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Selectivity assessment in host-guest complexes from single crystal X-ray diffraction data: The cavitand-alcohols case.

Rita De Zorzi,[a] Giovanna Brancatelli,[a] Monica Melegari,[b] Roberta Pinalli,[b] Enrico Dalcanale,[b] Silvano Geremia[a,*]

[a] Centro di Eccellenza in Biocristallografia, Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste, via Licio Giorgieri 1, 34127 Trieste (Italy)

[b] Dipartimento di Chimica, Università degli Studi di Parma and INSTM Udr Parma, Parco Area delle Scienze 17A, 43124 Parma (Italy)

Supporting Information

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Table S1: Unit cell parameters of crystals of cavitand 1 grown in presence of the 32 alcoholic binary mixtures.

Structure			$P\,2_1/c$	
	a (Å)	**b (Å)**	**c (Å)**	**β(°)**
MeOH:EtOH 4:6 (1)	12.2869	21.9113	17.6501	104.2735
MeOH:EtOH 4:6 (2)	12.3168	21.9755	17.6953	104.0978
MeOH:EtOH 6:4	12.3045	21.9400	17.6361	104.2101
MeOH:EtOH 8:2	12.2432	21.8836	17.6533	103.9962
MeOH:1-PrOH 2:8	12.2656	21.9235	17.7920	103.8710
MeOH:1-PrOH 4:6	12.2550	21.9946	17.7319	103.7852
MeOH:1-PrOH 6:4	12.2918	21.9386	17.8245	104.1782
MeOH:1-PrOH 8:2	12.2023	21.9788	17.7311	103.9392
MeOH:2-PrOH 2:8	12.3825	21.8372	17.7391	105.0385
MeOH:2-PrOH 4:6	12.2900	21.9072	17.7776	104.3076
MeOH:1-BuOH 2:8	12.2846	22.0579	17.7281	105.1994
EtOH:1-PrOH 2:8	12.3348	21.9096	17.7504	104.5037
EtOH:1-PrOH 4:6	12.3182	21.8896	17.6667	104.3783
EtOH:1-PrOH 6:4	12.3053	21.8672	17.6114	104.3707
EtOH:2-PrOH 2:8	12.3736	21.9300	17.6903	104.9088
EtOH:2-PrOH 4:6	12.3493	21.9209	17.6959	104.6636
EtOH:2-PrOH 6:4 (1)	12.3560	22.0006	17.6515	104.4803
EtOH:2-PrOH 6:4 (2)	12.3165	21.9261	17.6584	104.5299
1-PrOH:2-PrOH 2:8	12.4219	21.7781	17.8241	104.8786
1-PrOH:2-PrOH 4:6 (1)	12.3383	21.8612	17.8079	104.3235
1-PrOH:2-PrOH 4:6 (2)	12.3480	21.8835	17.7868	104.4537
1-PrOH:2-PrOH 6:4	12.3420	21.8601	17.8400	104.2637
1-PrOH:2-PrOH 8:2	12.3237	21.8917	17.8283	104.1339
1-PrOH:1-BuOH 2:8	12.3042	21.8544	17.8762	103.9091
1-PrOH:2-BuOH 2:8	12.4070	21.8138	17.8499	104.2039
1-PrOH:2-BuOH 4:6	12.3308	21.8214	17.8122	103.9154
2-PrOH:1-BuOH 2:8	12.3683	21.8461	17.8759	104.3928
2-PrOH:1-BuOH 6:4	12.4498	21.8497	17.7633	104.9914
2-PrOH:2-BuOH 2:8	12.5024	21.7654	17.8074	104.8721
2-PrOH:2-BuOH 4:6	12.4653	21.7958	17.7661	105.0446
1-BuOH:2-BuOH 4:6	12.4573	21.7456	17.8691	104.3873
1-BuOH:2-BuOH 6:4	12.4015	21.8886	17.9194	104.1694

Table S2. Occupancy factors for alcoholic guests *A* and *B* obtained by conventional structural refinement (x_A, x_B) of the host-guest crystal structures. As comparison, the computed occupancy factor of the alcohol *A* (x_w^A) is reported in the last column. For each structure the *R*-factor has been reported to attest the quality of the refined crystallographic model.

A	*B*	χ_A	x_A	x_B	*R*	x_w^A
MeOH	EtOH	0.4 (1)	0.37(2)	0.63(2)	0.0597	0.163(2)
MeOH	EtOH	0.4 (2)	0.37(2)	0.63(2)	0.0595	0.114(2)
MeOH	EtOH	0.6	0.37(2)	0.63(2)	0.0516	0.120(2)
MeOH	EtOH	0.8	0.44(4)	0.56(4)	0.1218	0.337(2)
MeOH	1-PrOH	0.2	0.46(1)	0.54(1)	0.0521	0.230(2)
MeOH	1-PrOH	0.4	0.56(1)	0.44(1)	0.0575	0.362(2)
MeOH	1-PrOH	0.6	0.47(1)	0.53(1)	0.0668	0.351(2)
MeOH	1-PrOH	0.8	0.40(2)	0.60(2)	0.0751	0.662(3)
MeOH	2-PrOH	0.2	0.34(1)	0.66(1)	0.0622	0.355(3)
MeOH	2-PrOH	0.4	0.61(1)	0.39(1)	0.0703	0.670(2)
MeOH	1-BuOH	0.2	0.65(2)	0.35(2)	0.0981	0.772(4)
EtOH	1-PrOH	0.2	0.75(2)	0.25(2)	0.0683	0.555(3)
EtOH	1-PrOH	0.4	0.83(1)	0.17(1)	0.0656	0.770(2)
EtOH	1-PrOH	0.6	0.89(1)	0.11(1)	0.1247	0.832(2)
EtOH	2-PrOH	0.2	0.65(1)	0.35(1)	0.0844	0.753(3)
EtOH	2-PrOH	0.4	0.73(1)	0.27(1)	0.0739	0.891(2)
EtOH	2-PrOH	0.6 (1)	0.77(1)	0.23(1)	0.0683	0.877(2)
EtOH	2-PrOH	0.6 (2)	0.75(1)	0.25(1)	0.0743	0.933(2)
1-PrOH	2-PrOH	0.2	0.30(1)	0.70(1)	0.0565	0.382(2)
1-PrOH	2-PrOH	0.4 (1)	0.44(1)	0.56(1)	0.0870	0.580(3)
1-PrOH	2-PrOH	0.4 (2)	0.49(1)	0.51(1)	0.0562	0.632(2)
1-PrOH	2-PrOH	0.6	0.56(1)	0.44(1)	0.0665	0.769(2)
1-PrOH	2-PrOH	0.8	0.76(1)	0.24(1)	0.0824	0.859(2)
1-PrOH	1-BuOH	0.2	0.41(2)	0.59(2)	0.0748	0.822(3)
1-PrOH	2-BuOH	0.2	0.63(1)	0.37(1)	0.0699	0.621(2)
1-PrOH	2-BuOH	0.4	0.76(1)	0.24(1)	0.0626	0.834(2)
2-PrOH	1-BuOH	0.2	0.45(1)	0.55(1)	0.0784	0.563(2)
2-PrOH	1-BuOH	0.6	0.82(1)	0.18(1)	0.0628	0.961(1)
2-PrOH	2-BuOH	0.2	0.38(2)	0.62(2)	0.0703	0.525(2)
2-PrOH	2-BuOH	0.4	0.71(2)	0.29(2)	0.0695	0.698(2)
1-BuOH	2-BuOH	0.4	0.31(2)	0.59(2)	0.0933	0.192(2)
1-BuOH	2-BuOH	0.6	0.45(1)	0.55(1)	0.0798	0.464(3)

Table S3. Ratios of the binding constants (K_A/K_B) for the cavitand Tiiii[H,CH_3,CH_3] site, calculated for each pair of alcohols. The K_A/K_B values are the mean values of the ratios reported in Table 2.

K_A/K_B		*Guest* A					
		MeOH	EtOH	1-PrOH	2-PrOH	1-BuOH	2-BuOH
Guest B	MeOH		5.68(7)	1.38(2)	0.381(3)	0.07(2)	
	EtOH	0.176(2)		0.225(3)	0.104(3)		
	1-PrOH	0.724(8)	4.44(6)		0.461(6)	0.054(1)	0.142(1)
	2-PrOH	2.62(2)	9.6(2)	2.17(2)		0.09(3)	0.254(3)
	1-BuOH	13.5(3)		18.5(4)	10.8(3)		2.14(3)
	2-BuOH			7.04(7)	3.94(4)	0.467(6)	

Figure S1. Structure and electron density map (contour level: 1σ) for the host-guest complex obtained in presence of the alcohol pair MeOH/1-PrOH 0.20:0.80.