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Supporting Information

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Encapsulated Carboxylic Acid Dimers with Compressed Hydrogen Bonds**

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Table S1. OHO hydrogen bond geometries and ^{1}H chemical shifts of carboxylic acid dimers in the solid state.

Compound	environment	Method	*T*/K	*p/kbar*	δ_{HH}/ppm	r_{OH}/Å	$r_{H...O}$/Å	$r_{O...O}$/Å	angle	q_1/Å	q_2/Å
BA	polycrystalline	NMR	298	0	12.7[1]						
BA	Crystal	XD[2]	295	0				2.627			
BA	Crystal	ND[3]	20	0		0.995	1.615	2.608	175.4	-0.310	2.610
BA	Crystal	ND[3]	50	0		0.990	1.628	2.616	175.4	-0.319	2.618
BA	Crystal	ND[3]	100	0		0.993	1.616	2.606	174.3	-0.312	2.609
BA	Crystal	ND[3]	125	0		1.001	1.615	2.616	180.0	-0.307	2.616
BA	Crystal	ND[3]	175	0		0.987	1.650	2.629	170.8	-0.331	2.637
BA-d_5	Crystal	ND[4]	5	0				2.657			
BA-d_5	Crystal	ND[4]	5	0.72				2.650			
BA-d_5	Crystal	ND[4]	5	2.0				2.637			
BA-d_5	Crystal	ND[4]	5	3.2				2.629			

XD: X-ray diffraction. ND: neutron diffraction

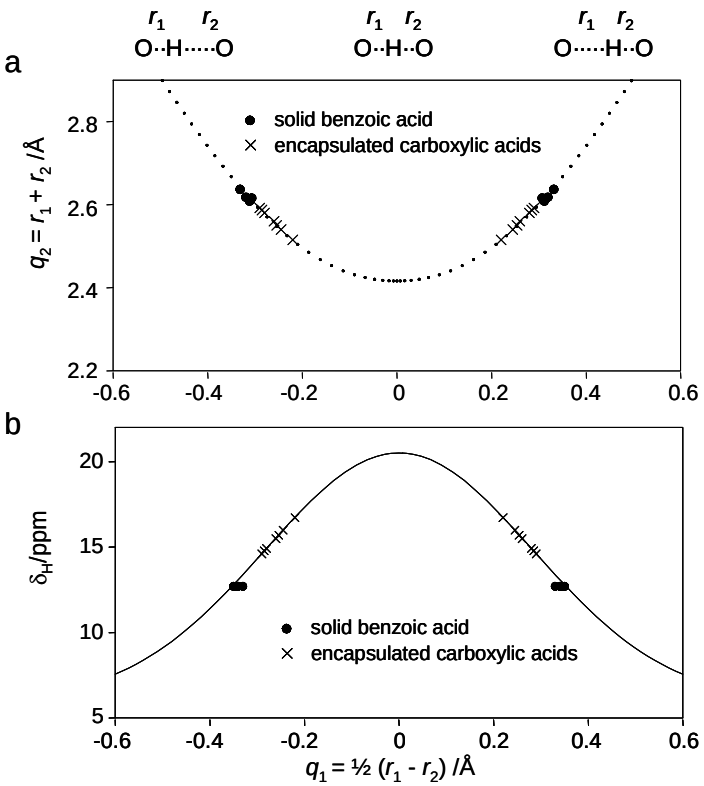

Figure S1. OHO hydrogen bond correlations according to Ref. 5. (a) Geometric hydrogen bond correlation. (b) ^{1}H NMR chemical shift-geometry correlation according to $\delta_H = 6 + 15.3\exp(-6.2q_1^2)$, see main text. The geometric data of solid benzoic acid stem from Ref. 3, the solid state chemical shift from Ref. 1. The data for encapsulated carboxylic acids were estimated as described in the main text.

[1] R. K. Harris,P. Jackson, L. H. Merwin, B. J. Say, G. S. Hägele, *J. Chem. Soc. Faraday Trans. I*, **1988**, *84*, 3649-3672.

[2] R. Feld, M. S . Lehmann, K. W. Muir, J. C. Speakmann, *Zeit. Krist.* **1981**, *157*, 215-231.

[3] C. C. Wilson, N. Shankland, A. J. Florence, *J. Chem. Soc. Faraday Trans.* **1996**, *92*, 5051-5057.

[4] D. F. Brougham, A. J. Horsewill, A. Ikram, R. M. Ibberson, P. J. McDonald, M. Pinter-Krainer, *J. Chem. Phys*. **1996**, *105*, 979–982.

[5] H. H. Limbach, P. M. Tolstoy, N. Perez-Hernandez, J. Guo, I. G. Shenderovich, G. S. Denisov, *Israel J. Chem.* **2009**, *49*, 199-216.