

A Thermodynamic Study of Selective Solvation in Solvent Mixtures

Rafel Cabot and Christopher A. Hunter*

SUPPLEMENTARY INFORMATION

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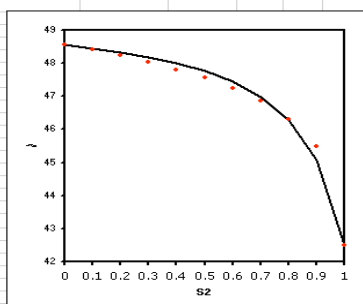
2. Fits to Equation 10.

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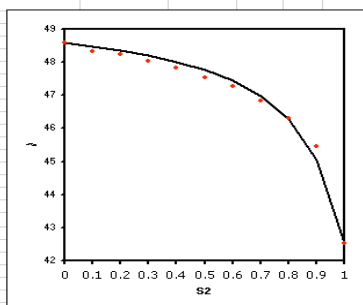
1. Fits to Equation 6.

1.1. Chloroform-Carbon tetrachloride

Expt	CHCl ₃		vol total / μ l	CCl ₄		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	$\Delta\rho$ / ppm	Kb 2 / M-1	error	
	S1	S2		vol S1 / μ l	vol S2 / μ l								-1.3659			4.49E-02
1	1	0	600	600	0	49.0296	18.4622	48.5474	12.50	0.00	0.000	48.5474	0.0000			
2	0.9	0.1	600	540	60	48.8636	18.4448	48.4047	11.25	4.15	0.016	48.4488	0.0019			
3	0.8	0.2	600	480	120	48.6984	18.4486	48.2298	10.00	8.29	0.036	48.3239	0.0100			
4	0.7	0.3	600	420	180	48.5007	18.4578	48.0223	8.75	12.44	0.060	48.1839	0.0259			
5	0.6	0.4	600	360	240	48.2786	18.4500	47.8098	7.50	16.58	0.090	48.0002	0.0367			
6	0.5	0.5	600	300	300	48.0211	18.4421	47.5590	6.25	20.73	0.150	47.7621	0.0412			
7	0.4	0.6	600	240	360	47.7137	18.4435	47.2502	5.00	24.87	0.182	47.4410	0.0364			
8	0.3	0.7	600	180	420	47.3188	18.4515	46.8473	3.75	29.02	0.258	46.9848	0.0189			
9	0.2	0.8	600	120	480	46.8931	18.5621	46.3110	2.50	33.16	0.373	46.2852	0.0007			
10	0.1	0.9	600	60	540	45.9498	18.4424	45.4874	1.25	37.31	0.573	45.0763	0.1690			
11	0	1	600	0	600	42.9470	18.4424	42.4946	0.00	41.45	1.000	42.4946	0.0000			
			total vol of stock	3300	3300			-8.06				ss residuals	0.3408			
<p>ρ 48.5474 42.4946 92 uncorrected 43.9505</p> <p>conc / M 12.498 41.451</p> <p>FW 119.38 153.82</p> <p>density 1.492 1.594</p> <p>N sites 1 4</p> <p>Phosphine Oxide</p> <p>FW 218.32 weight / g 0.0103 0.0095</p> <p>p 97% weight solvent / g 7.3000 7.1933</p> <p>V solvent / mL 4.8328 4.5127</p> <p>conc / mM 3.3532 3.3532</p> <p>External Reference</p> <p>Methylenediphosphonic acid</p> <p>Md / ppm 17.98</p> <p>FW 176.00</p> <p>weight / g 0.0177</p> <p>V / mL 2</p> <p>conc / mM 50.28</p>																

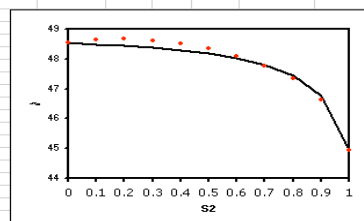


Expt	CHCl ₃		vol total / μ l	CCl ₄		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	$\Delta\rho$ / ppm	Kb 2 / M-1	error	
	S1	S2		vol S1 / μ l	vol S2 / μ l								-1.4171			4.67E-02
1	1	0	600	600	0	49.0376	18.4422	48.5754	12.50	0.00	0.000	48.5754	0.0000			
2	0.9	0.1	600	540	60	48.7939	18.4448	48.3291	11.25	4.15	0.017	48.4732	0.0208			
3	0.8	0.2	600	480	120	48.6396	18.4439	48.2357	10.00	8.29	0.037	48.3502	0.0131			
4	0.7	0.3	600	420	180	48.5000	18.4488	48.0312	8.75	12.44	0.062	48.1993	0.0283			
5	0.6	0.4	600	360	240	48.2873	18.4390	47.8293	7.50	16.58	0.094	48.0099	0.0330			
6	0.5	0.5	600	300	300	48.0128	18.4426	47.5502	6.25	20.73	0.154	47.7651	0.0462			
7	0.4	0.6	600	240	360	47.7341	18.4509	47.2632	5.00	24.87	0.189	47.4364	0.0300			
8	0.3	0.7	600	180	420	47.3124	18.4556	46.8368	3.75	29.02	0.266	46.9716	0.0182			
9	0.2	0.8	600	120	480	46.7817	18.4476	46.3141	2.50	33.16	0.383	46.2643	0.0029			
10	0.1	0.9	600	60	540	45.9219	18.4422	45.4597	1.25	37.31	0.552	45.0579	0.1615			
11	0	1	600	0	600	43.0227	18.4673	42.5354	0.00	41.45	1.000	42.5354	0.0000			
			total vol of stock	3300	3300			-8.04				ss residuals	0.3534			
<p>ρ 48.5754 42.5354 92 uncorrected 43.9526</p> <p>conc / M 12.498 41.451</p> <p>FW 119.38 153.82</p> <p>density 1.492 1.594</p> <p>N sites 1 4</p> <p>Phosphine Oxide</p> <p>FW 218.32 weight / g 0.0101 0.0113</p> <p>p 97% weight solvent / g 7.3791 8.8202</p> <p>V solvent / mL 4.9450 5.5334</p> <p>conc / mM 3.0733 3.0733</p> <p>External Reference</p> <p>Methylenediphosphonic acid</p> <p>Md / ppm 17.98</p> <p>FW 176.00</p> <p>weight / g 0.0177</p> <p>V / mL 2</p> <p>conc / mM 50.28</p>																

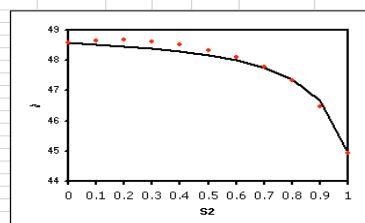


1.2. Chloroform-Acetone

Expt	CHCl ₃ Acetone		vol total / μ l	CHCl ₃ Acetone		ρ_{exp} / g / cm ³	ρ_{ref} / g / cm ³	ρ_{calc} / g / cm ³	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2		vol S1 / μ l	vol S2 / μ l												14132
1	1	0	600	600	0	49.0029	18.4444	48.5395	12.50	0.000	0.000	48.5395	0.0000				
2	0.9	0.1	600	540	60	49.0544	18.3372	48.5472	11.25	8.17	0.012	48.4552	0.0221				
3	0.8	0.2	600	480	120	49.1352	18.4469	48.6683	10.00	16.34	0.027	48.4424	0.0510				
4	0.7	0.3	600	420	180	49.0876	18.4534	48.6142	8.75	24.51	0.045	48.3769	0.0563				
5	0.6	0.4	600	360	240	48.9794	18.4470	48.5114	7.50	32.69	0.068	48.2933	0.0476				
6	0.5	0.5	600	300	300	48.8042	18.4469	48.3384	6.25	40.86	0.099	48.1628	0.0242				
7	0.4	0.6	600	240	360	48.5790	18.4555	48.1025	5.00	49.03	0.142	48.0302	0.0052				
8	0.3	0.7	600	180	420	48.2622	18.4622	47.7800	3.75	57.20	0.204	47.8055	0.0006				
9	0.2	0.8	600	120	480	47.8053	18.4483	47.3370	2.50	65.37	0.306	47.4420	0.0110				
10	0.1	0.9	600	60	540	47.3096	18.4484	46.6412	1.25	73.54	0.498	46.7536	0.0126				
11	0	1	600	0	600	45.4452	18.4727	44.9525	0.00	81.71	1.000	44.9525	0.0000				
			total vol of stock	3300	3300			-3.59			ss residuals	0.2338					
			ρ uncorrected														
			ρ	48.5385	44.9525												
			conc / M	12.439	81.716												
			FW	119.38	58.08												
			density	1.492	0.791												
			N sites	1	6												
			Phosphine Oxide														
			weight / g		CHCl ₃	Acetone											
			FW	218.32	0.0111	0.0119											
			p	97%	7.4123	4.2129	5.0416										
			V solvent / mL		4.9680	5.3261											
			conc / mM		9.9270	9.9270											
			External Reference														
			Methylenediphosphonic acid														
			M _d / ppm														
			FW														
			weight / g														
			V / mL														
			conc / mM														



Expt	CHCl ₃ Acetone		vol total / μ l	CHCl ₃ Acetone		ρ_{exp} / g / cm ³	ρ_{ref} / g / cm ³	ρ_{calc} / g / cm ³	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2		vol S1 / μ l	vol S2 / μ l												16316
1	1	0	600	600	0	49.0411	18.4433	48.5778	12.50	0.000	0.000	48.5778	0.0000				
2	0.9	0.1	600	540	60	49.1207	18.4438	48.6563	11.25	8.17	0.014	48.5285	0.0165				
3	0.8	0.2	600	480	120	49.1435	18.4441	48.6794	10.00	16.34	0.030	48.4688	0.0444				
4	0.7	0.3	600	420	180	49.0830	18.4496	48.6134	8.75	24.51	0.050	48.3948	0.0478				
5	0.6	0.4	600	360	240	48.9714	18.4446	48.5068	7.50	32.69	0.076	48.3009	0.0424				
6	0.5	0.5	600	300	300	48.8023	18.4432	48.3291	6.25	40.86	0.110	48.1777	0.0261				
7	0.4	0.6	600	240	360	48.5725	18.4538	48.0987	5.00	49.03	0.156	48.0089	0.0081				
8	0.3	0.7	600	180	420	48.2532	18.4579	47.7753	3.75	57.20	0.224	47.7636	0.0001				
9	0.2	0.8	600	120	480	47.7947	18.4469	47.3288	2.50	65.37	0.331	47.3744	0.0021				
10	0.1	0.9	600	60	540	46.3193	18.4472	46.4521	1.25	73.54	0.527	46.8522	0.0441				
11	0	1	600	0	600	45.4254	18.4686	44.9398	0.00	81.71	1.000	44.9398	0.0000				
			total vol of stock	3300	3300			-3.64			ss residuals	0.2315					
			ρ uncorrected														
			ρ	48.5778	44.9398												
			conc / M	12.438	81.716												
			FW	119.38	58.08												
			density	1.492	0.791												
			N sites	1	6												
			Phosphine Oxide														
			weight / g		CHCl ₃	Acetone											
			FW	218.32	0.0106	0.0108	4.9403										
			p	97%	7.3970	3.9956											
			V solvent / mL		4.9578	5.0513											
			conc / mM		9.4394	9.4394											
			External Reference														
			Methylenediphosphonic acid														
			M _d / ppm														
			FW														
			weight / g														
			V / mL														
			conc / mM														



1.3. Chloroform-Dichloromethane

Expt	CHCl ₃ DCM		vol total / μ l	CHCl ₃ DCM		δ_{exp} / ppm	δ_{ref} / ppm	δ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb 2 / M-1	error
	S1	S2		vol S1 / μ l	vol S2 / μ l											
1	1	0	600	600	0	48.7707	19.0399	48.7108	12.50	0.000	0.000	48.7108	0.0000			
2	0.9	0.1	600	540	60	48.7264	19.0375	48.6526	11.25	3.12	0.037	48.6404	0.0008			
3	0.8	0.2	600	480	120	48.6353	19.0386	48.5767	10.00	6.24	0.080	48.5594	0.0003	Δ alpha 0	-0.47	0
4	0.7	0.3	600	420	180	48.5431	19.0413	48.4818	8.75	9.36	0.130	48.4653	0.0003	Δ alpha 1	-0.51	0.8 CHCl ₃
5	0.6	0.4	600	360	240	48.4130	19.0392	48.3538	7.50	12.48	0.189	48.2546	0.0000	Δ alpha 2	-0.53	11 DCM
6	0.5	0.5	600	300	300	48.2889	19.0376	48.2414	6.25	15.60	0.259	48.2226	0.0004			
7	0.4	0.6	600	240	360	48.1386	19.0397	48.0789	5.00	18.72	0.344	48.0624	0.0003			
8	0.3	0.7	600	180	420	48.9360	19.0603	47.9557	3.75	21.84	0.449	47.8638	0.0001			
9	0.2	0.8	600	120	480	48.6745	19.0496	47.6049	2.50	24.96	0.583	47.6113	0.0000			
10	0.1	0.9	600	60	540	48.3044	19.0476	47.2368	1.25	28.08	0.759	47.2795	0.0018			
11	0	1	600	0	600	47.9189	19.0751	46.8238	0.00	31.20	1.000	46.8238	0.0000			
			total vol of stock	3300	3300			-1.88				ss residuals	0.0039			

ρ uncorrected			
ρ	48.7108	46.8238	46.2834
conc / M	12.498	31.202	
FW	118.38	84.93	
density	1.492	1.325	
N sites	1	2	

Phosphine Oxide		CHCl ₃	DCM	
FW	218.32	weight / g	0.0100	0.0110
p	97%	weight solvent / g	7.4264	7.2547
		V solvent / mL	4.9775	5.4742
		conc / mM	8.9262	8.9279

External Reference	
Methylenediphosphonic acid	
M _d / ppm	17.96
FW	176.00
weight / g	0.0177
V / mL	2
conc / mM	50.28

Expt	CHCl ₃ DCM		vol total / μ l	CHCl ₃ DCM		δ_{exp} / ppm	δ_{ref} / ppm	δ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb 2 / M-1	error
	S1	S2		vol S1 / μ l	vol S2 / μ l											
1	1	0	600	600	0	48.7767	19.0443	48.7124	12.50	0.000	0.000	48.7124	0.0000			
2	0.9	0.1	600	540	60	48.7001	19.0446	48.6355	11.25	3.12	0.039	48.6298	0.0000			
3	0.8	0.2	600	480	120	48.6225	19.0449	48.5576	10.00	6.24	0.083	48.5566	0.0000	Δ alpha 0	-0.46	0
4	0.7	0.3	600	420	180	48.5310	19.0487	48.4623	8.75	9.36	0.134	48.4602	0.0000	Δ alpha 1	-0.50	0.8 CHCl ₃
5	0.6	0.4	600	360	240	48.4094	19.0450	48.3444	7.50	12.48	0.194	48.2472	0.0000	Δ alpha 2	-0.52	11 DCM
6	0.5	0.5	600	300	300	48.2636	19.0450	48.2166	6.25	15.60	0.265	48.2131	0.0000			
7	0.4	0.6	600	240	360	48.1389	19.0471	48.0718	5.00	18.72	0.351	48.0511	0.0004			
8	0.3	0.7	600	180	420	48.9379	19.0680	47.8499	3.75	21.84	0.457	47.8517	0.0000			
9	0.2	0.8	600	120	480	48.6731	19.0557	47.5974	2.50	24.96	0.591	47.6001	0.0000			
10	0.1	0.9	600	60	540	48.3226	19.0544	47.2482	1.25	28.08	0.765	47.2728	0.0006			
11	0	1	600	0	600	47.9295	19.0790	46.8295	0.00	31.20	1.000	46.8295	0.0000			
			total vol of stock	3300	3300			-1.88				ss residuals	0.0011			

ρ uncorrected			
ρ	48.7124	46.8295	46.6776
conc / M	12.498	31.202	
FW	118.38	84.93	
density	1.492	1.325	
N sites	1	2	

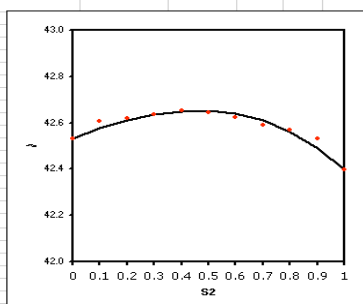
Phosphine Oxide		CHCl ₃	DCM	
FW	218.32	weight / g	0.0104	0.0108
p	97%	weight solvent / g	7.4162	6.9027
		V solvent / mL	4.9706	5.2106
		conc / mM	9.2961	9.2944

External Reference	
Methylenediphosphonic acid	
M _d / ppm	17.96
FW	176.00
weight / g	0.0177
V / mL	2
conc / mM	50.28

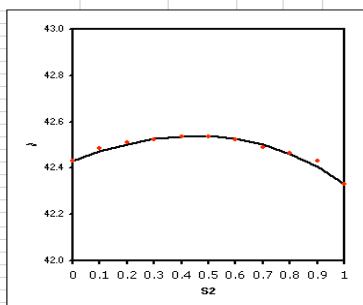
2. Fits to Equation 10.

2.1. Benzene-Carbon tetrachloride

Expt	C6H6		vol total / μ l	CCl4		δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	$\Delta\rho$ / ppm	Kb 2 / M-1	error	
	S1	S2		vol S1 / μ l	vol S2 / μ l								1.6595			1.06E+00
1	1	0	600	600	0	42.9894	18.4468	42.5316	67.14	0.00	0.000	42.5316	0.0000			
2	0.9	0.1	600	540	60	43.0719	18.4456	42.6063	60.42	4.15	0.068	42.5760	0.0009			
3	0.8	0.2	600	480	120	43.0860	18.4462	42.6198	53.71	8.29	0.141	42.6113	0.0001			
4	0.7	0.3	600	420	180	43.1117	18.4538	42.6379	47.00	12.44	0.219	42.6366	0.0000	Δ alpha 0	0.01	0
5	0.6	0.4	600	360	240	43.1196	18.4459	42.6537	40.28	16.58	0.304	42.6506	0.0000	Δ alpha 1	0.02	2.2
6	0.5	0.5	600	300	300	43.1005	19.4470	42.6425	33.57	20.73	0.395	42.6519	0.0001	Δ alpha 2	0.01	0.6
7	0.4	0.6	600	240	360	43.0994	18.4558	42.6236	26.85	24.87	0.495	42.6388	0.0002		a2-a1	0.0
8	0.3	0.7	600	180	420	43.0702	18.4537	42.5905	20.14	29.02	0.604	42.6093	0.0004			
9	0.2	0.8	600	120	480	43.0443	18.4564	42.5679	13.43	33.16	0.723	42.5612	0.0000			
10	0.1	0.9	600	60	540	43.0067	18.4537	42.5330	6.71	37.31	0.855	42.4916	0.0017			
11	0	1	600	0	600	42.9277	18.4507	42.3970	0.00	41.45	1.000	42.3970	0.0000			
			total vol of stock	3300	3300				-0.13				ss residuals	0.0034		
92 uncorrected																
ρ	42.5316	42.3970	40.7375													
conc / M	67.136	41.451														
FW	78.11	153.82														
density	0.874	1.594														
N sites	6	4														
Phosphine Oxide				C6H6	CCl4											
FW	218.32		weight / g	0.0102	0.0113											
p	97%		weight solvent / g	4.3744	8.9384											
			V solvent / mL	5.0050	5.5448											
			conc / mM	3.0546	3.0546											
External Reference																
Methylenediphosphonic acid																
δ / ppm	17.98															
FW	176.00															
weight / g	0.0177															
V / mL	2															
conc / mM	50.28															

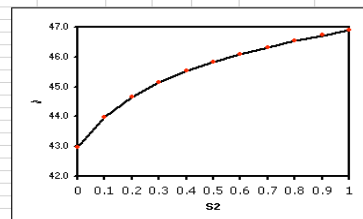


Expt	C6H6		vol total / μ l	CCl4		δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	$\Delta\rho$ / ppm	Kb 2 / M-1	error	
	S1	S2		vol S1 / μ l	vol S2 / μ l								1.9336			1.19E+00
1	1	0	600	600	0	42.8377	18.4467	42.4310	67.14	0.00	0.000	42.4310	0.0000			
2	0.9	0.1	600	540	60	42.9496	18.4461	42.4835	60.42	4.15	0.075	42.4713	0.0001			
3	0.8	0.2	600	480	120	42.9779	18.4463	42.5116	53.71	8.29	0.155	42.5029	0.0001	Δ alpha 0	0.04	0
4	0.7	0.3	600	420	180	42.9931	18.4511	42.5220	47.00	12.44	0.239	42.5251	0.0000	Δ alpha 1	0.05	2.2
5	0.6	0.4	600	360	240	43.0000	19.4445	42.5355	40.28	16.58	0.328	42.5371	0.0000	Δ alpha 2	0.04	0.6
6	0.5	0.5	600	300	300	43.0002	18.4436	42.5368	33.57	20.73	0.423	42.5378	0.0000			
7	0.4	0.6	600	240	360	42.9896	18.4475	42.5221	26.85	24.87	0.524	42.5263	0.0000		a2-a1	0.0
8	0.3	0.7	600	180	420	42.9660	18.4568	42.4992	20.14	29.02	0.631	42.5013	0.0001			
9	0.2	0.8	600	120	480	42.9299	18.4468	42.4633	13.43	33.16	0.746	42.4614	0.0000			
10	0.1	0.9	600	60	540	42.9255	19.4424	42.4291	6.71	37.31	0.863	42.4051	0.0005			
11	0	1	600	0	600	42.8222	18.4716	42.3306	0.00	41.45	1.000	42.3306	0.0000			
			total vol of stock	3300	3300				-0.10				ss residuals	0.0010		
92 uncorrected																
ρ	42.4310	42.3306	40.3970													
conc / M	67.136	41.451														
FW	78.11	153.82														
density	0.874	1.594														
N sites	6	4														
Phosphine Oxide				C6H6	CCl4											
FW	218.32		weight / g	0.0115	0.0119											
p	97%		weight solvent / g	4.3570	8.2227											
			V solvent / mL	4.9051	5.1565											
			conc / mM	10.2494	10.2494											
External Reference																
Methylenediphosphonic acid																
δ / ppm	17.98															
FW	176.00															
weight / g	0.0177															
V / mL	2															
conc / mM	50.28															

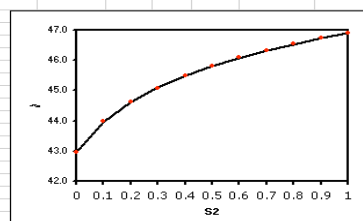


2.2. Benzene-Dichloromethane

Expt	Benzene DCM		vol total / μ l	Benzene DCM		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb 2 / M-1	error
	S1	S2		vol S1 / μ l	vol S2 / μ l											
1	1	0	600	600	0	44.0413	19.0382	42.9831	67.14	0.000	0.000	42.9831	0.0000			
2	0.9	0.1	600	540	60	45.0585	19.0392	43.9923	60.42	3.12	0.295	43.9908	0.0001			
3	0.8	0.2	600	480	120	45.7046	19.0383	44.6463	53.71	6.24	0.485	44.6511	0.0000			
4	0.7	0.3	600	420	180	46.1968	19.0399	45.1369	47.00	9.36	0.618	45.1427	0.0000			
5	0.6	0.4	600	360	240	46.5951	19.0479	45.5272	40.28	12.48	0.715	45.5259	0.0000			
6	0.5	0.5	600	300	300	46.8947	19.0392	45.8295	33.57	15.60	0.790	45.8386	0.0000			
7	0.4	0.6	600	240	360	47.1576	19.0402	46.0976	26.85	18.72	0.850	46.1028	0.0000			
8	0.3	0.7	600	180	420	47.3887	19.0408	46.3279	20.14	21.84	0.898	46.3321	0.0000			
9	0.2	0.8	600	120	480	47.6205	19.0478	46.5527	13.43	24.96	0.938	46.5357	0.0002			
10	0.1	0.9	600	60	540	47.8050	19.0479	46.7371	6.71	28.08	0.971	46.7196	0.0002			
11	0	1	600	0	600	47.9806	19.0725	46.8891	0.00	31.20	1.000	46.8991	0.0000			
			total vol of stock	3300	3300			3.31			ss residuals		0.0008			
<p>ρ 42.9831 46.8881 conc / M 67.136 31.202 FW 78.11 84.93 density 0.874 1.325 N sites 6 2</p> <p>Phosphine Oxide weight / g Benzene 0.0101 DCM 0.0102 FW 218.32 weight solvent / g 4.3818 6.7087 p 97% V solvent / mL 5.0135 5.0631 conc / mM 8.9507 8.9507</p> <p>External Reference Methylenediphosphonic acid M_d / ppm 17.96 FW 176.00 weight / g 0.0177 V / mL 2 conc / mM 50.28</p>																

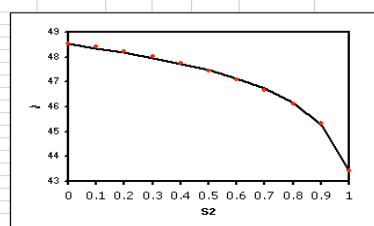


Expt	Benzene DCM		vol total / μ l	Benzene DCM		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb 2 / M-1	error
	S1	S2		vol S1 / μ l	vol S2 / μ l											
1	1	0	600	600	0	44.0111	19.0397	42.9514	67.14	0.000	0.000	42.9514	0.0000			
2	0.9	0.1	600	540	60	45.0576	19.0474	43.9902	60.42	3.12	0.315	43.9840	0.0007			
3	0.8	0.2	600	480	120	45.6970	19.0568	44.6202	53.71	6.24	0.509	44.6280	0.0001			
4	0.7	0.3	600	420	180	46.1669	19.0601	45.0888	47.00	9.36	0.640	45.1133	0.0007			
5	0.6	0.4	600	360	240	46.5841	19.0432	45.5009	40.28	12.48	0.734	45.4939	0.0000			
6	0.5	0.5	600	300	300	46.9707	19.0526	45.7981	33.57	15.60	0.805	45.8063	0.0001			
7	0.4	0.6	600	240	360	47.1513	19.0434	46.0879	26.85	18.72	0.861	46.0781	0.0001			
8	0.3	0.7	600	180	420	47.3974	19.0564	46.3210	20.14	21.84	0.906	46.3165	0.0000			
9	0.2	0.8	600	120	480	47.6161	19.0486	46.5475	13.43	24.96	0.943	46.5318	0.0002			
10	0.1	0.9	600	60	540	47.8007	19.0389	46.7416	6.71	28.08	0.974	46.7299	0.0001			
11	0	1	600	0	600	47.9894	19.0469	46.8145	0.00	31.20	1.000	46.8145	0.0000			
			total vol of stock	3300	3300			3.36			ss residuals		0.0021			
<p>ρ 42.9514 46.8145 conc / M 67.136 31.202 FW 78.11 84.93 density 0.874 1.325 N sites 6 2</p> <p>Phosphine Oxide weight / g Benzene 0.0102 DCM 0.0098 FW 218.32 weight solvent / g 4.3736 6.4354 p 97% V solvent / mL 5.0041 4.8569 conc / mM 9.0563 9.0563</p> <p>External Reference Methylenediphosphonic acid M_d / ppm 17.96 FW 176.00 weight / g 0.0177 V / mL 2 conc / mM 50.28</p>																

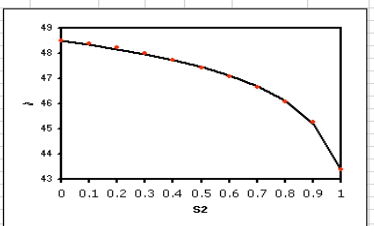


2.3. Chloroform-1,4-Dioxane

Expt	CHCl ₃ 1,4-Dioxane		CHCl ₃ 1,4-Dioxane		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2	vol total / μ l	vol S1 / μ l												vol S2 / μ l
1	1	0	600	600	0	48.9864	18.4467	48.5197	12.50	0.00	0.000	48.5197	0.0000			
2	0.9	0.1	600	540	60	48.9635	18.4443	48.2987	11.25	9.39	0.017	48.3479	0.0028			
3	0.8	0.2	600	480	120	48.7003	18.4433	48.2370	10.00	18.78	0.037	48.1624	0.0056			
4	0.7	0.3	600	420	180	48.4896	18.4497	48.0199	8.75	28.16	0.061	47.9586	0.0038			
5	0.6	0.4	600	360	240	48.2293	18.4450	47.7639	7.50	37.55	0.092	47.7295	0.0012			
6	0.5	0.5	600	300	300	47.9228	18.4464	47.4574	6.25	46.94	0.132	47.4639	0.0000			
7	0.4	0.6	600	240	360	47.5676	18.4542	47.0934	5.00	56.33	0.166	47.1128	0.0024			
8	0.3	0.7	600	180	420	47.1397	18.4569	46.6628	3.75	65.72	0.262	46.7315	0.0047			
9	0.2	0.8	600	120	480	46.5895	18.4464	46.1221	2.50	75.11	0.378	46.1587	0.0013			
10	0.1	0.9	600	60	540	45.8012	18.4475	45.3337	1.25	84.49	0.577	45.2507	0.0063			
11	0	1	600	0	600	43.9391	18.4732	43.4459	0.00	93.88	1.000	43.4459	0.0000			
total vol of stock			3300	3300				-5.07				ss residuals	0.0285			
22 uncorrected																
ρ	48.5197	43.4459	44.4969													
conc / M	12.498	93.893														
FW	119.38	88.11														
density	1.492	1.034														
N sites	1	8														
Phosphine Oxide			CHCl ₃	1,4-Dioxane												
FW	218.32	weight / g	0.0098	0.0197												
p	97%	weight solvent / g	7.3490	8.1593	5.0416											
		V solvent / mL	4.9256	7.8910												
		conc / mM	8.8398	8.8398												
External Reference																
Methylenediphosphonic acid																
M _d / ppm	17.36															
FW	176.00															
weight / g	0.0177															
V / mL	2															
conc / mM	50.28															

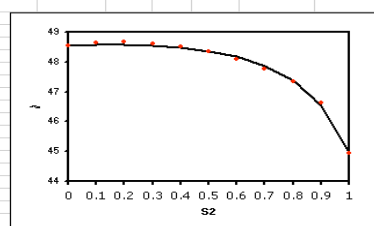


Expt	CHCl ₃ 1,4-Dioxane		CHCl ₃ 1,4-Dioxane		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2	vol total / μ l	vol S1 / μ l												vol S2 / μ l
1	1	0	600	600	0	48.9832	18.4463	48.5169	12.50	0.00	0.000	48.5169	0.0000			
2	0.9	0.1	600	540	60	48.8548	18.4482	48.3868	11.25	9.39	0.016	48.3413	0.0021			
3	0.8	0.2	600	480	120	48.6928	18.4481	48.2247	10.00	18.78	0.036	48.1521	0.0053			
4	0.7	0.3	600	420	180	48.4797	18.4535	48.0062	8.75	28.16	0.060	47.9446	0.0038			
5	0.6	0.4	600	360	240	48.2060	18.4485	47.7375	7.50	37.55	0.091	47.7117	0.0007			
6	0.5	0.5	600	300	300	47.9056	18.4469	47.4367	6.25	46.94	0.131	47.4423	0.0000			
7	0.4	0.6	600	240	360	47.5503	18.4560	47.0743	5.00	56.33	0.184	47.1174	0.0019			
8	0.3	0.7	600	180	420	47.1193	18.4629	46.6364	3.75	65.72	0.259	46.7018	0.0043			
9	0.2	0.8	600	120	480	46.5629	18.4540	46.0888	2.50	75.11	0.375	46.1236	0.0012			
10	0.1	0.9	600	60	540	45.7536	18.4497	45.2839	1.25	84.49	0.575	45.2064	0.0060			
11	0	1	600	0	600	43.8869	18.4729	43.3746	0.00	93.88	1.000	43.3746	0.0000			
total vol of stock			3300	3300				-5.14				ss residuals	0.0282			
22 uncorrected																
ρ	48.5169	43.3746	44.4659													
conc / M	12.498	93.893														
FW	119.38	88.11														
density	1.492	1.034														
N sites	1	8														
Phosphine Oxide			CHCl ₃	1,4-Dioxane												
FW	218.32	weight / g	0.0100	0.0128												
p	97%	weight solvent / g	7.3776	6.5995	4.9403											
		V solvent / mL	4.9447	6.3787												
		conc / mM	8.9854	8.9854												
External Reference																
Methylenediphosphonic acid																
M _d / ppm	17.36															
FW	176.00															
weight / g	0.0177															
V / mL	2															
conc / mM	50.28															

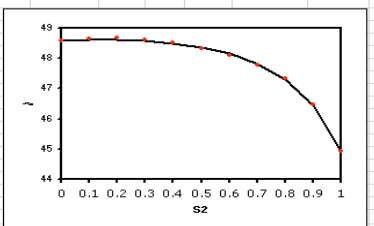


2.4. Chloroform-Acetone

Expt	CHCl ₃ Acetone		CHCl ₃ Acetone		δ _{exp} / ppm	δ _{exp} ref / ppm	δ _{exp} / ppm	[S1]	[S2]	[A-S2]	δ calc	error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2	vol total / μl	vol S1 / μl												vol S2 / μl
1	1	0	600	600	0	49.0029	18.4444	48.5395	12.50	0.000	0.000	48.5395	0.0000			
2	0.9	0.1	600	540	60	49.0544	18.3372	48.5472	11.25	8.17	0.023	48.5639	0.0063			
3	0.8	0.2	600	480	120	49.1352	18.4469	48.6683	10.00	16.34	0.051	48.5676	0.0101			
4	0.7	0.3	600	420	180	49.0876	18.4534	48.6142	8.75	24.51	0.084	48.5430	0.0051			
5	0.6	0.4	600	360	240	48.9794	18.4470	48.5114	7.50	32.69	0.125	48.4804	0.0010			
6	0.5	0.5	600	300	300	48.8042	18.4469	48.3384	6.25	40.86	0.176	48.3649	0.0007			
7	0.4	0.6	600	240	360	48.5730	18.4555	48.1025	5.00	49.03	0.243	48.1730	0.0050			
8	0.3	0.7	600	180	420	48.2622	18.4622	47.7800	3.75	57.20	0.333	47.8644	0.0071			
9	0.2	0.8	600	120	480	47.8053	18.4483	47.3370	2.50	65.37	0.461	47.3652	0.0008			
10	0.1	0.9	600	60	540	47.3096	18.4484	46.6412	1.25	73.54	0.658	46.5214	0.0144			
11	0	1	600	0	600	45.4452	18.4727	44.9525	0.00	81.71	1.000	44.9525	0.0000			
			total vol of stock	3300	3300							ss residuals	0.0511			
			92 uncorrected													
ρ	48.5385	44.9525	43.5393													
conc / M	12.439	81.716														
FW	119.38	58.08														
density	1.492	0.791														
N sites	1	6														
Phosphine Oxide				CHCl ₃	Acetone											
FW	218.32		weight / g	0.0111	0.0119											
p	97%		weight solvent / g	7.4123	4.2129	5.0416										
			V solvent / mL	4.9680	5.3261											
			conc / mM	9.9270	9.9270											
External Reference																
Methylenediphosphonic acid																
M _d / ppm	17.36															
FW	176.00															
weight / g	0.0177															
V / mL	2															
conc / mM	50.28															

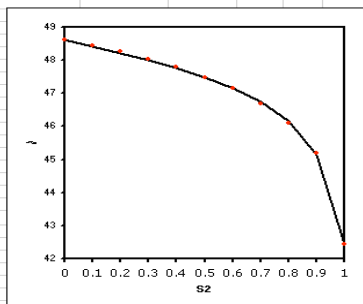


Expt	CHCl ₃ Acetone		CHCl ₃ Acetone		δ _{exp} / ppm	δ _{exp} ref / ppm	δ _{exp} / ppm	[S1]	[S2]	[A-S2]	δ calc	error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2	vol total / μl	vol S1 / μl												vol S2 / μl
1	1	0	600	600	0	49.0411	18.4433	48.5778	12.50	0.000	0.000	48.5778	0.0000			
2	0.9	0.1	600	540	60	49.1207	18.4438	48.6563	11.25	8.17	0.027	48.6049	0.0027			
3	0.8	0.2	600	480	120	49.1435	18.4441	48.6794	10.00	16.34	0.058	48.6068	0.0053			
4	0.7	0.3	600	420	180	49.0830	18.4496	48.6134	8.75	24.51	0.096	48.5762	0.0014			
5	0.6	0.4	600	360	240	48.9714	18.4446	48.5068	7.50	32.69	0.141	48.5024	0.0000			
6	0.5	0.5	600	300	300	48.8023	18.4432	48.3291	6.25	40.86	0.196	48.3639	0.0009			
7	0.4	0.6	600	240	360	48.5725	18.4538	48.0987	5.00	49.03	0.270	48.1544	0.0031			
8	0.3	0.7	600	180	420	48.2532	18.4579	47.7753	3.75	57.20	0.365	47.8162	0.0017			
9	0.2	0.8	600	120	480	47.7947	18.4469	47.3288	2.50	65.37	0.496	47.2854	0.0019			
10	0.1	0.9	600	60	540	46.3193	18.4472	46.4521	1.25	73.54	0.689	46.4269	0.0006			
11	0	1	600	0	600	45.4254	18.4686	44.9398	0.00	81.71	1.000	44.9398	0.0000			
			total vol of stock	3300	3300							ss residuals	0.0178			
			92 uncorrected													
ρ	48.5778	44.9398	43.2492													
conc / M	12.438	81.716														
FW	119.38	58.08														
density	1.492	0.791														
N sites	1	6														
Phosphine Oxide				CHCl ₃	Acetone											
FW	218.32		weight / g	0.0106	0.0108											
p	97%		weight solvent / g	7.3970	3.9956	4.9403										
			V solvent / mL	4.9578	5.0513											
			conc / mM	9.4994	9.4994											
External Reference																
Methylenediphosphonic acid																
M _d / ppm	17.36															
FW	176.00															
weight / g	0.0177															
V / mL	2															
conc / mM	50.28															

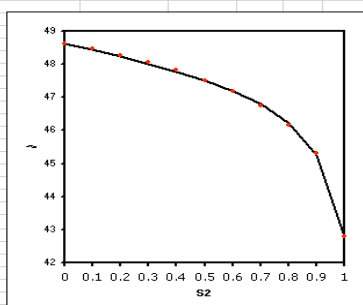


2.5. Chloroform-Benzene

Expt	CHCl ₃ C ₆ H ₆		CHCl ₃ C ₆ H ₆		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2	vol total / μ l	vol S1 / μ l												vol S2 / μ l
1	1	0	600	600	0	48.0787	18.4496	48.6091	12.50	0.00	0.000	48.6091	0.0000			
2	0.9	0.1	600	540	60	48.3939	18.4479	48.4520	11.25	6.71	0.011	48.4639	0.0012			
3	0.8	0.2	600	480	120	48.7336	18.4488	48.2648	10.00	13.43	0.023	48.2137	0.0026	Δ alpha 0	-0.96	0
4	0.7	0.3	600	420	180	48.9196	18.4520	48.0476	8.75	20.14	0.039	47.9953	0.0027	Δ alpha 1	-1.05	0.8 CHCl ₃
5	0.6	0.4	600	360	240	48.2626	18.4455	47.7971	7.50	26.85	0.060	47.7554	0.0017	Δ alpha 2	-1.23	2.2 C ₆ H ₆
6	0.5	0.5	600	300	300	47.8359	18.4484	47.4675	6.25	33.57	0.087	47.4832	0.0002			
7	0.4	0.6	600	240	360	47.6278	18.4565	47.1933	5.00	40.28	0.125	47.1937	0.0001			
8	0.3	0.7	600	180	420	47.1758	18.4674	46.6884	3.75	47.00	0.182	46.7468	0.0034			
9	0.2	0.8	600	120	480	46.5849	18.4557	46.1032	2.50	53.71	0.277	46.1569	0.0023			
10	0.1	0.9	600	60	540	45.6620	18.4514	45.1906	1.25	60.42	0.463	45.1320	0.0034			
11	0	1	600	0	600	42.9344	18.4760	42.4384	0.00	67.14	1.000	42.4384	0.0000			
			total vol of stock	3300	3300							ss residuals	0.0178			
			ρ uncorrected													
			ρ													
			conc / M													
			FW													
			density													
			N sites													
			Phosphine Oxide													
			weight / g													
			weight solvent / g													
			V solvent / mL													
			conc / mM													
			External Reference													
			Methylenediphosphonic acid													
			M _d / ppm													
			FW													
			weight / g													
			V / mL													
			conc / mM													

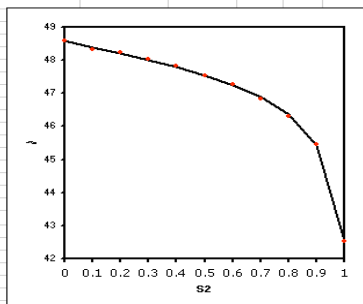


Expt	CHCl ₃ C ₆ H ₆		CHCl ₃ C ₆ H ₆		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb 2 / M-1	error	
	S1	S2	vol total / μ l	vol S1 / μ l												vol S2 / μ l
1	1	0	600	600	0	48.3936	18.4405	48.6211	12.50	0.00	0.000	48.6211	0.0000			
2	0.9	0.1	600	540	60	48.3234	18.4398	48.4895	11.25	6.71	0.011	48.4316	0.0014			
3	0.8	0.2	600	480	120	48.7354	18.4409	48.2745	10.00	13.43	0.025	48.2312	0.0019	Δ alpha 0	-0.95	0
4	0.7	0.3	600	420	180	48.5217	18.4496	48.0521	8.75	20.14	0.041	48.0162	0.0013	Δ alpha 1	-1.03	0.8 CHCl ₃
5	0.6	0.4	600	360	240	48.2784	18.4407	47.8177	7.50	26.85	0.063	47.7802	0.0014	Δ alpha 2	-1.21	2.2 C ₆ H ₆
6	0.5	0.5	600	300	300	47.9829	18.4429	47.5206	6.25	33.57	0.092	47.5100	0.0001			
7	0.4	0.6	600	240	360	47.5099	18.3112	47.1787	5.00	40.28	0.132	47.1964	0.0003			
8	0.3	0.7	600	180	420	47.2159	18.4528	46.7431	3.75	47.00	0.191	46.7943	0.0026			
9	0.2	0.8	600	120	480	46.6380	18.4465	46.1715	2.50	53.71	0.288	46.2247	0.0028			
10	0.1	0.9	600	60	540	45.7744	18.4430	45.3114	1.25	60.42	0.476	45.2509	0.0037			
11	0	1	600	0	600	43.2811	18.4671	42.7940	0.00	67.14	1.000	42.7940	0.0000			
			total vol of stock	3300	3300							ss residuals	0.0155			
			ρ uncorrected													
			ρ													
			conc / M													
			FW													
			density													
			N sites													
			Phosphine Oxide													
			weight / g													
			weight solvent / g													
			V solvent / mL													
			conc / mM													
			External Reference													
			Methylenediphosphonic acid													
			M _d / ppm													
			FW													
			weight / g													
			V / mL													
			conc / mM													

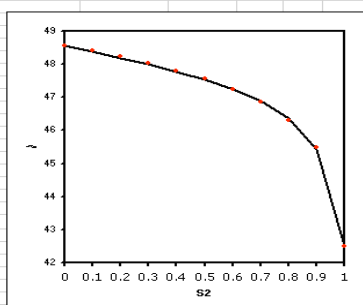


2.6. Chloroform-Carbon tetrachloride

Expt	CHCl3		CCl4		vol total / μ l	vol S1 / μ l	vol S2 / μ l	δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb2 / M-1	error
	S1	S2	S1	S2														
1	1	0	600	0	600	600	0	43.0376	18.4422	43.5754	12.50	0.00	0.000	43.5754	0.0000			
2	0.9	0.1	600	540	600	540	60	43.7339	18.4449	43.2291	11.25	4.15	0.008	43.2949	0.0043			
3	0.8	0.2	600	480	600	480	120	48.6996	18.4439	48.2397	10.00	8.29	0.019	48.2055	0.0009	Δ alpha 0	-0.90	0
4	0.7	0.3	600	420	600	420	180	48.5000	18.4488	48.0312	8.75	12.44	0.032	48.0040	0.0007	Δ alpha 1	-0.98	0.8 CHCl3
5	0.6	0.4	600	360	600	360	240	48.2873	18.4390	47.8283	7.50	16.58	0.048	47.7849	0.0019	Δ alpha 2	-0.96	0.6 CCl4
6	0.5	0.5	600	300	600	300	300	48.0129	18.4426	47.5902	6.25	20.73	0.071	47.5293	0.0001			
7	0.4	0.6	600	240	600	240	360	47.7341	18.4509	47.2832	5.00	24.87	0.103	47.2596	0.0002	a2-a1	-1.0	
8	0.3	0.7	600	180	600	180	420	47.3124	18.4566	46.8368	3.75	29.02	0.151	46.8951	0.0023			
9	0.2	0.8	600	120	600	120	480	46.7817	18.4476	46.3141	2.50	33.16	0.234	46.3612	0.0022			
10	0.1	0.9	600	60	600	60	540	45.9219	18.4422	45.4597	1.25	37.31	0.407	45.4186	0.0017			
11	0	1	600	0	600	0	600	43.0227	18.4673	42.5354	0.00	41.45	1.000	42.5354	0.0000			
total vol of stock						3300	3300			-6.04				ss residuals	0.0144			
ρ 2 uncorrected																		
ρ	43.5754	42.5354			43.9525													
conc / M	12.499	41.451																
FW	119.38	153.82																
density	1.492	1.534																
N sites	1	4																
Phosphine Oxide																		
			CHCl3	CCl4														
weight / g			0.0101	0.0113														
FW	218.32		7.3791	8.8202														
p	97%		4.9458	5.5334														
			9.0733	9.0733														
External Reference																		
Methylenediphosphonic acid																		
δ / ppm	17.98																	
FW	176.00																	
weight / g	0.0177																	
V / mL	2																	
conc / mM	50.28																	

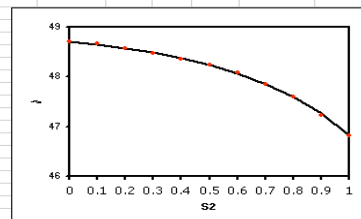


Expt	CHCl3		CCl4		vol total / μ l	vol S1 / μ l	vol S2 / μ l	δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb2 / M-1	error
	S1	S2	S1	S2														
1	1	0	600	0	600	600	0	43.0296	18.4622	43.5474	12.50	0.00	0.000	43.5474	0.0000			
2	0.9	0.1	600	540	600	540	60	48.8636	18.4449	48.4047	11.25	4.15	0.008	48.2722	0.0011			
3	0.8	0.2	600	480	600	480	120	48.6984	18.4486	48.2298	10.00	8.29	0.018	48.1883	0.0017	Δ alpha 0	-0.91	0
4	0.7	0.3	600	420	600	420	180	48.5007	18.4578	48.0229	8.75	12.44	0.031	47.9322	0.0009	Δ alpha 1	-0.99	0.8 CHCl3
5	0.6	0.4	600	360	600	360	240	48.2786	18.4500	47.8096	7.50	16.58	0.047	47.7786	0.0009	Δ alpha 2	-0.96	0.6 CCl4
6	0.5	0.5	600	300	600	300	300	48.0211	18.4421	47.5590	6.25	20.73	0.069	47.5395	0.0004			
7	0.4	0.6	600	240	600	240	360	47.7137	18.4435	47.2502	5.00	24.87	0.101	47.2554	0.0000	a2-a1	-1.0	
8	0.3	0.7	600	180	600	180	420	47.3188	18.4515	46.8473	3.75	29.02	0.148	46.8952	0.0023			
9	0.2	0.8	600	120	600	120	480	46.8931	18.5621	46.3110	2.50	33.16	0.230	46.3756	0.0042			
10	0.1	0.9	600	60	600	60	540	45.9498	18.4424	45.4874	1.25	37.31	0.402	45.4319	0.0031			
11	0	1	600	0	600	0	600	42.9470	18.4424	42.4946	0.00	41.45	1.000	42.4946	0.0000			
total vol of stock						3300	3300			-8.06				ss residuals	0.0148			
ρ 2 uncorrected																		
ρ	43.5474	42.4946			43.9505													
conc / M	12.498	41.451																
FW	119.38	153.82																
density	1.492	1.534																
N sites	1	4																
Phosphine Oxide																		
			CHCl3	CCl4														
weight / g			0.0103	0.0096														
FW	218.32		7.3000	7.1933														
p	97%		4.8328	4.5127														
			9.3532	9.3532														
External Reference																		
Methylenediphosphonic acid																		
δ / ppm	17.98																	
FW	176.00																	
weight / g	0.0177																	
V / mL	2																	
conc / mM	50.28																	

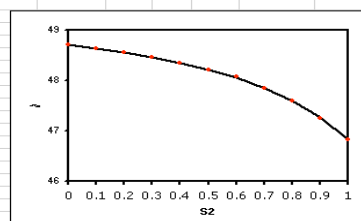


2.7. Chloroform-Dichloromethane

Expt	CHCl3		DCM		CHCl3		DCM		δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJmol	Kb2 / M-1	error		
	S1	S2	vol total / μ l	vol S1 / μ l	vol S2 / μ l	vol S1 / μ l	vol S2 / μ l	0.5404												1.77E-01	0.0116
1	1	0	600	600	0	43.7707	19.0399	48.7108	12.50	0.000	0.000	48.7108	0.0000								
2	0.9	0.1	600	540	60	43.7264	19.0375	48.6526	11.25	3.12	0.047	48.6511	0.0003								
3	0.8	0.2	600	480	120	43.6353	19.0386	48.5767	10.00	6.24	0.100	48.5772	0.0000								
4	0.7	0.3	600	420	180	43.5431	19.0413	48.4818	8.75	9.36	0.159	48.4861	0.0000								
5	0.6	0.4	600	360	240	43.4130	19.0392	48.3538	7.50	12.48	0.228	48.3742	0.0004								
6	0.5	0.5	600	300	300	43.2889	19.0376	48.2414	6.25	15.60	0.307	48.2366	0.0000								
7	0.4	0.6	600	240	360	43.1386	19.0397	48.0789	5.00	18.72	0.389	48.0669	0.0001								
8	0.3	0.7	600	180	420	43.0360	19.0603	47.9557	3.75	21.84	0.508	47.8562	0.0000								
9	0.2	0.8	600	120	480	43.8745	19.0496	47.6049	2.50	24.96	0.639	47.5323	0.0002								
10	0.1	0.9	600	60	540	43.3044	19.0476	47.2368	1.25	28.08	0.799	47.2571	0.0004								
11	0	1	600	0	600	47.9189	19.0751	46.8238	0.00	31.20	1.000	46.8238	0.0000								
			total vol of stock		3300	3300			-1.88			ss residuals		0.0015							
ρ uncorrected																					
ρ	48.7108	46.8238			46.2834																
conc / M	12.498	31.202																			
FW	118.38	84.93																			
density	1.492	1.325																			
N sites	1	2																			
Phosphine Oxide			CHCl3		DCM																
FW	218.32	weight / g	0.0100	0.0110																	
p	97%	weight solvent / g	7.4264	7.2547	7.2533																
		V solvent / mL	4.9775	5.4752	5.4742																
		conc / mM	8.9262	8.9262	8.9279																
External Reference																					
Methylenediphosphonic acid																					
δ / ppm	17.98																				
FW	176.00																				
weight / g	0.0177																				
V / mL	2																				
conc / mM	50.28																				

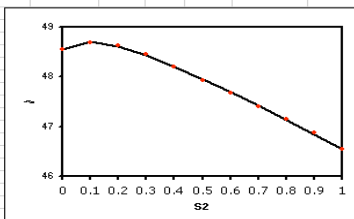


Expt	CHCl3		DCM		CHCl3		DCM		δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJmol	Kb2 / M-1	error		
	S1	S2	vol total / μ l	vol S1 / μ l	vol S2 / μ l	vol S1 / μ l	vol S2 / μ l	0.1519												1.56E-01	0.0089
1	1	0	600	600	0	43.7767	19.0443	48.7124	12.50	0.000	0.000	48.7124	0.0000								
2	0.9	0.1	600	540	60	43.7001	19.0446	48.6355	11.25	3.12	0.042	48.6431	0.0001								
3	0.8	0.2	600	480	120	43.6225	19.0449	48.5576	10.00	6.24	0.089	48.5620	0.0000								
4	0.7	0.3	600	420	180	43.5310	19.0487	48.4623	8.75	9.36	0.143	48.4666	0.0000								
5	0.6	0.4	600	360	240	43.4094	19.0450	48.3444	7.50	12.48	0.206	48.3533	0.0001								
6	0.5	0.5	600	300	300	43.2636	19.0450	48.2166	6.25	15.60	0.291	48.2175	0.0000								
7	0.4	0.6	600	240	360	43.1389	19.0471	48.0718	5.00	18.72	0.369	48.0526	0.0004								
8	0.3	0.7	600	180	420	43.0379	19.0680	47.8499	3.75	21.84	0.476	47.8493	0.0000								
9	0.2	0.8	600	120	480	43.8731	19.0557	47.5974	2.50	24.96	0.609	47.5940	0.0000								
10	0.1	0.9	600	60	540	43.3226	19.0544	47.2482	1.25	28.08	0.778	47.2695	0.0003								
11	0	1	600	0	600	47.9295	19.0790	46.8295	0.00	31.20	1.000	46.8295	0.0000								
			total vol of stock		3300	3300			-1.88			ss residuals		0.0009							
ρ uncorrected																					
ρ	48.7124	46.8295			46.6776																
conc / M	12.498	31.202																			
FW	118.38	84.93																			
density	1.492	1.325																			
N sites	1	2																			
Phosphine Oxide			CHCl3		DCM																
FW	218.32	weight / g	0.0104	0.0108																	
p	97%	weight solvent / g	7.4162	6.9027	6.904																
		V solvent / mL	4.9706	5.2096	5.2106																
		conc / mM	9.2961	9.2961	9.2944																
External Reference																					
Methylenediphosphonic acid																					
δ / ppm	17.96																				
FW	176.00																				
weight / g	0.0177																				
V / mL	2																				
conc / mM	50.28																				

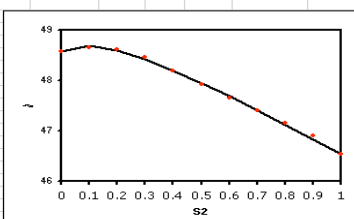


2.8. Chloroform-DMSO

Expt	CHCl3		DMSO		CHCl3		DMSO		δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb2 / M-1	error
	S1	S2	vol total / μ l	vol S1 / μ l	vol S2 / μ l	vol S1 / μ l	vol S2 / μ l	3.02E-01											
1	1	0	600	600	0	49.0295	18.4446	48.5609	12.50	0.00	0.000	48.5609	0.0000						
2	0.9	0.1	600	540	60	49.1473	18.4450	48.6523	11.25	8.45	0.404	48.7013	0.0004						
3	0.8	0.2	600	480	120	49.0931	18.4437	48.6294	10.00	16.89	0.604	48.6122	0.0003						
4	0.7	0.3	600	420	180	48.9284	18.4534	48.4950	8.75	25.34	0.723	48.4323	0.0005						
5	0.6	0.4	600	360	240	48.6666	18.4429	48.2037	7.50	33.79	0.802	48.2073	0.0000						
6	0.5	0.5	600	300	300	48.3977	18.4430	47.9347	6.25	42.24	0.899	47.9966	0.0005						
7	0.4	0.6	600	240	360	48.1390	18.4500	47.6890	5.00	50.68	0.901	47.6999	0.0005						
8	0.3	0.7	600	180	420	47.8919	18.4564	47.4055	3.75	59.13	0.934	47.4126	0.0001						
9	0.2	0.8	600	120	480	47.6165	18.4485	47.1480	2.50	67.58	0.961	47.1278	0.0004						
10	0.1	0.9	600	60	540	47.3513	18.4500	46.8813	1.25	76.03	0.982	46.8376	0.0019						
11	0	1	600	0	600	47.0356	18.4722	46.5434	0.00	84.47	1.000	46.5434	0.0000						
			total vol of stock			3300	3300				-2.02	ss residuals		0.0045					
ρ uncorrected																			
ρ	48.5609	46.5434			49.6875														
conc / M	12.498	84.475																	
FW	119.38	78.13																	
density	1.492	1.1																	
N sites	1	8																	
			CHCl3		DMSO														
FW	218.32	weight / g	0.0105	0.0097															
p	97%	weight solvent / g	7.4294	5.0601															
		V solvent / mL	4.9795	4.6001															
		conc / mM	9.3688	9.3688															
External Reference																			
Methylenediphosphonic acid																			
δ / ppm	17.98																		
FW	176.00																		
weight / g	0.0177																		
V / mL	2																		
conc / mM	50.28																		

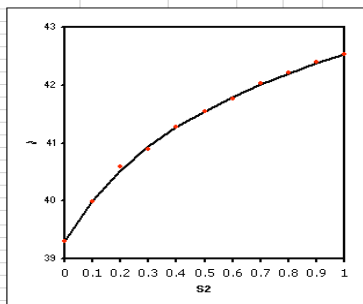


Expt	CHCl3		DMSO		CHCl3		DMSO		δ_{exp} / ppm	δ_{ref} / ppm	δ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb2 / M-1	error
	S1	S2	vol total / μ l	vol S1 / μ l	vol S2 / μ l	vol S1 / μ l	vol S2 / μ l	3.29E-01											
1	1	0	600	600	0	49.0492	18.4525	48.5727	12.50	0.00	0.000	48.5727	0.0000						
2	0.9	0.1	600	540	60	49.1218	18.4550	48.6630	11.25	8.45	0.384	48.6901	0.0007						
3	0.8	0.2	600	480	120	49.1218	18.4621	48.6197	10.00	16.89	0.584	48.5996	0.0004						
4	0.7	0.3	600	420	180	48.9437	18.4630	48.4607	8.75	25.34	0.706	48.4218	0.0015						
5	0.6	0.4	600	360	240	48.6669	18.4572	48.1937	7.50	33.79	0.789	48.1991	0.0001						
6	0.5	0.5	600	300	300	48.3959	18.4545	47.9213	6.25	42.24	0.849	47.9504	0.0008						
7	0.4	0.6	600	240	360	48.1398	18.4637	47.6561	5.00	50.68	0.894	47.6952	0.0008						
8	0.3	0.7	600	180	420	47.8861	18.4671	47.3990	3.75	59.13	0.929	47.4089	0.0001						
9	0.2	0.8	600	120	480	47.6234	18.4572	47.1462	2.50	67.58	0.957	47.1247	0.0005						
10	0.1	0.9	600	60	540	47.3636	18.4420	46.9016	1.25	76.03	0.981	46.8348	0.0045						
11	0	1	600	0	600	47.0432	18.4626	46.5406	0.00	84.47	1.000	46.5406	0.0000						
			total vol of stock			3300	3300				-2.03	ss residuals		0.0095					
ρ uncorrected																			
ρ	48.5727	46.5406			49.7022														
conc / M	12.498	84.475																	
FW	119.38	78.13																	
density	1.492	1.1																	
N sites	1	8																	
			CHCl3		DMSO														
FW	218.32	weight / g	0.0124	0.0110															
p	97%	weight solvent / g	7.3683	4.8191															
		V solvent / mL	4.9385	4.3910															
		conc / mM	11.658	11.658															
External Reference																			
Methylenediphosphonic acid																			
δ / ppm	17.98																		
FW	176.00																		
weight / g	0.0177																		
V / mL	2																		
conc / mM	50.28																		

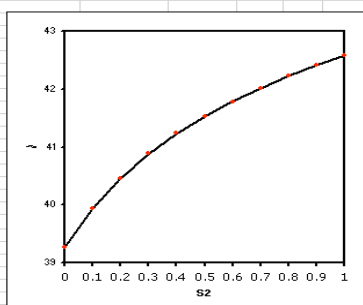


2.9. Cyclohexane-Benzene

												$\Delta\rho$ / ppm	Kb2 / M-1	error																																	
												0.6573	4.88E+00	0.0272																																	
Expt	C6H12	Benzene	vol total / μ l	C6H12	Benzene	vol S1 / μ l	vol S2 / μ l	ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	beta																														
1	1	0	600	600	0	600	0	39.7670	18.4470	39.3000	11.07	0.00	0.000	39.3000	0.0000																																
2	0.9	0.1	600	540	60	40.4474	19.4473	39.3601	39.37	6.71	0.247	40.005	0.0005																																		
3	0.8	0.2	600	480	120	41.0510	18.4460	40.5950	88.86	13.43	0.425	40.5245	0.0037			Δ alpha 0	0.38																														
4	0.7	0.3	600	420	180	41.3684	18.4532	40.8952	77.75	20.14	0.558	40.9350	0.0016			Δ alpha 1	0.39																														
5	0.6	0.4	600	360	240	41.7374	18.4493	41.2681	66.84	26.85	0.663	41.2699	0.0000			Δ alpha 2	0.48																														
6	0.5	0.5	600	300	300	42.0140	18.4476	41.5464	55.54	33.57	0.747	41.5016	0.0000				0.3																														
7	0.4	0.6	600	240	360	42.2369	18.4501	41.7858	44.43	40.29	0.836	41.7945	0.0008				2.2																														
8	0.3	0.7	600	180	420	42.5074	18.4577	42.0297	33.32	47.00	0.873	42.0082	0.0005			a2-a1	0.4																														
9	0.2	0.8	600	120	480	42.8322	18.4535	42.2187	22.21	53.71	0.922	42.1994	0.0004																																		
10	0.1	0.9	600	60	540	42.8677	18.4478	42.3999	11.11	60.42	0.964	42.3728	0.0007																																		
11	0	1	600	0	600	43.0186	18.4667	42.5319	0.00	67.14	1.000	42.5319	0.0000																																		
total vol of stock				3300	3300					3.23			ss residuals		0.0081																																
<table border="1"> <thead> <tr> <th colspan="3"></th> <th colspan="2">ρ2 uncorrected</th> </tr> </thead> <tbody> <tr> <td>ρ</td> <td>39.3000</td> <td>42.5319</td> <td colspan="2">41.8746</td> </tr> <tr> <td>conc / M</td> <td>11.074</td> <td>67.136</td> <td colspan="2"></td> </tr> <tr> <td>FW</td> <td>84.16</td> <td>78.11</td> <td colspan="2"></td> </tr> <tr> <td>density</td> <td>0.779</td> <td>0.874</td> <td colspan="2"></td> </tr> <tr> <td>N sites</td> <td>12</td> <td>6</td> <td colspan="2"></td> </tr> </tbody> </table>																					ρ 2 uncorrected		ρ	39.3000	42.5319	41.8746		conc / M	11.074	67.136			FW	84.16	78.11			density	0.779	0.874			N sites	12	6		
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		C6H12	Benzene																																												
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												$\Delta\rho$ / ppm	Kb2 / M-1	error																																	
												0.6301	4.35E+00	0.0052																																	
Expt	C6H12	Benzene	vol total / μ l	C6H12	Benzene	vol S1 / μ l	vol S2 / μ l	ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	beta																														
1	1	0	600	600	0	600	0	39.5675	18.2762	39.2713	11.07	0.00	0.000	39.2713	0.0000																																
2	0.9	0.1	600	540	60	40.4108	18.4523	39.9385	99.97	6.71	0.226	39.9405	0.0000																																		
3	0.8	0.2	600	480	120	40.9251	18.4527	40.4524	88.86	13.43	0.397	40.4609	0.0001			Δ alpha 0	0.35																														
4	0.7	0.3	600	420	180	41.3678	18.4570	40.8908	77.75	20.14	0.530	40.8811	0.0001			Δ alpha 1	0.36																														
5	0.6	0.4	600	360	240	41.7124	18.4556	41.2368	66.84	26.85	0.637	41.2310	0.0000			Δ alpha 2	0.45																														
6	0.5	0.5	600	300	300	42.0064	18.4581	41.5293	55.54	33.57	0.724	41.5293	0.0000				0.3																														
7	0.4	0.6	600	240	360	42.2642	18.4585	41.7857	44.43	40.28	0.798	41.7889	0.0000				2.2																														
8	0.3	0.7	600	180	420	42.4130	18.3823	42.0107	33.32	47.00	0.860	42.0185	0.0001			a2-a1	0.4																														
9	0.2	0.8	600	120	480	42.7058	18.4599	42.2259	22.21	53.71	0.913	42.2246	0.0000																																		
10	0.1	0.9	600	60	540	42.8526	18.4561	42.4185	11.11	60.42	0.959	42.4118	0.0000																																		
11	0	1	600	0	600	43.0839	18.4603	42.5639	0.00	67.14	1.000	42.5636	0.0000																																		
total vol of stock				3300	3300					3.31			ss residuals		0.0003																																
<table border="1"> <thead> <tr> <th colspan="3"></th> <th colspan="2">ρ2 uncorrected</th> </tr> </thead> <tbody> <tr> <td>ρ</td> <td>39.2713</td> <td>42.5319</td> <td colspan="2">41.9536</td> </tr> <tr> <td>conc / M</td> <td>11.074</td> <td>67.136</td> <td colspan="2"></td> </tr> <tr> <td>FW</td> <td>84.16</td> <td>78.11</td> <td colspan="2"></td> </tr> <tr> <td>density</td> <td>0.779</td> <td>0.874</td> <td colspan="2"></td> </tr> <tr> <td>N sites</td> <td>12</td> <td>6</td> <td colspan="2"></td> </tr> </tbody> </table>																					ρ 2 uncorrected		ρ	39.2713	42.5319	41.9536		conc / M	11.074	67.136			FW	84.16	78.11			density	0.779	0.874			N sites	12	6		
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		C6H12	Benzene																																												
Phosphine Oxide	weight / g	0.0119	0.0112																																												
FW	218.32	3.8680	4.0844																																												
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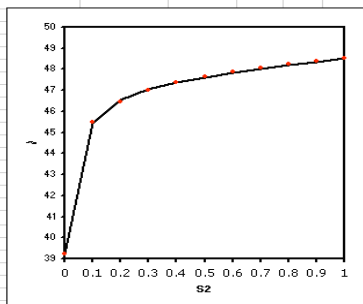
2.10. Cyclohexane-Carbon tetrachloride

Expt	C6H12		CCl4		vol total / μ l	C6H12		CCl4		δ_{exp} / ppm	δ_{ref} / ppm	δ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb2 / M-1	error	
	S1	S2	vol S1 / μ l	vol S2 / μ l		δ_{exp} / ppm	δ_{ref} / ppm	δ_{exp} / ppm	[S1]												[S2]
1	1	0	600	600	0	39.9366	18.4441	39.4725	111.07	0.00	0.000	39.4725	0.0000								
2	0.9	0.1	600	540	60	40.8427	18.4452	40.1785	99.97	4.15	0.237	40.1723	0.0000								
3	0.8	0.2	600	480	120	41.1272	18.4482	40.6590	88.86	8.29	0.487	40.6641	0.0000								
4	0.7	0.3	600	420	180	41.5051	18.4483	41.0368	77.75	12.44	0.620	41.0429	0.0000								
5	0.6	0.4	600	360	240	41.8260	18.4517	41.3543	66.84	16.58	0.717	41.3534	0.0000								
6	0.5	0.5	600	300	300	42.1066	18.4505	41.8351	55.54	20.73	0.792	41.8195	0.0002								
7	0.4	0.6	600	240	360	42.3416	18.4745	41.9471	44.43	24.57	0.851	41.9552	0.0001								
8	0.3	0.7	600	180	420	42.5682	18.4524	42.0958	33.32	29.02	0.899	42.0691	0.0007								
9	0.2	0.8	600	120	480	42.7090	18.4659	42.2231	22.21	33.16	0.938	42.2668	0.0019								
10	0.1	0.9	600	60	540	42.9372	18.4575	42.4597	11.11	37.31	0.972	42.4523	0.0001								
11	0	1	600	0	600	43.0981	18.4500	42.6201	0.00	41.45	1.000	42.6201	0.0000								
total vol of stock						3300	3300														
ρ 2 uncorrected																					
ρ 39.4725 42.6281 41.4243																					
conc / M 111.074 41.451																					
FW 84.16 153.82																					
density 0.779 1.534																					
N sites 12 4																					
Phosphine Oxide																					
weight / g C6H12 CCl4																					
FW 218.32 0.0111 0.0111																					
p 97% weight solvent / g 3.8740 7.9270 8.2222																					
V solvent / mL 4.9730 4.9730																					
conc / mM 9.9170 9.9170 9.561																					
External Reference																					
Methylenediphosphonic acid																					
M _d / ppm 17.98																					
FW 176.00																					
weight / g 0.0177																					
V / mL 2																					
conc / mM 50.28																					

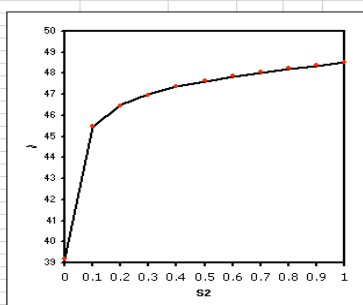
Expt	C6H12		CCl4		vol total / μ l	C6H12		CCl4		δ_{exp} / ppm	δ_{ref} / ppm	δ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	ρ error	ΔG / kJ/mol	Kb2 / M-1	error	
	S1	S2	vol S1 / μ l	vol S2 / μ l		δ_{exp} / ppm	δ_{ref} / ppm	δ_{exp} / ppm	[S1]												[S2]
1	1	0	600	600	0	39.9366	18.4478	39.5276	111.07	0.00	0.000	39.5276	0.0000								
2	0.9	0.1	600	540	60	40.6163	18.4482	40.1481	99.97	4.15	0.211	40.1063	0.0017								
3	0.8	0.2	600	480	120	41.0374	18.4511	40.5863	88.86	8.29	0.375	40.5647	0.0009								
4	0.7	0.3	600	420	180	41.3867	18.4582	40.9085	77.75	12.44	0.507	40.9384	0.0009								
5	0.6	0.4	600	360	240	41.7200	18.4508	41.2432	66.84	16.58	0.615	41.2501	0.0000								
6	0.5	0.5	600	300	300	41.9691	18.4524	41.4957	55.54	20.73	0.706	41.9562	0.0004								
7	0.4	0.6	600	240	360	42.2183	18.4540	41.7443	44.43	24.57	0.783	41.7443	0.0000								
8	0.3	0.7	600	180	420	42.4366	18.4637	41.9529	33.32	29.02	0.849	41.9451	0.0001								
9	0.2	0.8	600	120	480	42.6218	18.4569	42.1449	22.21	33.16	0.906	42.1232	0.0005								
10	0.1	0.9	600	60	540	42.7903	18.4510	42.2192	11.11	37.31	0.956	42.2627	0.0013								
11	0	1	600	0	600	42.9273	18.4603	42.4270	0.00	41.45	1.000	42.4270	0.0000								
total vol of stock						3300	3300														
ρ 2 uncorrected																					
ρ 39.5276 42.4270 42.1399																					
conc / M 111.074 41.451																					
FW 84.16 153.82																					
density 0.779 1.534																					
N sites 12 4																					
Phosphine Oxide																					
weight / g C6H12 CCl4																					
FW 218.32 0.0111 0.0117																					
p 97% weight solvent / g 3.8740 8.3555 8.2222																					
V solvent / mL 4.9730 5.2419																					
conc / mM 9.9170 9.9170 9.561																					
External Reference																					
Methylenediphosphonic acid																					
M _d / ppm 17.98																					
FW 176.00																					
weight / g 0.0177																					
V / mL 2																					
conc / mM 50.28																					

2.11. Cyclohexane-Chloroform

Expt	C6H12		CHCl3		vol total / μ l	C6H12		CHCl3		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb2 / M-1	error	
	S1	S2	vol S1 / μ l	vol S2 / μ l		vol S1 / μ l	vol S2 / μ l	1.2021	2.50E-02												0.0382
1	1	0	600	0	600	0	39.6722	18.4441	39.2081	11.07	0.00	0.000	39.2081	0.0000							
2	0.9	0.1	600	60	660	540	45.3679	18.4424	45.5045	39.37	1.25	0.758	45.4608	0.0019							
3	0.8	0.2	600	120	720	480	46.9377	18.4453	46.4724	88.86	2.50	0.876	46.5353	0.0040							
4	0.7	0.3	600	180	780	420	47.4643	18.4525	46.9918	77.75	3.75	0.923	47.0432	0.0026							
5	0.6	0.4	600	240	840	360	47.8333	18.4468	47.3665	66.84	5.00	0.949	47.3736	0.0001							
6	0.5	0.5	600	300	900	300	48.0244	18.3543	47.6501	55.54	6.25	0.966	47.6257	0.0006							
7	0.4	0.6	600	240	840	360	48.3447	18.4520	47.8727	44.43	7.50	0.977	47.8364	0.0013							
8	0.3	0.7	600	180	780	420	48.5406	18.4568	48.0638	33.32	8.75	0.985	48.0225	0.0017							
9	0.2	0.8	600	120	720	480	48.7109	18.4507	48.2402	22.21	10.00	0.991	48.1929	0.0022							
10	0.1	0.9	600	60	660	540	48.8576	18.4450	48.3926	11.11	11.25	0.996	48.2525	0.0016							
11	0	1	600	0	600	0	49.0095	18.4769	48.5046	0.00	12.50	1.000	48.5046	0.0000							
total vol of stock						3300	3300					3.30			ss residuals	0.0160					
ρ uncorrected																					
ρ	39.2081	48.5046			47.3025																
conc / M	11.074	12.438																			
FW	84.16	119.38																			
density	0.779	1.492																			
N sites	12	1																			
Phosphine Oxide																					
						C6H12	CHCl3														
FW	218.32		weight / g			0.0119	0.0109														
p	97%		weight solvent / g			3.8685	6.7866														
			V solvent / mL			4.9680	4.5487														
			conc / mM			10.6468	10.6468														
External Reference																					
Methylenediphosphonic acid																					
ρ / ppm	17.98																				
FW	176.00																				
weight / g	0.0177																				
V / mL	2																				
conc / mM	50.28																				

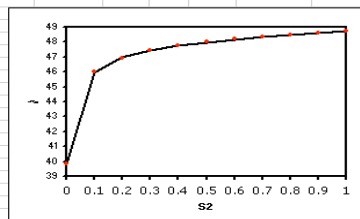


Expt	C6H12		CHCl3		vol total / μ l	C6H12		CHCl3		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{exp} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb2 / M-1	error	
	S1	S2	vol S1 / μ l	vol S2 / μ l		vol S1 / μ l	vol S2 / μ l	1.2421	2.51E-02												0.0401
1	1	0	600	0	600	0	39.6331	18.4459	39.1652	11.07	0.00	0.000	39.1652	0.0000							
2	0.9	0.1	600	60	660	540	45.9542	18.4488	45.4854	39.37	1.25	0.758	45.4331	0.0027							
3	0.8	0.2	600	120	720	480	46.9087	18.4465	46.4422	88.86	2.50	0.876	46.5100	0.0046							
4	0.7	0.3	600	180	780	420	47.4526	18.4526	46.9800	77.75	3.75	0.924	47.0210	0.0017							
5	0.6	0.4	600	240	840	360	47.8304	18.4465	47.3639	66.84	5.00	0.950	47.3548	0.0001							
6	0.5	0.5	600	300	900	300	48.1076	18.4466	47.6390	55.54	6.25	0.966	47.6106	0.0006							
7	0.4	0.6	600	240	840	360	48.3430	18.4562	47.8668	44.43	7.50	0.977	47.8250	0.0017							
8	0.3	0.7	600	180	780	420	48.5362	18.4591	48.0571	33.32	8.75	0.985	48.0149	0.0018							
9	0.2	0.8	600	120	720	480	48.7103	18.4501	48.2402	22.21	10.00	0.991	48.1891	0.0026							
10	0.1	0.9	600	60	660	540	48.8609	18.4473	48.3936	11.11	11.25	0.996	48.2526	0.0017							
11	0	1	600	0	600	0	49.0036	18.4750	48.5026	0.00	12.50	1.000	48.5026	0.0000							
total vol of stock						3300	3300					3.34			ss residuals	0.0177					
ρ uncorrected																					
ρ	39.1652	48.5046			47.2665																
conc / M	11.074	12.438																			
FW	84.16	119.38																			
density	0.779	1.492																			
N sites	12	1																			
Phosphine Oxide																					
						C6H12	CHCl3														
FW	218.32		weight / g			0.0124	0.0102														
p	97%		weight solvent / g			3.8752	6.1053														
			V solvent / mL			4.9746	4.0520														
			conc / mM			11.0750	11.0750														
External Reference																					
Methylenediphosphonic acid																					
ρ / ppm	17.98																				
FW	176.00																				
weight / g	0.0177																				
V / mL	2																				
conc / mM	50.28																				

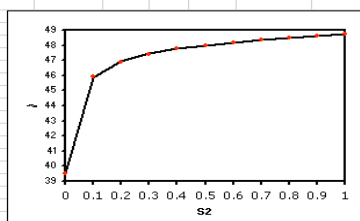


2.12. Dodecane-Chloroform

Expt	Dodecane		CHCl ₃		vol total / μ l	Dodecane		CHCl ₃		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb2 / M-1	error	
	S1	S2	vol S1 / μ l	vol S2 / μ l		vol S1 / μ l	vol S2 / μ l	ρ_{exp} / ppm	ρ_{ref} / ppm												ρ_{calc} / ppm
1	1	0	600	0	600	0	40.8946	19.0383	39.8363	114.48	0.000	0.000	39.8363	0.0000							
2	0.9	0.1	600	60	660	60	47.0412	19.0372	45.9040	103.04	1.25	0.759	45.9418	0.0018							
3	0.8	0.2	600	120	720	120	47.9599	19.0365	46.9034	91.59	2.50	0.876	46.9719	0.0047							
4	0.7	0.3	600	180	780	180	48.4702	19.0399	47.4103	80.14	3.75	0.924	47.4483	0.0014							
5	0.6	0.4	600	240	840	240	48.8036	19.0377	47.7459	68.63	5.00	0.950	47.7513	0.0000							
6	0.5	0.5	600	300	900	300	49.0629	19.0362	48.0047	57.24	6.25	0.966	47.9790	0.0007							
7	0.4	0.6	600	360	960	360	49.2839	19.0394	48.2075	45.79	7.50	0.977	48.1641	0.0018							
8	0.3	0.7	600	420	1020	420	49.4304	19.0583	48.3521	34.35	8.75	0.985	48.3263	0.0007							
9	0.2	0.8	600	480	1080	480	49.5776	19.0490	48.5086	22.90	10.00	0.991	48.4732	0.0013							
10	0.1	0.9	600	540	1140	540	49.6835	19.0408	48.6327	11.45	11.25	0.996	48.6095	0.0005							
11	0	1	600	600	1200	600	49.8060	19.0475	48.7395	0.00	12.50	1.000	48.7395	0.0000							
total vol of stock					3300	3300				9.90							ss residuals	0.0130			
ρ uncorrected																					
ρ	39.8363	48.7395			47.7597																
conc / M	114.484	12.438																			
FW	170.33	119.38																			
density	0.75	1.492																			
N sites	26	1																			
Phosphine Oxide																					
					Dodecane	CHCl ₃															
FW	218.32		weight / g		0.0107	0.0117															
p	97%		weight solvent / g		3.7470	8.1507	8.1618														
			V solvent / mL		4.9960	5.4629	5.4704														
			conc / mM		9.9157	9.9157	9.9227														
External Reference																					
Methylenediphosphonic acid																					
M_d / ppm	17.96																				
FW	176.00																				
weight / g	0.0177																				
V / mL	2																				
conc / mM	50.28																				

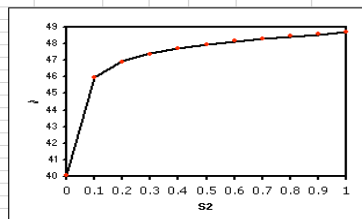


Expt	Dodecane		CHCl ₃		vol total / μ l	Dodecane		CHCl ₃		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb2 / M-1	error		
	S1	S2	vol S1 / μ l	vol S2 / μ l		vol S1 / μ l	vol S2 / μ l	ρ_{exp} / ppm	ρ_{ref} / ppm												ρ_{calc} / ppm	Δ alpha 0
1	1	0	600	0	600	0	40.8940	19.0399	39.4041	114.48	0.000	0.000	39.4041	0.0000								
2	0.9	0.1	600	60	660	60	46.9882	19.0477	45.9205	103.04	1.25	0.759	45.8800	0.0018								
3	0.8	0.2	600	120	720	120	47.9564	19.0482	46.8982	91.59	2.50	0.876	46.9506	0.0039								
4	0.7	0.3	600	180	780	180	48.4747	19.0581	47.3966	80.14	3.75	0.924	47.4414	0.0020								
5	0.6	0.4	600	240	840	240	48.8212	19.0474	47.7538	68.63	5.00	0.950	47.7507	0.0000								
6	0.5	0.5	600	300	900	300	49.0631	19.0459	48.0023	57.24	6.25	0.966	47.9900	0.0005								
7	0.4	0.6	600	360	960	360	49.2700	19.0566	48.1934	45.79	7.50	0.977	48.1670	0.0007								
8	0.3	0.7	600	420	1020	420	49.4361	19.0438	48.3723	34.35	8.75	0.985	48.3289	0.0019								
9	0.2	0.8	600	480	1080	480	49.5748	19.0410	48.5138	22.90	10.00	0.991	48.4747	0.0015								
10	0.1	0.9	600	540	1140	540	49.6853	19.0490	48.6263	11.45	11.25	0.996	48.6096	0.0003								
11	0	1	600	600	1200	600	49.8257	19.0700	48.7387	0.00	12.50	1.000	48.7387	0.0000								
total vol of stock					3300	3300				9.25							ss residuals	0.0124				
ρ uncorrected																						
ρ	39.4041	48.7387			47.7907																	
conc / M	114.484	12.438																				
FW	170.33	119.38																				
density	0.75	1.492																				
N sites	26	1																				
Phosphine Oxide																						
					Dodecane	CHCl ₃																
FW	218.32		weight / g		0.0112	0.0102																
p	97%		weight solvent / g		3.7297	6.7572	6.7426															
			V solvent / mL		4.9729	4.5289	4.5192															
			conc / mM		10.0665	10.0665	10.0291															
External Reference																						
Methylenediphosphonic acid																						
M_d / ppm	17.96																					
FW	176.00																					
weight / g	0.0177																					
V / mL	2																					
conc / mM	50.28																					



2.13. Octane-Chloroform

Expt	Octane		CHCl3		vol total / μ l	Octane		CHCl3		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb2 / M-1	error		
	S1	S2	vol S1 / μ l	vol S2 / μ l		vol S1 / μ l	vol S2 / μ l	ρ_{exp} / ppm	ρ_{ref} / ppm												ρ_{calc} / ppm	ΔG / kJ/mol
1	1	0	600	0	600	0	41.099	19.0380	40.0519	10.78	0.00	0.000	40.0519	0.0000								
2	0.9	0.1	600	60	600	60	47.0439	19.0467	45.3752	93.70	1.25	0.752	45.3381	0.0014								
3	0.8	0.2	600	120	600	120	47.9672	19.0467	46.9005	88.62	2.50	0.872	46.9551	0.0030								
4	0.7	0.3	600	180	600	180	48.4508	19.0535	47.3773	77.54	3.75	0.921	47.4255	0.0023								
5	0.6	0.4	600	240	600	240	48.7999	19.0481	47.7318	66.47	5.00	0.948	47.7237	0.0001								
6	0.5	0.5	600	300	600	300	48.0337	19.0454	47.9683	55.39	6.25	0.965	47.9459	0.0005								
7	0.4	0.6	600	240	600	360	48.2226	19.0560	48.1566	44.31	7.50	0.976	48.1276	0.0008								
8	0.3	0.7	600	180	600	420	49.3827	19.0614	48.3113	33.23	8.75	0.985	48.2855	0.0007								
9	0.2	0.8	600	120	600	480	49.5332	19.0511	48.4621	22.16	10.00	0.991	48.4280	0.0012								
10	0.1	0.9	600	60	600	540	49.6587	19.0494	48.5893	11.08	11.25	0.996	48.5600	0.0009								
11	0	1	600	0	600	600	49.7758	19.0712	48.6846	0.00	12.50	1.000	48.6846	0.0000								
					total vol of stock		3300	3300			8.83		ss residuals		0.0108							
92 uncorrected																						
ρ		40.0519	48.6846			47.7439																
conc / M		110.777	12.438																			
FW		114.23	119.38																			
density		0.703	1.492																			
N sites		18	1																			
Phosphine Oxide																						
				Octane		CHCl3																
FW		218.32		weight / g	0.0133	0.0178																
p		97%		weight solvent / g	3.5230	10.0068	10.0008															
				V solvent / mL	5.0114	6.7070	6.7029															
				conc / mM	11.7916	11.7916	11.7908															
External Reference																						
Methylenediphosphonic acid																						
M^d / ppm		17.98																				
FW		176.00																				
weight / g		0.0177																				
V / mL		2																				
conc / mM		50.28																				



Expt	Octane		CHCl3		vol total / μ l	Octane		CHCl3		ρ_{exp} / ppm	ρ_{ref} / ppm	ρ_{calc} / ppm	[S1]	[S2]	[A-S2]	ρ calc	error	ΔG / kJ/mol	Kb2 / M-1	error		
	S1	S2	vol S1 / μ l	vol S2 / μ l		vol S1 / μ l	vol S2 / μ l	ρ_{exp} / ppm	ρ_{ref} / ppm												ρ_{calc} / ppm	ΔG / kJ/mol
1	1	0	600	0	600	0	41.1675	19.0420	40.1055	10.78	0.00	0.000	40.1055	0.0000								
2	0.9	0.1	600	60	600	60	47.0620	19.0414	45.9676	99.70	1.25	0.745	45.9266	0.0017								
3	0.8	0.2	600	120	600	120	47.9667	19.0415	46.9052	88.62	2.50	0.868	46.9652	0.0036								
4	0.7	0.3	600	180	600	180	48.4679	19.0443	47.4036	77.54	3.75	0.918	47.4464	0.0018								
5	0.6	0.4	600	240	600	240	48.8083	19.0392	47.7491	66.47	5.00	0.946	47.7506	0.0000								
6	0.5	0.5	600	300	600	300	49.0489	19.0402	47.9097	55.39	6.25	0.963	47.9763	0.0002								
7	0.4	0.6	600	240	600	360	49.2444	19.0415	48.1829	44.31	7.50	0.975	48.1603	0.0005								
8	0.3	0.7	600	180	600	420	49.4336	19.0421	48.3715	33.23	8.75	0.984	48.3194	0.0027								
9	0.2	0.8	600	120	600	480	49.5707	19.0412	48.5095	22.16	10.00	0.991	48.4627	0.0022								
10	0.1	0.9	600	60	600	540	49.6866	19.0404	48.6262	11.08	11.25	0.996	48.5950	0.0010								
11	0	1	600	0	600	600	49.7866	19.0469	48.7197	0.00	12.50	1.000	48.7197	0.0000								
					total vol of stock		3300	3300			8.81		ss residuals		0.0137							
92 uncorrected																						
ρ		40.1055	48.7197			47.7970																
conc / M		110.777	12.438																			
FW		114.23	119.38																			
density		0.703	1.492																			
N sites		18	1																			
Phosphine Oxide																						
				Octane		CHCl3																
FW		218.32		weight / g	0.0109	0.0143																
p		97%		weight solvent / g	3.5286	9.8248	9.836															
				V solvent / mL	5.0193	6.8260	6.8225															
				conc / mM	9.6495	9.6495	9.6375															
External Reference																						
Methylenediphosphonic acid																						
M^d / ppm		17.98																				
FW		176.00																				
weight / g		0.0177																				
V / mL		2																				
conc / mM		50.28																				

