Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Cycloaddition of CO_2 and Epoxides Catalyzed by Imidazolium Bromides at Mild Conditions: Influence of the Cation on Catalyst Activity

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Supporting Information

Single Crystal X-Ray Structure Determination of Compound 10 (CCDC 928238)

General:

Data were collected on an X-ray single crystal diffractometer equipped with a CCD detector (Bruker APEX II, *κ*-CCD), a rotating anode (Bruker AXS, FR591) with MoK_α radiation ($\lambda = 0.71073$ Å), and a Montel mirror by using the APEX 2 software package.[S1] The measurements were performed on a single crystal coated with perfluorinated ether. The crystal was fixed on the top of a glass fiber and transferred to the diffractometer. The crystal was frozen under a stream of cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects, scan speed, and background using SAINT.[S2] Absorption corrections, including odd and even ordered spherical harmonics were performed using SADABS.[S2] Space group assignments were based upon systematic absences, *E* statistics, and successful refinement of the structures. Structures were solved by direct methods with the aid of successive difference Fourier maps,[S1] and were refined against all data using SHELXL-97[S3] in conjunction with SHELXLE.[S4] If not mentioned otherwise, non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in ideal positions using the SHELXL riding model. Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(F_o^2 - F_c^2)^2$ with SHELXL-97[S3] weighting scheme. Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from *International Tables for Crystallography*.[S6] Images of the crystal structures were generated by PLATON.[S5]

[1] APEX suite of crystallographic software. "**APEX 2"** Version 2008.4. Bruker AXS Inc., Madison, Wisconsin, USA (2008).

[2] SAINT, Version 7.56a and SADABS Version 2008/1. Bruker AXS Inc., Madison, Wisconsin, USA (2008).

[3] Sheldrick, G. M. "**SHELXL-97**", University of Göttingen, Göttingen, Germany, (1998).

[4] Huebschle, C. B.; Sheldrick, G. M.; Dittrich, B. (2011). "**SHELXLE**" J. Appl. Cryst., 44, (2011) 1281 - 1284.

[5] Spek, A. L. "**PLATON**", A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, (2010).

[6] International Tables for Crystallography, Vol. C, Tables 6.1.1.4 (pp. 500-502), 4.2.6.8 (pp. 219-222), and 4.2.4.2 (pp. 193-199), Wilson, A. J. C., Ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1992.

Special:

Compound 10

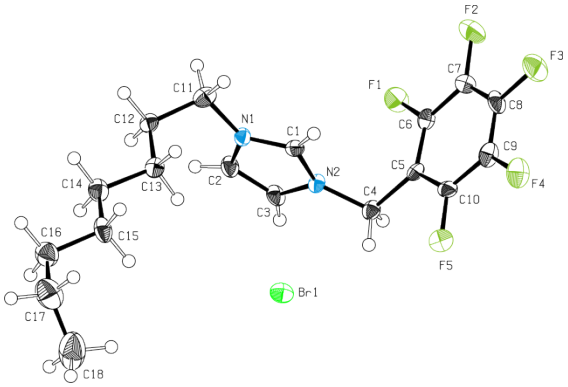

Figure F1 – Ortep drawing drawing of compound **10** with 50% ellipsoids. [5]

Table S1 – Sample and crystal data for Compound **10**.

Chemical formula	$C_{18}H_{22}BrF_5N_2$	
Formula weight	441.29	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal size	0.040 x 0.150 x 0.330 mm	
Crystal habit	clear colourless plate	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 7.8536(3) Å	α = 90°
	b = 8.5571(3) Å	β = 90.415(2)°
	c = 29.1438(9) Å	γ = 90°
Volume	1958.53(12) $Å^3$	
Z	4	
Density (calculated)	1.497 g/cm^3	
Absorption coefficient	2.148 mm^{-1}	
F(000)	896	

Table S2 – Data collection and structure refinement for Compound **10**.

Diffractometer	Bruker Kappa APEX II CCD
Radiation source	FR591 rotating anode, Mo
Theta range for data collection	1.40 to 25.36°
Index ranges	-9<=h<=9, -10<=k<=9, -34<=l<=34

Reflections collected	15259	
Independent reflections	3572 [R(int) = 0.0790]	
Coverage of independent reflections	99.5%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9267 and 0.5420	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 1997)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	3572 / 0 / 236	
Goodness-of-fit on F^2	1.112	
Δ/σ_{max}	0.001	
Final R indices	2270 data; I>2σ(I)	R1 = 0.0793, wR2 = 0.0824
	all data	R1 = 0.1433, wR2 = 0.0927
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0000P)^2+4.8085P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.245 and -0.962 eÅ^{-3}	
R.M.S. deviation from mean	0.121 eÅ^{-3}	

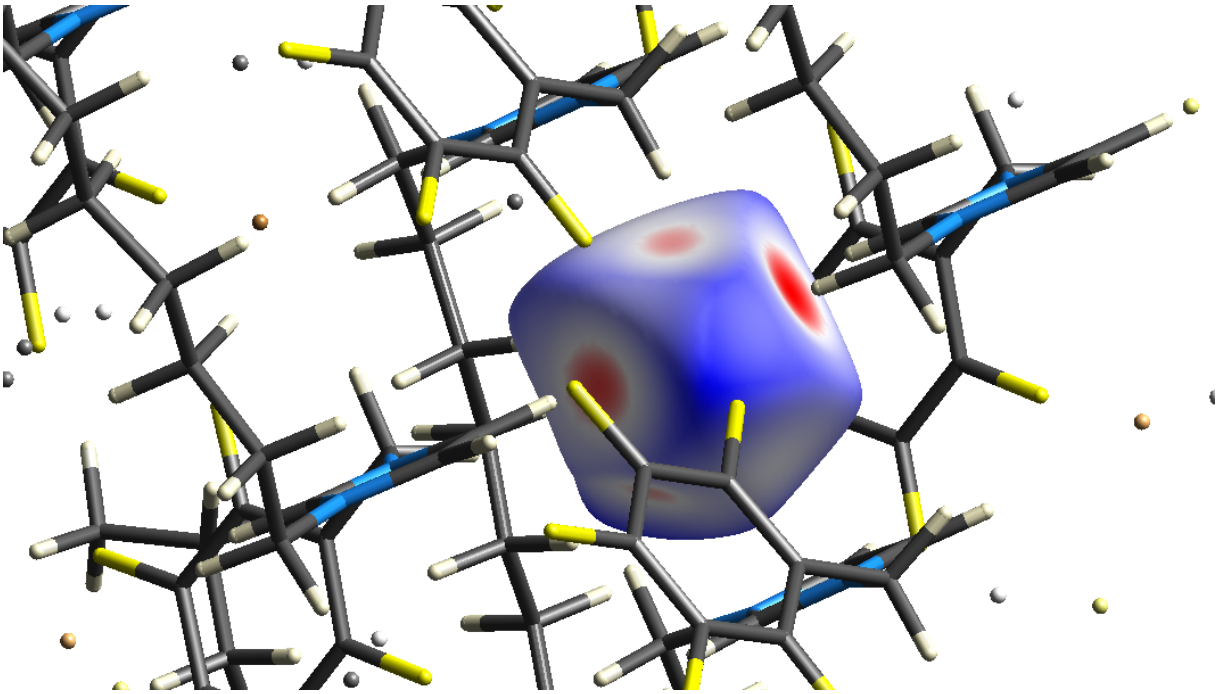

Figure F2 – Hirshfeld surface analysis of **10**.