Supporting information

Title: Hydrogen sulfide gas capture by organic superbase 1, 8-diazabicyclo-[5.4.0]-undec-7-ene through salt formation: Salt synthesis, characterization and application for CO_2 capture

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Table S1. ¹H NMR shifts and signal assignments in spectra of DBU and solid [DBU-H₂S] adduct (DMSO-d⁶ as internal standard)

DBU			solid [DBU-H ₂ S] adduct			
H ^{n (a)}	nН	δ, ppm	H ⁿ	nН	δ, ppm	
DBU 3, 4, 5	6	1.45-1.54	DBU 3, 4	4	1.56-1.57	
DBU 10	2	1.65	DBU 5	2	1.63-1.64	
DBU 6	2	2.24	DBU 10	2	1.86	
DBU 9	2	3.07	DBU 6	2	2.90-2.93	
DBU 11, 2	4	3.14-3.16	DBU 9	2	3.17	
			DBU 11	2	3.47	
			DBU 2	2	3.53-3.55	
			-SH/-NH	2	4.49	
^a Numbering of pro	4	$ \begin{array}{c} 2 & 11 \\ N & 10 \\ 7 & 8 \\ 6 & 9 \end{array} $				

Table S2. ¹³C NMR shifts and signal assignments in spectra of DBU and solid [DBU-H₂S] adduct (DMSO-d⁶ as internal standard)

DBU			solid [DBU-H ₂ S] adduct			
C ^{<i>n</i> (a)}	Rel. Int.	δ, ppm	C ⁿ	Rel. Int.	δ, ppm	
DBU 10	1	22.37	DBU 10	1	19.01	
DBU 5	1	25.82	DBU 5	1	23.45	
DBU 3	1	28.14	DBU 3	1	26.05	
DBU 4	1	29.13	DBU 4	1	28.16	
DBU 6	1	36.37	DBU 6	1	30.30	
DBU 9	1	43.49	DBU 9	1	36.70	
DBU 11	1	47.51	DBU 11	1	47.71	
DBU 2	1	51.82	DBU 2	1	52.88	
DBU 7	1	159.57	DBU 7	0.5	164.76	
	3 4	N 7 8 9				
^a Numbering of	of carbon atoms =	6				

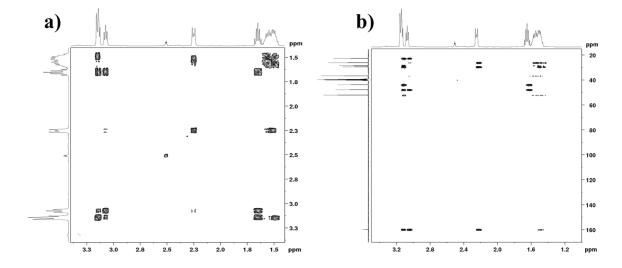


Figure S1 a) ¹H-¹³C COSY NMR and, b) ¹H-¹³C HMBC NMR of DBU (in solvent d⁶ - DMSO)

Figure S2 a) ¹H-¹³C COSY NMR and, b) ¹H-¹³C HMBC NMR solid [DBU-H₂S] adduct (in solvent d⁶ - DMSO)

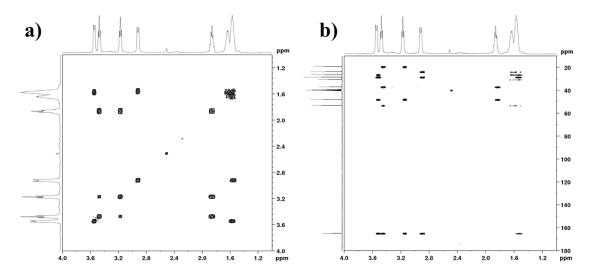


Figure S3 ¹H NMR spectra (in CDCl₃) of CO₂ treated aqueous solution of [DBUH][SH] salt with different water concentrations, a) DBU, b) [DBUH][SH] salt, with different water concentrations such as c) 5 wt.%, d) 10 wt.%, e) 14 wt.%, f) 18 wt.%, and g) 21 wt.%, CO₂ gas flow rate = 15 ml/min.

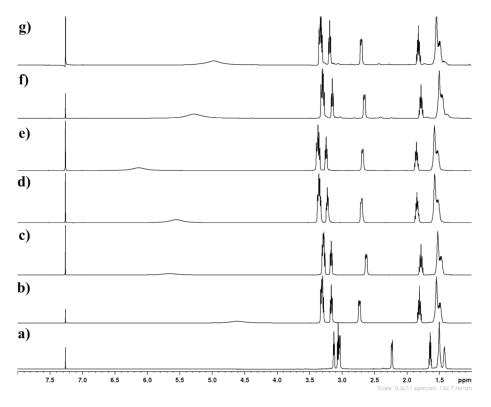


Figure S4 ¹H NMR spectra (in $CDCI_3$) of CO_2 treated aqueous solution of [DBUH][SH] salt (14 wt.% H₂O with different gas flow rates a) DBU, b) [DBUH][SH] salt, with different gas flow rates such as c) 5 ml/min, d) 10 ml/min, e) 15 ml/min, f) 20 ml/min, and g) 25 ml/min.

