Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Hydrogen Bonding Properties of Non-Polar Solvents

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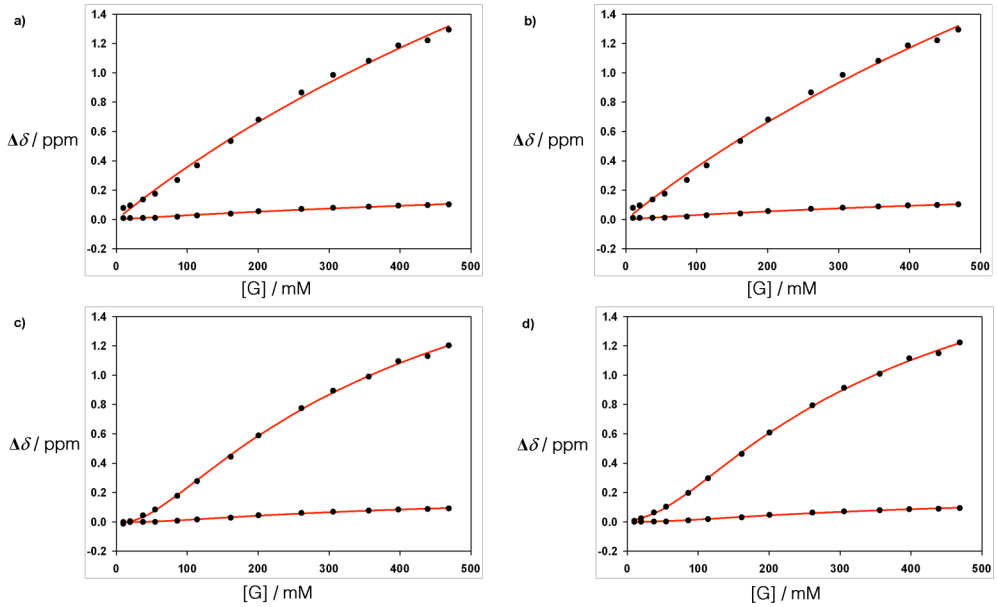
SUPPLEMENTARY INFORMATION

1. Self association of 13. ^{1}H NMR dilution experiment for hexafluoroisopropanol (**13**). The data for the CH and the OH signals were simultaneously fit to different binding isotherms: a) isodesmic polymerisation; b) isodesmic polymerisation plus cyclic dimer; c) isodesmic polymerisation plus cyclic trimer; d) isodesmic polymerisation plus cyclic tetramer. The corresponding fits for non-isodesmic polymerisation, isodesmic polymerisation plus cyclic pentamer, and isodesmic polymerisation plus cyclic hexamer are indistinguishable from (d).

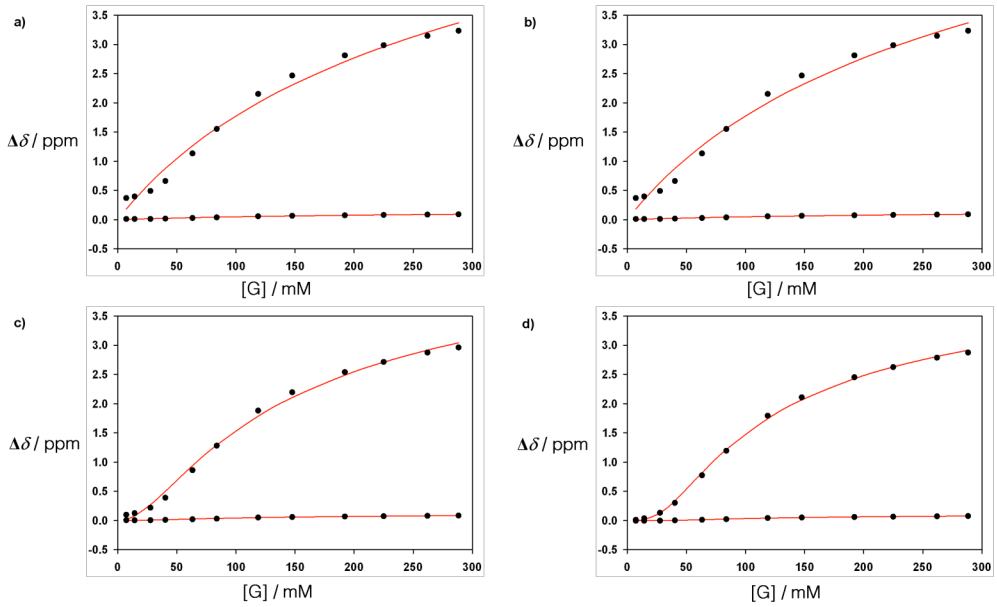


Quality of fit (% error between calculated and experimental chemical shifts changes)

Isotherm	***K*** **/ M^{-1}**	***α***	***EM*** **/ M**	**(1/*N*) *EM K*^{N}**	**% error**
Isodesmic polymerisation	0.4				3.7
Non-isodesmic polymerisation	4	7			1.0
Isodesmic polymerisation plus cyclic dimer	nd		-	0.2 M^{-1}	3.7
Isodesmic polymerisation plus cyclic trimer	nd		-	4 M^{-2}	1.2
Isodesmic polymerisation plus cyclic tetramer	0.6		2800	21 M^{-3}	1.1
Isodesmic polymerisation plus cyclic pentamer	1		280	260 M^{-4}	1.0
Isodesmic polymerisation plus cyclic hexamer	4		38	14,000 M^{-5}	1.1

nd no polymer detected

2. Self association of 14. ^{1}H NMR dilution experiment for of trifluoroethanol (**14**). The data for the CH_2 and the OH signals were simultaneously fit to different binding isotherms: a) isodesmic polymerisation; b) isodesmic polymerisation plus cyclic dimer; c) isodesmic polymerisation plus cyclic trimer; d) isodesmic polymerisation plus cyclic tetramer. The corresponding fits for non-isodesmic polymerisation, isodesmic polymerisation plus cyclic pentamer, and isodesmic polymerisation plus cyclic hexamer are indistinguishable from (d).



Quality of fit (% error between calculated and experimental chemical shifts changes)

Isotherm	***K*** **/ M^{-1}**	***α***	**(1/*N*) *EM K*^{N}**	**% error**
Isodesmic polymerisation	3			7.2
Non-isodesmic polymerisation	13	15		1.2
Isodesmic polymerisation plus cyclic dimer	nd		1 M^{-1}	7.2
Isodesmic polymerisation plus cyclic trimer	nd		25 M^{-2}	3.8
Isodesmic polymerisation plus cyclic tetramer	nd		390 M^{-3}	1.7
Isodesmic polymerisation plus cyclic pentamer	nd		6,100 M^{-4}	1.0
Isodesmic polymerisation plus cyclic hexamer	nd		97,000 M^{-5}	1.5

nd no polymer detected

3. Association constants for 1:1 H-bonded complexes measured in alkanes

Reference	T	Solvent	HB Donor	HB Acceptor	K_a / M^{-1}
1	300	cyclohexane	Pyrrole	tetrahydrofuran	4.00E-01
2	298	cyclohexane	2-Chloroethanol	cyclopentanone	2.40E+01
3	298	cyclohexane	4-fluorophenol	c-propylamine	1.50E+01
4	296	cyclohexane	t-Butyl sulphide	pyridine N-oxide	7.35E-01
5	295	cyclohexane	N-methylaniline	N,N-dimethylacetamide	8.00E+00
1	300	cyclohexane	Pyrrole	diethyl ether	5.00E-01
2	298	cyclohexane	2,2,2-trichloroethanol	cyclopentanone	6.00E+01
4	296	cyclohexane	Isopropyl sulphide	pyridine N-oxide	6.50E-01
1	300	cyclohexane	Diphenylamine	tetrahydrofuran	4.00E-01
1	300	cyclohexane	Diphenylamine	diethyl ether	2.80E-01
1	300	cyclohexane	Carbazole	tetrahydrofuran	1.50E+00
6	296	cyclohexane	N-methylaniline	tributyl phosphate	7.30E+00
7	296	cyclohexane	Phenol	tetrahydrothiophene	8.50E+00
8	298	cyclohexane	4-chlorophenol	triethylamine	1.55E+03
8	298	cyclohexane	4-chlorophenol	isopropylamine	2.42E+03
9	298	cyclohexane	Pyrrole	EtCN	1.10E+01
10	298	cyclohexane	4-chlorophenol	tetrahydrothiophene	1.00E+01
8	298	cyclohexane	4-chlorophenol	1,4-dioxane	5.60E+01
10	298	cyclohexane	hexafluoropropan-2-ol	tetrahydrothiophene	1.47E+01
8	298	cyclohexane	4-chlorophenol	n-butylamine	2.04E+03
11	295	cyclohexane	Chloroform	tributylamine	2.80E-01
12	298	cyclohexane	Pyrrole	triethylamine	4.40E+00
13	300	cyclohexane	Chloroform	triethylamine	4.30E-01
14	298	cyclohexane	4-nitrophenol	diethyl ether	2.50E+01
15	297	cyclohexane	1-naphthol	benzene	1.60E-01
16	298	cyclohexane	N-methylaniline	Ph2CO	1.40E+00
1	300	cyclohexane	Pyrrole	1,4-dioxane	8.00E-01
4	296	cyclohexane	Dichloromethane	pyridine N-oxide	2.41E+00
3	298	cyclohexane	4-fluorophenol	3-bromopyridine	1.30E+01
11	294	cyclohexane	Chloroform	tributyl phosphate	5.20E+00
17	293	cyclohexane	Chloroform	triethyl phosphate	5.60E+00
5	295	cyclohexane	Aniline	N,N-dimethylacetamide	1.00E+01
17	293	cyclohexane	Chloroform	HMPA	1.30E+01
8	298	cyclohexane	4-chlorophenol	morpholine	5.24E+02
10	298	cyclohexane	4-t-butylphenol	tetrahydrothiophene	3.40E+00
5	295	cyclohexane	N-methylaniline	benzophenone	1.10E+00
8	298	cyclohexane	4-chlorophenol	tripropylamine	2.64E+02
5	295	cyclohexane	N-methylaniline	acetone	1.20E+00
18	301	cyclohexane	Chloroform	dibutyl ether	2.40E-01
5	295	cyclohexane	N-methylaniline	ethyl acetate	9.60E-01
1	300	cyclohexane	Diphenylamine	1,4-dioxane	5.80E-01
3	298	cyclohexane	4-fluorophenol	triethylamine	9.80E+01
5	295	cyclohexane	Aniline	anisole	7.30E-01
19	298	cyclohexane	N-methylaniline	cyclohexyldimethylamine	5.60E-01
4	296	cyclohexane	Chloroform	pyridine N-oxide	4.73E+00
5	295	cyclohexane	N-methylaniline	cyclohexanone	1.20E+00

4	296	cyclohexane	2,2,2-Trichloroethanol	pyridine N-oxide	3.30E+02
15	297	cyclohexane	1-naphthol	toluene	2.40E-01
6	296	cyclohexane	Aniline	tributyl phosphate	9.70E+00
13	310	cyclohexane	Chloroform	quinuclidine	1.20E+00
12	298	cyclohexane	Pyrrole	pyridine	5.50E+00
7	294	cyclohexane	3-trifluoromethylphenol	tetrahydrothiophene	6.00E+00
3	298	cyclohexane	4-fluorophenol	dimethyl sulphoxide	3.60E+02
5	295	cyclohexane	Aniline	dipropyl ether	5.00E-01
4	296	cyclohexane	2,2,2-Trifluoroethanol	pyridine N-oxide	7.88E+02
8	298	cyclohexane	4-chlorophenol	tributylamine	2.45E+02
4	296	cyclohexane	4-fluorophenol	pyridine N-oxide	1.87E+03
20	300	cyclohexane	4-chlorophenol	tetrahydrofuran	2.60E+01
20	300	cyclohexane	3-methylphenol	1,4-dioxane	1.20E+01
18	301	cyclohexane	Chloroform	1-methyl-2-pyrrolidone	3.20E+00
5	295	cyclohexane	Aniline	ethyl acetate	1.60E+00
14	298	cyclohexane	4-chlorophenol	triethylamine	1.94E+02
21	298	cyclohexane	4-t-butylphenol	N,N-dimethylacetamide	2.74E+02
20	300	cyclohexane	4-chlorophenol	diethyl ether	1.40E+01
14	298	cyclohexane	Phenol	triethylamine	8.50E+01
22	285	cyclohexane	3-nitrophenol	diethyl ether	1.13E+02
3	298	cyclohexane	4-fluorophenol	1,4-dioxane	6.70E+00
23	298	cyclohexane	Chloroform	c-hexylamine	1.10E+00
5	295	cyclohexane	N-methylaniline	anisole	3.60E-01
4	296	cyclohexane	Propan-1-ol	pyridine N-oxide	1.94E+01
4	296	cyclohexane	PhC<>CH	pyridine N-oxide	1.23E+00
14	298	cyclohexane	4-nitrophenol	triethylamine	1.26E+03
24	298	cyclohexane	N-methylaniline	pyridine	1.31E+00
15	297	cyclohexane	1-naphthol	4-methylpyridine	9.10E+01
13	300	cyclohexane	Chloroform	2,6-dimethylpyridine	8.00E-01
15	297	cyclohexane	1-naphthol	p-xylene	4.80E-01
25	298	cyclohexane	3-fluorophenol	ethyl acetate	3.40E+01
5	295	cyclohexane	N-methylaniline	dipropyl ether	3.10E-01
4	296	cyclohexane	Phenol	pyridine N-oxide	9.47E+02
20	300	cyclohexane	1-naphthol	1,4-dioxane	1.30E+01
21	298	cyclohexane	4-chlorophenol	triethylamine	2.26E+02
14	298	cyclohexane	4-nitro-3-trifluoromethylphenol	triethylamine	6.17E+03
4	296	cyclohexane	Pentafluorophenol	pyridine N-oxide	4.85E+03
10	298	cyclohexane	4-t-butylphenol	tetrahydrofuran	2.50E+01
4	296	cyclohexane	Hexafluoropropan-2-ol	pyridine N-oxide	5.40E+03
24	298	cyclohexane	N-methylaniline	N,N-dimethylaniline	4.60E-01
20	300	cyclohexane	2-naphthol	1,4-dioxane	1.30E+01
15	297	cyclohexane	1-naphthol	pyridine	6.70E+01
24	298	cyclohexane	Aniline	benzene	2.70E-01
3	298	cyclohexane	4-fluorophenol	HMPA	6.30E+03
25	298	cyclohexane	3-fluorophenol	pyridine	2.62E+02
14	298	cyclohexane	3,4-dichlorophenol	triethylamine	5.56E+02
26	293	cyclohexane	Chloroform	pentan-3-one	7.30E-01
5	295	cyclohexane	N-methylaniline	tetrahydrofuran	7.80E-01
14	298	cyclohexane	4-cyanophenol	triethylamine	9.26E+02
20	300	cyclohexane	1-naphthol	tetrahydrofuran	2.00E+01

4	296	cyclohexane	t-Butyl alcohol	pyridine N-oxide	1.80E+01
1	300	cyclohexane	Carbazole	1,4-dioxane	2.50E+00
18	301	cyclohexane	Chloroform	diethyl sulphide	2.20E-01
21	298	cyclohexane	4-t-butylphenol	pyridine	7.20E+01
24	298	cyclohexane	Aniline	pyridine	1.70E+00
13	300	cyclohexane	Chloroform	tetrahydrofuran	5.40E-01
18	301	cyclohexane	Chloroform	cyclohexanone	1.00E+00
20	300	cyclohexane	2-naphthol	diethyl ether	1.10E+01
9	293	cyclohexane	Pyrrole	tetrahydropyran	4.80E+00
4	296	cyclohexane	Propan-2-ol	pyridine N-oxide	1.87E+01
21	298	cyclohexane	3-trifluoromethylphenol	ethyl acetate	4.30E+01
15	297	cyclohexane	1-naphthol	m-xylene	5.30E-01
21	298	cyclohexane	3-trifluoromethylphenol	pyridine	4.00E+02
20	300	cyclohexane	1-naphthol	diethyl ether	1.10E+01
20	300	cyclohexane	2-naphthol	tetrahydrofuran	2.20E+01
9	298	cyclohexane	Pyrrole	1,4-dioxane	1.70E+00
21	298	cyclohexane	3-trifluoromethylphenol	cyclohexanone	7.10E+01
7	298	cyclohexane	3-fluorophenol	diethyl sulphide	2.60E+00
24	298	cyclohexane	Aniline	N,N-dimethylaniline	7.10E-01
13	283	cyclohexane	Chloroform	pyridine	1.40E+00
23	298	cyclohexane	Chloroform	aniline	5.10E-01
4	296	cyclohexane	4-Chlorophenol	pyridine N-oxide	2.23E+03
18	301	cyclohexane	Chloroform	ethyl acetate	6.70E-01
18	301	cyclohexane	Chloroform	1,4-dioxane	5.80E-01
21	298	cyclohexane	4-t-butylphenol	triethylamine	1.06E+02
15	297	cyclohexane	1-naphthol	o-xylene	5.00E-01
15	297	cyclohexane	1-naphthol	3-methylpyridine	7.90E+01
14	298	cyclohexane	3,5-dichlorophenol	triethylamine	9.08E+02
14	298	cyclohexane	3-nitrophenol	triethylamine	1.04E+03
4	296	cyclohexane	Ethanol	pyridine N-oxide	1.89E+01
21	298	cyclohexane	4-chlorophenol	pyridine	2.11E+02
7	293	cyclohexane	3-trifluoromethylphenol	diethyl sulphide	4.90E+00
20	300	cyclohexane	4-chlorophenol	1,4-dioxane	1.60E+01
15	297	cyclohexane	1-naphthol	2-methylpyridine	8.70E+01
27	293	cyclohexane	Dichloromethane	HMPA	1.40E+00
4	296	cyclohexane	Pyrrole	pyridine N-oxide	4.03E+01
7	295	cyclohexane	Phenol	dibutyl ether	8.50E+00
16	298	cyclohexane	Aniline	Ph2CO	9.00E-01
24	298	cyclohexane	N-methylaniline	benzene	1.40E-01
7	298	cyclohexane	Phenol	diethyl sulphide	2.00E+00
3	298	cyclohexane	4-fluorophenol	pyridine	1.07E+02
5	295	cyclohexane	Aniline	tetrahydrofuran	1.20E+00
3	298	cyclohexane	4-fluorophenol	N,N-dimethylformamide	2.00E+02
3	298	cyclohexane	4-fluorophenol	benzonitrile	1.00E+01
15	297	cyclohexane	1-naphthol	mesitylene	9.70E-01
20	300	cyclohexane	3-methylphenol	diethyl ether	1.00E+01
18	301	cyclohexane	Chloroform	tetrahydrothiophene	2.80E-01
13	300	cyclohexane	Chloroform	acetone	6.70E-01
20	300	cyclohexane	3-methylphenol	tetrahydrofuran	1.90E+01
4	296	cyclohexane	Methanol	pyridine N-oxide	2.53E+01

25	298	cyclohexane	3-fluorophenol	dibutyl ether	1.70E+01
3	298	cyclohexane	4-fluorophenol	4-N,N-dimethylaminopyridine	1.40E+03
28	298	isooctane	t-butyl alcohol	triethylamine	1.00E+00
28	298	isooctane	propan-2-ol	triethylamine	1.40E+00
29	313	n-heptane	Cl2CHCN	pentamethylbenzene	1.50E+00
30	298	n-heptane	t-butyl alcohol	cyclohexanone	7.50E-01
28	298	isooctane	Methanol	triethylamine	3.40E+00
28	298	isooctane	Ethanol	triethylamine	2.60E+00
31	294	isooctane	2-naphthol	1,4-dioxane	2.10E+01
32	298	n-heptane	1-naphthol	n-butylamine	1.28E+02
32	298	n-heptane	3-methylphenol	n-butylamine	8.60E+01
29	313	n-heptane	Cl2CHCN	mesitylene	7.00E-01
32	298	n-heptane	2-naphthol	n-butylamine	1.46E+02
20	293	isooctane	1-naphthol	1,4-dioxane	1.80E+01
31	293	isooctane	Phenol	1,4-dioxane	1.64E+01
29	313	n-heptane	Dichloromethane	1,4-dioxane	2.00E-01
7	295	n-hexane	hexafluoropropan-2-ol	tetrahydrothiophene	6.40E+00
32	298	n-heptane	3-methylphenol	triethylamine	6.60E+01
32	298	n-heptane	1-naphthol	triethylamine	1.02E+02
33	298	n-heptane	Phenol	triethylamine	8.90E+01
29	313	n-heptane	Cl2CHCN	toluene	3.80E-01
32	298	n-heptane	2-naphthol	triethylamine	1.17E+02
34	298	n-hexane	2,2,2-trifluoroethanol	triethylamine	7.10E+01
35	298	n-hexane	hexafluoropropan-2-ol	pyridine	7.31E+02
36	304	n-hexane	Chloroform	acetone	9.00E-01
29	313	n-heptane	Dichloromethane	benzene	1.20E-01
36	304	n-hexane	CHBr3	acetone	4.50E-01
29	313	n-heptane	Cl2CHCN	benzene	3.10E-01
34	298	n-hexane	2,2,2-trifluoroethanol	2,4,6-trimethylpyridine	1.05E+02
36	304	n-hexane	CHCl2Br	acetone	8.00E-01
29	313	n-heptane	Dichloromethane	mesitylene	1.70E-01
37	298	n-heptane	Phenol	pyridine	8.00E+01
29	313	n-heptane	Cl2CHCN	1,4-dioxane	1.40E+00
34	298	n-hexane	2,2,2-trifluoroethanol	pyridine	5.90E+01
29	313	n-heptane	Dichloromethane	toluene	1.50E-01
50	298	octane	2-tBuPhenol	Bu3PO	8.00E+00
50	298	cis-decalin	2-tBuPhenol	Bu3PO	1.00E+00
50	298	cyclohexane	2-tBuPhenol	Bu3PO	6.80E+00
50	298	octane	Phenol	Bu3PO	2.80E+01
50	298	cyclohexane	Phenol	Bu3PO	4.00E+02
50	298	cyclohexane	4-Fphenol	Bu3PO	5.40E+01
50	298	cyclohexane	4-Fphenol	ClMe Phosphonate	2.34E+02
50	298	octane	Phenol	ClMe Phosphonate	1.50E+01
50	298	cyclohexane	Phenol	iPr Phosphonate	1.80E+01
50	298	cis-decalin	Phenol	ClMe Phosphonate	1.00E+00
50	298	cyclohexane	Phenol	ClMe Phosphonate	8.00E+01
50	298	octane	2-tBuPhenol	ClMe Phosphonate	1.00E+01
50	298	cyclohexane	Pyrrole	Bu3PO	1.70E+01
50	298	cyclohexane	2-tBuPhenol	ClMe Phosphonate	1.40E+00
50	298	cis-decalin	2-tBuPhenol	ClMe Phosphonate	1.00E+00

50	298	octane	Pyrrole	Bu3PO	3.68E+03
50	298	cis-decalin	Phenol	Bu3PO	1.00E+00
50	298	cyclohexane	4-Fphenol	iPr Phosphonate	3.20E+00
50	298	cyclohexane	2-tBuPhenol	iPr Phosphonate	6.30E+01
50	298	cis-decalin	Pyrrole	Bu3PO	1.00E+00
50	298	cyclohexane	Pyrrole	iPr Phosphonate	1.30E+01
50	298	cyclohexane	Pyrrole	ClMe Phosphonate	1.00E+00
50	298	octane	Pyrrole	ClMe Phosphonate	1.30E+01
50	298	cis-decalin	Pyrrole	ClMe Phosphonate	1.00E+00
50	298	cyclohexane	4-NO2Phenol	Bu3PO	4.70E+01
50	298	cyclohexane	4-NO2Phenol	iPr Phosphonate	6.10E+01
50	298	cyclohexane	4-NO2Phenol	ClMe Phosphonate	1.26E+02

4. Association constants for 1:1 H-bonded complexes measured in perfluoro-*n*-hexane

Reference	T	HB Donor	HB Acceptor	K_a / M^{-1}
50	298	CF3Phenol	n-Bu3PO	4.70E+01
50	298	CF3CH2OH	n-Bu3PO	5.40E+01
50	298	(CF3)2CHOH	n-Bu3PO	6.10E+01
50	298	(CF3)2CHOH	DMF	3.20E+00
50	298	(CF3)3COH	DMF	1.80E+01
50	298	CF3Phenol	DMSO	6.30E+01
50	298	(CF3)3COH	Acetone	1.30E+01
50	298	CF3CH2OH	DMSO	1.26E+02
50	298	(CF3)2CHOH	Acetone	2.34E+02
50	298	CF3CH2OH	DMF	2.80E+01
50	298	(CF3)3COH	Me formate	8.00E+00
50	298	CF3Phenol	Acetone	3.68E+03
50	298	CF3CH2OH	Acetone	1.50E+01
50	298	(CF3)2CHOH	Me formate	1.00E+01
50	298	CF3CH2OH	Me formate	1.30E+01
50	298	CF3Phenol	Me formate	4.00E+02
50	298	(CF3)3COH	n-Bu3PO	6.80E+00
50	298	(CF3)3COH	DMSO	1.70E+01
50	298	(CF3)2CHOH	DMSO	8.00E+01
50	298	CF3Phenol	DMF	1.40E+00

5. Association constants for 1:1 H-bonded complexes measured in dichloromethane

Reference	T	HB Donor	HB Acceptor	K_a / M^{-1}
38	297	methanol	Triethylamine	6.80E+00
39	298	2-naphthol	Triethylamine	6.10E+01
39	293	1-naphthol	triethylamine	5.40E+01
3	298	4-fluorophenol	triethylamine	4.70E+01
40	298	phenol	pyridine	1.70E+01
3	298	4-fluorophenol	triphenylphosphine oxide	8.00E+01
3	298	4-fluorophenol	4-N,N-dimethylaminopyridine	1.26E+02
41	297	phenol	pyridine N-oxide	6.30E+01
3	298	4-fluorophenol	pyridine	1.80E+01
3	298	4-fluorophenol	cyclohexanone	3.20E+00
3	298	4-fluorophenol	dimethyl sulphoxide	2.80E+01
3	298	4-fluorophenol	1,4-dioxane	1.40E+00
3	298	4-fluorophenol	diphenyl sulphoxide	1.30E+01
3	298	4-fluorophenol	HMPA	2.34E+02
3	298	4-fluorophenol	N,N-dimethylformamide	1.50E+01
39	293	phenol	trimethylamine N-oxide	3.68E+03
41	297	phenol	pyrazine N-oxide	8.00E+00
41	297	phenol	pyridazine N-oxide	1.00E+01
41	297	phenol	pyrimidine N-oxide	1.30E+01
42	313	phenol	chloride	4.00E+02
42	313	phenol	bromide	1.00E+02
42	313	phenol	iodide	3.00E+01
42	313	phenol	picrate	2.00E+01
39	298	2-naphthol	trimethylamine N-oxide	6.31E+03
15	293	1-naphthol	trimethylamine N-oxide	6.56E+03

6. Association constants for 1:1 H-bonded complexes measured in 1,2-dichloroethane

Reference	T	HB Donor	HB Acceptor	K_a / M^{-1}
25	298	3-fluorophenol	triethylamine	8.20E+01
3	298	4-fluorophenol	triethylamine	5.00E+01
25	298	3-fluorophenol	Pyridine	3.20E+01
3	298	4-fluorophenol	Pyridine	2.00E+01
3	298	4-fluorophenol	4-N,N-dimethylaminopyridine	1.38E+02
25	298	3-fluorophenol	dibutyl ether	3.30E+00
3	298	4-fluorophenol	3-bromopyridine	5.30E+00
3	298	4-fluorophenol	N,N-dimethylformamide	1.90E+01
25	298	3-fluorophenol	dimethyl sulphoxide	7.30E+01
3	298	4-fluorophenol	dimethyl sulphoxide	4.50E+01
3	298	4-fluorophenol	HMPA	3.55E+02
25	298	3-fluorophenol	ethyl acetate	2.50E+00
3	298	4-fluorophenol	1,4-dioxane	1.20E+00
3	298	4-fluorophenol	cyclohexanone	3.30E+00
3	298	4-fluorophenol	triphenylphosphine oxide	1.10E+02
3	298	4-fluorophenol	benzonitrile	7.00E-01

7. Association constants for 1:1 H-bonded complexes measured in 1,1,1-trichloroethane

Reference	T	HB Donor	HB Acceptor	K_a / M^{-1}
43	298	Methanol	N-methylpyrrolidin-2-one	5.10E+00
43	298	Ethanol	N-methylpyrrolidin-2-one	1.62E+01
43	298	Propan-1-ol	N-methylpyrrolidin-2-one	1.29E+01
43	298	Propan-2-ol	N-methylpyrrolidin-2-one	8.13E+00
43	298	t-Butyl alcohol	N-methylpyrrolidin-2-one	2.50E+00
43	298	benzyl alcohol	N-methylpyrrolidin-2-one	7.94E+00
43	298	2-chloroethanol	N-methylpyrrolidin-2-one	8.50E+00
43	298	2,2,2-trifluoroethanol	N-methylpyrrolidin-2-one	1.00E+02
43	298	Hexafluoropropan-2-ol	N-methylpyrrolidin-2-one	6.76E+02
43	298	Phenol	N-methylpyrrolidin-2-one	1.38E+02
43	298	2-Methylphenol	N-methylpyrrolidin-2-one	5.62E+01
43	298	2,6-Dimethylphenol	N-methylpyrrolidin-2-one	1.20E+01
43	298	2-Isopropylphenol	N-methylpyrrolidin-2-one	8.91E+01
43	298	2-t-Butylphenol	N-methylpyrrolidin-2-one	7.08E+01
43	298	2-Chlorophenol	N-methylpyrrolidin-2-one	2.14E+02
43	298	2,6-Dichlorophenol	N-methylpyrrolidin-2-one	9.55E+00
43	298	2-Cyanophenol	N-methylpyrrolidin-2-one	4.90E+02
43	298	3-Dimethylaminophenol	N-methylpyrrolidin-2-one	6.17E+01
43	298	3-Methylphenol	N-methylpyrrolidin-2-one	7.76E+01
43	298	3-Chlorophenol	N-methylpyrrolidin-2-one	3.16E+02
43	298	4-Methoxyphenol	N-methylpyrrolidin-2-one	1.51E+02
43	298	4-Trifluoromethylphenol	N-methylpyrrolidin-2-one	6.31E+02
43	298	4-nitrophenol	N-methylpyrrolidin-2-one	1.32E+03
43	298	Acetic acid	N-methylpyrrolidin-2-one	1.10E+02
43	298	Benzoic acid	N-methylpyrrolidin-2-one	1.17E+02
43	298	Trifluoroacetic acid	N-methylpyrrolidin-2-one	3.55E+03
43	298	Pyrrole	N-methylpyrrolidin-2-one	8.91E+00
43	298	Indole	N-methylpyrrolidin-2-one	1.41E+01
43	298	Chloroform	N-methylpyrrolidin-2-one	2.51E+00
43	298	4-nitrophenol	Ethanol	2.57E+01
43	298	4-nitrophenol	Propan-2-ol	2.29E+01
43	298	4-nitrophenol	t-Butyl alcohol	2.82E+01
43	298	4-nitrophenol	Dibutyl ether	1.91E+01
43	298	4-nitrophenol	Tetrahydrofuran	4.90E+01
43	298	4-nitrophenol	Anisole	2.00E+00
43	298	4-nitrophenol	1,4-Dioxane	1.91E+01
43	298	4-nitrophenol	Acetone	4.07E+01
43	298	4-nitrophenol	Pentan-3-one	3.16E+01
43	298	4-nitrophenol	MeCOiPr	3.31E+01
43	298	4-nitrophenol	MeCOtBu	2.75E+01
43	298	4-nitrophenol	Cyclohexanone	5.01E+01
43	298	4-nitrophenol	Acetophenone	2.88E+01
43	298	4-nitrophenol	Ethyl acetate	2.69E+01
43	298	4-nitrophenol	y-Butyrolactone	4.68E+01
43	298	4-nitrophenol	N,N-Dimethylformamide	6.46E+02

43	298	4-nitrophenol	N,N-Diethylformamide	5.37E+02
43	298	4-nitrophenol	N,N-Dimethylthioacetamide	5.75E+01
43	298	4-nitrophenol	N-Methylpyrrolidin-2-one	1.32E+03
43	298	4-nitrophenol	N,N-Dimethylbenzamide	6.61E+02
43	298	4-nitrophenol	Tetramethylurea	1.55E+03
43	298	4-nitrophenol	Tetramethyl thiourea	9.12E+01
43	298	4-nitrophenol	phenyl dimethylcarbamate	1.23E+02
43	298	4-nitrophenol	Dimethyl sulphoxide	1.15E+03
43	298	4-nitrophenol	Tetramethylene sulfone	4.07E+01
43	298	4-nitrophenol	Triphenylphosphine oxide	7.08E+03
43	298	4-nitrophenol	Triethyl phosphate	1.48E+03
43	298	4-nitrophenol	Benzylamine	2.29E+02
43	298	4-nitrophenol	CF3CH2NH2	1.02E+01
43	298	4-nitrophenol	Pyridine	3.31E+02
43	298	4-nitrophenol	2-Methoxypyridine	1.91E+01
43	298	4-nitrophenol	2-Fluoropyridine	2.57E+01
43	298	4-nitrophenol	2-Chloropyridine	3.02E+01
43	298	4-nitrophenol	2-Cyanopyridine	1.00E+01
43	298	4-nitrophenol	3-Methylpyridine	4.47E+02
43	298	4-nitrophenol	3-Fluoropyridine	6.61E+01
43	298	4-nitrophenol	3-Chloropyridine	5.89E+01
43	298	4-nitrophenol	3-Bromopyridine	5.75E+01
43	298	4-nitrophenol	3-Cyanopyridine	2.57E+01
43	298	4-nitrophenol	4-Methylpyridine	6.03E+02
43	298	4-nitrophenol	4-Methoxypyridine	7.41E+02
43	298	4-nitrophenol	4-N,N-Dimethylaminopyridine	3.47E+03
43	298	4-nitrophenol	4-Acetylpyridine	1.58E+02
43	298	4-nitrophenol	Pyrazine	2.88E+01
43	298	4-nitrophenol	Pyrimidine	4.68E+01
43	298	4-nitrophenol	Pyridazine	3.39E+02
43	298	4-nitrophenol	Acetonitrile	1.70E+01
43	298	4-nitrophenol	chloroacetonitrile	4.07E+00
43	298	4-nitrophenol	PhCN	1.15E+01
43	298	4-nitrophenol	4-Methoxybenzonitrile	2.09E+01
43	298	4-nitrophenol	4-Chlorobenzonitrile	8.32E+00

8. Association constants for 1:1 H-bonded complexes measured in benzene

Reference	T	HB Donor	HB Acceptor	K_a / M^{-1}
2	298	Ethanol	cyclopentanone	9.30E+00
44	298	Phenol	pyridine	7.90E+01
45	298	2,2,2-trifluoroethanol	benzophenone	7.60E+00
37	298	Phenol	pyridine	3.60E+01
46	298	3-fluorophenol	triethylamine	1.20E+02
45	298	Ethanol	acetone	1.60E+00
47	298	butan-1-ol	pyridine	2.00E+00
46	298	3-fluorophenol	dimethyl sulphoxide	2.54E+02
47	298	propan-2-ol	pyridine	2.00E+00
25	298	3-fluorophenol	pyridine	5.30E+01
46	298	3-fluorophenol	ethyl acetate	5.00E+00
48	298	picric acid	tribenzylamine	1.69E+03
48	298	Benzoic acid	triethylamine	3.76E+03
48	298	Benzoic acid	diphenyl amidine	2.25E+05

9. Association constants for 1:1 H-bonded complexes measured in chlorobenzene

Reference	T	HB Donor	HB Acceptor	K_a / M^{-1}
3	298	4-fluorophenol	HMPA	1.15E+03
38	297	Methanol	triethylamine	6.00E+00
3	298	4-fluorophenol	4-N,N-dimethylaminopyridine	2.40E+02
3	298	4-fluorophenol	3-bromopyridine	1.20E+01
3	298	4-fluorophenol	triethylamine	6.90E+01
3	298	4-fluorophenol	pyridine	4.00E+01
3	298	4-fluorophenol	1,4-dioxane	3.50E+00
3	298	4-fluorophenol	N,N-dimethylformamide	5.50E+01
3	298	4-fluorophenol	dimethyl sulphoxide	1.60E+02
3	298	4-fluorophenol	benzonitrile	3.00E+00

10. Association constants for 1:1 H-bonded complexes measured in *o*-dichlorobenzene

Reference	T	HB Donor	HB Acceptor	K_a / M^{-1}
25	298	3-fluorophenol	Pyridine	1.16E+02
25	298	3-fluorophenol	dibutyl ether	7.40E+00
49	298	3-trifluoromethylphenol	N,N-dimethylacetamide	3.47E+02
3	298	4-fluorophenol	quinuclidine	4.70E+02
3	298	4-fluorophenol	triethylamine	8.50E+01
3	298	4-fluorophenol	4-N,N-dimethylaminopyridine	4.10E+02
3	298	4-fluorophenol	Pyridine	4.30E+01
3	298	4-fluorophenol	N,N-dimethylformamide	5.00E+01
3	298	4-fluorophenol	dimethyl sulphoxide	1.50E+02
3	298	4-fluorophenol	cyclohexanone	1.05E+01
3	298	4-fluorophenol	3-bromopyridine	8.90E+00
3	298	4-fluorophenol	HMPA	1.15E+03
3	298	4-fluorophenol	1,4-dioxane	2.80E+00
3	298	4-fluorophenol	benzonitrile	2.50E+00
3	298	4-fluorophenol	triphenylphosphine oxide	4.50E+02
46	298	3-fluorophenol	Triethylamine	1.58E+02
46	298	3-fluorophenol	ethyl acetate	1.00E+01
46	298	3-fluorophenol	dimethyl sulphoxide	3.21E+02

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