APPENDIX E

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

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

74 Experimental points
Glycine Pb(II) [LT]/[MT] = 800.6698
25 10 2003 Saturday Date when experiment was performed
pbgcl Files recorded during the experiment
DPP DCT ISE
0 1 0 indicators for mode of experiment
DCT EXPERIMENT
OH-titrant L-titrant M-titrant
1 0 0 indicaters for mode of titration

Titration No.:	with pH	protons NaOH/ml	L-sol/ml	M-sol/ml	Ip(obs)	Ip(exp)	Ip(corr)	Log[MF]	Log[LF]	Ep(obs)/mV	Init Ep/mV	Shift/mV	ECFC/mV	CCFC/mV	[LT]	[MT]
1	5.243	0.015	0	0	1.992	2.041881	0.975571	-4.31341	-5.48817	-376.74	-371.43	5.309998	5.627715	6.496849	6.45E-02	8.06E-05
2	5.317	0.03	0	0	1.995	2.040862	0.977528	-4.31975	-5.4143	-376.98	-371.43	5.550018	5.841995	6.677871	6.45E-02	8.05E-05
3	5.36	0.04	0	0	1.991	2.040184	0.975892	-4.32391	-5.3714	-377.23	-371.43	5.800018	6.113508	6.796553	6.45E-02	8.05E-05
4	5.413	0.05	0	0	1.98	2.039506	0.970823	-4.32953	-5.3185	-377.42	-371.43	5.990021	6.370413	6.958683	6.44E-02	8.05E-05
5	5.469	0.06	0	0	1.979	2.038829	0.970655	-4.33616	-5.2626	-377.81	-371.43	6.380005	6.762619	7.15046	6.44E-02	8.05E-05
6	5.536	0.07	0	0	1.984	2.038152	0.973431	-4.3451	-5.1957	-378.15	-371.43	6.720001	7.065935	7.410832	6.44E-02	8.04E-05
7	5.61	0.08	0	0	1.976	2.037475	0.969828	-4.35644	-5.12182	-378.51	-371.43	7.080017	7.47359	7.74196	0.0643786	8.04E-05
8	5.691	0.09	0	0	1.965	2.036799	0.964749	-4.37084	-5.04093	-378.9	-371.43	7.470001	7.931024	8.163488	6.44E-02	8.04E-05
9	5.778	0.1	0	0	1.966	2.036124	0.96556	-4.38892	-4.95406	-379.67	-371.43	8.240021	8.690246	8.693963	6.43E-02	8.04E-05
10	5.869	0.11	0	0	1.955	2.035449	0.960476	-4.4111	-4.86321	-380.39	-371.43	8.960022	9.478065	9.345909	6.43E-02	8.03E-05
11	5.963	0.12	0	0	1.95	2.034774	0.958338	-4.43795	-4.76936	-381.28	-371.43	9.850006	10.39669	10.13593	6.43E-02	8.03E-05
12	6.056	0.13	0	0	1.941	2.0341	0.95423	-4.46887	-4.67653	-382.43	-371.43	11	11.60185	11.04614	6.43E-02	8.03E-05
13	6.145	0.14	0	0	1.928	2.033426	0.948154	-4.50284	-4.5877	-383.37	-371.43	11.94	12.62393	12.04692	6.43E-02	8.02E-05
14	6.227	0.15	0	0	1.921	2.032753	0.945024	-4.53819	-4.50589	-384.52	-371.43	13.09	13.81639	13.08808	6.42E-02	8.02E-05
15	6.305	0.16	0	0	1.913	2.03208	0.9414	-4.57554	-4.42808	-385.71	-371.43	14.28	15.05575	14.18887	0.0642081	8.02E-05
16	6.38	0.17	0	0	1.905	2.031407	0.937774	-4.61499	-4.35328	-386.81	-371.43	15.38	16.20534	15.35133	6.42E-02	8.02E-05
17	6.449	0.18	0	0	1.895	2.030735	0.93316	-4.65436	-4.28448	-387.84	-371.43	16.41	17.2987	16.51164	6.42E-02	8.01E-05
18	6.51	0.19	0	0	1.891	2.030063	0.931498	-4.69162	-4.22369	-388.94	-371.43	17.51001	18.4216	17.60975	0.0641444	8.01E-05
19	6.57	0.2	0	0	1.873	2.029392	0.922936	-4.73051	-4.1639	-389.96	-371.43	18.53	19.56021	18.75579	6.41E-02	8.01E-05
20	6.624	0.21	0	0	1.859	2.028722	0.916341	-4.76738	-4.11011	-390.89	-371.43	19.46002	20.58237	19.84208	0.064102	8.01E-05
21	6.673	0.22	0	0	1.853	2.028051	0.913685	-4.80234	-4.06133	-391.92	-371.43	20.49002	21.64965	20.872	6.41E-02	8.00E-05
22	6.72	0.23	0	0	1.837	2.027382	0.906095	-4.8372	-4.01455	-392.75	-371.43	21.32001	22.58681	21.89881	6.41E-02	8.00E-05
23	6.761	0.24	0	0	1.822	2.026712	0.898993	-4.86864	-3.97376	-393.53	-371.43	22.10001	23.46789	22.82475	6.40E-02	8.00E-05
24	6.802	0.25	0	0	1.808	2.026043	0.89238	-4.90104	-3.93298	-394.38	-371.43	22.95001	24.41274	23.77875	6.40E-02	8.00E-05
25	6.872	0.265	0	0	1.798	2.025041	0.887883	-4.95849	-3.86335	-395.87	-371.43	24.44	25.96763	25.47177	6.40E-02	7.99E-05
26	6.932	0.28	0	0	1.789	2.024039	0.883876	-5.00984	-3.80371	-397.06	-371.43	25.63	27.21574	26.98435	6.40E-02	7.99E-05
27	6.985	0.295	0	0	1.776	2.023039	0.877887	-5.05678	-3.75108	-398.3	-371.43	26.87	28.54307	28.36645	6.39E-02	7.98E-05
28	7.033	0.31	0	0	1.762	2.022039	0.871398	-5.10055	-3.70344	-399.4	-371.43	27.97	29.73839	29.6547	6.39E-02	7.98E-05
29	7.078	0.325	0	0	1.741	2.02104	0.861438	-5.14265	-3.65881	-400.41	-371.43	28.98001	30.89608	30.8937	6.39E-02	7.98E-05
30	7.135	0.345	0	0	1.734	2.019711	0.858539	-5.19745	-3.60232	-401.88	-371.43	30.45001	32.40938	32.50626	6.38E-02	7.97E-05
31	7.189	0.365	0	0	1.7	2.018382	0.842259	-5.25088	-3.54884	-403.02	-371.43	31.59	33.79531	34.0783	0.0637753	7.97E-05
32	7.241	0.385	0	0	1.679	2.017056	0.832401	-5.30373	-3.49738	-404.36	-371.43	32.92999	35.28654	35.63308	6.37E-02	7.96E-05
33	7.285	0.405	0	0	1.662	2.015731	0.824515	-5.34952	-3.45391	-405.47	-371.43	34.04001	36.51885	36.97917	6.37E-02	7.95E-05
34	7.328	0.425	0	0	1.643	2.014408	0.815624	-5.39524	-3.41146	-406.62	-371.43	35.19	37.80811	38.32305	6.36E-02	7.95E-05
35	7.38	0.45	0	0	1.622	2.012757	0.80586	-5.45182	-3.36016	-408.1	-371.43	36.67001	39.44284	39.98616	6.36E-02	7.94E-05
36	7.426	0.475	0	0	1.606	2.011108	0.798565	-5.50307	-3.31486	-409.2	-371.43	37.77002	40.65967	41.49177	6.35E-02	7.94E-05
37	7.471	0.5	0	0	1.573	2.009463	0.782796	-5.55434	-3.27059	-410.21	-371.43	38.78	41.92585	42.99766	6.35E-02	7.93E-05
38	7.519	0.53	0	0	1.55	2.007491	0.772108	-5.61027	-3.22346	-411.67	-371.43	40.24002	43.56248	44.63955	6.34E-02	7.92E-05
39	7.563	0.565	0	0	1.531	2.005196	0.763516	-5.6627	-3.18041	-413.15	-371.43	41.72	45.18621	46.1756	6.34E-02	7.91E-05
40	7.61	0.6	0	0	1.514	2.002906	0.755902	-5.71998	-3.13444	-414.62	-371.43	43.19	46.78498	47.85538	6.33E-02	7.90E-05
41	7.652	0.635	0	0	1.483	2.000621	0.74127	-5.77231	-3.09346	-416.05	-371.43	44.62	48.46608	49.38859	0.0632141	7.90E-05
42	7.694	0.675	0	0	1.455	1.998016	0.728222	-5.82574	-3.05261	-417.79	-371.43	46.36002	50.43423	50.95223	0.0631318	7.88E-05
43	7.738	0.72	0	0	1.447	1.995094	0.725279	-5.88293	-3.00991	-419.48	-371.43	48.05002	52.17626	52.62511	6.30E-02	7.87E-05
44	7.778	0.765	0	0	1.417	1.992181	0.711281	-5.93602	-2.97121	-420.86	-371.43	49.42999	53.80659	54.17686	0.0629474	7.86E-05
45	7.819	0.815	0	0	1.378	1.988953	0.692827	-5.99156	-2.93166	-422.65	-371.43	51.22	55.9343	55.79886	6.28E-02	7.85E-05
46	7.858	0.87	0	0	1.345	1.985415	0.67744	-6.04544	-2.89421	-423.45	-371.43	52.02002	57.02283	57.36969	6.27E-02	7.84E-05
47	7.911	0.96	0	0	1.307	1.979652	0.660217	-6.1203	-2.84365	-425.68	-371.43	54.25	59.58364	59.54663	6.26E-02	7.81E-05
48	7.966	1.05	0	0	1.264	1.973923	0.640349	-6.20015	-2.79127	-427.89	-371.43	56.46002	62.18618	61.87149	6.24E-02	7.79E-05
49	8.014	1.14	0	0	1.219	1.968227	0.619339	-6.27158	-2.74587	-429.45	-371.43	58.02002	64.17474	63.94719	6.22E-02	7.77E-05
50	8.057	1.23	0	0	1.196	1.962563	0.609407	-6.33694	-2.70545	-431.09	-371.43	59.66	66.02241	65.84361	6.20E-02	7.74E-05
51	8.114	1.35	0	0	1.157	1.955063	0.591797	-6.42569	-2.65207	-432.75	-371.43	61.32001	68.0591	68.41966	6.18E-02	7.72E-05
52	8.162	1.47	0	0	1.113	1.947619	0.571467	-6.50212	-2.60758	-434.69	-371.43	63.26001	70.44817	70.63127	6.15E-02	7.69E-05
53	8.203	1.59	0	0	1.068	1.940232	0.55045	-6.56855	-2.56998	-436.56	-371.43	65.13	72.79954	72.54741	6.13E-02	7.66E-05
54	8.253	1.74	0	0	1.039	1.931077	0.538042	-6.65112	-2.52439	-438.58	-371.43	67.14999	75.11241	74.92913	6.10E-02	7.62E-05
55	8.294	1.89	0	0	0.998	1.922007	0.519249	-6.71981	-2.48756	-440.73	-371.43	69.30002	77.71916	76.90041	6.07E-02	7.58E-05
56	8.342	2.07	0	0	0.959	1.911235	0.50177	-6.80155	-2.44474	-442.4	-371.43	70.97	79.82903	79.24628	6.04E-02	7.54E-05
57	8.402	2.33	0	0	0.904	1.895888	0.476821	-6.90529	-2.39209	-445.24	-371.43	73.81	83.32419	82.21122	5.99E-02	7.48E-05
58	8.464	2.63	0	0	0.859	1.878483	0.457284	-7.01417	-2.33863	-447.87	-371.43	76.44	86.49165	85.31344	5.94E-02	7.41E-05
59	8.537	3.03	0	0	0.819	1.855767	0.441327	-7.14409	-2.27706	-450.05	-371.43	78.62	89.12793	89.00017	5.86E-02	7.32E-05
60	8.596	3.43	0	0	0.779	1.833594	0.424849	-7.24953	-2.22898	-452.71	-371.43	81.28	92.27677	91.9645	0.0579365	7.24E-05
61	8.652	3.83	0	0	0.739	1.811945	0.407849	-7.35022	-2.18423	-455.59	-371.43	84.16	95.68137	94.79038	5.73E-02	7.15E-05
62	8.704	4.23	0	0	0.708	1.7908	0.395354	-7.44384	-2.14363	-457.12	-371.43	85.69	97.61109	97.40888	5.66E-02	7.07E-05
63	8.788	4.93	0	0	0.664	1.754962	0.378356	-7.59471	-2.08009	-460.5	-371.43	89.07001	101.5556	101.612	5.55E-02	6.93E-05
64	8.839	5.53	0	0	0.644	1.725366	0.373254	-7.68345	-2.04456	-462.45	-371.43	91.02002	103.6801	104.0182	5.45E-02	6.81E-05
65	8.892	6.13	0	0	0.602	1.696751	0.354796	-7.77555	-2.0081	-464.5	-371.43	93.07001	106.3816	106.5279	5.36E-02	6.70E-05
66	8.942	6.73	0	0	0.576	1.66907	0.345102	-7.86122	-1.97488	-466.46	-371.43	95.03	108.6974	108.8505	0.052738	6.59E-05
67	9.014	7.63	0	0	0.543	1.629202	0.333292	-7.98233	-1.9289	-468.73	-371.43	97.30002	111.4148	112.1225	5.15E-02	6.43E-05
68	9.076	8.53	0	0	0.512	1.591193	0.321771	-8.08257	-1.8922	-471	-371.43	99.57001	114.1367	114.7841	5.03E-02	6.28E-05
69	9.172	10.13	0	0	0.463	1.527828	0.303045	-8.22972	-1.84051	-474.51	-371.43	103.08	118.417	118.6148	4.83E-02	6.03E-05
70	9.257	11.73	0	0	0.423	1.469315	0.287889	-8.35141	-1.79978	-476.92	-371.43	105.49	121.4861	121.7127	4.64E-02	5.80E-05
71	9.338	13.33	0	0	0.393	1.41512	0.277715	-8.46059	-1.7646	-478.84	-371.43	107.41	123.8682	124.4594	4.47E-02	5.58E-05
72	9.415	14.93	0	0	0.373	1.36478	0.273304	-8.55778	-1.73468	-481.87	-371.43	110.44	127.1039	126.8692	4.31E-02	5.39E-05
73	9.486	16.53	0	0	0.352	1.317898	0.267092	-8.64092	-1.71072	-483.81	-371.43	112.38	129.3393	128.8793	4.16E-02	5.20E-05
74	9.556	18.13	0	0	0.313	1.27413	0.245658	-8.71845	-1.68962	-484.17	-371.43	112.74	130.774	130.7389	0.040259	5.03E-05

0.3374033 Overall fit of CCFC in ECFC/mV

ini-VT/ml	ini-LT/M	ini-MT/M	ini-Ep/mV	ini-Ip
30.048	0.06455	8.06E-05	-3.71E+02	2.0429

2 No. of protonation constants
LogKa:
9.54
2.39

4 No. of ML and M(HL) complexes

Log(Beta)	M	L	H	Refined	RefInd
10.456	1	1	1	1	1
3.49E-02	Stand. deviation in Log(beta)				
1.22E-03	COVAR for this log				
4.582	1	1	0	1	1
1.27E-02	Stand. deviation in Log(beta)				
1.61E-04	COVAR for this log				
7.289	1	2	0	1	1
3.21E-02	Stand. deviation in Log(beta)				
1.03E-03	COVAR for this log				
9.256	1	3	0	1	1
5.13E-02	Stand. deviation in Log(beta)				
2.63E-03	COVAR for this log				

8	No. of MOH and ML(OH) complexes					
Log(Beta)	M	L	OH	Refined	RefInd	
6	1	0	1	0	0	
10.3	1	0	2	0	0	
13.3	1	0	3	0	0	
7.6	2	0	1	0	0	
31.7	3	0	4	0	0	
35.1	4	0	4	0	0	
67.4	6	0	8	0	0	
15.01351	1	2	2	1	0	
0	Stand. deviation in Log(beta)					
0.3290193	COVAR for this log					
Temp.	I-strength	pKw	SLOPE	n-ELECTRONS		
25	0.5	13.74	29.57985	2		
AMAX	APOS	ANEG				
6	1	6				
Software	indicators					
1	1	1	1	1	1	
0						