

APPENDIX F

Experimental data from DCP studies of Pb(II)–Sarcosine–OH system

DCP data for Pb-Sarcosine-OH system from refinement by 3D-CFC

56 Experimental points																
Sarcosine	Lead	[LT]/[MT] = 401.627														
4	8	2004 Wednesday Date when experiment was performed														
Pbsar	Files recorded during the experiment															
DPP	DCT	ISE	0 indicators for mode of experiment													
DCT	EXPERIMENT															
OH-titrant	L-titrant	M-titrant	0 indicators for mode of titration													
Titration	with	protons														
No.:	pH	NaOH/ml	L-sol/ml	M-sol/ml	lp(obs)	lp(exp)	lp(corr)	Log[MF]	Log[LF]	Ep(obs)/mV	Init Ep/mV	Shift/mV	ECFC/mV	CCFC/mV	[LT]	[MT]
1	5.063	0	0	0	2.94	3.0298	0.970361	-4.221462	-6.43142	-454.86	-452.83	2.029999	2.416507	3.668172	0.03209	0.0000799
2	5.149	0.01	0	0	2.938	3.028792	0.970024	-4.222161	-6.345474	-454.89	-452.83	2.060028	2.451004	3.684575	3.21E-02	7.99E-05
3	5.273	0.02	0	0	2.932	3.027795	0.968365	-4.223338	-6.221516	-455.14	-452.83	2.310028	2.722993	3.715104	3.21E-02	7.98E-05
4	5.431	0.03	0	0	2.92	3.026778	0.964722	-4.225305	-6.063568	-455.49	-452.83	2.660004	3.121381	3.769025	3.21E-02	7.98E-05
5	5.625	0.04	0	0	2.899	3.025772	0.958103	-4.228803	-5.869644	-455.78	-452.83	2.950012	3.499842	3.868205	3.20E-02	7.98E-05
6	5.855	0.05	0	0	2.868	3.024767	0.948172	-4.235387	-5.63975	-456.14	-452.83	3.310028	3.993699	4.05871	3.20E-02	7.98E-05
7	6.096	0.06	0	0	2.829	3.023762	0.935589	-4.246944	-5.398895	-456.36	-452.83	3.529999	4.385291	4.396308	3.20E-02	7.97E-05
8	6.317	0.07	0	0	2.791	3.022758	0.923329	-4.264349	-5.178076	-457.06	-452.83	4.230011	5.254763	4.906854	3.20E-02	7.97E-05
9	6.518	0.08	0	0	2.754	3.021755	0.911391	-4.288889	-4.97729	-458.16	-452.83	5.330017	6.521946	5.628503	3.20E-02	7.97E-05
10	6.689	0.09	0	0	2.722	3.020752	0.9011	-4.319069	-4.806529	-458.82	-452.83	5.990021	7.327828	6.516959	3.20E-02	7.97E-05
11	6.832	0.1	0	0	2.694	3.01975	0.892127	-4.352922	-4.663786	-460.03	-452.83	7.200012	8.666387	7.514055	3.20E-02	7.96E-05
12	7.004	0.115	0	0	2.661	3.018249	0.881637	-4.40657	-4.492192	-461.45	-452.83	8.620026	10.23834	9.094563	3.20E-02	7.96E-05
13	7.15	0.13	0	0	2.632	3.016748	0.872463	-4.465175	-4.346632	-463.1	-452.83	10.27002	12.02272	10.8217	3.20E-02	7.96E-05
14	7.269	0.145	0	0	2.608	3.015249	0.864937	-4.52293	-4.228087	-464.26	-452.83	11.43002	13.29402	12.52368	3.19E-02	7.95E-05
15	7.371	0.16	0	0	2.586	3.013752	0.858067	-4.580073	-4.126559	-465.43	-452.83	12.60001	14.56645	14.20759	3.19E-02	7.95E-05
16	7.459	0.175	0	0	2.567	3.012257	0.852185	-4.635251	-4.039042	-467.57	-452.83	14.74002	16.79482	15.8337	3.19E-02	7.94E-05
17	7.538	0.19	0	0	2.55	3.010762	0.846962	-4.689506	-3.960544	-468.42	-452.83	15.99003	17.72381	17.43184	3.19E-02	7.94E-05
18	7.623	0.21	0	0	2.531	3.008772	0.841207	-4.75291	-3.876195	-471.07	-452.83	18.24002	20.46139	19.29884	3.19E-02	7.93E-05
19	7.696	0.23	0	0	2.514	3.006785	0.836109	-4.811521	-3.803852	-471.5	-452.83	18.67001	20.96947	21.02405	3.18E-02	7.93E-05
20	7.762	0.25	0	0	2.498	3.0048	0.831337	-4.867796	-3.738526	-472.76	-452.83	19.93002	22.30301	22.68019	3.18E-02	7.92E-05
21	7.832	0.275	0	0	2.481	3.002323	0.82636	-4.930872	-3.66936	-474.74	-452.83	21.91	24.36012	24.53538	3.18E-02	7.92E-05
22	7.893	0.3	0	0	2.466	2.99985	0.822041	-4.988658	-3.609195	-475.47	-452.83	22.64001	25.15745	26.2341	3.18E-02	7.91E-05
23	7.947	0.325	0	0	2.452	2.99738	0.818048	-5.04199	-3.556031	-477.15	-452.83	24.32001	26.9	27.80106	3.17E-02	7.90E-05
24	8.005	0.355	0	0	2.436	2.994423	0.813512	-5.101532	-3.499041	-478.63	-452.83	25.80002	28.45143	29.54983	0.0317153	7.90E-05
25	8.065	0.39	0	0	2.419	2.990979	0.808765	-5.16558	-3.440225	-480.63	-452.83	27.80002	30.52662	31.42937	3.17E-02	7.89E-05
26	8.119	0.425	0	0	2.404	2.987544	0.804674	-5.225345	-3.38742	-482.33	-452.83	29.5	32.29174	33.18244	3.16E-02	7.88E-05
27	8.173	0.465	0	0	2.387	2.983628	0.800033	-5.287116	-3.334775	-484.26	-452.83	31.43002	34.29608	34.99276	3.16E-02	7.87E-05
28	8.228	0.51	0	0	2.371	2.979234	0.795842	-5.352093	-3.281317	-486.55	-452.83	33.72	36.65352	36.89585	3.16E-02	7.86E-05
29	8.282	0.56	0	0	2.353	2.974367	0.791093	-5.41792	-3.229025	-488.02	-452.83	35.19	38.20042	38.82199	3.15E-02	7.84E-05
30	8.337	0.615	0	0	2.335	2.969032	0.786452	-5.487047	-3.17595	-490.55	-452.83	37.72	40.80601	40.84371	3.14E-02	7.83E-05
31	8.389	0.675	0	0	2.317	2.963234	0.781916	-5.554347	-3.126017	-492.41	-452.83	39.58002	42.74033	42.8093	3.14E-02	7.81E-05
32	8.44	0.74	0	0	2.298	2.956978	0.777145	-5.622207	-3.077272	-494.67	-452.83	41.84003	45.07896	44.78946	3.13E-02	7.80E-05
33	8.495	0.815	0	0	2.278	2.949792	0.772258	-5.697489	-3.024948	-496.51	-452.83	43.68002	47	46.98502	0.0312426	7.79E-05
34	8.546	0.895	0	0	2.258	2.942166	0.767462	-5.769261	-2.976759	-498.41	-452.83	45.58002	48.98002	49.07477	3.12E-02	7.76E-05
35	8.598	0.99	0	0	2.237	2.933161	0.762659	-5.844419	-2.928013	-500.72	-452.83	47.89001	51.37067	51.25855	3.11E-02	7.74E-05
36	8.648	1.09	0	0	2.216	2.92374	0.757933	-5.918836	-2.881474	-502.94	-452.83	50.11002	53.67051	53.41256	3.10E-02	7.71E-05
37	8.699	1.205	0	0	2.194	2.912982	0.75318	-5.996354	-2.834424	-505.43	-452.83	52.60001	56.24132	55.66407	3.09E-02	7.68E-05
38	8.748	1.33	0	0	2.171	2.901378	0.748265	-6.072998	-2.789671	-507.73	-452.83	54.90002	58.62544	57.87993	3.07E-02	7.65E-05
39	8.797	1.47	0	0	2.148	2.88849	0.743641	-6.151657	-2.745396	-509.5	-452.83	56.67001	60.47507	60.14944	3.06E-02	7.62E-05
40	8.846	1.62	0	0	2.124	2.874808	0.738832	-6.23247	-2.701557	-511.78	-452.83	58.95001	62.83841	62.4789	3.04E-02	7.58E-05
41	8.897	1.805	0	0	2.098	2.858112	0.734051	-6.318867	-2.656671	-513.94	-452.83	61.11002	65.08181	64.95967	3.03E-02	7.54E-05
42	8.947	1.99	0	0	2.071	2.841608	0.728813	-6.406174	-2.613096	-516.48	-452.83	63.64999	67.17379	67.46782	3.01E-02	7.49E-05
43	8.996	2.22	0	0	2.044	2.821353	0.724475	-6.494018	-2.571447	-518.54	-452.83	65.70999	69.85048	69.97434	2.99E-02	7.44E-05
44	9.047	2.465	0	0	2.014	2.800093	0.719262	-6.588428	-2.528633	-521.36	-452.83	68.53	72.76326	72.66982	2.97E-02	7.38E-05
45	9.096	2.725	0	0	1.984	2.777879	0.714214	-6.682028	-2.488307	-524.05	-452.83	71.22	75.54374	75.33616	2.94E-02	7.33E-05
46	9.147	3.01	0	0	1.952	2.753931	0.708805	-6.782791	-2.447071	-526.91	-452.83	74.07999	78.50138	78.20547	2.92E-02	7.28E-05
47	9.197	3.33	0	0	1.92	2.727528	0.703934	-6.884799	-2.407766	-529.45	-452.83	76.62003	81.13	81.09913	0.0288885	7.19E-05
48	9.248	3.7	0	0	1.885	2.697624	0.698763	-6.99228	-2.368887	-532.49	-452.83	79.66	84.2647	84.13676	2.86E-02	7.11E-05
49	9.299	4.09	0	0	1.849	2.666806	0.693339	-7.103619	-2.330973	-535.08	-452.83	82.25003	86.95484	87.28254	2.82E-02	7.03E-05
50	9.35	4.51	0	0	1.811	2.634395	0.687444	-7.218779	-2.294204	-538.02	-452.83	85.19003	90.00452	90.53188	2.79E-02	6.95E-05
51	9.399	4.935	0	0	1.773	2.602391	0.681297	-7.333083	-2.259921	-541.23	-452.83	88.39999	93.32988	93.75594	2.76E-02	6.88E-05
52	9.45	5.44	0	0	1.732	2.565358	0.675149	-7.455269	-2.225874	-544.1	-452.83	91.26999	96.31631	97.18607	2.72E-02	6.77E-05
53	9.499	5.935	0	0	1.691	2.530068	0.668362	-7.576158	-2.194161	-547.61	-452.83	94.78	99.95513	100.584	2.68E-02	6.67E-05
54	9.55	6.505	0	0	1.646	2.490614	0.660891	-7.704783	-2.162784	-551.51	-452.83	98.68002	104.0007	104.1868	2.64E-02	6.57E-05
55	9.601	7.08	0	0	1.6	2.452043	0.652517	-7.83647	-2.132516	-555.75	-452.83	102.92	108.4044	107.8816	2.60E-02	6.47E-05
56	9.651	7.685	0	0	1.553	2.412727	0.64367	-7.967863	-2.104395	-559.83	-452.83	107	112.6597	111.5546	0.0255543	6.38E-05

0.437448 Overall fit of CCFC in ECFC/mV

ini-VT/ml ini-LT/M ini-MT/M ini-Ep/mV ini-lp
30.048 0.03209 7.99E-05 -4.53E+02 3.0298

2 No. of protonation constants

LogKa: