SUPPLEMENTARY INFORMATION

Solute-Solvent Interactions in cryosolutions: A study of halothane/ammonia complexes

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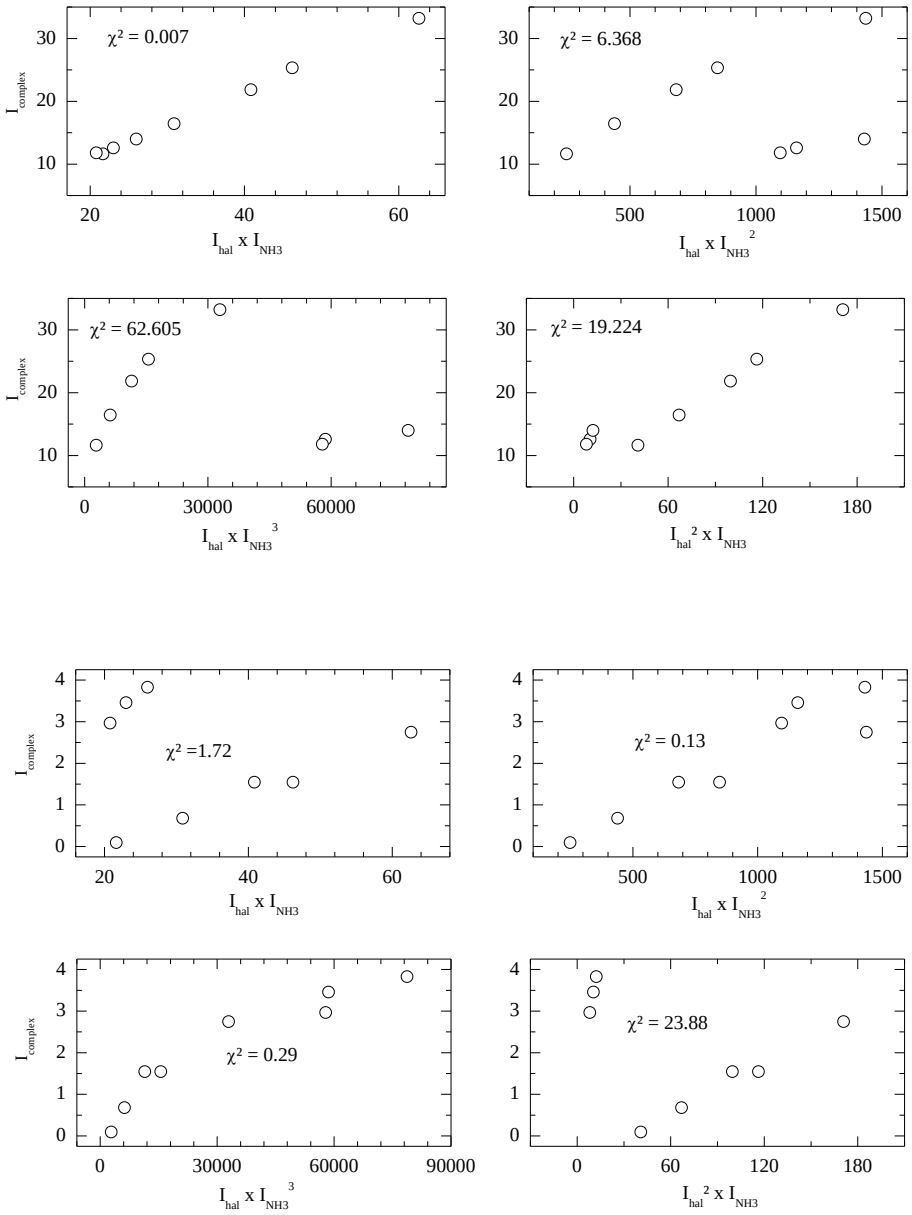

Fig. SF1 Scatter plots for the integrated intensity of the 2956 (upper four plots) and 2920 cm^{-1} complex band (lower four plots) versus the product of the intensities of monomer halothane and NH_3. The data presented are based upon a series of 8 different solutions recorded at 213 K in which the mole fractions of halothane and NH_3 were varied between 2.0×10^{-4} and 1.1×10^{-2} and between 1.8×10^{-4} and 2.4×10^{-2}. The monomer intensities were approximated by numerically integrating the ν_1 and ν_4 absorption bands appearing in monomer halothane and monomer NH_3, respectively.

Table ST1 MP2/6-311++G(d,p) harmonic frequencies (ν_i) in cm^{-1}, IR intensities (ε_i) in km mol^{-1}, Raman scattering activities (S_i) in $Å^4$ amu^{-1}, for halothane, NH_3 and the 1:1 and 1:2 complexes of halothane with NH_3. The complexation shifts $\Delta\nu$, in cm^{-1}, are also given.

			monomer			1:1 *complex*			
			ν_i	ε_i	S_i	ν_i	ε_i	S_i	$\Delta\nu$
halothane	A	ν_1	3186.15	3.4	61.9	3122.60	172.8	180.3	-63.55
		ν_2	1365.19	80.2	3.2	1408.02	46.4	3.5	42.83
		ν_3	1305.88	197.2	0.7	1308.02	192.7	1.0	2.14
		ν_4	1258.91	15.3	4.2	1317.84	39.8	3.1	58.93
		ν_5	1211.79	233.2	2.3	1205.31	216.9	2.4	-6.48
		ν_6	1159.69	221.9	2.6	1171.70	215.2	2.0	12.01
		ν_7	890.05	36.8	1.6	890.60	36.4	1.35	0.55
		ν_8	848.46	74.6	3.1	845.83	83.5	3.8	-2.63
		ν_9	737.45	19.1	8.9	734.88	26.2	11.0	-2.57
		ν_{10}	676.66	27.0	1.2	676.30	29.5	1.0	-0.36
		ν_{11}	560.92	4.3	2.0	560.30	4.3	2.0	-0.62
		ν_{12}	525.56	5.0	1.7	526.37	8.0	1.6	0.81
		ν_{13}	374.75	0.5	2.9	374.98	0.7	2.8	0.23
		ν_{14}	320.25	0.6	3.1	320.41	1.0	3.0	0.16
		ν_{15}	238.81	0.4	2.4	241.67	1.3	2.3	2.86
		ν_{16}	207.49	0.7	1.0	206.39	4.1	1.0	-1.10
		ν_{17}	164.31	1.0	0.5	163.72	0.4	0.4	-0.59
		ν_{18}	78.00	0.0	0.2	79.17	0.0	0.2	1.17
NH_3	A	ν_1	3529.51	1.7	136.3	3523.65	0	117.4	-5.86
		ν_2	1069.31	206.6	5.8	1128.17	258.7	7.1	58.86
	E	ν_3	3681.02	11.8	89.4	3669.55	22	83.4	-11.47
		ν_4	1665.35	29.0	18.4	1665.26	54.8	14.8	-0.09
VdW	A	ν_1				232.50	43.5	0.4	
		ν_2				225.74	43.8	0.5	
		ν_3				110.19	0.9	0.1	
		ν_4				14.90	2.1	0.8	
		ν_5				12.98	2.4	0.3	

ν_6	7.75	0.2	0.1

			monomer		1:2 *complex*		
			ν_i	ε_i	ν_i	ε_i	$\Delta\nu$
halothane	A	ν_1	3186.15	3.4	3076.36	245.5	-109.79
		ν_2	1365.19	80.2	1409.43	43.2	44.24
		ν_3	1305.88	197.2	1305.86	200.1	-0.02
		ν_4	1258.91	15.3	1331.3	27.1	72.39
		ν_5	1211.79	233.2	1210.54	217.52	-1.25
		ν_6	1159.69	221.9	1175.85	249.45	16.16
		ν_7	890.05	36.8	891.11	41.8	1.06
		ν_8	848.46	74.6	843.22	83.4	-5.24
		ν_9	737.45	19.1	733.78	25.2	-3.67
		ν_{10}	676.66	27.0	677.21	37.06	0.55
		ν_{11}	560.92	4.3	560.39	4.9	-0.53
		ν_{12}	525.56	5.0	526.51	8.2	0.95
		ν_{13}	374.75	0.5	374.58	0.2	-0.17
		ν_{14}	320.25	0.6	320	2.3	-0.25
		ν_{15}	238.81	0.4	242	1.6	3.19
		ν_{16}	207.49	0.7	207.37	3.1	-0.12
		ν_{17}	164.31	1.0	164.72	0.9	0.41
		ν_{18}	78.00	0.0	79.86	0.1	1.86
NH_3 (CH bonded)	A	ν_1	3529.51	1.7	3478.08	74	-51.43
		ν_2	1069.31	206.6	1154	232.7	84.69
	E	ν_3	3681.02	11.8	3625.38	62.2	-55.64
		ν_3	3681.02	11.8	3670.44	7.4	-10.58
		ν_4	1665.35	29.0	1662.2	19.2	-3.15
		ν_4	1665.35	29.0	1693.24	10	27.89
NH_3 (NH bonded)	A	ν_1	3529.51	1.7	3522.02	1.7	-7.49
		ν_2	1069.31	206.6	1129.63	189.1	60.32
	E	ν_3	3681.02	11.8	3664.75	7.7	-16.27
		ν_3	3681.02	11.8	3670.79	9.3	-10.23
		ν_4	1665.35	29.0	1660.21	41.5	-5.14
		ν_4	1665.35	29.0	1666.2	34.6	0.85
VdW	A	ν_1			445.21	62.3	
		ν_2			297.29	67.2	

v_3	210.63	1.4
v_4	194.67	105.5
v_5	143.08	16.9
v_6	142.16	1.2
v_7	120.73	5.6
v_8	48.93	1.0
v_9	40.07	0.0
v_{10}	30.77	0.8
v_{11}	28.36	0.3
v_{12}	23.14	0.1