Electronic Supplementary Information

Selectivity of Aliphatic Alcohols by Host-Guest Chemistry

Nicole M. Sykes, Hong Su, Edwin Weber, Susan A. Bourne and Luigi R. Nassimbeni

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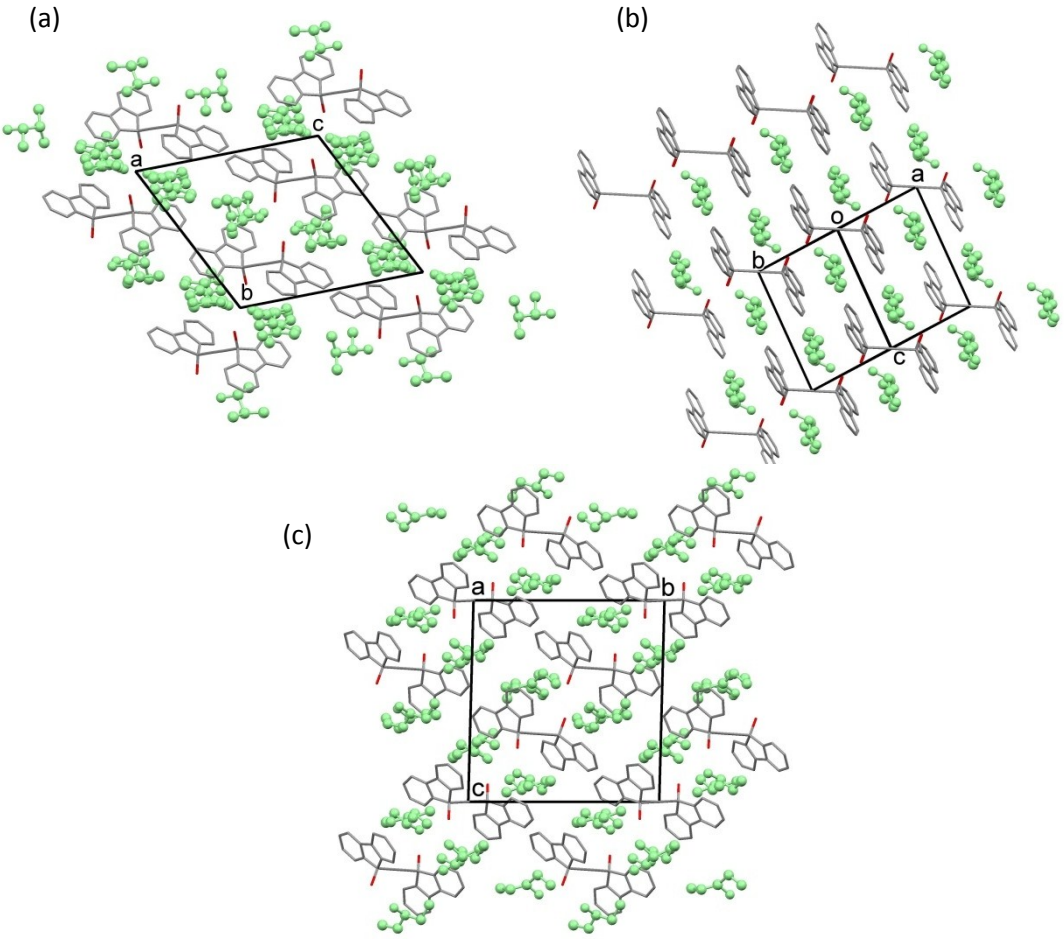
1. CSD analysis of 9,9'-(ethyne-1,2-diyl)-bis(fluoren-9-ol)

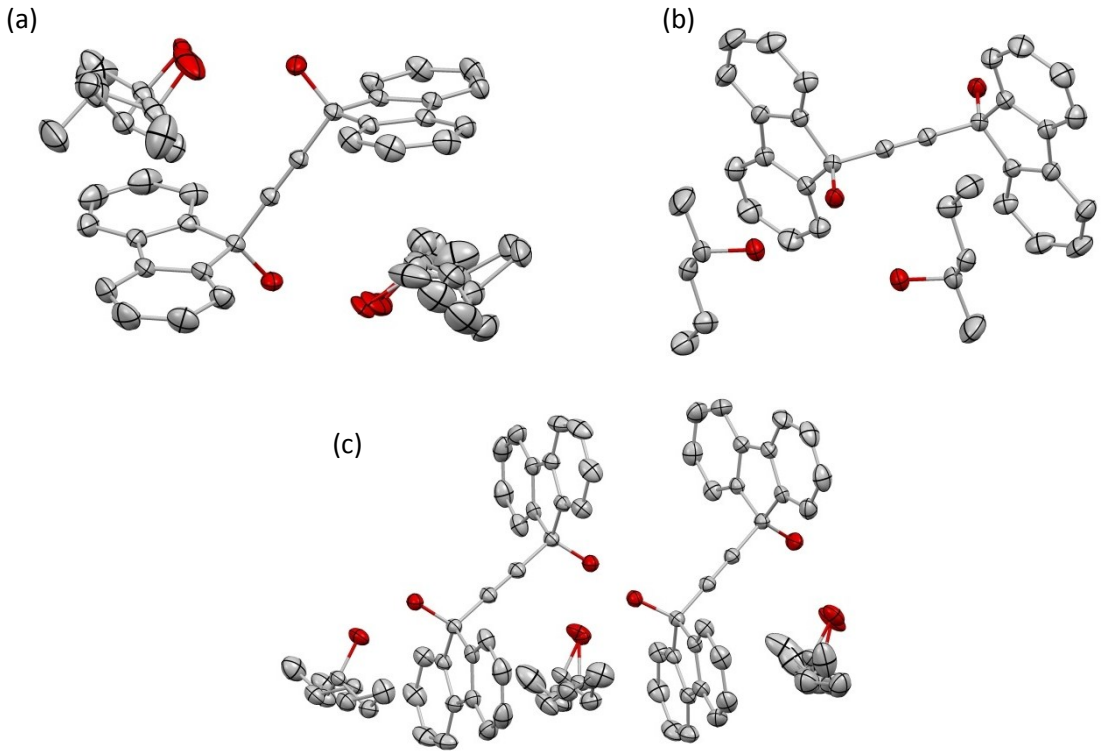
Guest	REFCODE	Reference
2,6-dimethylpiperidine	CANFUV	N. M. Sykes, H. Su, E .Weber, S. A. Bourne and L. R. Nassimbeni, Cryst. Growth Des., 2017, 17, 819-826.
2-methylpiperidine	CANGC	
3,5-methylpiperidine	CANGEG	
3-methylpiperidine	CANGIK	
4-methylpiperidine	CANGOQ	
2-picoline	CISPEA	L. R. Nassimbeni, G. Ramon and E. Weber, *J. Therm. Anal. Cal*., 2007, **90**, 31-37.
3-picoline	CISPIE	
4-picoline	CISPOK	
Pyridine	CISPUQ	
Acetonitrile and water	DEZBOA	T. le Roux, L. R. Nassimbeni and E. Weber, *Chem. Commun*., 2007, 1124-1126.
Ethanol	DEZBUG	
Ethanol and acetonitrile	DEZCAN	
Ethanol and acetonitrile	DIFDEC	
Ethanol and acetonitrile	DIFDIG	
Acetonitrile and water	DEZBOA01	T. le Roux, L. R. Nassimbeni and E. Weber, *New J. Chem.*, 2008**, 32***,* 856-863.
Acetonitrile	ROBGAR	
Ethanol	DEZBUG01	
Acetonitrile and water	DEZCAN01	
Ethanol and Acetonitrile	DIFDEC01	
Ethanol and Acetonitrile	DIFDIG01	
Ethanol	GIZPOV	

1-propanol Cyclohexanol Tetrahydrofuran	IFAHOM IFHAUS IFAJAA	E. Weber, S. Nitsche, A. Wierig, I. Csoregh; *Eur.J.Org.Chem,* 2002, 856
9H-fluoren-9-one	QIZLES	J. Gabriel Garcia, F. R. Fronczek; Private Communication (2014)
9H-fluoren-9-one	QIZLES01	Varshni Singh, F. R. Fronczek, S. F. Watkins; Private Communication (2012)
Caffeine Caffeine and Methanol Methanol	UPIWAS UPIWEW UPIWIA	A. Jacobs, L. Nassimbeni, K. L. Nohako, G. Ramon, B. K. Sebogisi; *J.Chem.Cryst*, 2011, **41**, 610

2. ORTEP and Packing Figures



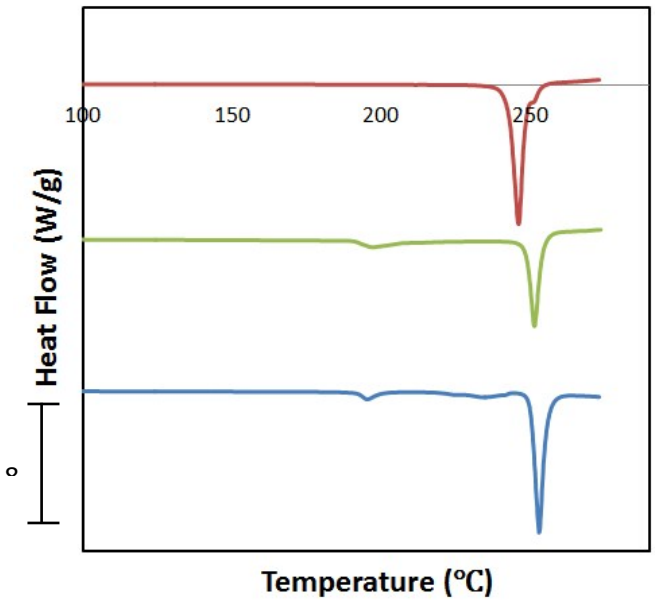
The packing of (a) **H·2(3MBUT)** viewed down [100] (b) **H·2(2PENT)** and (c) **3H·6(3PENT)** viewed down [100], with guest atoms shown in green.



ORTEP diagrams of (a) **H·2(3MBUT)** (b) **H·2(2PENT)** and (c) **3H·6(3PENT)**

3. Apohost polymorph DSC

DSC traces of **Apohost(α)** (red), **Apohost(β)** (green) and **H** as received from Professor Edwin Weber (blue).



4. DFT calculation

Relaxed potential energy scans were computed using density functional theory (DFT), employing the B3LYP hybrid exchange-correlation functional[1-3] and the def2-SVP basis set.[4] Dispersion effects were taken into account by adding the D3 correction of Grimme, with Becke-Johnson (BJ) dampening.[5,6] This level of theory is denoted B3LYP-D3/def2-SVP. The Gaussian 09 package was used.[7]

References

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3. P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch. *J. Phys. Chem*. 1994, **98**, 11623-11627.
4. F. Weigend, R. Ahlrichs. *Phys. Chem. Chem. Phys*. 2005, **7**, 3297-3305.
5. S. Grimme, J. Antony, S. Ehrlich, H. Krieg. *J. Chem. Phys*. 2010, **132**, 154104.
6. S. Grimme, S. Ehrlich, L. Goerigk. *J. Comput. Chem*. 2011, **32**, 1456-1465.
7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, Petersson, G. A.; Nakatsuji, H.; Caricato, M.; 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. Jr. 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, D. J. Fox. Gaussian 09, Revision D.01, Gaussian, Inc.: Wallingford CT, 2009.

5. Hirshfeld Analysis

Host selected as target in all cases

Apohost(α)

	Out %		
In %	**C**	**H**	**O**
C	6.8	20.5	0
H	16.3	46.9	4.2
O	0	5.3	0

Apohost(β) *cis-*

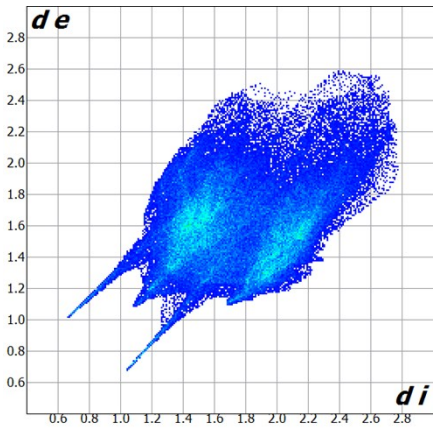
	Out %		
In %	**C**	**H**	**O**
C	5.2	21.9	0.2
H	20.2	46.3	1.5
O	0	4.8	0

Apohost(β) *trans-*

	Out %		
In %	**C**	**H**	**O**
C	9.2	18.1	0.1
H	8.5	48.9	10.2
O	0.4	4.6	0

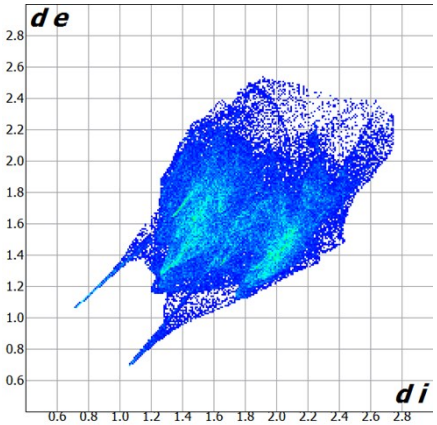
H·2(3MBUT)

	Out %		
In %	**C**	**H**	**O**
C	0	27.2	0.1
H	2.5	62.1	4.0
O	0	4.2	0



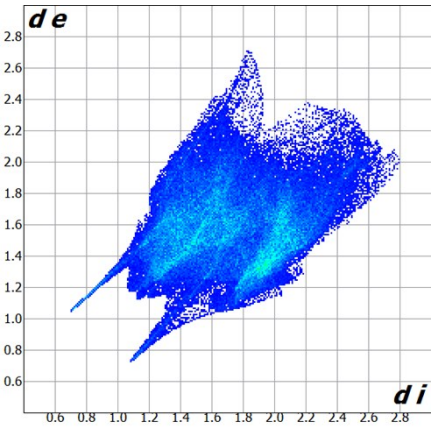
3H·6(3PENT) *trans-*

	Out %		
In %	**C**	**H**	**O**
C	0	26.4	0
H	3.7	60.3	3.8
O	0	5.3	0



3H·6(3PENT)
gauche-

	Out %		
In %	**C**	**H**	**O**
C	0	27.4	0
H	2.9	60.7	3.9
O	0	5.1	0



H·2(2PENT)

	Out %		
In %	**C**	**H**	**O**
C	0	26.8	0
H	2.0	62.8	3.9
O	0	4.5	0

H·2(1BUT)

	Out %		
In %	**C**	**H**	**O**
C	0.8	27.0	0
H	7.4	55.8	4.4
O	0	4.7	0