Chemistry

Characterizing the properties of anion-binding bis(cyclopeptides) with solvent-independent energy increments

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CONTENT

Table S1. Overview of Dataset Used for the Analysis

Entry	Comp.	No. of Linkers	Solvent	vol% Water	mol% Water	Anion	Method	log K_a	T / K	$\Delta G°_{exp}$ [a]	Ref.	$\Delta G°_{tr}$ [a]	α	β	π^*	$E_T(30)$
1	**1d**	1	D_2O/CD_3OD	50.0	69.0	SO_4^{2-}	NMR	5.54	298	-31.6	[1]	11.67	1.00	0.68	1.02	58.42
2	**1d**	1	D_2O/CD_3OD	50.0	69.0	I^-	NMR	3.95	298	-22.5		0.32	1.00	0.68	1.02	58.42
3	**1d**	1	D_2O/CD_3OD	50.0	69.0	I^-	NMR	4.04	298	-23.0		0.32	1.00	0.68	1.02	58.42
4	**1d**	1	D_2O/CD_3OD	50.0	69.0	I^-	NMR	4.05	298	-23.1		0.32	1.00	0.68	1.02	58.42
5	**1d**	1	D_2O/CD_3OD	50.0	69.0	Br^-	NMR	3.72	298	-21.2		1.77	1.00	0.68	1.02	58.42
6	**1d**	1	D_2O/CD_3OD	50.0	69.0	Cl^-	NMR	2.85	298	-16.3		2.89	1.00	0.68	1.02	58.42
7	**1d**	1	D_2O/CD_3OD	50.0	69.0	NO_3^-	NMR	2.11	298	-12.0		1.48	1.00	0.68	1.02	58.42
8	**1d**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	4.55	298	-26.0		11.56	1.00	0.68	1.02	58.44
9	**1d**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	3.79	298	-21.6		0.31	1.00	0.68	1.02	58.44
10	**1d**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	3.51	298	-20.0		0.31	1.00	0.68	1.02	58.44
11	**1d**	1	H_2O/CH_3OH	50.0	69.2	Br^-	ITC	3.45	298	-19.7		1.75	1.00	0.68	1.02	58.44
12	**1d**	1	H_2O/CH_3OH	50.0	69.2	Cl^-	ITC	2.51	298	-14.3		2.86	1.00	0.68	1.02	58.44
13	**1d**	1	H_2O/CH_3CN	33.3	59.1	I^-	ITC	3.52	298	-20.1	[2]	6.54	0.88	0.60	0.87	55.80
14	**1d**	1	H_2O/CH_3CN	33.3	59.1	SO_4^{2-}	ITC	5.30	298	-30.2		n.a.[b]	0.88	0.60	0.87	55.80
15	**1j**	1	H_2O/CH_3CN	33.0	58.8	I^-	ITC	4.46	298	-25.4		6.57	0.88	0.60	0.86	55.79
16	**1j**	1	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	6.73	298	-38.4		n.a.	0.88	0.60	0.86	55.79
17	**1l**	1	H_2O/CH_3CN	33.0	58.8	I^-	ITC	4.75	298	-27.1		6.57	0.88	0.60	0.86	55.79
18	**1l**	1	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	6.83	298	-39.0		n.a.	0.88	0.60	0.86	55.79
19	**1l**	1	H_2O/CH_3CN	58.0	80.0	I^-	ITC	4.65	298	-26.5	[3]	4.16	0.97	0.61	0.99	57.66
20	**1l**	1	H_2O/CH_3CN	50.0	74.3	I^-	ITC	4.73	298	-27.0		4.87	0.94	0.61	0.95	56.87
21	**1l**	1	H_2O/CH_3CN	33.0	58.8	I^-	ITC	4.85	298	-27.7		6.57	0.88	0.60	0.86	55.79
22	**1l**	1	H_2O/CH_3CN	25.0	49.1	I^-	ITC	4.99	298	-28.5		7.79	0.86	0.59	0.84	55.59
23	**1l**	1	H_2O/CH_3CN	70.0	87.1	SO_4^{2-}	ITC	5.45	298	-31.1		n.a.	1.02	0.62	1.04	59.07
24	**1l**	1	H_2O/CH_3CN	58.0	80.0	SO_4^{2-}	ITC	5.91	298	-33.7		n.a.	0.97	0.61	0.99	57.66
25	**1l**	1	H_2O/CH_3CN	50.0	74.3	SO_4^{2-}	ITC	6.06	298	-34.6		n.a.	0.94	0.61	0.95	56.87

26	**1l**	1	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	6.83	298	-39.0		n.a.	0.88	0.60	0.86	55.79
27	**1l**	1	H_2O/CH_3CN	25.0	49.1	SO_4^{2-}	ITC	7.29	298	-41.6		n.a.	0.86	0.59	0.84	55.59
28	**1d**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	3.79	298	-21.6		0.31	1.00	0.68	1.02	58.44
29	**1f**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	5.10	298	-29.1		11.56	1.00	0.68	1.02	58.44
30	**1f**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	4.00	298	-22.8		0.31	1.00	0.68	1.02	58.44
31	**1f**	1	H_2O/CH_3OH	50.0	69.2	Br^-	ITC	3.30	298	-18.8		1.75	1.00	0.68	1.02	58.44
32	**1f**	1	H_2O/CH_3OH	50.0	69.2	Cl^-	ITC	1.86	298	-10.6		2.86	1.00	0.68	1.02	58.44
33	**1g**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	5.32	298	-30.3		11.56	1.00	0.68	1.02	58.44
34	**1g**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	3.61	298	-20.6	[4]	0.31	1.00	0.68	1.02	58.44
35	**1g**	1	H_2O/CH_3OH	50.0	69.2	Br^-	ITC	3.03	298	-17.3		1.75	1.00	0.68	1.02	58.44
36	**1c**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	5.97	298	-34.1		11.56	1.00	0.68	1.02	58.44
37	**1c**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	4.43	298	-25.3		0.31	1.00	0.68	1.02	58.44
38	**1c**	1	H_2O/CH_3OH	50.0	69.2	Br^-	ITC	4.01	298	-22.9		1.75	1.00	0.68	1.02	58.44
39	**1c**	1	H_2O/CH_3OH	50.0	69.2	Cl^-	ITC	3.39	298	-19.3		2.86	1.00	0.68	1.02	58.44
40	**1c**	1	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	5.75	298	-32.8		n.a.	0.88	0.60	0.86	55.79
41	**1c**	1	H_2O/CH_3CN	33.0	58.8	I^-	ITC	4.05	298	-23.1		6.57	0.88	0.60	0.86	55.79
42	**1h**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	3.87	298	-22.1	[5]	11.56	1.00	0.68	1.02	58.44
43	**1h**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	2.68	298	-15.3		0.31	1.00	0.68	1.02	58.44
44	**1i**	1	H_2O/CH_3OH	35.0	54.7	SO_4^{2-}	ITC	5.67	298	-32.3		19.04	0.98	0.69	0.93	57.51
45	**1i**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	4.96	298	-28.3		11.56	1.00	0.68	1.02	58.44
46	**1i**	1	H_2O/CH_3OH	65.0	80.7	SO_4^{2-}	ITC	4.26	298	-24.3		6.56	1.05	0.65	1.07	59.59
47	**3i**	3	H_2O/CH_3OH	35.0	54.7	SO_4^{2-}	ITC	6.34	298	-36.2	[6]	19.04	0.98	0.69	0.93	57.51
48	**3i**	3	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	5.70	298	-32.5		11.56	1.00	0.68	1.02	58.44
49	**3i**	3	H_2O/CH_3OH	65.0	80.7	SO_4^{2-}	ITC	5.19	298	-29.6		6.56	1.05	0.65	1.07	59.59
50	**1k**	1	H_2O/CH_3CN	33.0	58.8	I^-	ITC	4.89	298	-27.9		6.57	0.88	0.60	0.86	55.79
51	**1k**	1	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	6.78	298	-38.7		n.a.	0.88	0.60	0.86	55.79
52	**2k**	2	H_2O/CH_3CN	33.0	58.8	I^-	ITC	6.04	298	-34.5	[7]	6.57	0.88	0.60	0.86	55.79
53	**2k**	2	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	8.67	298	-49.5		n.a.	0.88	0.60	0.86	55.79
54	**2k**	2	H_2O/CH_3CN	33.0	58.8	SeO_4^{2-}	ITC	8.04	298	-45.9		n.a.	0.88	0.60	0.86	55.79

55	**1l**	1	H_2O/CH_3CN	33.0	58.8	I^-	ITC	4.75	298	-27.1		6.57	0.88	0.60	0.86	55.79
56	**1l**	1	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	6.83	298	-39.0		n.a.	0.88	0.60	0.86	55.79
57	**2l**	2	H_2O/CH_3CN	33.0	58.8	I^-	ITC	5.08	298	-29.0		6.57	0.88	0.60	0.86	55.79
58	**2l**	2	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	7.59	298	-43.3		n.a.	0.88	0.60	0.86	55.79
59	**2l**	2	H_2O/CH_3CN	33.0	58.8	SeO_4^{2-}	ITC	6.60	298	-37.7		n.a.	0.88	0.60	0.86	55.79
60	**1b**	1	H_2O/CH_3OH	30.0	49.0	SO_4^{2-}	ITC	6.77	298	-38.6		22.35	0.98	0.68	0.90	57.23
61	**1b**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	5.87	298	-33.5		11.56	1.00	0.68	1.02	58.44
62	**1b**	1	H_2O/CH_3OH	70.0	84.0	SO_4^{2-}	ITC	5.07	298	-28.9		5.27	1.07	0.63	1.08	60.03
63	**1b**	1	H_2O/CH_3OH	95.0	97.7	SO_4^{2-}	ITC	3.70	298	-21.1		0.66	1.16	0.51	1.10	62.55
64	**1b**	1	H_2O/CH_3OH	20.0	36.0	I^-	ITC	4.96	298	-28.3	[8]	3.07	0.99	0.67	0.82	56.68
65	**1b**	1	H_2O/CH_3OH	30.0	49.0	I^-	ITC	4.73	298	-27.0		1.77	0.98	0.68	0.90	57.23
66	**1b**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	4.59	298	-26.2		0.31	1.00	0.68	1.02	58.44
67	**1b**	1	H_2O/CH_3OH	70.0	84.0	I^-	ITC	4.43	298	-25.3		-0.19	1.07	0.63	1.08	60.03
68	**1b**	1	H_2O/CH_3OH	90.0	95.3	I^-	ITC	4.12	298	-23.5		-0.16	1.14	0.54	1.10	62.01
69	**1b**	1	H_2O/CH_3OH	95.0	97.7	I^-	ITC	3.96	298	-22.6		-0.11	1.16	0.51	1.10	62.55
70	**1b**	1	H_2O/CH_3OH	30.0	49.0	SO_4^{2-}	ITC	6.76	298	-38.6		22.35	0.98	0.68	0.90	57.23
71	**1b**	1	H_2O/CH_3OH	50.0	69.2	SO_4^{2-}	ITC	5.87	298	-33.5		11.56	1.00	0.68	1.02	58.44
72	**1b**	1	H_2O/CH_3OH	70.0	84.0	SO_4^{2-}	ITC	5.04	298	-28.8		5.27	1.07	0.63	1.08	60.03
73	**1b**	1	H_2O/CH_3OH	95.0	97.7	SO_4^{2-}	ITC	3.69	298	-21.1		0.66	1.16	0.51	1.10	62.55
74	**1b**	1	H_2O/–	100.0	100.0	SO_4^{2-}	ITC	3.49	298	-19.9		0.00	1.17	0.47	1.09	1.09
75[c]	**1b**	1	H_2O/CH_3OH	0.0	0.0	I^-	ITC	6.14	298	-35.0		7.31	1.00	0.70	0.59	55.69
76[c]	**1b**	1	H_2O/CH_3OH	0.0	0.0	I^-	ITC	6.38	298	-36.4	[9]	7.31	1.00	0.70	0.59	55.69
77	**1b**	1	H_2O/CH_3OH	5.0	10.6	I^-	ITC	5.85	298	-33.4		6.02	1.01	0.70	0.67	55.84
78	**1b**	1	H_2O/CH_3OH	10.0	20.0	I^-	ITC	5.40	298	-30.8		4.89	1.01	0.68	0.73	56.10
79	**1b**	1	H_2O/CH_3OH	10.0	20.0	I^-	ITC	5.53	298	-31.5		4.89	1.01	0.68	0.73	56.10
80	**1b**	1	H_2O/CH_3OH	20.0	36.0	I^-	ITC	4.96	298	-28.3		3.07	0.99	0.67	0.82	56.68
81	**1b**	1	H_2O/CH_3OH	30.0	49.0	I^-	ITC	4.72	298	-26.9		1.77	0.98	0.68	0.90	57.23
82	**1b**	1	H_2O/CH_3OH	50.0	69.2	I^-	ITC	4.59	298	-26.2		0.31	1.00	0.68	1.02	58.44
83	**1b**	1	H_2O/CH_3OH	70.0	84.0	I^-	ITC	4.43	298	-25.3		-0.19	1.07	0.63	1.08	60.03

84	**1b**	1	H_2O/CH_3OH	90.0	95.3	I^-	ITC	4.10	298	-23.4	-0.16	1.14	0.54	1.10	62.01
85	**1b**	1	H_2O/CH_3OH	95.0	97.7	I^-	ITC	3.96	298	-22.6	-0.11	1.16	0.51	1.10	62.55
86	**1b**	1	H_2O/–	100.0	100.0	I^-	ITC	3.80	298	-21.7	0.00	1.17	0.47	1.09	1.09
87	**1b**	1	H_2O/CH_3CN	30.0	55.4	SO_4^{2-}	ITC	6.25	298	-35.7	n.a.	0.87	0.60	0.85	55.70
88	**1b**	1	H_2O/CH_3CN	50.0	74.3	SO_4^{2-}	ITC	5.24	298	-29.9	n.a.	0.94	0.61	0.95	56.87
89	**1b**	1	H_2O/CH_3CN	70.0	87.1	SO_4^{2-}	ITC	4.78	298	-27.3	n.a.	1.02	0.62	1.04	59.07
90	**1b**	1	H_2O/CH_3CN	80.0	92.1	SO_4^{2-}	ITC	4.48	298	-25.6	n.a.	1.06	0.60	1.08	60.37
91	**1b**	1	H_2O/CH_3CN	95.0	98.2	SO_4^{2-}	ITC	3.97	298	-22.6	n.a.	1.14	0.52	1.10	62.41
92[c]	**1b**	1	H_2O/CH_3CN	0.0	0.0	I^-	ITC	6.24	298	-35.6	20.33	0.25	0.47	0.73	45.99
93[c]	**1b**	1	H_2O/CH_3CN	0.0	0.0	I^-	ITC	6.25	298	-35.7	20.33	0.25	0.47	0.73	45.99
94	**1b**	1	H_2O/CH_3CN	5.0	13.2	I^-	ITC	5.55	298	-31.7	15.85	0.61	0.55	0.75	51.91
95	**1b**	1	H_2O/CH_3CN	20.0	42.0	I^-	ITC	4.74	298	-27.0	8.89	0.83	0.59	0.83	55.47
96	**1b**	1	H_2O/CH_3CN	20.0	42.0	I^-	ITC	4.72	298	-26.9	8.89	0.83	0.59	0.83	55.47
97	**1b**	1	H_2O/CH_3CN	30.0	55.4	I^-	ITC	4.35	298	-24.8	6.97	0.87	0.60	0.85	55.70
98	**1b**	1	H_2O/CH_3CN	50.0	74.3	I^-	ITC	4.20	298	-24.0	4.87	0.94	0.61	0.95	56.87
99	**1b**	1	H_2O/CH_3CN	70.0	87.1	I^-	ITC	4.23	298	-24.1	3.04	1.02	0.62	1.04	59.07
100	**1b**	1	H_2O/CH_3CN	80.0	92.1	I^-	ITC	4.22	298	-24.1	2.05	1.06	0.60	1.08	60.37
101	**1b**	1	H_2O/CH_3CN	95.0	98.2	I^-	ITC	3.94	298	-22.5	0.47	1.14	0.52	1.10	62.41
102	**1b**	1	H_2O/–	100.0	100.0	I^-	ITC	3.62	298	-20.7	0.00	1.17	0.47	1.09	1.09
103	**1b**	1	H_2O/–	100.0	100.0	Br^-	ITC	3.23	298	-18.4	0.00	1.17	0.47	1.09	1.09
104	**1b**	1	H_2O/–	100.0	100.0	Cl^-	ITC	2.15	298	-12.3	0.00	1.17	0.47	1.09	1.09
105	**1b**	1	H_2O/–	100.0	100.0	SO_4^{2-}	ITC	3.31	298	-18.9	0.00	1.17	0.47	1.09	1.09
106	**1b**	1	H_2O/CH_3OH	70.0	84.0	SO_4^{2-}	ITC	4.82	298	-27.5	5.27	1.07	0.63	1.08	60.03
107	**1b**	1	H_2O/CH_3OH	95.0	97.7	SO_4^{2-}	ITC	3.62	298	-20.7	0.66	1.16	0.51	1.10	62.55
108	**1b**	1	H_2O/CH_3OH	95.0	97.7	I^-	ITC	3.73	298	-21.3	-0.11	1.16	0.51	1.10	62.55
109	**1b**	1	H_2O/CH_3CN	70.0	87.1	SO_4^{2-}	ITC	4.66	298	-26.6	n.a.	1.02	0.62	1.04	59.07
110	**1b**	1	H_2O/CH_3CN	95.0	98.2	SO_4^{2-}	ITC	3.98	298	-22.7	n.a.	1.14	0.52	1.10	62.41
111	**1b**	1	H_2O/CH_3CN	95.0	98.2	I^-	ITC	3.77	298	-21.5	0.47	1.14	0.52	1.10	62.41
112[c]	**1b**	1	H_2O/DMSO	40.0	72.4	SO_4^{2-}	ITC	6.72	298	-38.3	46.58	0.49	0.64	1.10	53.56

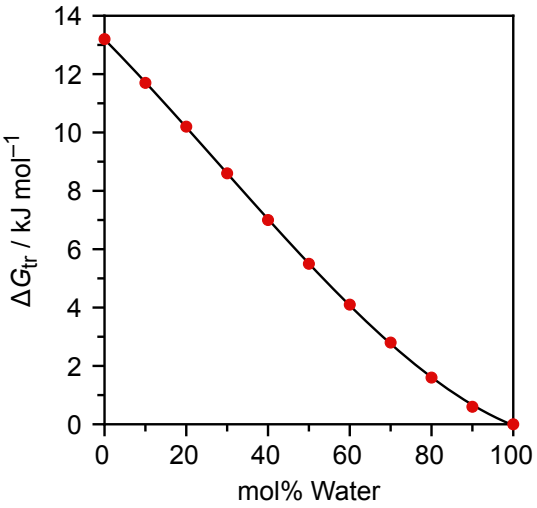
113[c]	**1b**	1	H_2O/DMSO	50.0	79.8	SO_4^{2-}	ITC	5.89	298	-33.6		32.31	0.59	0.61	1.12	55.30
114[c]	**1b**	1	H_2O/DMSO	70.0	90.2	SO_4^{2-}	ITC	4.85	298	-27.7		13.20	0.81	0.55	1.12	58.63
115[c]	**1b**	1	H_2O/DMSO	90.0	97.3	SO_4^{2-}	ITC	3.86	298	-22.0		2.54	1.05	0.50	1.10	61.68
116[c]	**1b**	1	H_2O/DMSO	0.0	0.0	I^-	ITC	3.21	298	-18.3		14.08	0.00	0.79	0.98	45.00
117[c]	**1b**	1	H_2O/DMSO	70.0	90.2	I^-	ITC	3.20	298	-18.3		1.33	0.81	0.55	1.12	58.63
118	**1e**	1	H_2O/CH_3CN	33.0	58.8	I^-	ITC	4.45	298	-25.4	[10]	6.57	0.88	0.60	0.86	55.79
119	**1e**	1	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	6.71	298	-38.3		n.a.	0.88	0.60	0.86	55.79
120	**3e**	3	D_2O/CD_3CN	33.0	61.3	I^-	NMR	3.00	298	-17.1		6.30	0.89	0.60	0.87	55.88
121	**3e**	3	H_2O/CH_3CN	33.0	58.8	SO_4^{2-}	ITC	4.31	298	-24.6		n.a.	0.88	0.60	0.86	55.79

[a] Gibbs free energies in kJ mol^{-1}; [b] n.a. – not available; [c] not considered in the statistical analysis.

Tables S2. Polynomial Fits of Transfer Energies and Solvent Property Parameters

$\Delta G°_{tr}$ of the Transfer of Chloride Anions from Water to Water/Methanol Mixtures[11]

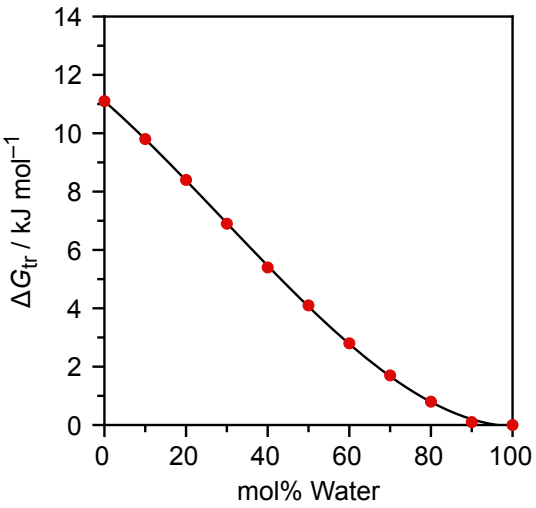
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	13.2
10.0	11.7
20.0	10.2
30.0	8.6
40.0	7.0
50.0	5.5
60.0	4.1
70.0	2.8
80.0	1.6
90.0	0.6
100.0	0.0



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	0	6.57E-06	-5.57E-04	-1.42E-01	1.32E+01

$\Delta G°_{tr}$ of the Transfer of Bromide Anions from Water to Water/Methanol Mixtures[11]

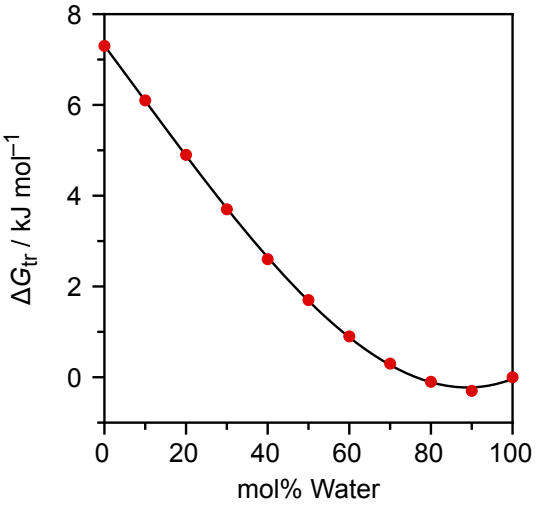
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	11.1
10.0	9.8
20.0	8.4
30.0	6.9
40.0	5.4
50.0	4.1
60.0	2.8
70.0	1.7
80.0	0.8
90.0	0.1
100.0	0.0



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	0	9.40E-06	-8.24E-04	-1.23E-01	1.11E+01

$\Delta G°_{tr}$ of the Transfer of Iodide Anions from Water to Water/Methanol Mixtures[11]

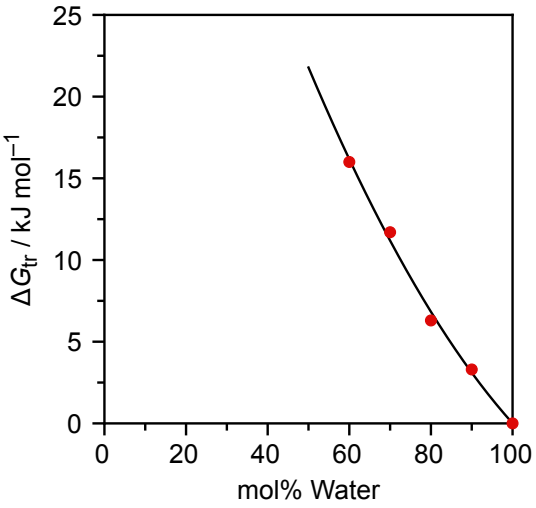
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	7.3
10.0	6.1
20.0	4.9
30.0	3.7
40.0	2.6
50.0	1.7
60.0	0.9
70.0	0.3
80.0	-0.1
90.0	-0.3
100.0	0.0



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	0	6.10E-06	-1.34E-04	-1.21E-01	7.31E+00

$\Delta G°_{tr}$ of the Transfer of Sulfate Anions from Water to Water/Methanol Mixtures[11]

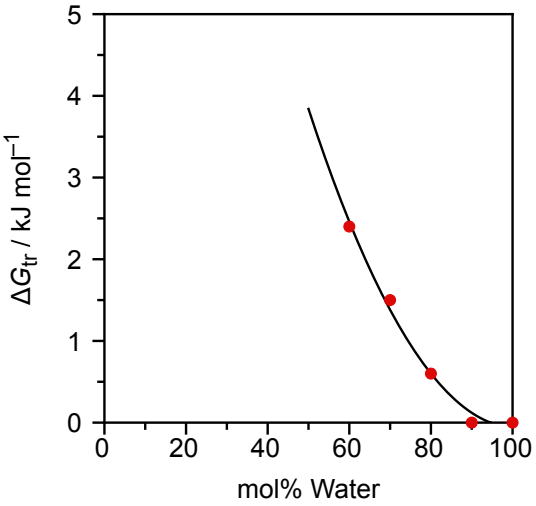
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	
10.0	
20.0	
30.0	
40.0	
50.0	
60.0	16.0
70.0	11.7
80.0	6.3
90.0	3.3
100.0	0.0



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	0	0	3.14E-03	-9.07E-01	5.93E+01

$\Delta G°_{tr}$ of the Transfer of Nitrate Anions from Water to Water/Methanol Mixtures[11]

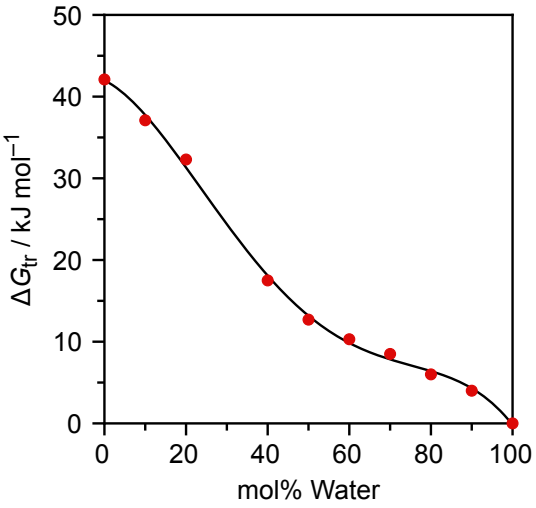
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	
10.0	
20.0	
30.0	
40.0	
50.0	
60.0	2.4
70.0	1.5
80.0	0.6
90.0	0.0
100.0	0.0



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	0	0	1.50E-03	-3.03E-01	1.52E+01

$\Delta G°_{tr}$ of the Transfer of Chloride Anions from Water to Water/Acetonitrile Mixtures[11]

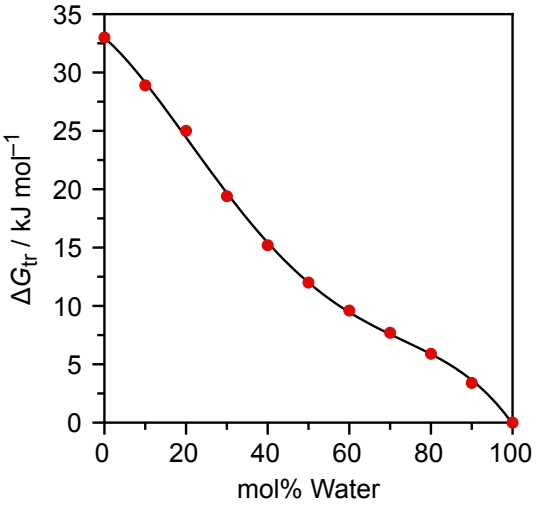
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	42.1
10.0	37.1
20.0	32.3
30.0	
40.0	17.5
50.0	12.7
60.0	10.3
70.0	8.5
80.0	6.0
90.0	4.0
100.0	0.0



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	-2.02E-06	4.00E-04	-2.16E-02	-2.46E-01	4.20E+01

$\Delta G°_{tr}$ of the Transfer of Bromide Anions from Water to Water/Acetonitrile Mixtures[11]

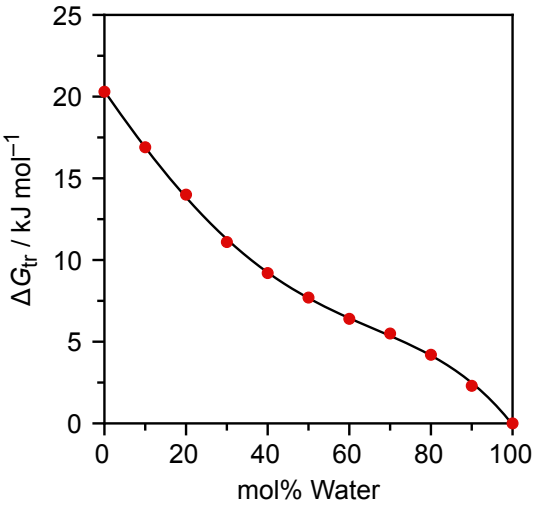
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	33.0
10.0	28.9
20.0	25.0
30.0	19.4
40.0	15.2
50.0	12.0
60.0	9.6
70.0	7.7
80.0	5.9
90.0	3.4
100.0	0.0



Polynomial			$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$				
a	b	c	d	e	f	g	h
0	0	0	-1.08E-06	2.03E-04	-9.72E-03	-3.05E-01	3.30E+01

$\Delta G°_{tr}$ of the Transfer of Iodide Anions from Water to Water/Acetonitrile Mixtures[11]

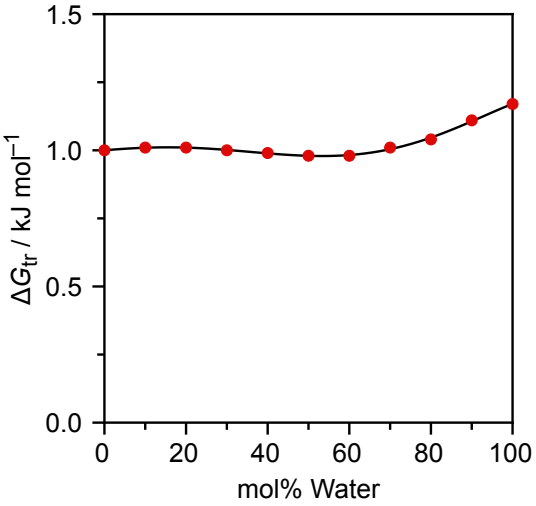
mol% Water (x)	$\Delta G°_{tr}$ / kJ mol^{-1} (y)
0.0	20.3
10.0	16.9
20.0	14.0
30.0	11.1
40.0	9.2
50.0	7.7
60.0	6.4
70.0	5.5
80.0	4.2
90.0	2.3
100.0	0.0



Polynomial			$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$				
a	b	c	d	e	f	g	h
0	0	0	-3.09E-07	3.50E-05	1.14E-03	-3.59E-01	2.03E+01

Kamlet-Taft Parameter α for Water/Methanol Mixtures[12]

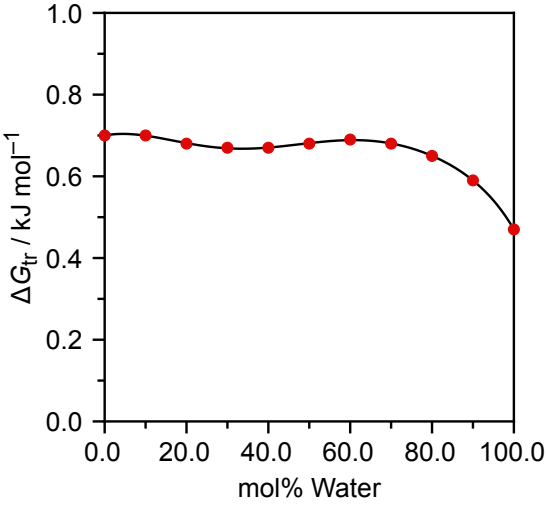
mol% Water (x)	α (y)
0.0	1.00
10.0	1.01
20.0	1.01
30.0	1.00
40.0	0.99
50.0	0.98
60.0	0.98
70.0	1.01
80.0	1.04
90.0	1.11
100.0	1.17



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	-1.92E-10	4.08E-08	-2.01E-06	-8.97E-06	1.18E-03	1.00E+00

Kamlet-Taft Parameter β for Water/Methanol Mixtures[12]

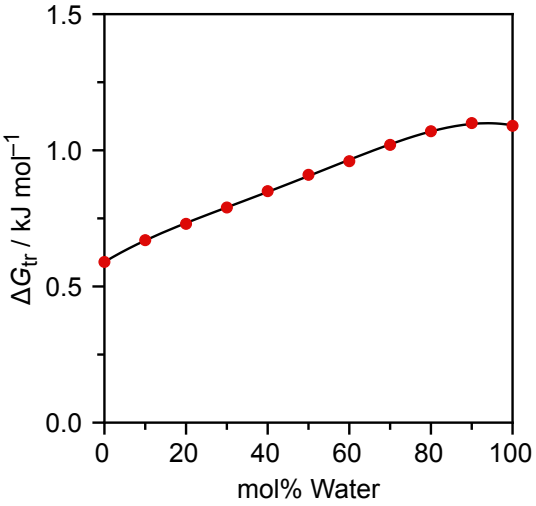
mol% Water (x)	β (y)
0.0	0.70
10.0	0.70
20.0	0.68
30.0	0.67
40.0	0.67
50.0	0.68
60.0	0.69
70.0	0.68
80.0	0.65
90.0	0.59
100.0	0.47



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
-1.11E-13	3.29E-11	-3.39E-09	1.04E-07	3.49E-06	-2.25E-04	1.77E-03	7.00E-01

Kamlet-Taft Parameter π^* for Water/Methanol Mixtures[12]

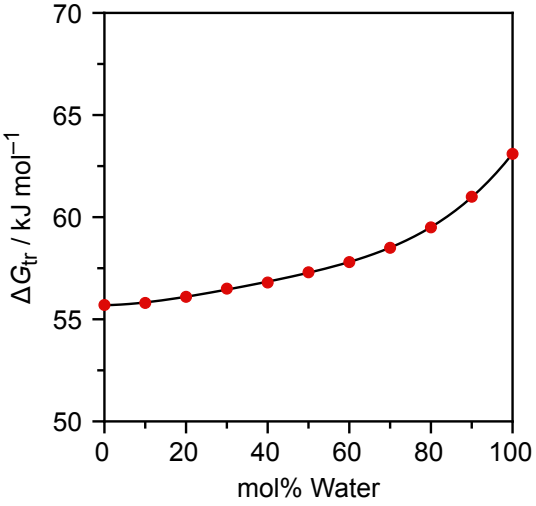
mol% Water (x)	π^* (y)
0.0	0.59
10.0	0.67
20.0	0.73
30.0	0.79
40.0	0.85
50.0	0.91
60.0	0.96
70.0	1.02
80.0	1.07
90.0	1.10
100.0	1.09



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	-1.31E-08	2.26E-06	-1.35E-04	9.06E-03	5.90E-01

Reichardt's $E_T(30)$ for Water/Methanol Mixtures[12]

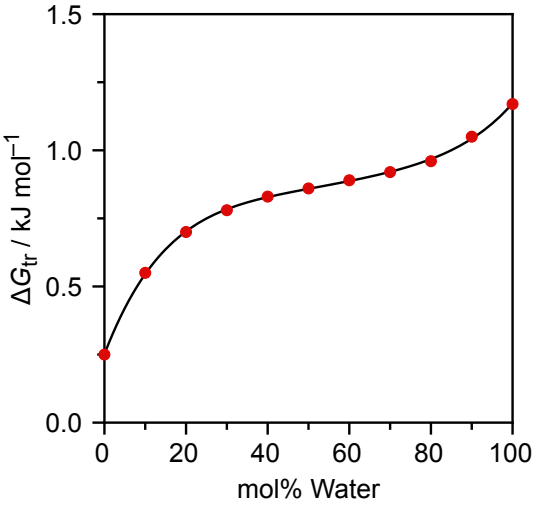
mol% Water (x)	$E_T(30)$ (y)
0.0	55.70
10.0	55.80
20.0	56.10
30.0	56.50
40.0	56.80
50.0	57.30
60.0	57.80
70.0	58.50
80.0	59.50
90.0	61.00
100.0	63.10



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	0	1.69E-07	-2.18E-05	1.26E-03	2.94E-03	5.57E+01

Kamlet-Taft Parameter α for Water/Acetonitrile Mixtures[12]

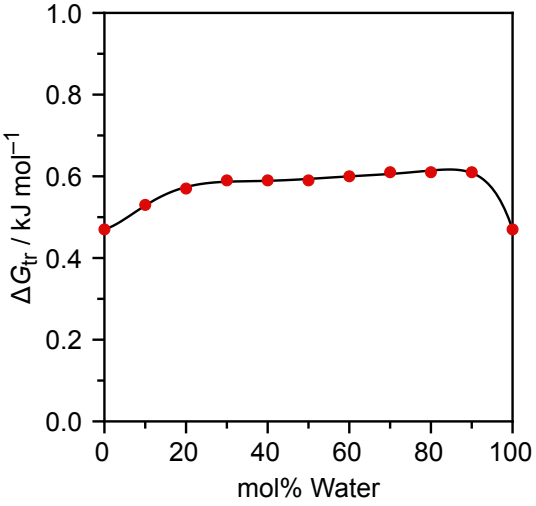
mol% Water (x)	α (y)
0.0	0.25
10.0	0.55
20.0	0.70
30.0	0.78
40.0	0.83
50.0	0.86
60.0	0.89
70.0	0.92
80.0	0.96
90.0	1.05
100.0	1.17



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	4.81E-10	-1.41E-07	1.75E-05	-1.12E-03	3.90E-02	2.51E-01

Kamlet-Taft Parameter β for Water/Acetonitrile Mixtures[12]

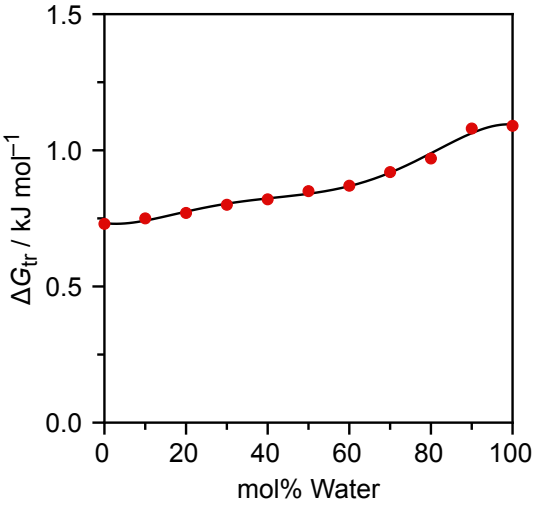
mol% Water (x)	β (y)
0.0	0.47
10.0	0.53
20.0	0.57
30.0	0.59
40.0	0.59
50.0	0.59
60.0	0.60
70.0	0.61
80.0	0.61
90.0	0.61
100.0	0.47



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
-4.90E-13	1.63E-10	-2.16E-08	1.45E-06	-4.90E-05	6.72E-04	2.75E-03	4.70E-01

Kamlet-Taft Parameter π^* for Water/Methanol Mixtures[12]

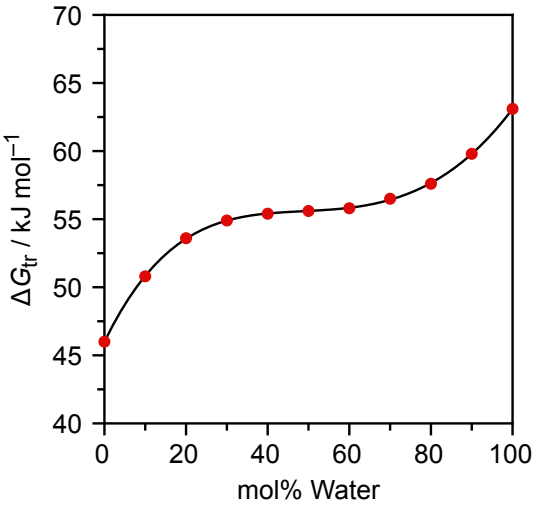
mol% Water (x)	π^* (y)
0.0	0.73
10.0	0.75
20.0	0.77
30.0	0.80
40.0	0.82
50.0	0.85
60.0	0.87
70.0	0.92
80.0	0.97
90.0	1.08
100.0	1.09



Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	-6.73E-10	1.58E-07	-1.24E-05	3.92E-04	-1.92E-03	7.33E-01

Reichardt's $E_T(30)$ for Water/Methanol Mixtures[12]

mol% Water (x)	$E_T(30)$ (y)
0.0	46.00
10.0	50.80
20.0	53.60
30.0	54.90
40.0	55.40
50.0	55.60
60.0	55.80
70.0	56.50
80.0	57.60
90.0	59.80
100.0	63.10



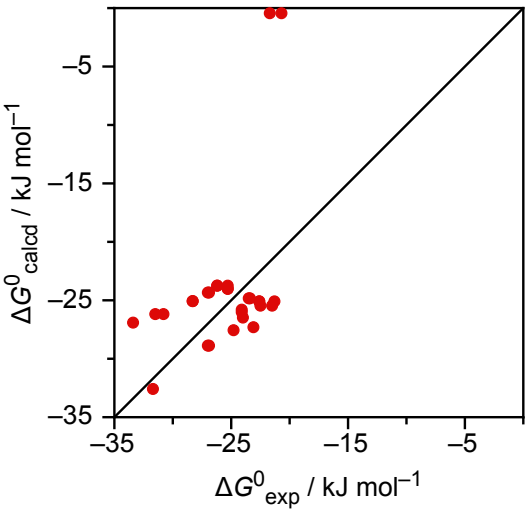
Polynomial	$y = a \times x^7 + b \times x^6 + c \times x^5 + d \times x^4 + e \times x^3 + f \times x^2 + g \times x + h$						
a	b	c	d	e	f	g	h
0	0	2.08E-09	-7.89E-07	1.63E-04	-1.50E-02	6.19E-01	4.60E+01

Tables S3. Comparison of the Experimental and Calculated Gibbs free Energies

Iodide Complexation / $E_T(30)$

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.74	-0.40				0.9424

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
37	-25.3	-23.75
41	-23.1	-27.30
64	-28.3	-25.07
65	-27.0	-24.33
66	-26.2	-23.75
67	-25.3	-24.01
68	-23.5	-24.83
69	-22.6	-25.09
77	-33.4	-26.91
78	-30.8	-26.18
79	-31.5	-26.18
80	-28.3	-25.07
81	-26.9	-24.33
82	-26.2	-23.75
83	-25.3	-24.01
84	-23.4	-24.83
85	-22.6	-25.09
86	-21.7	-0.44
94	-31.7	-32.58
95	-27.0	-28.88
96	-26.9	-28.88
97	-24.8	-27.56
98	-24.0	-26.48
99	-24.1	-26.01
100	-24.1	-25.80
101	-22.5	-25.46
102	-20.7	-0.44
108	-21.3	-25.09
111	-21.5	-25.46

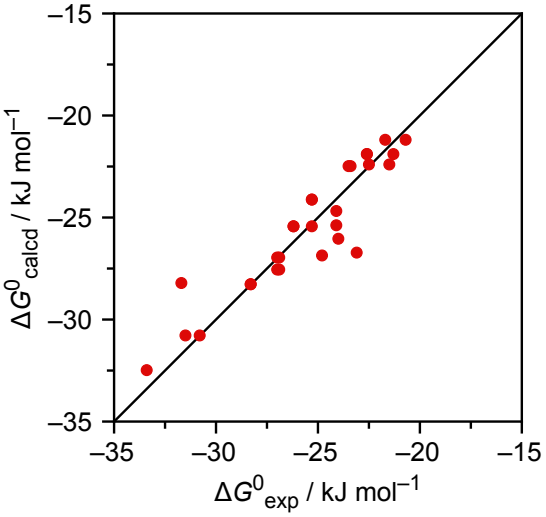


[a] e, a, b, and p in kJ mol^{-1}.

Iodide Complexation / α, β, π^*

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.65		-14.44	-27.77	8.03	0.9976

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
37	-25.3	-25.43
41	-23.1	-26.72
64	-28.3	-28.27
65	-27.0	-26.96
66	-26.2	-25.43
67	-25.3	-24.12
68	-23.5	-22.48
69	-22.6	-21.89
77	-33.4	-32.48
78	-30.8	-30.78
79	-31.5	-30.78
80	-28.3	-28.27
81	-26.9	-26.96
82	-26.2	-25.43
83	-25.3	-24.12
84	-23.4	-22.48
85	-22.6	-21.89
86	-21.7	-21.19
94	-31.7	-28.21
95	-27.0	-27.55
96	-26.9	-27.55
97	-24.8	-26.86
98	-24.0	-26.04
99	-24.1	-25.38
100	-24.1	-24.68
101	-22.5	-22.40
102	-20.7	-21.19
108	-21.3	-21.89
111	-21.5	-22.40

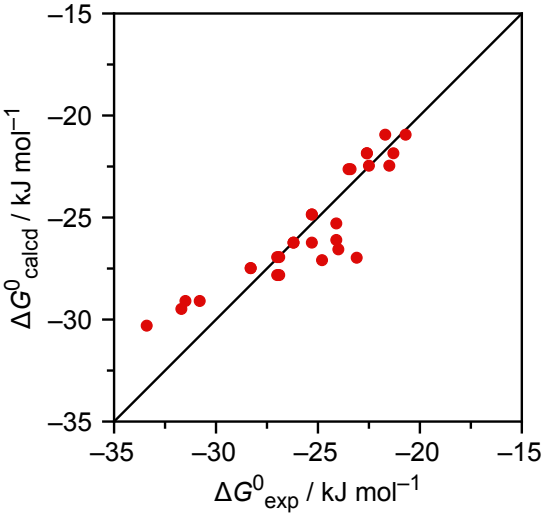


[a] e, a, b, and p in kJ mol^{-1}.

Iodide Complexation / α, β

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.62		-6.24	-29.00		0.9967

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
37	-25.3	-26.23
41	-23.1	-26.97
64	-28.3	-27.48
65	-27.0	-26.94
66	-26.2	-26.23
67	-25.3	-24.85
68	-23.5	-22.63
69	-22.6	-21.85
77	-33.4	-30.30
78	-30.8	-29.09
79	-31.5	-29.09
80	-28.3	-27.48
81	-26.9	-26.94
82	-26.2	-26.23
83	-25.3	-24.85
84	-23.4	-22.63
85	-22.6	-21.85
86	-21.7	-20.94
94	-31.7	-29.48
95	-27.0	-27.82
96	-26.9	-27.82
97	-24.8	-27.09
98	-24.0	-26.56
99	-24.1	-26.10
100	-24.1	-25.29
101	-22.5	-22.46
102	-20.7	-20.94
108	-21.3	-21.85
111	-21.5	-22.46

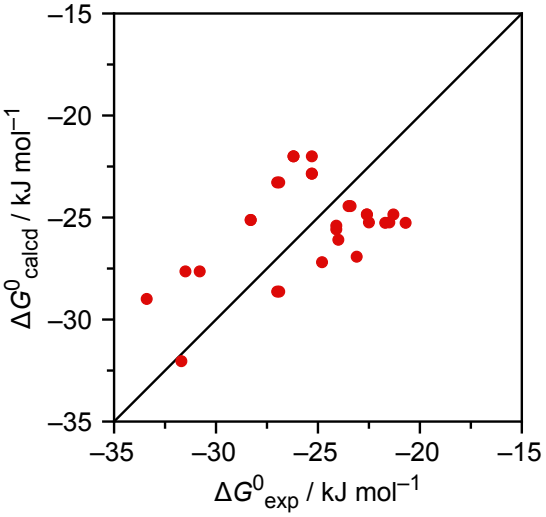


[a] e, a, b, and p in kJ mol^{-1}.

Iodide Complexation / α

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ a			
g	e	a	b	p	R^2
-1.19		-21.59			0.9862

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
37	-25.3	-22.00
41	-23.1	-26.92
64	-28.3	-25.12
65	-27.0	-23.28
66	-26.2	-22.00
67	-25.3	-22.85
68	-23.5	-24.44
69	-22.6	-24.85
77	-33.4	-28.99
78	-30.8	-27.64
79	-31.5	-27.64
80	-28.3	-25.12
81	-26.9	-23.28
82	-26.2	-22.00
83	-25.3	-22.85
84	-23.4	-24.44
85	-22.6	-24.85
86	-21.7	-25.26
94	-31.7	-32.04
95	-27.0	-28.63
96	-26.9	-28.63
97	-24.8	-27.19
98	-24.0	-26.09
99	-24.1	-25.58
100	-24.1	-25.40
101	-22.5	-25.24
102	-20.7	-25.26
108	-21.3	-24.85
111	-21.5	-25.24

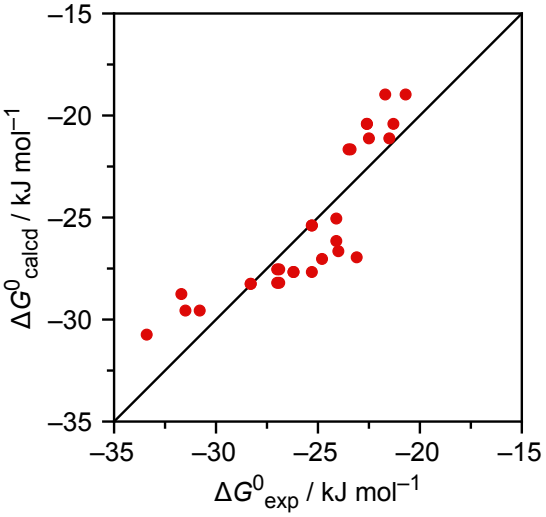


[a] e, a, b, and p in kJ mol^{-1}.

Iodide Complexation / β

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.42			-40.37		0.9950

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
37	-25.3	-27.67
41	-23.1	-26.95
64	-28.3	-28.25
65	-27.0	-28.20
66	-26.2	-27.67
67	-25.3	-25.39
68	-23.5	-21.66
69	-22.6	-20.41
77	-33.4	-30.74
78	-30.8	-29.56
79	-31.5	-29.56
80	-28.3	-28.25
81	-26.9	-28.20
82	-26.2	-27.67
83	-25.3	-25.39
84	-23.4	-21.66
85	-22.6	-20.41
86	-21.7	-18.97
94	-31.7	-28.75
95	-27.0	-27.54
96	-26.9	-27.54
97	-24.8	-27.03
98	-24.0	-26.65
99	-24.1	-26.15
100	-24.1	-25.05
101	-22.5	-21.12
102	-20.7	-18.97
108	-21.3	-20.41
111	-21.5	-21.12

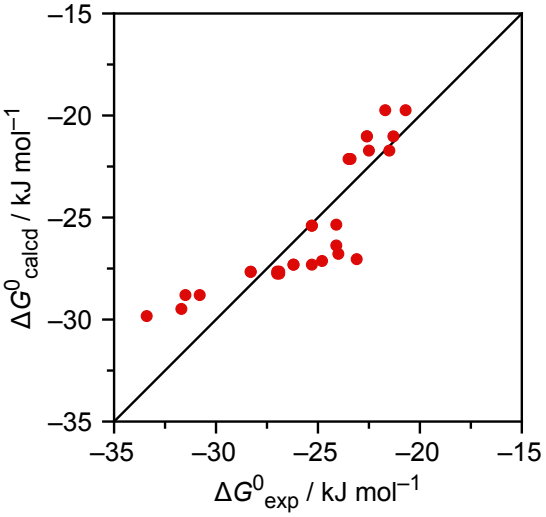


[a] e, a, b, and p in kJ mol^{-1}.

Iodide Complexation / β, π^*

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.50			-35.86	-2.65	0.9954

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
37	-25.3	-27.31
41	-23.1	-27.04
64	-28.3	-27.66
65	-27.0	-27.65
66	-26.2	-27.31
67	-25.3	-25.40
68	-23.5	-22.13
69	-22.6	-21.02
77	-33.4	-29.83
78	-30.8	-28.80
79	-31.5	-28.80
80	-28.3	-27.66
81	-26.9	-27.65
82	-26.2	-27.31
83	-25.3	-25.40
84	-23.4	-22.13
85	-22.6	-21.02
86	-21.7	-19.74
94	-31.7	-29.48
95	-27.0	-27.75
96	-26.9	-27.75
97	-24.8	-27.13
98	-24.0	-26.78
99	-24.1	-26.37
100	-24.1	-25.35
101	-22.5	-21.72
102	-20.7	-19.74
108	-21.3	-21.02
111	-21.5	-21.72

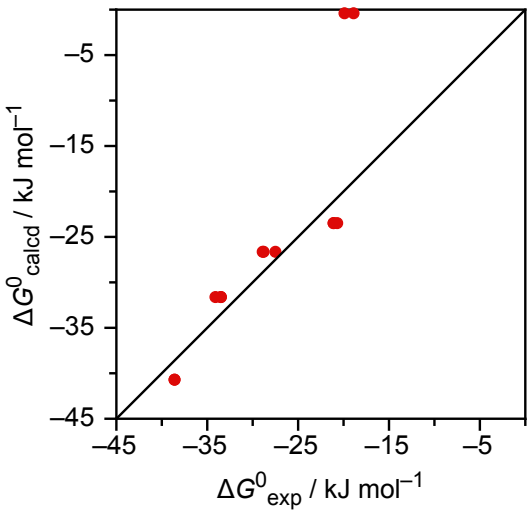


[a] e, a, b, and p in kJ mol^{-1}.

Sulfate Complexation / $E_T(30)$

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.88	-0.37				0.9288

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
36	-34.1	-31.61
60	-38.6	-40.70
61	-33.5	-31.61
62	-28.9	-26.64
63	-21.1	-23.48
70	-38.6	-40.70
71	-33.5	-31.61
72	-28.8	-26.64
73	-21.1	-23.48
74	-19.9	-0.40
105	-18.9	-0.40
106	-27.5	-26.64
107	-20.7	-23.48

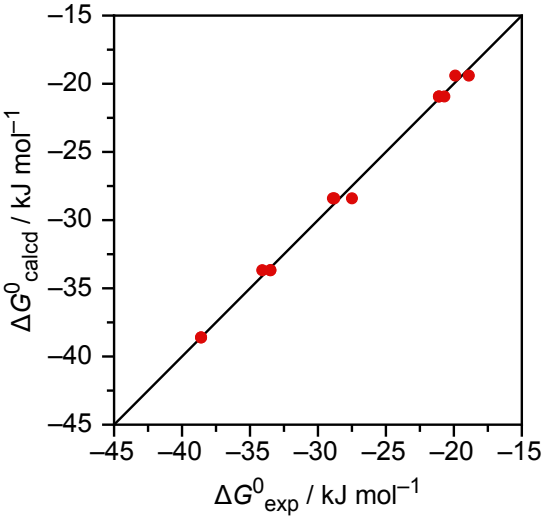


[a] e, a, b, and p in kJ mol^{-1}.

Sulfate Complexation / α, β, π^*

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-1.19		50.26	11.51	-76.71	0.9998

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
36	-34.1	-33.67
60	-38.6	-38.60
61	-33.5	-33.67
62	-28.9	-28.40
63	-21.1	-20.93
70	-38.6	-38.60
71	-33.5	-33.67
72	-28.8	-28.40
73	-21.1	-20.93
74	-19.9	-19.40
105	-18.9	-19.40
106	-27.5	-28.40
107	-20.7	-20.93

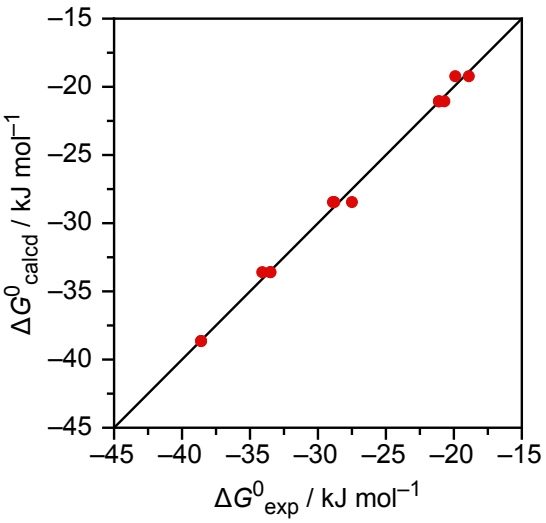


[a] e, a, b, and p in kJ mol^{-1}.

Sulfate Complexation / α, β

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.47		0.30	-41.64		0.9998

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
36	-34.1	-33.59
60	-38.6	-38.64
61	-33.5	-33.59
62	-28.9	-28.45
63	-21.1	-21.06
70	-38.6	-38.64
71	-33.5	-33.59
72	-28.8	-28.45
73	-21.1	-21.06
74	-19.9	-19.22
105	-18.9	-19.22
106	-27.5	-28.45
107	-20.7	-21.06

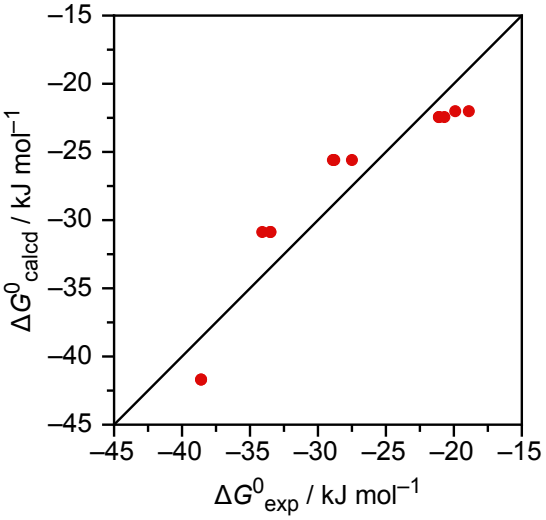


[a] e, a, b, and p in kJ mol^{-1}.

Sulfate Complexation / α

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-1.04		-18.81			0.9918

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
36	-34.1	-30.87
60	-38.6	-41.69
61	-33.5	-30.87
62	-28.9	-25.59
63	-21.1	-22.44
70	-38.6	-41.69
71	-33.5	-30.87
72	-28.8	-25.59
73	-21.1	-22.44
74	-19.9	-22.01
105	-18.9	-22.01
106	-27.5	-25.59
107	-20.7	-22.44

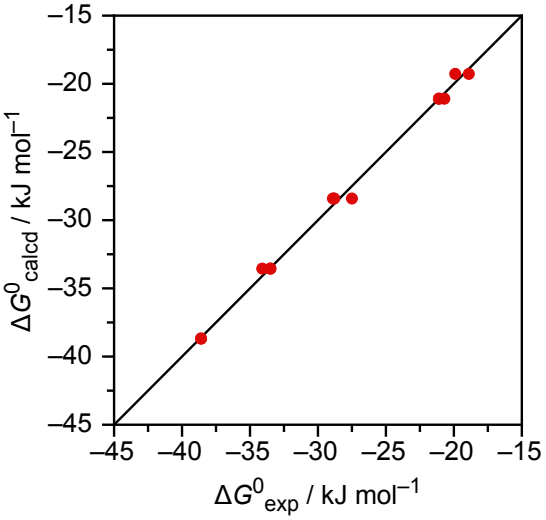


[a] e, a, b, and p in kJ mol^{-1}.

Sulfate Complexation / β

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.48			-41.00		0.9998

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
36	-34.1	-33.55
60	-38.6	-38.68
61	-33.5	-33.55
62	-28.9	-28.41
63	-21.1	-21.09
70	-38.6	-38.68
71	-33.5	-33.55
72	-28.8	-28.41
73	-21.1	-21.09
74	-19.9	-19.27
105	-18.9	-19.27
106	-27.5	-28.41
107	-20.7	-21.09

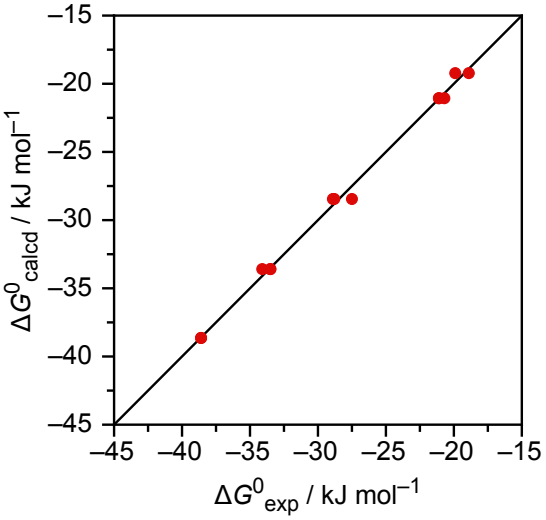


[a] e, a, b, and p in kJ mol^{-1}.

Sulfate Complexation / β, π^*

Linear Relationship		$\Delta G°_{calcd} = g\,\Delta G°_{tr} + e\,E_T(30) + a\,\alpha + b\,\beta + p\,\pi^*$ [a]			
g	e	a	b	p	R^2
-0.47			-41.92	0.44	0.9998

Entry	$\Delta G°_{exp}$	$\Delta G°_{calcd}$
36	-34.1	-33.59
60	-38.6	-38.64
61	-33.5	-33.59
62	-28.9	-28.45
63	-21.1	-21.06
70	-38.6	-38.64
71	-33.5	-33.59
72	-28.8	-28.45
73	-21.1	-21.06
74	-19.9	-19.22
105	-18.9	-19.22
106	-27.5	-28.45
107	-20.7	-21.06



[a] e, a, b, and p in kJ mol^{-1}.

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