1.335
N1–C5	1.389(3)	1.384(3)	1.372	1.373
N1–C31	1.457(3)	1.461(3)	1.437	1.438
C2–N3	1.324(3)	1.327(3)	1.324	1.324
N3–C4	1.385(3)	1.384(3)	1.372	1.372
N3–C6	1.473(3)	1.475(3)	1.451	1.453
C2–N1–C5	108.78(16)	109.01(17)	109.5	109.5
N3–C2–N1	108.64(17)	108.14(18)	107.6	107.6
C2–N3–C4	108.63(16)	108.93(17)	109.4	109.5
C5–C4–N3	107.39(18)	107.27(18)	107.0	107.1
C4–C5–N1	106.54(17)	106.63(19)	106.4	106.4
N1–C31–N1'	110.80(16)		110.9	

**S5. References**

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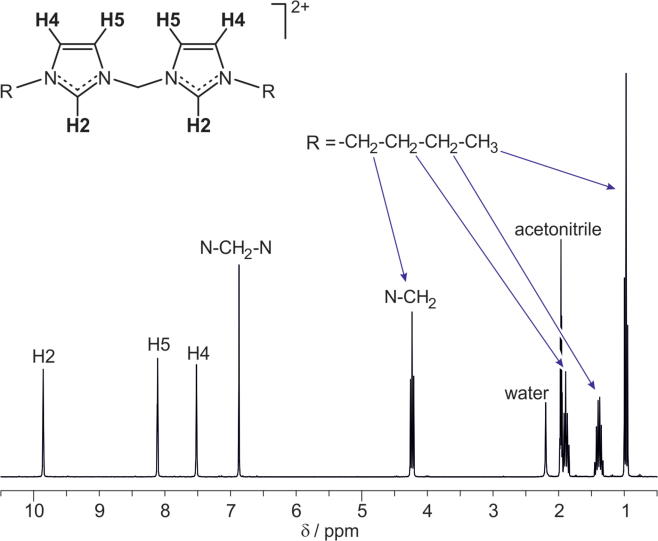


Figure S1

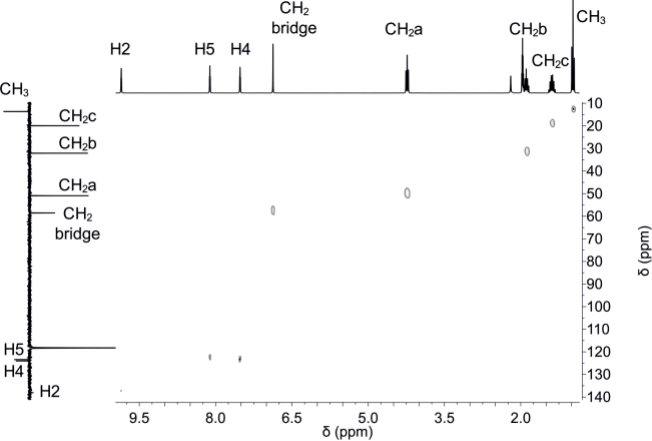


Figure S2

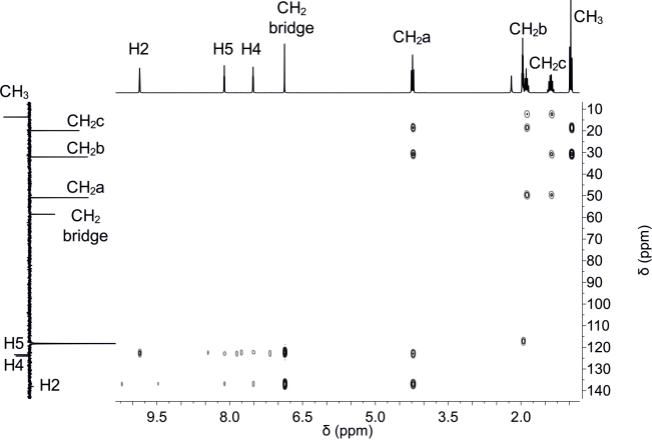


Figure S3

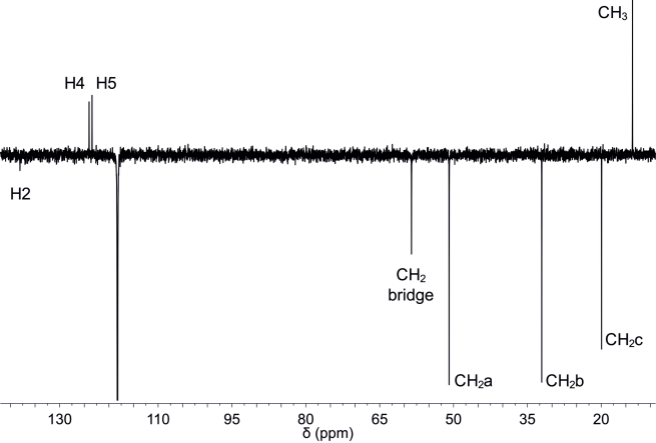


Figure S4