

APPENDIX G

Experimental data from GEP and DCP studies of Zn(II)–Glycine–OH
system

GEP data for Zn-Glycine-OH system

TASK	ZBAR		1 TITRATION	ZN(11)	WITH	GLY0	L:M	6 GEP						
MODL	ZN+2	GLY0	H		1									
CPLX		0	0	-13.74 H	+1(	-1)								
CPLX		0	0	-9.14 ZN+2(	1)	H	+1(	-1)						
CPLX		0	0	-16.38 ZN+2(	1)	H	+1(	-2)						
CPLX		0	0	-27.62 ZN+2(	1)	H	+1(	-3)						
CPLX		0	0	-40.16 ZN+2(	1)	H	+1(	-4)						
CPLX		0	0	-8.74 ZN+2(	2)	H	+1(	-1)						
CPLX		0	0	-27.06 ZN+2(	4)	H	+1(	-4)						
CPLX		0	0	10.69 ZN+2(	1)	GLY0(	1)	H	+1(	1)				
CPLX		0	0	9.54 GLY0(	1)	H	+1(	1)						
CPLX		0	0	11.93 GLY0(	1)	H	+1(	2)						
CPLX	1		0	4.843 ZN+2(	1)	GLY0(	1)							
CPLX	1		0	9.076 ZN+2(	1)	GLY0(	2)							
CPLX	1		0	11.38 ZN+2(	1)	GLY0(	3)							
CONC														
VESL	IVOL		25.5	0	0									
VESL	H		1	0.0000001	0	1								
VESL	ZN+2		0.0010961	0	0									
VESL	GLY0		0.0067257	1	0									
BUR1	H		1	-0.0517473	0	0								
ELEC														
ZERO	H		1	411.04	0									
GRAD	H		1	58.634	0									
DATA														
EMF	PH			ZBAR(H)		POINT		PA			ZBAR(M)			POINT
OBS	OBS	CALC	RESID	OBS	CALC	RESID	RESID	OBS	CALC	RESID	OBS	CALC	RESID	RESID
101	5.288	5.144	0.144	1	1	0	0.144	6.426	6.571	-0.145	0.01	0.02	-0.005	0.145
81.7	5.617	5.557	0.06	0.99	0.99	0	0.06	6.099	6.159	-0.06	0.04	0.04	-0.001	0.06
68.7	5.839	5.816	0.022	0.99	0.99	0	0.022	5.88	5.902	-0.022	0.08	0.08	0	0.022
66	5.885	5.866	0.019	0.99	0.99	0	0.019	5.835	5.854	-0.019	0.08	0.09	0	0.019
63.4	5.929	5.911	0.018	0.98	0.98	0	0.018	5.791	5.809	-0.018	0.09	0.09	0	0.018
61	5.97	5.952	0.017	0.98	0.98	0	0.017	5.751	5.768	-0.017	0.1	0.1	0	0.017
58.9	6.006	5.991	0.015	0.98	0.98	0	0.015	5.716	5.73	-0.015	0.11	0.11	0	0.015
56.9	6.04	6.027	0.013	0.98	0.98	0	0.013	5.682	5.695	-0.013	0.12	0.12	0	0.013
54.9	6.074	6.061	0.013	0.98	0.98	0	0.013	5.649	5.662	-0.013	0.13	0.13	0	0.013
53	6.106	6.092	0.014	0.98	0.98	0	0.014	5.617	5.632	-0.014	0.14	0.14	0	0.014
51.3	6.135	6.122	0.013	0.98	0.98	0	0.013	5.589	5.602	-0.013	0.15	0.15	0	0.013
49.6	6.164	6.15	0.014	0.97	0.97	0	0.014	5.561	5.575	-0.014	0.16	0.16	0	0.014
48	6.192	6.177	0.014	0.97	0.97	0	0.014	5.534	5.549	-0.014	0.17	0.17	0	0.014
46.5	6.217	6.203	0.014	0.97	0.97	0	0.014	5.509	5.524	-0.014	0.17	0.17	0	0.014
45.1	6.241	6.227	0.014	0.97	0.97	0	0.014	5.486	5.5	-0.014	0.18	0.18	0	0.014
43.8	6.263	6.251	0.012	0.97	0.97	0	0.012	5.465	5.477	-0.012	0.19	0.19	0	0.012
42.4	6.287	6.274	0.014	0.97	0.97	0	0.014	5.442	5.455	-0.014	0.2	0.2	0	0.014
41.3	6.306	6.295	0.011	0.97	0.97	0	0.011	5.424	5.434	-0.011	0.21	0.21	0	0.011
40.1	6.326	6.316	0.01	0.96	0.96	0	0.01	5.404	5.414	-0.01	0.22	0.22	0	0.01
38.9	6.347	6.336	0.01	0.96	0.96	0	0.01	5.384	5.395	-0.01	0.23	0.23	0	0.01
37.8	6.366	6.356	0.01	0.96	0.96	0	0.01	5.366	5.376	-0.01	0.24	0.24	0	0.01
36.7	6.384	6.375	0.009	0.96	0.96	0	0.009	5.348	5.358	-0.009	0.25	0.25	0	0.009
35.6	6.403	6.393	0.01	0.96	0.96	0	0.01	5.33	5.34	-0.01	0.26	0.26	0	0.01
34.6	6.42	6.411	0.009	0.96	0.96	0	0.009	5.314	5.323	-0.009	0.26	0.26	0	0.009
33.6	6.437	6.429	0.009	0.95	0.95	0	0.009	5.298	5.306	-0.009	0.27	0.27	0	0.009
32.6	6.454	6.446	0.009	0.95	0.95	0	0.009	5.282	5.29	-0.009	0.28	0.28	0	0.009
31.6	6.471	6.462	0.009	0.95	0.95	0	0.009	5.265	5.275	-0.009	0.29	0.29	0	0.009
30.6	6.488	6.478	0.01	0.95	0.95	0	0.01	5.249	5.259	-0.01	0.3	0.3	0	0.01
29.7	6.504	6.494	0.01	0.95	0.95	0	0.01	5.234	5.244	-0.01	0.31	0.31	0	0.01
28.8	6.519	6.509	0.01	0.95	0.95	0	0.01	5.22	5.23	-0.01	0.32	0.32	0	0.01
27.9	6.534	6.524	0.01	0.95	0.95	0	0.01	5.205	5.215	-0.01	0.33	0.33	0	0.01
26.9	6.551	6.539	0.013	0.94	0.94	0	0.013	5.189	5.202	-0.013	0.34	0.34	0	0.013
26.1	6.565	6.553	0.012	0.94	0.94	0	0.012	5.176	5.188	-0.012	0.35	0.35	0	0.012
25.2	6.58	6.567	0.013	0.94	0.94	0	0.013	5.161	5.175	-0.013	0.36	0.36	0	0.013
24.4	6.594	6.581	0.013	0.94	0.94	0	0.013	5.149	5.161	-0.013	0.36	0.36	0	0.013
23.6	6.608	6.595	0.013	0.94	0.94	0	0.013	5.136	5.149	-0.013	0.37	0.37	0	0.013
22.8	6.621	6.608	0.013	0.94	0.94	0	0.013	5.123	5.136	-0.013	0.38	0.38	0	0.013
22	6.635	6.621	0.014	0.94	0.94	0	0.014	5.11	5.124	-0.014	0.39	0.39	0	0.014
21.3	6.647	6.634	0.013	0.93	0.93	0	0.013	5.099	5.112	-0.013	0.4	0.4	0	0.013
20.5	6.661	6.647	0.014	0.93	0.93	0	0.014	5.086	5.1	-0.014	0.41	0.41	0	0.014
19.8	6.673	6.659	0.013	0.93	0.93	0	0.013	5.075	5.088	-0.013	0.42	0.42	0	0.013
19.1	6.685	6.672	0.013	0.93	0.93	0	0.013	5.064	5.076	-0.013	0.43	0.43	0	0.013
18.3	6.698	6.684	0.014	0.93	0.93	0	0.014	5.051	5.065	-0.014	0.44	0.44	0	0.014
17.6	6.71	6.696	0.014	0.93	0.93	0	0.014	5.04	5.054	-0.014	0.45	0.45	0	0.014
16.9	6.722	6.708	0.014	0.92	0.92	0	0.014	5.029	5.043	-0.014	0.45	0.45	0	0.014
16.2	6.734	6.719	0.015	0.92	0.92	0	0.015	5.017	5.032	-0.015	0.46	0.46	0	0.015
15.5	6.746	6.731	0.015	0.92	0.92	0	0.015	5.006	5.021	-0.015	0.47	0.47	0	0.015
14.9	6.756	6.742	0.014	0.92	0.92	0	0.014	4.997	5.011	-0.014	0.48	0.48	0	0.014
14.2	6.768	6.753	0.015	0.92	0.92	0	0.015	4.986	5	-0.015	0.49	0.49	0	0.015
13.5	6.78	6.764	0.016	0.92	0.92	0	0.016	4.975	4.99	-0.016	0.5	0.5	0	0.016
12.9	6.79	6.775	0.015	0.92	0.92	0	0.015	4.965	4.98	-0.015	0.51	0.51	0	0.015
12.2	6.802	6.786	0.016	0.91	0.91	0	0.016	4.954	4.97	-0.016	0.52	0.52	0	0.016
11.6	6.812	6.797	0.016	0.91	0.91	0	0.016	4.945	4.96	-0.016	0.53	0.53	0	0.016
10.9	6.824	6.807	0.017	0.91	0.91	0	0.017	4.933	4.95	-0.017	0.54	0.54	0	0.017
10.3	6.835	6.818	0.017	0.91	0.91	0	0.017	4.924	4.941	-0.017	0.54	0.54	0	0.017
9.7	6.845	6.828	0.017	0.91	0.91	0	0.017	4.915	4.931	-0.017	0.55	0.55	0	0.017
9.1	6.855	6.839	0.016	0.91	0.91	0	0.016	4.905	4.922	-0.016	0.56	0.56	0	0.016
8.5	6.865	6.849	0.017	0.9	0.9	0	0.017	4.896	4.912	-0.017	0.57	0.57	0	0.017
7.9	6.876	6.859	0.017	0.9	0.9	0	0.017	4.886	4.903	-0.017	0.58	0.58	0	0.017
7.4	6.884	6.869	0.015	0.9	0.9	0	0.015	4.879	4.894	-0.015	0.59	0.59	0	0.015
6.8	6.894	6.879	0.016	0.9	0.9	0	0.016	4.869	4.885	-0.016	0.6	0.6	0	0.016
6.3	6.903	6.889	0.014	0.9	0.9	0	0.014	4.861	4.876	-0.014	0.61	0.61	0	0.014
5.7	6.913	6.898	0.015	0.9	0.9	0	0.015	4.852	4.867	-0.015	0.62	0.62	0	0.015
5.1	6.923	6.908	0.015	0.9	0.9	0	0.015	4.843	4.858	-0.015	0.63	0.63	0	0.015
4.6	6.932	6.918	0.014	0.89	0.89	0	0.014	4.835	4.849	-0.014	0.63	0.63	0	0.014
4	6.942	6.927	0.015	0.89	0.89	0	0.015	4.825	4.84	-0.015	0.64	0.64	0	0.015

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3.5	6.951	6.937	0.014	0.89	0.89	0	0.014	4.818	4.832	-0.014	0.65	0.65	0	0.014
2.9	6.961	6.946	0.015	0.89	0.89	0	0.015	4.808	4.823	-0.015	0.66	0.66	0	0.015
2.4	6.969	6.955	0.014	0.89	0.89	0	0.014	4.801	4.814	-0.014	0.67	0.67	0	0.014
1.8	6.98	6.965	0.015	0.89	0.89	0	0.015	4.791	4.806	-0.015	0.68	0.68	-0.001	0.015
1.3	6.988	6.974	0.014	0.89	0.89	0	0.014	4.783	4.798	-0.014	0.69	0.69	-0.001	0.014
0.7	6.998	6.983	0.015	0.88	0.88	0	0.015	4.774	4.789	-0.015	0.7	0.7	-0.001	0.015
0	7.01	6.992	0.018	0.88	0.88	0	0.018	4.763	4.781	-0.018	0.71	0.71	-0.001	0.018
0	7.01	7.001	0.009	0.88	0.88	0	0.009	4.764	4.773	-0.009	0.72	0.72	0	0.009
-0.7	7.022	7.01	0.012	0.88	0.88	0	0.012	4.753	4.765	-0.012	0.72	0.72	0	0.012
-1.3	7.032	7.019	0.013	0.88	0.88	0	0.013	4.743	4.756	-0.013	0.73	0.73	-0.001	0.013
-1.8	7.041	7.028	0.013	0.88	0.88	0	0.013	4.736	4.748	-0.013	0.74	0.74	-0.001	0.013
-2.3	7.049	7.037	0.012	0.87	0.87	0	0.012	4.728	4.74	-0.012	0.75	0.75	0	0.012
-2.8	7.058	7.046	0.012	0.87	0.87	0	0.012	4.72	4.732	-0.012	0.76	0.76	0	0.012
-3.3	7.067	7.055	0.012	0.87	0.87	0	0.012	4.712	4.724	-0.012	0.77	0.77	0	0.012
-3.8	7.075	7.064	0.012	0.87	0.87	0	0.012	4.705	4.716	-0.012	0.78	0.78	0	0.012
-4.3	7.084	7.072	0.011	0.87	0.87	0	0.011	4.697	4.708	-0.011	0.79	0.79	0	0.011
-4.8	7.092	7.081	0.011	0.87	0.87	0	0.011	4.689	4.701	-0.011	0.8	0.8	0	0.011
-5.2	7.099	7.09	0.009	0.87	0.87	0	0.009	4.683	4.693	-0.009	0.8	0.8	0	0.009
-5.7	7.107	7.098	0.009	0.86	0.86	0	0.009	4.676	4.685	-0.009	0.81	0.81	0	0.009
-6.2	7.116	7.107	0.009	0.86	0.86	0	0.009	4.668	4.677	-0.009	0.82	0.82	0	0.009
-6.7	7.125	7.115	0.009	0.86	0.86	0	0.009	4.66	4.67	-0.009	0.83	0.83	0	0.009
-7.2	7.133	7.124	0.009	0.86	0.86	0	0.009	4.653	4.662	-0.009	0.84	0.84	0	0.009
-7.8	7.143	7.132	0.011	0.86	0.86	0	0.011	4.643	4.654	-0.011	0.85	0.85	-0.001	0.011
-8.3	7.152	7.141	0.011	0.86	0.86	0	0.011	4.636	4.647	-0.011	0.86	0.86	-0.001	0.011
-8.8	7.16	7.149	0.011	0.86	0.86	0	0.011	4.628	4.639	-0.011	0.87	0.87	-0.001	0.011
-9.3	7.169	7.158	0.011	0.85	0.85	0	0.011	4.62	4.631	-0.011	0.88	0.88	-0.001	0.011
-9.8	7.177	7.166	0.011	0.85	0.85	0	0.011	4.613	4.624	-0.011	0.88	0.88	-0.001	0.011
-10.3	7.186	7.175	0.011	0.85	0.85	0	0.011	4.605	4.616	-0.011	0.89	0.89	-0.001	0.011
-10.8	7.194	7.183	0.011	0.85	0.85	0	0.011	4.597	4.609	-0.011	0.9	0.9	-0.001	0.011
-11.2	7.201	7.191	0.01	0.85	0.85	0	0.01	4.591	4.601	-0.01	0.91	0.91	-0.001	0.01
-11.7	7.21	7.2	0.01	0.85	0.85	0	0.01	4.584	4.594	-0.01	0.92	0.92	-0.001	0.01
-12.2	7.218	7.208	0.01	0.84	0.84	0	0.01	4.576	4.586	-0.01	0.93	0.93	-0.001	0.01
-12.7	7.227	7.216	0.011	0.84	0.84	0	0.011	4.568	4.579	-0.011	0.94	0.94	-0.001	0.011
-13.1	7.234	7.225	0.009	0.84	0.84	0	0.009	4.562	4.571	-0.009	0.95	0.95	-0.001	0.009
-13.6	7.242	7.233	0.009	0.84	0.84	0	0.009	4.555	4.564	-0.009	0.96	0.96	-0.001	0.009
-14	7.249	7.241	0.008	0.84	0.84	0	0.008	4.549	4.557	-0.008	0.96	0.96	0	0.008
-14.5	7.258	7.249	0.008	0.84	0.84	0	0.008	4.541	4.549	-0.008	0.97	0.97	-0.001	0.008
-15	7.266	7.258	0.008	0.84	0.84	0	0.008	4.533	4.542	-0.008	0.98	0.98	-0.001	0.008
-15.4	7.273	7.266	0.007	0.83	0.83	0	0.007	4.527	4.534	-0.007	0.99	0.99	0	0.007
-15.9	7.281	7.274	0.007	0.83	0.83	0	0.007	4.52	4.527	-0.007	1	1	0	0.007
-16.4	7.29	7.282	0.008	0.83	0.83	0	0.008	4.512	4.52	-0.008	1.01	1.01	-0.001	0.008
-16.9	7.298	7.291	0.008	0.83	0.83	0	0.008	4.504	4.512	-0.008	1.02	1.02	-0.001	0.008
-17.3	7.305	7.299	0.007	0.83	0.83	0	0.007	4.498	4.505	-0.007	1.03	1.03	0	0.007
-17.8	7.314	7.307	0.007	0.83	0.83	0	0.007	4.491	4.498	-0.007	1.03	1.03	0	0.007
-18.3	7.322	7.315	0.007	0.83	0.83	0	0.007	4.483	4.49	-0.007	1.04	1.04	-0.001	0.007
-18.9	7.333	7.323	0.009	0.82	0.82	0	0.009	4.474	4.483	-0.009	1.05	1.05	-0.001	0.009
-19.4	7.341	7.332	0.01	0.82	0.82	0	0.01	4.466	4.476	-0.01	1.06	1.06	-0.001	0.01
-19.8	7.348	7.34	0.008	0.82	0.82	0	0.008	4.46	4.468	-0.008	1.07	1.07	-0.001	0.008
-20.3	7.356	7.348	0.009	0.82	0.82	0	0.009	4.453	4.461	-0.009	1.08	1.08	-0.001	0.009
-20.8	7.365	7.356	0.009	0.82	0.82	0	0.009	4.445	4.454	-0.009	1.09	1.09	-0.001	0.009
-21.3	7.374	7.364	0.009	0.82	0.82	0	0.009	4.437	4.446	-0.009	1.09	1.1	-0.001	0.009
-21.7	7.38	7.373	0.008	0.81	0.81	0	0.008	4.431	4.439	-0.008	1.1	1.1	-0.001	0.008
-22.2	7.389	7.381	0.008	0.81	0.81	0	0.008	4.424	4.432	-0.008	1.11	1.11	-0.001	0.008
-22.6	7.396	7.389	0.007	0.81	0.81	0	0.007	4.418	4.425	-0.007	1.12	1.12	-0.001	0.007
-23.1	7.404	7.397	0.007	0.81	0.81	0	0.007	4.41	4.417	-0.007	1.13	1.13	-0.001	0.007
-23.6	7.413	7.405	0.007	0.81	0.81	0	0.007	4.403	4.41	-0.007	1.14	1.14	-0.001	0.007
-24	7.42	7.414	0.006	0.81	0.81	0	0.006	4.397	4.403	-0.006	1.15	1.15	-0.001	0.006
-24.5	7.428	7.422	0.006	0.81	0.81	0	0.006	4.389	4.395	-0.006	1.16	1.16	-0.001	0.006
-24.9	7.435	7.43	0.005	0.8	0.8	0	0.005	4.383	4.388	-0.005	1.16	1.16	0	0.005
-25.4	7.443	7.438	0.005	0.8	0.8	0	0.005	4.375	4.38	-0.005	1.17	1.17	0	0.005
-25.9	7.452	7.447	0.005	0.8	0.8	0	0.005	4.368	4.373	-0.005	1.18	1.18	0	0.005
-26.4	7.461	7.455	0.006	0.8	0.8	0	0.006	4.36	4.366	-0.006	1.19	1.19	-0.001	0.006
-26.8	7.467	7.463	0.004	0.8	0.8	0	0.004	4.354	4.358	-0.004	1.2	1.2	0	0.004
-27.3	7.476	7.472	0.004	0.8	0.8	0	0.004	4.347	4.351	-0.004	1.21	1.21	0	0.004
-27.8	7.484	7.48	0.005	0.79	0.79	0	0.005	4.339	4.344	-0.005	1.22	1.22	0	0.005
-28.2	7.491	7.488	0.003	0.79	0.79	0	0.003	4.333	4.336	-0.003	1.22	1.22	0	0.003
-28.7	7.5	7.497	0.003	0.79	0.79	0	0.003	4.325	4.329	-0.003	1.23	1.23	0	0.003
-29.2	7.508	7.505	0.003	0.79	0.79	0	0.003	4.318	4.321	-0.003	1.24	1.24	0	0.003
-29.7	7.517	7.513	0.004	0.79	0.79	0	0.004	4.31	4.314	-0.004	1.25	1.25	0	0.004
-31.6	7.549	7.547	0.002	0.78	0.78	0	0.002	4.281	4.284	-0.002	1.28	1.28	0	0.002
-33.6	7.583	7.581	0.002	0.78	0.78	0	0.002	4.251	4.253	-0.002	1.32	1.32	0	0.002
-35.7	7.619	7.615	0.004	0.77	0.77	0	0.004	4.219	4.223	-0.004	1.35	1.35	-0.001	0.004
-37.8	7.655	7.65	0.005	0.76	0.76	0	0.005	4.187	4.192	-0.005	1.38	1.38	-0.001	0.005
-39.9	7.691	7.685	0.006	0.76	0.76	0	0.006	4.155	4.16	-0.006	1.41	1.42	-0.001	0.006
-42	7.727	7.721	0.006	0.75	0.75	0	0.006	4.123	4.129	-0.006	1.45	1.45	-0.001	0.006
-44	7.761	7.757	0.004	0.75	0.75	0	0.004	4.092	4.096	-0.004	1.48	1.48	-0.001	0.004
-46.2	7.798	7.794	0.005	0.74	0.74	0	0.005	4.059	4.063	-0.005	1.51	1.51	-0.001	0.005
-48.4	7.836	7.831	0.005	0.73	0.73	0	0.005	4.025	4.03	-0.005	1.54	1.54	-0.001	0.005
-50.7	7.875	7.868	0.007	0.73	0.73	0	0.007	3.99	3.996	-0.007	1.57	1.57	-0.001	0.007
-52.9	7.912	7.907	0.006	0.72	0.72	0	0.006	3.956	3.962	-0.006	1.6	1.6	-0.001	0.006
-55	7.948	7.945	0.003	0.72	0.72	0	0.003	3.924	3.927	-0.003	1.63	1.63	-0.001	0.003
-57.4	7.989	7.984	0.005	0.71	0.71	0	0.005	3.887	3.892	-0.005	1.65	1.65	-0.001	0.005
-59.7	8.028	8.024	0.005	0.7	0.7	0	0.005	3.852	3.857	-0.005	1.68	1.68	-0.002	0.005
-62	8.068	8.063	0.005	0.7	0.7	0	0.005	3.817	3.822	-0.005	1.7	1.71	-0.002	0.005
-64.3	8.107	8.103	0.004	0.69	0.69	0	0.004	3.782	3.786	-0.004	1.73	1.73	-0.002	0.004
-66.5	8.144	8.142	0.002	0.69	0.69	0	0.002	3.748	3.751	-0.002	1.75	1.75	-0.001	0.002
-68.8	8.184	8.182												

APPENDIX G

-75.5	8.298	8.298	0	0.66	0.66	0	0	3.612	3.612	0	1.84	1.84	0	0
-77.6	8.334	8.335	-0.002	0.66	0.66	0	0.002	3.58	3.578	0.002	1.86	1.86	0.001	0.002
-79.8	8.371	8.372	-0.001	0.65	0.65	0	0.001	3.547	3.546	0.001	1.87	1.87	0.001	0.001
-81.8	8.405	8.408	-0.003	0.64	0.64	0	0.003	3.517	3.515	0.003	1.89	1.89	0.002	0.003
-83.9	8.441	8.443	-0.002	0.64	0.64	0	0.002	3.486	3.484	0.002	1.9	1.9	0.001	0.002
-85.9	8.475	8.477	-0.002	0.63	0.63	0	0.002	3.456	3.455	0.002	1.92	1.92	0.001	0.002
-87.8	8.508	8.51	-0.002	0.63	0.63	0	0.002	3.428	3.426	0.002	1.93	1.93	0.002	0.003
-89.6	8.538	8.542	-0.003	0.62	0.62	0	0.003	3.402	3.399	0.003	1.95	1.94	0.003	0.004
-91.5	8.571	8.573	-0.002	0.61	0.61	0	0.002	3.374	3.372	0.002	1.96	1.96	0.002	0.003
-93.3	8.601	8.603	-0.001	0.61	0.61	0	0.001	3.348	3.347	0.001	1.97	1.97	0.001	0.002
-95.1	8.632	8.632	0	0.6	0.6	0	0	3.322	3.322	0	1.98	1.98	0	0.001
-96.7	8.659	8.66	0	0.6	0.6	0	0	3.299	3.299	0	1.99	1.99	0.001	0.001
-98.3	8.687	8.687	-0.001	0.59	0.59	0	0.001	3.276	3.276	0.001	2	2	0.001	0.001
-99.8	8.712	8.714	-0.001	0.59	0.59	0	0.001	3.256	3.254	0.001	2.01	2.01	0.002	0.002
-101.4	8.74	8.74	0	0.58	0.58	0	0	3.233	3.233	0	2.02	2.02	0	0
-102.9	8.765	8.765	0.001	0.57	0.57	0	0.001	3.212	3.213	-0.001	2.03	2.03	-0.001	0.001
-104.3	8.789	8.789	0	0.57	0.57	0	0	3.193	3.193	0	2.04	2.04	0	0
-105.6	8.811	8.813	-0.001	0.56	0.56	0	0.001	3.176	3.175	0.001	2.05	2.05	0.002	0.002
-107	8.835	8.836	0	0.56	0.56	0	0	3.157	3.157	0	2.06	2.05	0.001	0.001
-108.4	8.859	8.858	0.001	0.55	0.55	0	0.001	3.138	3.139	-0.001	2.06	2.06	-0.002	0.002
-109.6	8.879	8.88	-0.001	0.54	0.54	0	0.001	3.123	3.122	0.001	2.07	2.07	0.001	0.001
-110.9	8.902	8.901	0	0.54	0.54	0	0	3.106	3.106	0	2.08	2.08	0	0
-112.1	8.922	8.922	0	0.53	0.53	0	0	3.09	3.09	0	2.09	2.09	0	0
-113.3	8.943	8.943	0	0.53	0.53	0	0	3.075	3.075	0	2.09	2.09	0	0
-114.5	8.963	8.963	0	0.52	0.52	0	0	3.06	3.06	0	2.1	2.1	0	0.001
-115.7	8.984	8.982	0.001	0.51	0.51	0	0.001	3.045	3.046	-0.001	2.11	2.11	-0.002	0.002
-116.8	9.002	9.002	0.001	0.51	0.51	0	0.001	3.031	3.032	-0.001	2.11	2.12	-0.001	0.001
-118	9.023	9.021	0.002	0.5	0.5	0	0.002	3.016	3.018	-0.002	2.12	2.12	-0.005	0.005
-119.2	9.043	9.039	0.004	0.5	0.5	0	0.004	3.001	3.005	-0.004	2.12	2.13	-0.009	0.01
-120.4	9.064	9.057	0.006	0.49	0.49	0	0.006	2.986	2.992	-0.006	2.12	2.14	-0.015	0.016
-121.5	9.082	9.075	0.007	0.48	0.48	0	0.007	2.973	2.98	-0.007	2.13	2.14	-0.018	0.019
-122.6	9.101	9.093	0.008	0.48	0.48	0	0.008	2.96	2.968	-0.008	2.13	2.15	-0.021	0.023
-123.6	9.118	9.11	0.008	0.47	0.47	0	0.008	2.948	2.957	-0.008	2.14	2.16	-0.021	0.022
-124.7	9.137	9.127	0.01	0.47	0.47	0	0.01	2.935	2.945	-0.01	2.14	2.16	-0.026	0.028
-125.7	9.154	9.144	0.01	0.46	0.46	0	0.01	2.924	2.934	-0.01	2.14	2.17	-0.027	0.029
-126.7	9.171	9.161	0.01	0.46	0.46	0	0.01	2.913	2.923	-0.01	2.15	2.18	-0.029	0.031
-127.7	9.188	9.177	0.011	0.45	0.45	0	0.011	2.902	2.913	-0.011	2.15	2.18	-0.032	0.034
-128.7	9.205	9.193	0.012	0.44	0.44	0	0.012	2.891	2.903	-0.012	2.16	2.19	-0.035	0.037
-129.7	9.222	9.209	0.013	0.44	0.44	0	0.013	2.88	2.893	-0.013	2.16	2.2	-0.039	0.041
-130.6	9.238	9.225	0.012	0.43	0.43	0	0.012	2.871	2.883	-0.013	2.17	2.2	-0.039	0.041
-131.6	9.255	9.241	0.014	0.43	0.43	0	0.014	2.86	2.874	-0.014	2.17	2.21	-0.044	0.046
-132.5	9.27	9.256	0.014	0.42	0.42	0	0.014	2.851	2.865	-0.014	2.17	2.22	-0.045	0.047
-133.4	9.285	9.272	0.014	0.41	0.41	0	0.014	2.842	2.856	-0.014	2.18	2.23	-0.046	0.048
-134.3	9.301	9.287	0.014	0.41	0.41	0	0.014	2.833	2.847	-0.014	2.19	2.23	-0.047	0.049
-135.2	9.316	9.302	0.014	0.4	0.4	0	0.014	2.824	2.838	-0.014	2.19	2.24	-0.049	0.051
-136.1	9.331	9.317	0.015	0.4	0.4	0	0.015	2.815	2.83	-0.015	2.2	2.25	-0.052	0.054
-136.9	9.345	9.332	0.013	0.39	0.39	0	0.013	2.808	2.822	-0.014	2.21	2.25	-0.048	0.05
-137.7	9.359	9.346	0.012	0.39	0.38	0	0.012	2.802	2.814	-0.013	2.22	2.26	-0.045	0.047
-138.6	9.374	9.361	0.013	0.38	0.38	0	0.013	2.793	2.807	-0.013	2.22	2.27	-0.049	0.051
-139.4	9.388	9.375	0.012	0.37	0.37	0	0.012	2.787	2.799	-0.012	2.23	2.28	-0.047	0.049
-140.2	9.401	9.39	0.011	0.37	0.37	0	0.011	2.78	2.792	-0.012	2.24	2.28	-0.045	0.046
-141	9.415	9.404	0.011	0.36	0.36	0	0.011	2.774	2.785	-0.011	2.25	2.29	-0.043	0.044
-141.9	9.43	9.418	0.012	0.36	0.36	0	0.012	2.766	2.778	-0.012	2.25	2.3	-0.048	0.05
-142.7	9.444	9.433	0.011	0.35	0.35	0	0.011	2.759	2.771	-0.012	2.26	2.31	-0.047	0.049
-143.5	9.458	9.447	0.011	0.34	0.34	0	0.011	2.753	2.764	-0.011	2.27	2.32	-0.046	0.047
-144.3	9.471	9.461	0.011	0.34	0.34	0	0.011	2.747	2.758	-0.011	2.28	2.33	-0.045	0.047
-145.1	9.485	9.475	0.01	0.33	0.33	0	0.01	2.741	2.752	-0.011	2.29	2.34	-0.045	0.046
-145.8	9.497	9.488	0.008	0.33	0.33	0	0.008	2.737	2.746	-0.009	2.31	2.35	-0.037	0.038
-146.6	9.511	9.502	0.008	0.32	0.32	0	0.008	2.732	2.74	-0.008	2.32	2.36	-0.037	0.038
-147.4	9.524	9.516	0.008	0.32	0.32	0	0.008	2.726	2.734	-0.008	2.33	2.37	-0.037	0.038
-148.2	9.538	9.53	0.008	0.31	0.31	0	0.008	2.721	2.729	-0.008	2.34	2.38	-0.037	0.038
-148.9	9.55	9.543	0.006	0.3	0.3	0	0.006	2.717	2.724	-0.007	2.36	2.39	-0.029	0.03
-149.7	9.563	9.557	0.006	0.3	0.3	0	0.006	2.712	2.719	-0.007	2.37	2.4	-0.03	0.031
-150.5	9.577	9.571	0.006	0.29	0.29	0	0.006	2.707	2.714	-0.007	2.38	2.41	-0.031	0.031
-151.2	9.589	9.584	0.005	0.29	0.29	0	0.005	2.704	2.709	-0.005	2.4	2.42	-0.023	0.024
-152	9.603	9.598	0.005	0.28	0.28	0	0.005	2.699	2.704	-0.005	2.41	2.44	-0.024	0.025
-152.7	9.615	9.611	0.003	0.28	0.28	0	0.003	2.696	2.7	-0.004	2.43	2.45	-0.017	0.017
-153.5	9.628	9.625	0.004	0.27	0.27	0	0.004	2.692	2.696	-0.004	2.44	2.46	-0.018	0.019
-154.2	9.64	9.638	0.002	0.26	0.26	0	0.002	2.69	2.692	-0.002	2.47	2.48	-0.011	0.011
-155	9.654	9.651	0.002	0.26	0.26	0	0.002	2.686	2.688	-0.003	2.48	2.49	-0.013	0.013
-155.7	9.666	9.665	0.001	0.25	0.25	0	0.001	2.684	2.685	-0.001	2.5	2.51	-0.005	0.005
-156.5	9.679	9.678	0.001	0.25	0.25	0	0.001	2.68	2.681	-0.001	2.52	2.53	-0.007	0.007
-157.2	9.691	9.691	0	0.24	0.24	0	0	2.678	2.678	0	2.54	2.54	0	0
-158	9.705	9.705	0	0.24	0.24	0	0	2.675	2.675	0	2.56	2.56	-0.002	0.002
-158.8	9.719	9.718	0.001	0.23	0.23	0	0.001	2.672	2.673	-0.001	2.58	2.58	-0.005	0.005
-159.6	9.732	9.731	0.001	0.23	0.23	0	0.001	2.669	2.671	-0.001	2.6	2.6	-0.007	0.007
-160.4	9.746	9.744	0.002	0.22	0.22	0	0.002	2.667	2.668	-0.002	2.62	2.63	-0.01	0.01
-161.2	9.76	9.757	0.002	0.21	0.21	0	0.002	2.664	2.667	-0.002	2.64	2.65	-0.013	0.013
-162	9.773	9.77	0.003	0.21	0.21	0	0.003	2.662	2.665	-0.003	2.66	2.67	-0.016	0.016
-162.9	9.789	9.783	0.005	0.2	0.2	0	0.005	2.658	2.664	-0.006	2.67	2.7	-0.03	0.03
-163.7	9.802	9.796	0.006	0.2	0.2	0	0.006	2.657	2.663	-0.006	2.69	2.73	-0.033	0.034
-164.5	9.816	9.809	0.006	0.19	0.19	0	0.006	2.655	2.662	-0.007	2.72	2.76	-0.037	0.038
-165.3	9.829	9.822	0.007	0.19	0.19	0	0.007	2.654	2.662	-0.008	2.75	2.79	-0.042	0.043
-166.1	9.843	9.835	0.008	0.18	0.18	0	0.008	2.654	2.662	-0.009	2.77	2.82	-0.046	0.047
-166.9	9.857	9.848	0.008	0.18	0.18	0	0.008	2.653	2.663	-0.01	2.8	2.85	-0.051	0.052
-167.7	9.87	9.861	0.009	0.17	0.17	0	0.009	2.653	2.664	-0.01	2.83	2.89	-0.057	0.057
-168.4	9.882	9.874	0.008	0.17	0.17	0	0.008	2.656	2.665</					

DCP data for Zn-Glycine-OH system from refinement by 3D-CFC (From $E'_{1/2}$ data below pH 7.5)

27 Experimental points																																
Glycine	Zinc	[L]/[MT] = 242.0317																														
17	6	2004 Thursday Date when experiment was performed																														
zng-	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 indicators 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[L/F]	Ep(obs)/mV	IniEp/mV	Shift/mV	ECFC/mV	CCFC/mV	[LT]	[MT]																
1	4.876	0.02	0	0	2.875	3.026586	0.949915	-3.9833	-6.25136	-982.6	-982.6	-2.44E-05	0.66006	0.400909	2.59E-02	1.07E-04																
2	4.953	0.03	0	0	2.846	3.025381	0.940708	-3.98616	-6.17431	-982.6	-982.6	-2.44E-05	0.785183	0.480273	2.59E-02	1.07E-04																
3	5.02	0.038	0	0	2.823	3.024417	0.933403	-3.98907	-6.1073	-982.8	-982.6	0.199988	1.085343	0.562229	2.59E-02	1.07E-04																
4	5.102	0.046	0	0	2.816	3.023455	0.931385	-3.99326	-6.02528	-982.3	-982.6	-0.30001	0.613146	0.682226	2.59E-02	1.07E-04																
5	5.194	0.054	0	0	2.821	3.022492	0.933336	-3.99901	-5.93329	-982.4	-982.6	-0.19998	0.686303	0.848335	0.025914	1.07E-04																
6	5.304	0.062	0	0	2.818	3.02153	0.93264	-4.00774	-5.82331	-982.2	-982.6	-0.39999	0.495871	1.102394	2.59E-02	1.07E-04																
7	5.437	0.07	0	0	2.8	3.020569	0.926978	-4.02188	-5.69038	-982.4	-982.6	-0.19998	0.774117	1.516621	2.59E-02	1.07E-04																
8	5.586	0.078	0	0	2.77	3.019609	0.917337	-4.04427	-5.54152	-983.3	-982.6	0.699988	1.808378	2.17461	2.59E-02	1.07E-04																
9	5.749	0.086	0	0	2.763	3.018649	0.91531	-4.08024	-5.37875	-984.9	-982.6	2.300025	3.436835	3.23472	2.59E-02	1.07E-04																
10	5.911	0.094	0	0	2.761	3.01769	0.914938	-4.13335	-5.21709	-987.1	-982.6	4.499976	5.642006	4.801613	2.59E-02	1.07E-04																
11	6.06	0.102	0	0	2.953	3.016731	0.978874	-4.2036	-5.06852	-989.4	-982.6	6.800025	7.074324	6.875414	2.59E-02	1.07E-04																
12	6.198	0.11	0	0	2.988	3.015773	0.990791	-4.29237	-4.93102	-992.1	-982.6	9.499975	9.618829	9.497325	2.59E-02	1.07E-04																
13	6.315	0.118	0	0	3.001	3.014816	0.995417	-4.38869	-4.81452	-994.8	-982.6	12.19999	12.25899	12.34213	2.58E-02	1.07E-04																
14	6.425	0.126	0	0	3.005	3.013859	0.997061	-4.49823	-4.70502	-998.5	-982.6	15.9	15.93781	15.57846	2.58E-02	1.07E-04																
15	6.527	0.134	0	0	2.982	3.012902	0.989743	-4.61631	-4.60352	-1001.9	-982.6	19.30002	19.43246	19.06702	2.58E-02	1.07E-04																
16	6.641	0.144	0	0	2.958	3.011708	0.982167	-4.76595	-4.49009	-1005.9	-982.6	23.30002	23.53118	23.48848	2.58E-02	1.07E-04																
17	6.748	0.154	0	0	2.923	3.010514	0.97093	-4.92153	-4.38364	-1010.3	-982.6	27.69999	28.07896	28.08519	2.58E-02	1.07E-04																
18	6.85	0.164	0	0	2.87	3.009322	0.953703	-5.08138	-4.28217	-1014.1	-982.6	31.49998	32.10893	32.80848	2.58E-02	1.07E-04																
19	6.923	0.174	0	0	2.806	3.00813	0.932805	-5.20154	-4.20962	-1017.8	-982.6	35.19999	36.09357	36.35792	2.58E-02	1.07E-04																
20	7.01	0.184	0	0	2.769	3.006939	0.92087	-5.35001	-4.12313	-1021.3	-982.6	38.69999	39.759	40.74456	2.58E-02	1.07E-04																
21	7.091	0.194	0	0	2.734	3.00575	0.90959	-5.49248	-4.04264	-1025.8	-982.6	43.20005	44.4174	44.95358	2.58E-02	1.06E-04																
22	7.166	0.204	0	0	2.716	3.004561	0.903959	-5.62736	-3.96817	-1029.9	-982.6	47.30003	48.59715	48.93842	2.58E-02	1.06E-04																
23	7.236	0.214	0	0	2.652	3.003373	0.883007	-5.75537	-3.89871	-1033.4	-982.6	50.80003	52.3984	52.71995	2.58E-02	1.06E-04																
24	7.309	0.226	0	0	2.632	3.001949	0.876764	-5.89065	-3.82635	-1037.3	-982.6	54.70005	56.38958	56.71516	2.57E-02	1.06E-04																
25	7.377	0.238	0	0	2.593	3.000526	0.864182	-6.01799	-3.75902	-1041.3	-982.6	58.70005	60.57527	60.47583	2.57E-02	1.06E-04																
26	7.44	0.25	0	0	2.561	2.999105	0.853922	-6.1369	-3.69671	-1045	-982.6	62.4	64.42866	63.98717	2.57E-02	1.06E-04																
27	7.503	0.264	0	0	2.561	2.997448	0.854394	-6.25652	-3.63451	-1050	-982.6	67.4	69.42156	67.51842	2.57E-02	1.06E-04																

0.329294 Overall fit of CCFC in ECFC/mV

ini-VT/ml	ini-LT/M	ini-MT/M	ini-Ep/mV	ini-IP
25.08	0.02597	1.07E-04	-982.6	3.029

2 No. of protonation constants

LogKa:
9.54
2.39

3 No. of ML and M(HL) complexes

Log(Beta)	M	L	H	Refined	RefInd
4.737	1	1	0	1	1
4.72E-02	Stand. deviation in Log(beta)				
2.23E-03	COVAR for this log				
9.516	1	2	0	1	1
1.60E-02	Stand. deviation in Log(beta)				
2.55E-04	COVAR for this log				
10.5	1	3	0	0	0

7 No. of MOH and ML(OH) complexes

Log(Beta)	M	L	OH	Refined	RefInd
4.7	1	0	1	0	0
11.1	1	0	2	0	0
13.6	1	0	3	0	0
14.8	1	0	4	0	0
5	2	0	1	0	0
27.9	4	0	4	0	0
9.85	1	1	1	0	0

Temp.	I-strength	pKw	SLOPE	n-ELECTRONS
25	0.5	13.74	29.58	2

AMAX	APOS	ANEG
4	1	4

Software	indicators				
1	1	1	1	1	1
0					