

APPENDIX B

Experimental data from GEP studies of the protonation equilibria of the
ligand Glycine

GEP titration raw Data from *Autotitrator VI* used in GEP experiment for Protonation Constants for Glycine

Start date&time 04-Nov-03 02:55:55
PARAMETERS SET

Pause time for Equilibration(s) 45
Max.time of equilibration (min) 5
Sampling rate of pH meter(s) 1
Max. # readings to Save 20
Criterion of Stability 0.15
STOP CONDITIONS
Stop pH 12
Stop mV -260
Stop Volume(mL) 30

COMMENT Determination of Protonation consts.:Glycine
0.0594g Glycine in 14.008ml HNO3(−0.05M) i and 30mL 0.5M NaNO3
Titrant:−0.05M NaOH

Volume increment (mL)	Total Vol. Added (mL)	Final reading (mV)	FinalStd Dev	pH	T(°C)	Total #readings	Elapsed Time(s)	Comment	Last readings (mV)
0.1	0	280.4	0.04216	2.219	25.9	10	10 Not Timed-out		280.4
0.1	0.1	280	0	2.225	25.9	10	10 Not Timed-out		280
0.1	0.2	279.7	0	2.23	25.9	10	10 Not Timed-out		279.7
0.1	0.3	279.4	0	2.236	25.9	10	10 Not Timed-out		279.4
0.1	0.4	279.1	0.04216	2.241	25.9	10	10 Not Timed-out		279.1
0.1	0.5	278.7	0	2.247	25.9	10	10 Not Timed-out		278.7
0.1	0.6	278.4	0	2.253	25.9	10	10 Not Timed-out		278.4
0.1	0.7	278.1	0.04216	2.258	25.9	10	10 Not Timed-out		278
0.1	0.8	277.7	0	2.264	25.9	10	10 Not Timed-out		277.7
0.1	0.9	277.4	0	2.27	25.9	10	10 Not Timed-out		277.4
0.1	1	277	0.05164	2.277	25.9	10	10 Not Timed-out		277
0.1	1.1	276.7	0	2.282	25.9	10	10 Not Timed-out		276.7
0.1	1.2	276.4	0	2.287	25.9	10	10 Not Timed-out		276.4
0.1	1.3	276	0	2.294	25.9	10	10 Not Timed-out		276
0.1	1.4	275.7	0	2.299	25.9	10	10 Not Timed-out		275.7
0.1	1.5	275.3	0	2.305	25.9	10	10 Not Timed-out		275.3
0.1	1.6	275	0	2.311	25.9	10	10 Not Timed-out		275
0.1	1.7	274.6	0	2.317	25.9	10	10 Not Timed-out		274.6
0.1	1.8	274.3	0	2.323	25.9	10	10 Not Timed-out		274.3
0.1	1.9	273.9	0	2.329	25.9	10	10 Not Timed-out		273.9
0.1	2	273.6	0	2.335	25.9	10	10 Not Timed-out		273.6
0.1	2.1	273.2	0	2.34	25.9	10	10 Not Timed-out		273.2
0.1	2.2	272.9	0.03162	2.347	25.9	10	10 Not Timed-out		272.9
0.1	2.3	272.5	0	2.353	25.9	10	10 Not Timed-out		272.5
0.1	2.4	272.1	0	2.36	25.9	10	10 Not Timed-out		272.1
0.1	2.5	271.8	0.03162	2.366	25.9	10	10 Not Timed-out		271.8
0.1	2.6	271.4	0	2.371	25.9	10	10 Not Timed-out		271.4
0.1	2.7	271	0	2.378	25.9	10	10 Not Timed-out		271
0.1	2.8	270.7	0	2.384	25.9	10	10 Not Timed-out		270.7
0.1	2.9	270.3	0	2.39	25.9	10	10 Not Timed-out		270.3
0.1	3	269.9	0.03162	2.397	25.9	10	10 Not Timed-out		269.9
0.1	3.1	269.6	0.03162	2.403	25.9	10	10 Not Timed-out		269.6
0.1	3.2	269.2	0	2.41	25.9	10	10 Not Timed-out		269.2
0.1	3.3	268.8	0	2.415	25.9	10	10 Not Timed-out		268.8
0.1	3.4	268.4	0	2.422	25.9	10	10 Not Timed-out		268.4
0.1	3.5	268	0	2.429	25.9	10	10 Not Timed-out		268
0.1	3.6	267.7	0.04216	2.435	25.9	10	10 Not Timed-out		267.7
0.1	3.7	267.3	0	2.442	25.9	10	10 Not Timed-out		267.3
0.1	3.8	266.9	0	2.448	25.9	10	10 Not Timed-out		266.9
0.1	3.9	266.5	0	2.454	25.9	10	10 Not Timed-out		266.5
0.1	4	266.1	0	2.461	25.9	10	10 Not Timed-out		266.1
0.1	4.1	265.7	0	2.468	25.9	10	10 Not Timed-out		265.7
0.1	4.2	265.3	0	2.475	25.9	10	10 Not Timed-out		265.3
0.1	4.3	264.9	0	2.481	25.9	10	10 Not Timed-out		264.9

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0.1	4.4		264.5	0	2.488	25.9	10	10	Not Timed-out	264.5	264.5	264.5	264.5	264.5	264.5	264.5	264.5	264.5	264.5
0.1	4.5		264.1	0	2.495	25.9	10	10	Not Timed-out	264.1	264.1	264.1	264.1	264.1	264.1	264.1	264.1	264.1	264.1
0.1	4.6		263.7	0	2.502	25.9	10	10	Not Timed-out	263.7	263.7	263.7	263.7	263.7	263.7	263.7	263.7	263.7	263.7
0.1	4.7		263.3	0	2.509	25.9	10	10	Not Timed-out	263.3	263.3	263.3	263.3	263.3	263.3	263.3	263.3	263.3	263.3
0.1	4.8		262.9	0	2.516	25.9	10	10	Not Timed-out	262.9	262.9	262.9	262.9	262.9	262.9	262.9	262.9	262.9	262.9
0.1	4.9		262.5	0	2.523	25.9	10	10	Not Timed-out	262.5	262.5	262.5	262.5	262.5	262.5	262.5	262.5	262.5	262.5
0.1	5		262.1	0.05164	2.53	25.9	10	10	Not Timed-out	262	262	262	262	262	262	262	262	262	262
0.1	5.1		261.6	0	2.537	25.9	10	10	Not Timed-out	261.6	261.6	261.6	261.6	261.6	261.6	261.6	261.6	261.6	261.6
0.1	5.2		261.2	0	2.544	25.9	10	10	Not Timed-out	261.2	261.2	261.2	261.2	261.2	261.2	261.2	261.2	261.2	261.2
0.1	5.3		260.8	0	2.552	25.9	10	10	Not Timed-out	260.8	260.8	260.8	260.8	260.8	260.8	260.8	260.8	260.8	260.8
0.1	5.4		260.4	0.03162	2.559	25.9	10	10	Not Timed-out	260.4	260.4	260.3	260.4	260.4	260.4	260.4	260.4	260.4	260.4
0.1	5.5		259.9	0	2.566	25.9	10	10	Not Timed-out	259.9	259.9	259.9	259.9	259.9	259.9	259.9	259.9	259.9	259.9
0.1	5.6		259.5	0	2.574	25.9	10	10	Not Timed-out	259.5	259.5	259.5	259.5	259.5	259.5	259.5	259.5	259.5	259.5
0.1	5.7		259	0.05164	2.581	25.9	10	10	Not Timed-out	259	259	259	259	259	259	259	259	259	259
0.1	5.8		258.6	0	2.589	25.9	10	10	Not Timed-out	258.6	258.6	258.6	258.6	258.6	258.6	258.6	258.6	258.6	258.6
0.1	5.9		258.2	0.03162	2.597	25.9	10	10	Not Timed-out	258.2	258.2	258.1	258.2	258.2	258.2	258.2	258.2	258.2	258.2
0.1	6		257.7	0	2.604	25.9	10	10	Not Timed-out	257.7	257.7	257.7	257.7	257.7	257.7	257.7	257.7	257.7	257.7
0.1	6.1		257.3	0.04216	2.612	25.9	10	10	Not Timed-out	257.3	257.3	257.2	257.3	257.3	257.3	257.3	257.3	257.3	257.3
0.1	6.2		256.8	0	2.619	26	10	10	Not Timed-out	256.8	256.8	256.8	256.8	256.8	256.8	256.8	256.8	256.8	256.8
0.1	6.3		256.3	0	2.627	26	10	10	Not Timed-out	256.3	256.3	256.3	256.3	256.3	256.3	256.3	256.3	256.3	256.3
0.1	6.4		255.9	0	2.635	26	10	10	Not Timed-out	255.9	255.9	255.9	255.9	255.9	255.9	255.9	255.9	255.9	255.9
0.1	6.5		255.4	0	2.643	26	10	10	Not Timed-out	255.4	255.4	255.4	255.4	255.4	255.4	255.4	255.4	255.4	255.4
0.1	6.6		254.9	0	2.652	26	10	10	Not Timed-out	254.9	254.9	254.9	254.9	254.9	254.9	254.9	254.9	254.9	254.9
0.1	6.7		254.4	0.0483	2.659	26	10	10	Not Timed-out	254.4	254.4	254.4	254.4	254.4	254.4	254.4	254.4	254.4	254.4
0.1	6.8		254	0	2.668	26	10	10	Not Timed-out	254	254	254	254	254	254	254	254	254	254
0.1	6.9		253.5	0	2.676	26	10	10	Not Timed-out	253.5	253.5	253.5	253.5	253.5	253.5	253.5	253.5	253.5	253.5
0.1	7		253	0	2.684	26	10	10	Not Timed-out	253	253	253	253	253	253	253	253	253	253
0.1	7.1		252.5	0	2.692	26	10	10	Not Timed-out	252.5	252.5	252.5	252.5	252.5	252.5	252.5	252.5	252.5	252.5
0.1	7.2		252	0	2.701	26	10	10	Not Timed-out	252	252	252	252	252	252	252	252	252	252
0.1	7.3		251.5	0	2.709	26	10	10	Not Timed-out	251.5	251.5	251.5	251.5	251.5	251.5	251.5	251.5	251.5	251.5
0.1	7.4		251	0	2.718	26	10	10	Not Timed-out	251	251	251	251	251	251	251	251	251	251
0.1	7.5		250.4	0.03162	2.728	26	10	10	Not Timed-out	250.4	250.4	250.4	250.4	250.4	250.4	250.4	250.4	250.4	250.4
0.1	7.6		249.9	0	2.737	26	10	10	Not Timed-out	249.9	249.9	249.9	249.9	249.9	249.9	249.9	249.9	249.9	249.9
0.1	7.7		249.4	0	2.745	26	10	10	Not Timed-out	249.4	249.4	249.4	249.4	249.4	249.4	249.4	249.4	249.4	249.4
0.1	7.8		248.9	0.0483	2.755	26	10	10	Not Timed-out	248.9	248.9	248.9	248.9	248.9	248.9	248.9	248.9	248.9	248.9
0.1	7.9		248.3	0	2.764	26	10	10	Not Timed-out	248.3	248.3	248.3	248.3	248.3	248.3	248.3	248.3	248.3	248.3
0.1	8		247.8	0	2.773	26	10	10	Not Timed-out	247.8	247.8	247.8	247.8	247.8	247.8	247.8	247.8	247.8	247.8
0.1	8.1		247.2	0	2.783	26	10	10	Not Timed-out	247.2	247.2	247.2	247.2	247.2	247.2	247.2	247.2	247.2	247.2
0.1	8.2		246.6	0	2.793	26	10	10	Not Timed-out	246.6	246.6	246.6	246.6	246.6	246.6	246.6	246.6	246.6	246.6
0.1	8.3		246.1	0	2.802	26	10	10	Not Timed-out	246.1	246.1	246.1	246.1	246.1	246.1	246.1	246.1	246.1	246.1
0.1	8.4		245.5	0	2.811	26	10	10	Not Timed-out	245.5	245.5	245.5	245.5	245.5	245.5	245.5	245.5	245.5	245.5
0.1	8.5		244.9	0	2.821	26	10	10	Not Timed-out	244.9	244.9	244.9	244.9	244.9	244.9	244.9	244.9	244.9	244.9
0.1	8.6		244.3	0	2.832	26	10	10	Not Timed-out	244.3	244.3	244.3	244.3	244.3	244.3	244.3	244.3	244.3	244.3
0.1	8.7		243.6	0	2.842	26	10	10	Not Timed-out	243.6	243.6	243.6	243.6	243.6	243.6	243.6	243.6	243.6	243.6
0.1	8.8		243	0	2.852	26	10	10	Not Timed-out	243	243	243	243	243	243	243	243	243	243
0.1	8.9		242.4	0	2.862	26	10	10	Not Timed-out	242.4	242.4	242.4	242.4	242.4	242.4	242.4	242.4	242.4	242.4
0.1	9		241.7	0	2.873	26	10	10	Not Timed-out	241.7	241.7	241.7	241.7	241.7	241.7	241.7	241.7	241.7	241.7
0.1	9.1		241.1	0	2.885	26	10	10	Not Timed-out	241.1	241.1	241.1	241.1	241.1	241.1	241.1	241.1	241.1	241.1
0.1	9.2		240.4	0	2.896	26.1	10	10	Not Timed-out	240.4	240.4	240.4	240.4	240.4	240.4	240.4	240.4	240.4	240.4
0.1	9.3		239.8	0	2.907	26	10	10	Not Timed-out	239.8	239.8	239.8	239.8	239.8	239.8	239.8	239.8	239.8	239.8
0.1	9.4		239.1	0	2.919	26.1	10	10	Not Timed-out	239.1	239.1	239.1	239.1	239.1	239.1	239.1	239.1	239.1	239.1
0.1	9.5		238.4	0	2.93	26.1	10	10	Not Timed-out	238.4	238.4	238.4	238.4	238.4	238.4	238.4	238.4	238.4	238.4
0.1	9.6		237.7	0	2.941	26.1	10	10	Not Timed-out	237.7	237.7	237.7	237.7	237.7	237.7	237.7	237.7	237.7	237.7
0.1	9.7		237	0	2.954	26.1	10	10	Not Timed-out	237	237	237	237	237	237	237	237	237	237
0.1	9.8		236.3	0	2.966	26.1	10	10	Not Timed-out	236.3	236.3	236.3	236.3	236.3	236.3	236.3	236.3	236.3	236.3
0.1	9.9		235.6	0.0483	2.979	26.1	10	10	Not Timed-out	235.6	235.6	235.6	235.6	235.6	235.6	235.6	235.6	235.6	235.6
0.1	10		234.8	0	2.991	26.1	10	10	Not Timed-out	234.8	234.8	234.8	234.8	234.8	234.8	234.8	234.8	234.8	234.8
0.1	10.1		234	0	3.004	26.1	10	10	Not Timed-out	234	234	234	234	234	234	234	234	234	234
0.1	10.2		233.2	0.04216	3.018	26.1	10	10	Not Timed-out	233.2	233.2	233.2	233.2	233.2	233.2	233.2	233.2	233.2	233.2
0.1	10.3		232.4	0.0483	3.031	26.1	10	10	Not Timed-out	232.4	232.4	232.5	232.4	232.4	232.5	232.4	232.4	232.4	232.4
0.1	10.4		231.6	0	3.045	26.1	10	10	Not Timed-out	231.6	231.6	231.6	231.6	231.6	231.6	231.6	231.6	231.6	231.6
0.1	10.5		230.8	0.04216	3.06	26.1	10	10	Not Timed-out	230.8	230.8	230.8	230.7	230.8	230.7	230.8	230.8	230.8	230.8
0.1	10.6		229.9	0	3.075	26.2	10	10	Not Timed-out	229.9	229.9	229.9	229.9	229.9	229.9	229.9	229.9	229.9	229.9
0.1	10.7		229	0	3.089	26.1	10	10	Not Timed-out	229	229	229	229	229	229	229	229	229	229
0.1	10.8		228.1	0	3.105	26.2	10	10	Not Timed-out	228.1	228.1	228.1	228.1	228.1	228.1	228.1	228.1	228.1	228.1
0.1	10.9		227.2	0	3.121	26.2	10	10	Not Timed-out	227.2	227.2	227.2	227.2	227.2	227.2	227.2	227.2	227.2	227.2
0.1	11		226.2	0	3.138	26.2	10	10	Not Timed-out	226.2	226.2	226.2	226.2	226.2	226.2	226.2	226.2	226.2	226.2
0.1	11.1		225.2	0	3.155	26.2	10	10	Not Timed-out	225.2	225.2	225.2	225.2	225.2	225.2	225.2	225.2	225.2	225.2
0.1	11.2		224.2	0	3.171	26.2	10	10	Not Timed-out	224.2	224.2	224.2	224.2	224.2	224.2	224.2	224.2	224.2	224.2

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0.1	25.1	-167.9	0	9.776	26.3	10	10 Not Timed-out	-167.9	-167.9	-167.9	-167.9	-167.9	-167.9	-167.9	-167.9	-167.9	-167.9
0.1	25.2	-168.5	0	9.787	26.3	10	10 Not Timed-out	-168.5	-168.5	-168.5	-168.5	-168.5	-168.5	-168.5	-168.5	-168.5	-168.5
0.1	25.3	-169.2	0.04216	9.798	26.3	10	10 Not Timed-out	-169.3	-169.2	-169.2	-169.3	-169.2	-169.2	-169.2	-169.2	-169.2	-169.2
0.1	25.4	-169.9	0	9.809	26.3	10	10 Not Timed-out	-169.9	-169.9	-169.9	-169.9	-169.9	-169.9	-169.9	-169.9	-169.9	-169.9
0.1	25.5	-170.6	0.05164	9.82	26.3	10	10 Not Timed-out	-170.6	-170.6	-170.5	-170.6	-170.6	-170.6	-170.5	-170.5	-170.6	-170.6
0.1	25.6	-171.2	0	9.831	26.3	10	10 Not Timed-out	-171.2	-171.2	-171.2	-171.2	-171.2	-171.2	-171.2	-171.2	-171.2	-171.2
0.1	25.7	-171.9	0	9.842	26.3	10	10 Not Timed-out	-171.9	-171.9	-171.9	-171.9	-171.9	-171.9	-171.9	-171.9	-171.9	-171.9
0.1	25.8	-172.6	0.0527	9.853	26.3	10	10 Not Timed-out	-172.5	-172.5	-172.6	-172.5	-172.6	-172.5	-172.6	-172.6	-172.6	-172.6
0.1	25.9	-173.2	0	9.864	26.3	10	10 Not Timed-out	-173.2	-173.2	-173.2	-173.2	-173.2	-173.2	-173.2	-173.2	-173.2	-173.2
0.1	26	-173.9	0	9.876	26.3	10	10 Not Timed-out	-173.9	-173.9	-173.9	-173.9	-173.9	-173.9	-173.9	-173.9	-173.9	-173.9
0.1	26.1	-174.6	0	9.888	26.3	10	10 Not Timed-out	-174.6	-174.6	-174.6	-174.6	-174.6	-174.6	-174.6	-174.6	-174.6	-174.6
0.1	26.2	-175.3	0	9.899	26.3	10	10 Not Timed-out	-175.3	-175.3	-175.3	-175.3	-175.3	-175.3	-175.3	-175.3	-175.3	-175.3
0.1	26.3	-176	0	9.91	26.3	10	10 Not Timed-out	-176	-176	-176	-176	-176	-176	-176	-176	-176	-176
0.1	26.4	-176.7	0	9.923	26.3	10	10 Not Timed-out	-176.7	-176.7	-176.7	-176.7	-176.7	-176.7	-176.7	-176.7	-176.7	-176.7
0.1	26.5	-177.4	0	9.935	26.3	10	10 Not Timed-out	-177.4	-177.4	-177.4	-177.4	-177.4	-177.4	-177.4	-177.4	-177.4	-177.4
0.1	26.6	-178.1	0.03162	9.946	26.3	10	10 Not Timed-out	-178.1	-178.1	-178.2	-178.1	-178.1	-178.1	-178.1	-178.1	-178.1	-178.1
0.1	26.7	-178.9	0.05164	9.959	26.3	10	10 Not Timed-out	-178.9	-178.9	-178.9	-178.9	-178.8	-178.8	-178.9	-178.8	-178.8	-178.8
0.1	26.8	-179.6	0	9.971	26.3	10	10 Not Timed-out	-179.6	-179.6	-179.6	-179.6	-179.6	-179.6	-179.6	-179.6	-179.6	-179.6
0.1	26.9	-180.3	0	9.984	26.3	10	10 Not Timed-out	-180.3	-180.3	-180.3	-180.3	-180.3	-180.3	-180.3	-180.3	-180.3	-180.3
0.1	27	-181.1	0	9.996	26.3	10	10 Not Timed-out	-181.1	-181.1	-181.1	-181.1	-181.1	-181.1	-181.1	-181.1	-181.1	-181.1
0.1	27.1	-181.8	0.03162	10.009	26.3	10	10 Not Timed-out	-181.8	-181.8	-181.9	-181.8	-181.8	-181.8	-181.8	-181.8	-181.8	-181.8
0.1	27.2	-182.6	0	10.022	26.3	10	10 Not Timed-out	-182.6	-182.6	-182.6	-182.6	-182.6	-182.6	-182.6	-182.6	-182.6	-182.6
0.1	27.3	-183.4	0.03162	10.035	26.3	10	10 Not Timed-out	-183.4	-183.4	-183.4	-183.4	-183.4	-183.4	-183.4	-183.4	-183.4	-183.4
0.1	27.4	-184.1	0	10.047	26.3	10	10 Not Timed-out	-184.1	-184.1	-184.1	-184.1	-184.1	-184.1	-184.1	-184.1	-184.1	-184.1
0.1	27.5	-184.9	0.04216	10.061	26.3	10	10 Not Timed-out	-185	-184.9	-184.9	-184.9	-184.9	-184.9	-184.9	-185	-184.9	-184.9
0.1	27.6	-185.7	0.0483	10.074	26.3	10	10 Not Timed-out	-185.7	-185.7	-185.7	-185.7	-185.8	-185.8	-185.7	-185.8	-185.7	-185.7
0.1	27.7	-186.5	0.05164	10.088	26.3	10	10 Not Timed-out	-186.5	-186.5	-186.5	-186.5	-186.6	-186.5	-186.6	-186.5	-186.6	-186.6
0.1	27.8	-187.4	0.03162	10.102	26.3	10	10 Not Timed-out	-187.4	-187.4	-187.4	-187.4	-187.4	-187.4	-187.4	-187.3	-187.4	-187.4
0.1	27.9	-188.2	0	10.115	26.3	10	10 Not Timed-out	-188.2	-188.2	-188.2	-188.2	-188.2	-188.2	-188.2	-188.2	-188.2	-188.2
0.1	28	-189	0	10.13	26.3	10	10 Not Timed-out	-189	-189	-189	-189	-189	-189	-189	-189	-189	-189
0.1	28.1	-189.9	0	10.144	26.3	10	10 Not Timed-out	-189.9	-189.9	-189.9	-189.9	-189.9	-189.9	-189.9	-189.9	-189.9	-189.9
0.1	28.2	-190.7	0	10.158	26.3	10	10 Not Timed-out	-190.7	-190.7	-190.7	-190.7	-190.7	-190.7	-190.7	-190.7	-190.7	-190.7
0.1	28.3	-191.6	0	10.173	26.3	10	10 Not Timed-out	-191.6	-191.6	-191.6	-191.6	-191.6	-191.6	-191.6	-191.6	-191.6	-191.6
0.1	28.4	-192.5	0.04216	10.188	26.3	10	10 Not Timed-out	-192.4	-192.5	-192.4	-192.5	-192.5	-192.5	-192.5	-192.5	-192.5	-192.5
0.1	28.5	-193.3	0.04216	10.203	26.3	10	10 Not Timed-out	-193.3	-193.3	-193.3	-193.3	-193.3	-193.4	-193.3	-193.3	-193.3	-193.4
0.1	28.6	-194.2	0.03162	10.217	26.3	10	10 Not Timed-out	-194.2	-194.2	-194.3	-194.2	-194.2	-194.2	-194.2	-194.2	-194.2	-194.2
0.1	28.7	-195.1	0.04216	10.233	26.3	10	10 Not Timed-out	-195.1	-195.2	-195.1	-195.1	-195.2	-195.1	-195.1	-195.1	-195.1	-195.1
0.1	28.8	-196	0.03162	10.248	26.3	10	10 Not Timed-out	-196	-196	-196	-196.1	-196	-196	-196	-196	-196	-196
0.1	28.9	-196.9	0.0527	10.264	26.3	10	10 Not Timed-out	-196.9	-196.9	-196.9	-197	-197	-197	-197	-196.9	-197	-197
0.1	29	-197.9	0	10.279	26.3	10	10 Not Timed-out	-197.9	-197.9	-197.9	-197.9	-197.9	-197.9	-197.9	-197.9	-197.9	-197.9
0.1	29.1	-198.8	0	10.294	26.3	10	10 Not Timed-out	-198.8	-198.8	-198.8	-198.8	-198.8	-198.8	-198.8	-198.8	-198.8	-198.8
0.1	29.2	-199.8	0	10.311	26.3	10	10 Not Timed-out	-199.8	-199.8	-199.8	-199.8	-199.8	-199.8	-199.8	-199.8	-199.8	-199.8
0.1	29.3	-200.7	0	10.327	26.3	10	10 Not Timed-out	-200.7	-200.7	-200.7	-200.7	-200.7	-200.7	-200.7	-200.7	-200.7	-200.7
0.1	29.4	-201.7	0	10.343	26.3	10	10 Not Timed-out	-201.7	-201.7	-201.7	-201.7	-201.7	-201.7	-201.7	-201.7	-201.7	-201.7
0.1	29.5	-202.6	0.03162	10.359	26.3	10	10 Not Timed-out	-202.6	-202.7	-202.6	-202.6	-202.6	-202.6	-202.6	-202.6	-202.6	-202.6
0.1	29.6	-203.6	0	10.375	26.3	10	10 Not Timed-out	-203.6	-203.6	-203.6	-203.6	-203.6	-203.6	-203.6	-203.6	-203.6	-203.6
0.1	29.7	-204.6	0	10.391	26.3	10	10 Not Timed-out	-204.6	-204.6	-204.6	-204.6	-204.6	-204.6	-204.6	-204.6	-204.6	-204.6
0.1	29.8	-205.5	0.04216	10.407	26.3	10	10 Not Timed-out	-205.5	-205.6	-205.5	-205.5	-205.6	-205.5	-205.5	-205.5	-205.5	-205.5
0.1	29.9	-206.6	0	10.424	26.3	10	10 Not Timed-out	-206.6	-206.6	-206.6	-206.6	-206.6	-206.6	-206.6	-206.6	-206.6	-206.6
0.1	30	-207.6	0	10.44	26.3	10	10 Not Timed-out	-207.6	-207.6	-207.6	-207.6	-207.6	-207.6	-207.6	-207.6	-207.6	-207.6
0.1	30.1	-208.6	0	10.457	26.3	10	10 Not Timed-out	-208.6	-208.6	-208.6	-208.6	-208.6	-208.6	-208.6	-208.6	-208.6	-208.6
0.1	30.2	-209.5	0.05164	10.473	26.3	10	10 Not Timed-out	-209.6	-209.5	-209.5	-209.5	-209.6	-209.5	-209.6	-209.5	-209.6	-209.5
0.1	30.3	-210.5	0	10.49	26.3	10	10 Not Timed-out	-210.5	-210.5	-210.5	-210.5	-210.5	-210.5	-210.5	-210.5	-210.5	-210.5
0.1	30.4	-211.5	0	10.506	26.3	10	10 Not Timed-out	-211.5	-211.5	-211.5	-211.5	-211.5	-211.5	-211.5	-211.5	-211.5	-211.5

A Stop Condition met
End Date&Time

04-Nov-03

09:23:16

GEP data for protonation constants of the ligand glycine from refinement by ESTA

TASK	ZBAR	1 GLY0	PROTONATION												
MODL	GLY0	H	1												
CPLX		0	0	-13.74	H	+1(	-1)								
CPLX		1	0	9.573	GLY0(	1)	H	+1(	1)						
CPLX		1	0	11.92	GLY0(	1)	H	+1(	2)						
CONC															
VESL	IVOL	44.008	0	0											
VESL	H	1	0.0154802	0		0									
VESL	GLY0	0.0179799	1	0											
BUR1	H	1	-0.0488315	0		0									
ELEC															
ZERO	H	1	411.46	0											
GRAD	H	1	58.523	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	
280.4	2.239	2.248	-0.008	1.54	1.55	-0.006	0.01	0	0	0	0	0	0	0	0
280	2.246	2.253	-0.007	1.54	1.54	-0.005	0.008	0	0	0	0	0	0	0	0
279.7	2.251	2.258	-0.007	1.54	1.54	-0.005	0.009	0	0	0	0	0	0	0	0
279.4	2.257	2.264	-0.007	1.53	1.54	-0.005	0.009	0	0	0	0	0	0	0	0
279.1	2.262	2.269	-0.008	1.53	1.53	-0.005	0.009	0	0	0	0	0	0	0	0
278.7	2.269	2.275	-0.006	1.53	1.53	-0.004	0.007	0	0	0	0	0	0	0	0
278.4	2.274	2.28	-0.006	1.52	1.53	-0.004	0.008	0	0	0	0	0	0	0	0
278.1	2.279	2.286	-0.007	1.52	1.52	-0.005	0.008	0	0	0	0	0	0	0	0
277.7	2.286	2.291	-0.005	1.52	1.52	-0.004	0.007	0	0	0	0	0	0	0	0
277.4	2.291	2.297	-0.006	1.51	1.52	-0.004	0.007	0	0	0	0	0	0	0	0
277	2.298	2.302	-0.004	1.51	1.52	-0.003	0.005	0	0	0	0	0	0	0	0
276.7	2.303	2.308	-0.005	1.51	1.51	-0.003	0.006	0	0	0	0	0	0	0	0
276.4	2.308	2.313	-0.005	1.51	1.51	-0.003	0.006	0	0	0	0	0	0	0	0
276	2.315	2.319	-0.004	1.5	1.51	-0.003	0.005	0	0	0	0	0	0	0	0
275.7	2.32	2.324	-0.005	1.5	1.5	-0.003	0.005	0	0	0	0	0	0	0	0
275.3	2.327	2.33	-0.003	1.5	1.5	-0.002	0.004	0	0	0	0	0	0	0	0
275	2.332	2.336	-0.004	1.49	1.5	-0.002	0.005	0	0	0	0	0	0	0	0
274.6	2.339	2.341	-0.003	1.49	1.49	-0.002	0.003	0	0	0	0	0	0	0	0
274.3	2.344	2.347	-0.003	1.49	1.49	-0.002	0.004	0	0	0	0	0	0	0	0
273.9	2.351	2.353	-0.002	1.48	1.49	-0.001	0.003	0	0	0	0	0	0	0	0
273.6	2.356	2.359	-0.003	1.48	1.48	-0.002	0.003	0	0	0	0	0	0	0	0
273.2	2.362	2.364	-0.002	1.48	1.48	-0.001	0.002	0	0	0	0	0	0	0	0
272.9	2.368	2.37	-0.003	1.47	1.48	-0.002	0.003	0	0	0	0	0	0	0	0
272.5	2.374	2.376	-0.002	1.47	1.47	-0.001	0.002	0	0	0	0	0	0	0	0
272.1	2.381	2.382	-0.001	1.47	1.47	0	0.001	0	0	0	0	0	0	0	0
271.8	2.386	2.388	-0.002	1.47	1.47	-0.001	0.002	0	0	0	0	0	0	0	0
271.4	2.393	2.394	-0.001	1.46	1.46	0	0.001	0	0	0	0	0	0	0	0
271	2.4	2.4	0	1.46	1.46	0	0	0	0	0	0	0	0	0	0
270.7	2.405	2.406	-0.001	1.46	1.46	0	0.001	0	0	0	0	0	0	0	0
270.3	2.412	2.412	0	1.45	1.45	0	0	0	0	0	0	0	0	0	0
269.9	2.419	2.418	0.001	1.45	1.45	0	0.001	0	0	0	0	0	0	0	0
269.6	2.424	2.424	0	1.45	1.45	0	0	0	0	0	0	0	0	0	0
269.2	2.431	2.43	0.001	1.44	1.44	0	0.001	0	0	0	0	0	0	0	0
268.8	2.438	2.436	0.001	1.44	1.44	0.001	0.001	0	0	0	0	0	0	0	0
268.4	2.445	2.443	0.002	1.44	1.43	0.001	0.002	0	0	0	0	0	0	0	0
268	2.451	2.449	0.002	1.43	1.43	0.001	0.003	0	0	0	0	0	0	0	0
267.7	2.456	2.455	0.001	1.43	1.43	0.001	0.001	0	0	0	0	0	0	0	0
267.3	2.463	2.462	0.002	1.43	1.42	0.001	0.002	0	0	0	0	0	0	0	0
266.9	2.47	2.468	0.002	1.42	1.42	0.001	0.003	0	0	0	0	0	0	0	0
266.5	2.477	2.474	0.003	1.42	1.42	0.001	0.003	0	0	0	0	0	0	0	0
266.1	2.484	2.481	0.003	1.41	1.41	0.001	0.003	0	0	0	0	0	0	0	0
265.7	2.491	2.487	0.003	1.41	1.41	0.002	0.004	0	0	0	0	0	0	0	0
265.3	2.497	2.494	0.004	1.41	1.41	0.002	0.004	0	0	0	0	0	0	0	0
264.9	2.504	2.5	0.004	1.4	1.4	0.002	0.004	0	0	0	0	0	0	0	0
264.5	2.511	2.507	0.004	1.4	1.4	0.002	0.005	0	0	0	0	0	0	0	0
264.1	2.518	2.514	0.004	1.4	1.4	0.002	0.005	0	0	0	0	0	0	0	0
263.7	2.525	2.52	0.005	1.39	1.39	0.002	0.005	0	0	0	0	0	0	0	0
263.3	2.532	2.527	0.005	1.39	1.39	0.002	0.005	0	0	0	0	0	0	0	0
262.9	2.538	2.534	0.005	1.39	1.38	0.002	0.005	0	0	0	0	0	0	0	0
262.5	2.545	2.541	0.005	1.38	1.38	0.002	0.005	0	0	0	0	0	0	0	0
262.1	2.552	2.547	0.005	1.38	1.38	0.002	0.005	0	0	0	0	0	0	0	0
261.6	2.561	2.554	0.006	1.38	1.37	0.002	0.007	0	0	0	0	0	0	0	0
261.2	2.568	2.561	0.006	1.37	1.37	0.002	0.007	0	0	0	0	0	0	0	0
260.8	2.574	2.568	0.006	1.37	1.37	0.002	0.006	0	0	0	0	0	0	0	0
260.4	2.581	2.576	0.006	1.36	1.36	0.002	0.006	0	0	0	0	0	0	0	0
259.9	2.59	2.583	0.007	1.36	1.36	0.003	0.008	0	0	0	0	0	0	0	0
259.5	2.597	2.59	0.007	1.36	1.35	0.002	0.007	0	0	0	0	0	0	0	0
259	2.605	2.597	0.008	1.35	1.35	0.003	0.008	0	0	0	0	0	0	0	0
258.6	2.612	2.604	0.007	1.35	1.35	0.003	0.008	0	0	0	0	0	0	0	0
258.2	2.619	2.612	0.007	1.35	1.34	0.002	0.007	0	0	0	0	0	0	0	0
257.7	2.627	2.619	0.008	1.34	1.34	0.003	0.009	0	0	0	0	0	0	0	0
257.3	2.634	2.627	0.007	1.34	1.33	0.003	0.008	0	0	0	0	0	0	0	0
256.8	2.643	2.634	0.008	1.33	1.33	0.003	0.009	0	0	0	0	0	0	0	0
256.3	2.651	2.642	0.009	1.33	1.33	0.003	0.01	0	0	0	0	0	0	0	0
255.9	2.658	2.65	0.008	1.33	1.32	0.003	0.009	0	0	0	0	0	0	0	0
255.4	2.667	2.658	0.009	1.32	1.32	0.003	0.01	0	0	0	0	0	0	0	0
254.9	2.675	2.665	0.01	1.32	1.32	0.003	0.01	0	0	0	0	0	0	0	0
254.4	2.684	2.673	0.01	1.31	1.31	0.003	0.011	0	0	0	0	0	0	0	0
254	2.691	2.681	0.009	1.31	1.31	0.003	0.01	0	0	0	0	0	0	0	0
253.5	2.699	2.689	0.01	1.31	1.3	0.003	0.01	0	0	0	0	0	0	0	0

APPENDIX B

253	2.708	2.698	0.01	1.3	1.3	0.003	0.01	0	0	0	0	0	0	0
252.5	2.716	2.706	0.01	1.3	1.3	0.003	0.011	0	0	0	0	0	0	0
252	2.725	2.714	0.01	1.29	1.29	0.003	0.011	0	0	0	0	0	0	0
251.5	2.733	2.723	0.011	1.29	1.29	0.003	0.011	0	0	0	0	0	0	0
251	2.742	2.731	0.011	1.29	1.28	0.003	0.011	0	0	0	0	0	0	0
250.4	2.752	2.74	0.012	1.28	1.28	0.003	0.013	0	0	0	0	0	0	0
249.9	2.761	2.749	0.012	1.28	1.28	0.003	0.012	0	0	0	0	0	0	0
249.4	2.769	2.758	0.012	1.27	1.27	0.003	0.012	0	0	0	0	0	0	0
248.9	2.778	2.766	0.011	1.27	1.27	0.003	0.012	0	0	0	0	0	0	0
248.3	2.788	2.776	0.012	1.27	1.26	0.003	0.013	0	0	0	0	0	0	0
247.8	2.797	2.785	0.012	1.26	1.26	0.003	0.012	0	0	0	0	0	0	0
247.2	2.807	2.794	0.013	1.26	1.26	0.003	0.013	0	0	0	0	0	0	0
246.6	2.817	2.803	0.014	1.25	1.25	0.003	0.014	0	0	0	0	0	0	0
246.1	2.826	2.813	0.013	1.25	1.25	0.003	0.013	0	0	0	0	0	0	0
245.5	2.836	2.823	0.013	1.25	1.24	0.003	0.014	0	0	0	0	0	0	0
244.9	2.846	2.832	0.014	1.24	1.24	0.003	0.014	0	0	0	0	0	0	0
244.3	2.856	2.842	0.014	1.24	1.23	0.003	0.014	0	0	0	0	0	0	0
243.6	2.868	2.853	0.016	1.23	1.23	0.003	0.016	0	0	0	0	0	0	0
243	2.879	2.863	0.016	1.23	1.23	0.003	0.016	0	0	0	0	0	0	0
242.4	2.889	2.873	0.016	1.23	1.22	0.003	0.016	0	0	0	0	0	0	0
241.7	2.901	2.884	0.017	1.22	1.22	0.003	0.017	0	0	0	0	0	0	0
241.1	2.911	2.895	0.016	1.22	1.21	0.003	0.017	0	0	0	0	0	0	0
240.4	2.923	2.905	0.018	1.21	1.21	0.003	0.018	0	0	0	0	0	0	0
239.8	2.933	2.917	0.017	1.21	1.21	0.003	0.017	0	0	0	0	0	0	0
239.1	2.945	2.928	0.017	1.2	1.2	0.003	0.018	0	0	0	0	0	0	0
238.4	2.957	2.939	0.018	1.2	1.2	0.003	0.018	0	0	0	0	0	0	0
237.7	2.969	2.951	0.018	1.2	1.19	0.003	0.018	0	0	0	0	0	0	0
237	2.981	2.963	0.018	1.19	1.19	0.003	0.018	0	0	0	0	0	0	0
236.3	2.993	2.975	0.018	1.19	1.18	0.003	0.018	0	0	0	0	0	0	0
235.6	3.005	2.988	0.017	1.18	1.18	0.003	0.017	0	0	0	0	0	0	0
234.8	3.019	3	0.018	1.18	1.18	0.003	0.018	0	0	0	0	0	0	0
234	3.032	3.013	0.019	1.17	1.17	0.003	0.019	0	0	0	0	0	0	0
233.2	3.046	3.027	0.019	1.17	1.17	0.003	0.019	0	0	0	0	0	0	0
232.4	3.06	3.04	0.019	1.17	1.16	0.003	0.02	0	0	0	0	0	0	0
231.6	3.073	3.054	0.019	1.16	1.16	0.003	0.019	0	0	0	0	0	0	0
230.8	3.087	3.068	0.019	1.16	1.15	0.002	0.019	0	0	0	0	0	0	0
229.9	3.102	3.083	0.019	1.15	1.15	0.002	0.02	0	0	0	0	0	0	0
229	3.118	3.098	0.02	1.15	1.15	0.002	0.02	0	0	0	0	0	0	0
228.1	3.133	3.113	0.02	1.14	1.14	0.002	0.02	0	0	0	0	0	0	0
227.2	3.149	3.129	0.019	1.14	1.14	0.002	0.019	0	0	0	0	0	0	0
226.2	3.166	3.145	0.02	1.13	1.13	0.002	0.02	0	0	0	0	0	0	0
225.2	3.183	3.162	0.02	1.13	1.13	0.002	0.021	0	0	0	0	0	0	0
224.2	3.2	3.18	0.02	1.13	1.12	0.002	0.02	0	0	0	0	0	0	0
223.1	3.219	3.197	0.021	1.12	1.12	0.002	0.021	0	0	0	0	0	0	0
222	3.237	3.216	0.021	1.12	1.11	0.002	0.022	0	0	0	0	0	0	0
220.9	3.256	3.235	0.021	1.11	1.11	0.002	0.021	0	0	0	0	0	0	0
219.7	3.277	3.255	0.022	1.11	1.11	0.002	0.022	0	0	0	0	0	0	0
218.5	3.297	3.276	0.022	1.1	1.1	0.002	0.022	0	0	0	0	0	0	0
217.2	3.319	3.297	0.022	1.1	1.1	0.002	0.022	0	0	0	0	0	0	0
215.9	3.342	3.32	0.022	1.09	1.09	0.002	0.022	0	0	0	0	0	0	0
214.5	3.366	3.343	0.023	1.09	1.09	0.002	0.023	0	0	0	0	0	0	0
213.1	3.389	3.368	0.022	1.09	1.08	0.001	0.022	0	0	0	0	0	0	0
211.6	3.415	3.393	0.022	1.08	1.08	0.001	0.022	0	0	0	0	0	0	0
210	3.442	3.421	0.022	1.08	1.07	0.001	0.022	0	0	0	0	0	0	0
208.3	3.471	3.45	0.022	1.07	1.07	0.001	0.022	0	0	0	0	0	0	0
206.5	3.502	3.48	0.022	1.07	1.07	0.001	0.022	0	0	0	0	0	0	0
204.5	3.536	3.513	0.023	1.06	1.06	0.001	0.023	0	0	0	0	0	0	0
202.4	3.572	3.548	0.024	1.06	1.06	0.001	0.024	0	0	0	0	0	0	0
200.2	3.61	3.586	0.024	1.05	1.05	0.001	0.024	0	0	0	0	0	0	0
197.9	3.649	3.627	0.022	1.05	1.05	0.001	0.022	0	0	0	0	0	0	0
195.2	3.695	3.672	0.023	1.04	1.04	0.001	0.023	0	0	0	0	0	0	0
192.3	3.745	3.722	0.022	1.04	1.04	0.001	0.022	0	0	0	0	0	0	0
189.1	3.8	3.778	0.021	1.03	1.03	0.001	0.021	0	0	0	0	0	0	0
185.5	3.861	3.842	0.019	1.03	1.03	0	0.019	0	0	0	0	0	0	0
181.3	3.933	3.916	0.017	1.03	1.03	0	0.017	0	0	0	0	0	0	0
176.3	4.018	4.005	0.013	1.02	1.02	0	0.013	0	0	0	0	0	0	0
170.1	4.124	4.115	0.009	1.02	1.02	0	0.009	0	0	0	0	0	0	0
162	4.263	4.263	0	1.01	1.01	0	0	0	0	0	0	0	0	0
150.7	4.456	4.485	-0.029	1.01	1.01	0	0.029	0	0	0	0	0	0	0
130.7	4.797	4.954	-0.157	1	1	0	0.157	0	0	0	0	0	0	0
57.8	6.043	7.054	-1.01	1	1	0	1.01	0	0	0	0	0	0	0
-17.2	7.325	7.537	-0.212	0.99	0.99	0	0.212	0	0	0	0	0	0	0
-37.3	7.668	7.762	-0.094	0.98	0.98	0	0.094	0	0	0	0	0	0	0
-48.3	7.856	7.911	-0.055	0.98	0.98	0	0.055	0	0	0	0	0	0	0
-56.1	7.989	8.023	-0.034	0.97	0.97	0	0.034	0	0	0	0	0	0	0
-62.3	8.095	8.114	-0.018	0.97	0.97	0	0.018	0	0	0	0	0	0	0
-67.3	8.181	8.189	-0.008	0.96	0.96	0	0.008	0	0	0	0	0	0	0
-71.4	8.251	8.254	-0.003	0.95	0.95	0	0.003	0	0	0	0	0	0	0
-75	8.312	8.311	0.001	0.95	0.95	0	0.001	0	0	0	0	0	0	0
-78.2	8.367	8.362	0.005	0.94	0.94	0	0.005	0	0	0	0	0	0	0
-81.1	8.417	8.409	0.008	0.94	0.94	0	0.008	0	0	0	0	0	0	0
-83.7	8.461	8.451	0.01	0.93	0.93	0	0.01	0	0	0	0	0	0	0
-86	8.5	8.49	0.01	0.92	0.92	0	0.01	0	0	0	0	0	0	0
-88.2	8.538	8.527	0.011	0.92	0.92	0	0.011	0	0	0	0	0	0	0
-90.3	8.574	8.56	0.013	0.91	0.91	0	0.013	0	0	0	0	0	0	0
-92.2	8.606	8.592	0.014	0.9	0.9	0	0.014	0	0	0	0	0	0	0
-94.2	8.64	8.622	0.018	0.9	0.9	0	0.018	0	0	0	0	0	0	0
-95.9	8.669	8.651	0.018	0.89	0.89	0	0.018	0	0	0	0	0	0	0

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-97.5	8.697	8.678	0.019	0.89	0.89	0	0.019	0	0	0	0	0	0	0
-99.1	8.724	8.704	0.02	0.88	0.88	0	0.02	0	0	0	0	0	0	0
-100.5	8.748	8.729	0.019	0.87	0.87	0	0.019	0	0	0	0	0	0	0
-102	8.774	8.752	0.021	0.87	0.87	0	0.021	0	0	0	0	0	0	0
-103.3	8.796	8.775	0.021	0.86	0.86	0	0.021	0	0	0	0	0	0	0
-104.7	8.82	8.797	0.023	0.86	0.86	0	0.023	0	0	0	0	0	0	0
-105.9	8.84	8.818	0.022	0.85	0.85	0	0.022	0	0	0	0	0	0	0
-107.2	8.862	8.839	0.024	0.84	0.84	0	0.024	0	0	0	0	0	0	0
-108.4	8.883	8.859	0.024	0.84	0.84	0	0.024	0	0	0	0	0	0	0
-109.5	8.902	8.878	0.024	0.83	0.83	0	0.024	0	0	0	0	0	0	0
-110.6	8.921	8.897	0.024	0.83	0.83	0	0.024	0	0	0	0	0	0	0
-111.7	8.939	8.915	0.024	0.82	0.82	0	0.024	0	0	0	0	0	0	0
-112.8	8.958	8.933	0.026	0.81	0.81	0	0.026	0	0	0	0	0	0	0
-113.8	8.975	8.95	0.025	0.81	0.81	0	0.025	0	0	0	0	0	0	0
-114.8	8.992	8.967	0.026	0.8	0.8	0	0.026	0	0	0	0	0	0	0
-115.8	9.009	8.983	0.026	0.79	0.79	0	0.026	0	0	0	0	0	0	0
-116.7	9.025	8.999	0.025	0.79	0.79	0	0.025	0	0	0	0	0	0	0
-117.7	9.042	9.015	0.027	0.78	0.78	0	0.027	0	0	0	0	0	0	0
-118.6	9.057	9.031	0.027	0.78	0.78	0	0.027	0	0	0	0	0	0	0
-119.5	9.073	9.046	0.027	0.77	0.77	0	0.027	0	0	0	0	0	0	0
-120.4	9.088	9.061	0.027	0.76	0.76	0	0.027	0	0	0	0	0	0	0
-121.2	9.102	9.075	0.027	0.76	0.76	0	0.027	0	0	0	0	0	0	0
-122.1	9.117	9.09	0.028	0.75	0.75	0	0.028	0	0	0	0	0	0	0
-122.9	9.131	9.104	0.027	0.75	0.75	0	0.027	0	0	0	0	0	0	0
-123.7	9.144	9.118	0.027	0.74	0.74	0	0.027	0	0	0	0	0	0	0
-124.5	9.158	9.131	0.027	0.73	0.73	0	0.027	0	0	0	0	0	0	0
-125.3	9.172	9.145	0.027	0.73	0.73	0	0.027	0	0	0	0	0	0	0
-126.1	9.185	9.158	0.028	0.72	0.72	0	0.028	0	0	0	0	0	0	0
-126.9	9.199	9.171	0.028	0.72	0.72	0	0.028	0	0	0	0	0	0	0
-127.7	9.213	9.184	0.029	0.71	0.71	0	0.029	0	0	0	0	0	0	0
-128.4	9.225	9.197	0.028	0.7	0.7	0	0.028	0	0	0	0	0	0	0
-129.1	9.237	9.209	0.027	0.7	0.7	0	0.027	0	0	0	0	0	0	0
-129.9	9.25	9.222	0.029	0.69	0.69	0	0.029	0	0	0	0	0	0	0
-130.6	9.262	9.234	0.028	0.68	0.68	0	0.028	0	0	0	0	0	0	0
-131.4	9.276	9.246	0.03	0.68	0.68	0	0.03	0	0	0	0	0	0	0
-132.1	9.288	9.258	0.03	0.67	0.67	0	0.03	0	0	0	0	0	0	0
-132.8	9.3	9.27	0.03	0.67	0.67	0	0.03	0	0	0	0	0	0	0
-133.5	9.312	9.282	0.03	0.66	0.66	0	0.03	0	0	0	0	0	0	0
-134.2	9.324	9.294	0.03	0.65	0.65	0	0.03	0	0	0	0	0	0	0
-134.8	9.334	9.306	0.028	0.65	0.65	0	0.028	0	0	0	0	0	0	0
-135.5	9.346	9.317	0.029	0.64	0.64	0	0.029	0	0	0	0	0	0	0
-136.1	9.356	9.329	0.028	0.64	0.64	0	0.028	0	0	0	0	0	0	0
-136.8	9.368	9.34	0.028	0.63	0.63	0	0.028	0	0	0	0	0	0	0
-137.4	9.379	9.351	0.027	0.62	0.62	0	0.027	0	0	0	0	0	0	0
-138.1	9.39	9.363	0.028	0.62	0.62	0	0.028	0	0	0	0	0	0	0
-138.7	9.401	9.374	0.027	0.61	0.61	0	0.027	0	0	0	0	0	0	0
-139.4	9.413	9.385	0.028	0.61	0.61	0	0.028	0	0	0	0	0	0	0
-140	9.423	9.396	0.027	0.6	0.6	0	0.027	0	0	0	0	0	0	0
-140.6	9.433	9.407	0.027	0.59	0.59	0	0.027	0	0	0	0	0	0	0
-141.3	9.445	9.418	0.028	0.59	0.59	0	0.028	0	0	0	0	0	0	0
-141.9	9.455	9.428	0.027	0.58	0.58	0	0.027	0	0	0	0	0	0	0
-142.5	9.466	9.439	0.026	0.58	0.58	0	0.026	0	0	0	0	0	0	0
-143.1	9.476	9.45	0.026	0.57	0.57	0	0.026	0	0	0	0	0	0	0
-143.7	9.486	9.461	0.025	0.56	0.56	0	0.025	0	0	0	0	0	0	0
-144.3	9.496	9.471	0.025	0.56	0.56	0	0.025	0	0	0	0	0	0	0
-144.9	9.507	9.482	0.025	0.55	0.55	0	0.025	0	0	0	0	0	0	0
-145.6	9.519	9.493	0.026	0.55	0.54	0	0.026	0	0	0	0	0	0	0
-146.2	9.529	9.503	0.026	0.54	0.54	0	0.026	0	0	0	0	0	0	0
-146.8	9.539	9.514	0.025	0.53	0.53	0	0.025	0	0	0	0	0	0	0
-147.4	9.549	9.524	0.025	0.53	0.53	0	0.025	0	0	0	0	0	0	0
-147.9	9.558	9.535	0.023	0.52	0.52	0	0.023	0	0	0	0	0	0	0
-148.5	9.568	9.545	0.023	0.52	0.51	0	0.023	0	0	0	0	0	0	0
-149.2	9.58	9.556	0.024	0.51	0.51	0	0.024	0	0	0	0	0	0	0
-149.8	9.59	9.566	0.024	0.5	0.5	0	0.024	0	0	0	0	0	0	0
-150.3	9.599	9.577	0.022	0.5	0.5	0	0.022	0	0	0	0	0	0	0
-150.9	9.609	9.587	0.022	0.49	0.49	0	0.022	0	0	0	0	0	0	0
-151.5	9.619	9.598	0.022	0.48	0.48	0	0.022	0	0	0	0	0	0	0
-152.1	9.63	9.608	0.022	0.48	0.48	0	0.022	0	0	0	0	0	0	0
-152.7	9.64	9.619	0.021	0.47	0.47	0	0.021	0	0	0	0	0	0	0
-153.3	9.65	9.629	0.021	0.47	0.47	0	0.021	0	0	0	0	0	0	0
-153.9	9.66	9.64	0.021	0.46	0.46	0	0.021	0	0	0	0	0	0	0
-154.5	9.671	9.65	0.021	0.45	0.45	0	0.021	0	0	0	0	0	0	0
-155.1	9.681	9.661	0.02	0.45	0.45	0	0.02	0	0	0	0	0	0	0
-155.7	9.691	9.671	0.02	0.44	0.44	0	0.02	0	0	0	0	0	0	0
-156.3	9.701	9.682	0.02	0.44	0.44	0	0.02	0	0	0	0	0	0	0
-156.8	9.71	9.692	0.018	0.43	0.43	0	0.018	0	0	0	0	0	0	0
-157.4	9.72	9.703	0.017	0.43	0.42	0	0.017	0	0	0	0	0	0	0
-158	9.731	9.713	0.017	0.42	0.42	0	0.017	0	0	0	0	0	0	0
-158.6	9.741	9.724	0.017	0.41	0.41	0	0.017	0	0	0	0	0	0	0
-159.2	9.751	9.735	0.016	0.41	0.41	0	0.016	0	0	0	0	0	0	0
-159.8	9.761	9.746	0.016	0.4	0.4	0	0.016	0	0	0	0	0	0	0
-160.4	9.772	9.756	0.015	0.4	0.39	0	0.015	0	0	0	0	0	0	0
-161	9.782	9.767	0.015	0.39	0.39	0	0.015	0	0	0	0	0	0	0
-161.6	9.792	9.778	0.014	0.38	0.38	0	0.014	0	0	0	0	0	0	0
-162.2	9.802	9.789	0.013	0.38	0.38	0	0.013	0	0	0	0	0	0	0
-162.9	9.814	9.8	0.014	0.37	0.37	0	0.014	0	0	0	0	0	0	0
-163.5	9.825	9.811	0.014	0.37	0.37	0	0.014	0	0	0	0	0	0	0
-164.1	9.835	9.822	0.013	0.36	0.36	0	0.013	0	0	0	0	0	0	0

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-164.7	9.845	9.833	0.012	0.35	0.35	0	0.012	0	0	0	0	0	0	0
-165.3	9.855	9.844	0.011	0.35	0.35	0	0.011	0	0	0	0	0	0	0
-166	9.867	9.856	0.012	0.34	0.34	0	0.012	0	0	0	0	0	0	0
-166.6	9.877	9.867	0.011	0.34	0.34	0	0.011	0	0	0	0	0	0	0
-167.2	9.888	9.878	0.009	0.33	0.33	0	0.009	0	0	0	0	0	0	0
-167.9	9.9	9.89	0.01	0.32	0.32	0	0.01	0	0	0	0	0	0	0
-168.5	9.91	9.901	0.009	0.32	0.32	0	0.009	0	0	0	0	0	0	0
-169.2	9.922	9.913	0.009	0.31	0.31	0	0.009	0	0	0	0	0	0	0
-169.9	9.934	9.925	0.009	0.31	0.31	0	0.009	0	0	0	0	0	0	0
-170.6	9.946	9.937	0.009	0.3	0.3	0	0.009	0	0	0	0	0	0	0
-171.2	9.956	9.949	0.007	0.3	0.3	0	0.007	0	0	0	0	0	0	0
-171.9	9.968	9.961	0.007	0.29	0.29	0	0.007	0	0	0	0	0	0	0
-172.6	9.98	9.973	0.007	0.28	0.28	0	0.007	0	0	0	0	0	0	0
-173.2	9.99	9.985	0.005	0.28	0.28	0	0.005	0	0	0	0	0	0	0
-173.9	10.002	9.998	0.005	0.27	0.27	0	0.005	0	0	0	0	0	0	0
-174.6	10.014	10.01	0.004	0.27	0.27	0	0.004	0	0	0	0	0	0	0
-175.3	10.026	10.023	0.003	0.26	0.26	0	0.003	0	0	0	0	0	0	0
-176	10.038	10.036	0.003	0.26	0.26	0	0.003	0	0	0	0	0	0	0
-176.7	10.05	10.048	0.002	0.25	0.25	0	0.002	0	0	0	0	0	0	0
-177.4	10.062	10.062	0	0.24	0.24	0	0	0	0	0	0	0	0	0
-178.1	10.074	10.075	-0.001	0.24	0.24	0	0.001	0	0	0	0	0	0	0
-178.9	10.088	10.088	0	0.23	0.23	0	0	0	0	0	0	0	0	0
-179.6	10.1	10.102	-0.002	0.23	0.23	0	0.002	0	0	0	0	0	0	0
-180.3	10.112	10.115	-0.004	0.22	0.22	0	0.004	0	0	0	0	0	0	0
-181.1	10.125	10.129	-0.004	0.22	0.22	0	0.004	0	0	0	0	0	0	0
-181.8	10.137	10.143	-0.006	0.21	0.21	0	0.006	0	0	0	0	0	0	0
-182.6	10.151	10.157	-0.006	0.21	0.21	0	0.006	0	0	0	0	0	0	0
-183.4	10.165	10.172	-0.007	0.2	0.2	0	0.007	0	0	0	0	0	0	0
-184.1	10.177	10.186	-0.01	0.19	0.2	-0.001	0.01	0	0	0	0	0	0	0
-184.9	10.19	10.201	-0.011	0.19	0.19	-0.001	0.011	0	0	0	0	0	0	0
-185.7	10.204	10.216	-0.012	0.18	0.18	-0.001	0.012	0	0	0	0	0	0	0
-186.5	10.218	10.231	-0.013	0.18	0.18	-0.001	0.013	0	0	0	0	0	0	0
-187.4	10.233	10.246	-0.013	0.17	0.17	-0.001	0.013	0	0	0	0	0	0	0
-188.2	10.247	10.262	-0.015	0.17	0.17	-0.001	0.015	0	0	0	0	0	0	0
-189	10.26	10.277	-0.017	0.16	0.16	-0.001	0.017	0	0	0	0	0	0	0
-189.9	10.276	10.293	-0.018	0.16	0.16	-0.001	0.018	0	0	0	0	0	0	0
-190.7	10.289	10.309	-0.02	0.15	0.15	-0.002	0.02	0	0	0	0	0	0	0
-191.6	10.305	10.325	-0.021	0.15	0.15	-0.002	0.021	0	0	0	0	0	0	0
-192.5	10.32	10.342	-0.022	0.14	0.14	-0.002	0.022	0	0	0	0	0	0	0
-193.3	10.334	10.359	-0.025	0.14	0.14	-0.002	0.025	0	0	0	0	0	0	0
-194.2	10.349	10.375	-0.026	0.13	0.14	-0.002	0.026	0	0	0	0	0	0	0
-195.1	10.364	10.392	-0.028	0.13	0.13	-0.003	0.028	0	0	0	0	0	0	0
-196	10.38	10.41	-0.03	0.12	0.13	-0.003	0.03	0	0	0	0	0	0	0
-196.9	10.395	10.427	-0.032	0.12	0.12	-0.003	0.032	0	0	0	0	0	0	0
-197.9	10.412	10.445	-0.032	0.11	0.12	-0.003	0.032	0	0	0	0	0	0	0
-198.8	10.428	10.462	-0.035	0.11	0.11	-0.004	0.035	0	0	0	0	0	0	0
-199.8	10.445	10.48	-0.035	0.11	0.11	-0.004	0.035	0	0	0	0	0	0	0
-200.7	10.46	10.498	-0.038	0.1	0.11	-0.004	0.038	0	0	0	0	0	0	0
-201.7	10.477	10.516	-0.039	0.1	0.1	-0.005	0.039	0	0	0	0	0	0	0
-202.6	10.493	10.534	-0.041	0.09	0.1	-0.005	0.042	0	0	0	0	0	0	0
-203.6	10.51	10.552	-0.042	0.09	0.09	-0.006	0.043	0	0	0	0	0	0	0
-204.6	10.527	10.57	-0.043	0.09	0.09	-0.006	0.044	0	0	0	0	0	0	0
-205.5	10.542	10.588	-0.046	0.08	0.09	-0.007	0.047	0	0	0	0	0	0	0
-206.6	10.561	10.606	-0.045	0.08	0.08	-0.007	0.046	0	0	0	0	0	0	0
-207.6	10.578	10.624	-0.046	0.07	0.08	-0.007	0.047	0	0	0	0	0	0	0
-208.6	10.595	10.642	-0.047	0.07	0.08	-0.008	0.048	0	0	0	0	0	0	0
-209.5	10.611	10.66	-0.05	0.07	0.08	-0.008	0.05	0	0	0	0	0	0	0
-210.5	10.628	10.678	-0.05	0.06	0.07	-0.009	0.051	0	0	0	0	0	0	0
-211.5	10.645	10.696	-0.051	0.06	0.07	-0.009	0.052	0	0	0	0	0	0	0

AVERAGE OF SUM OF SQUARES
OF RESIDUALS: 3.96E-03 9.94E-06 3.97E-03 0.00E+00 0.00E+00 0.00E+00

NUMBER OF TITRATIONS = 1

TOTAL NUMBER OF POINTS = 305