Crystallization and temperature-dependent structure deflection of C_6mimBr Ionic Liquid Intercalated in Laponite

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Supporting information

Computational method

Density functional theory (DFT) calculations were performed with the Gaussian-09 C1 package[1] using the B3LYP functional, a hybrid Hartree–Fock/DFT method that incorporates Becke's three-parameter functional (B3) with the Lee, Yang and Parr correlation functional.[2, 3] The 6-31++G(d) basis sets were used. Geometry is fully optimized in aqueous solution. Solvation effects were taken into account using the conductor-like screening model (COSMO) method.[4, 5] No symmetry constraints were imposed during the structural optimizations. Frequency calculations were carried out to verify the structure at the energy minima.

The optimized structure of C_6mim^+ is shown in Figure S1. As shown in Figure S1, the molecular dimensions of C_6mim^+ are 10.8×4.2×3.6 in Å.

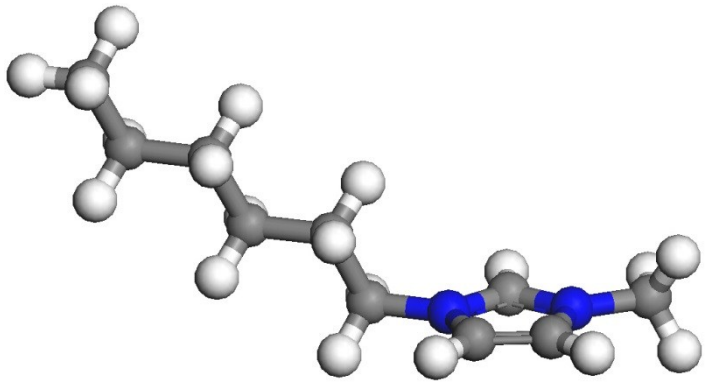

Figure S1 Optimized structure of C_6mim^+. Grey, blue and white spheres denote carbon, nitrogen and hydrogen atoms.

Optimized Cartesian x, y and z coordinates of C_6mim^+

N	9.82706200	3.85280300	10.06654000
C	9.70054500	5.05882000	10.92180600
H	9.89881100	5.92321300	10.28108600
H	10.50453200	5.00384600	11.66110400
C	8.32925400	5.16195200	11.59765000
H	8.15257200	4.25845600	12.19662400

H	7.54342700	5.19496600	10.83127000
C	8.23493500	6.41003400	12.48985500
H	8.43176400	7.30745000	11.88553900
H	9.02389600	6.37197200	13.25505000
C	6.86746400	6.54829700	13.17520000
H	6.66782300	5.64755200	13.77441100
H	6.07911600	6.59029200	12.40913900
C	10.50583200	2.74153700	10.37560000
H	11.08047100	2.58818200	11.27719000
N	10.36333600	1.85091400	9.38423600
C	10.96178600	0.50825800	9.33767000
H	10.16949600	-0.24076200	9.27528100
H	11.54246200	0.34791500	10.24682700
H	11.61874400	0.43284900	8.46854800
C	9.56291500	2.41370400	8.40659300
H	9.30902700	1.88480800	7.50018300
C	9.22660600	3.66525600	8.83511700
H	8.62223400	4.42958500	8.37056100
C	6.76627100	7.78844200	14.07502900
C	5.39970500	7.92301700	14.75627200
H	6.96736800	8.68771200	13.47546200
H	7.55497400	7.74565000	14.83964700
H	5.18449300	7.05515100	15.39210600
H	4.59264100	8.00380800	14.01745800
H	5.36074000	8.81622100	15.38934500

References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Wallingford CT, 2009.
2. A. D. Becke, *Physical Review A*, 1988, **38**, 3098.
3. C. Lee, W. Yang and R. G. Parr, *Physical Review B*, 1988, **37**, 785.
4. A. Klamt and G. Schuurmann, *Journal of the Chemical Society, Perkin Transactions 2*, 1993, 799.
5. C. C. Pye and T. Ziegler, *Theor Chem Acc*, 1999, **101**, 396.