

Supporting Information

Phase Equilibria for the Glycine–Methanol–NH₄Cl–H₂O System

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Table S1. The Parameters of HKF Equation of State ^a (eq 12) for Species ^b

species	$a_1 (\times 10)$	$a_2 (\times 10^{-2})$	a_3	$a_4 (\times 10^{-4})$	c_1	$c_2 (\times 10^{-4})$	$\omega (\times 10^{-5})$
H ⁺	0	0	0	0	0	0	0
NH ₄ ⁺	3.8763	2.3448	8.5605	-2.8759	17.45	-0.0210	1.5020
⁺ NH ₃ CH ₂ COOH	7.6046	7.0825	10.9119	-3.0717	^{40.901} ₁	-3.4185	-0.2330
OH ⁻	1.2527	0.0738	1.8423	-2.7821	4.15	-10.346	1.7246
Cl ⁻	4.0320	4.8010	5.5630	-2.8470	-4.4	-5.7140	1.4560
NH ₂ CH ₂ COO ⁻	7.6046	7.0825	10.9119	-3.0717	^{14.199} ₈	-3.4185	-0.2330
⁺ NH ₃ CH ₂ COO ⁻	7.6046	7.0825	10.9119	-3.0717	^{14.199} ₈	-3.4185	-0.2330

^a Units: (a_1) cal·bar⁻¹·mol⁻¹; (a_2) cal·mol⁻¹; (a_3) cal·K·bar⁻¹·mol⁻¹; (a_4) cal·K·mol⁻¹; (c_1) cal·K⁻¹·mol⁻¹; (c_2) cal·K·mol⁻¹; (ω) cal·mol⁻¹.

^b The data were taken from the Public databank of OLI (version 9.1).

Table S2. Relevant Thermodynamic Data for the Main Species in the Glycine–NH₄Cl–H₂O System ^a

species	$\Delta G_{f,298.2K}^0$ kJ·mol ⁻¹	$\Delta H_{f,298.2K}^0$ kJ·mol ⁻¹	$\Delta S_{f,298.2K}^0$ J·mol ⁻¹ ·K ⁻¹	$\Delta C_{p,298.2K}^0$ J·mol ⁻¹ ·K ⁻¹	$\Delta V_{f,298.2K}^0$ L·mol ⁻¹
NH ₄ ⁺	-79.4542	-133.260	111.169	65.8562	0.01813
⁺ NH ₃ CH ₂ COOH	-384.133	-519.624	184.256		
OH ⁻	-157.298	-229.987	-10.711	-137.193	-0.00418
Cl ⁻	-131.290	-167.080	56.735	-123.177	0.01779
NH ₂ CH ₂ COO ⁻	-315.045	-471.600	113.602	0	0.04377
H ₂ O	-237.190	-285.830	69.95	75.3	0.01806
⁺ NH ₃ CH ₂ COO ⁻	-370.704	-515.377	153.458	39.33	0.04319
NH ₄ Cl(s)	-203.092	-314.553	95.86	86.441	0.03503
NH ₂ CH ₂ COOH(s)	-368.933	-528.500	103.5	99.2	0.06788

^a The data were taken from the Public databank of OLI (version 9.1).

Table S3. Empirical Parameters of Equation 13 ^a for Species ^b

species	A	B	C	D
NH ₂ CH ₂ COOH(s)	0.82609 ₆	-345.0285	0.0017942 ₅	2.44634 × 10 ⁻⁶
NH ₄ Cl(s)	-3.787	0	0.023471	-2.2061 × 10 ⁻⁵

^a $\log K = A + \frac{B}{T} + CT + DT^2$

^b The data were taken from the Public databank of OLI (version 9.1).

Table S4. Experimental Solubility in the Glycine–NH₄Cl–H₂O System at the Temperature Range from 283.2 to 353.2 K and at the Pressure $p = 0.1$ MPa ^a

$m(\text{NH}_4\text{Cl})$, mol·kg ⁻¹	$m(\text{Glycine})$, mol·kg ⁻¹	ρ^b , g·mL ⁻¹	Solid ^c	$m(\text{NH}_4\text{Cl})$, mol·kg ⁻¹	$m(\text{Glycine})$, mol·kg ⁻¹	ρ^b , g·mL ⁻¹	Solid ^c
$T = 283.2$ K				$T = 323.2$ K			
0.0000	2.3331	1.0640	G	0.0000	5.0641	1.1019	G
0.2083	2.3837	1.0703	G	0.2083	5.1034	1.1129	G
0.4998	2.4715	1.0771	G	0.4998	5.0961	1.1186	G
1.0110	2.6512	1.0882	G	1.0110	5.2947	1.1284	G
1.5035	2.7800	1.0962	G	1.5035	5.3405	1.1348	G
2.0039	2.8294	1.1037	G	2.0039	5.4154	1.1403	G
2.5012	2.8911	1.1108	G	2.5012	5.6298	1.1477	G
3.0011	2.9663	1.1175	G	3.0011	5.7121	1.1523	G
4.0313	3.1129	1.1305	G	4.0313	5.8720	1.1606	G
5.0260	3.3394	1.1421	G	5.0260	6.2456	1.1696	G
5.9965	3.4284	1.1526	G	5.9965	6.3565	1.1759	G
6.2861	3.4706	1.1557	G	9.2530	7.1565	1.1925	G
6.9723	3.1910	1.1622	G + N	11.2342	7.3844	1.1996	G + N
6.2708	0.0000	1.0841	N	9.2905	0.0000	1.0739	N
6.2917	0.5003	1.0959	N	9.5105	0.5003	1.0850	N
6.4572	1.0004	1.1084	N	9.6107	1.0004	1.0953	N
6.5798	1.5002	1.1198	N	9.7266	1.5002	1.1052	N
6.7512	2.5002	1.1412	N	9.9554	2.5002	1.1239	N
6.8731	3.1650	1.1545	N	11.0770	6.9649	1.1928	N
$T = 293.2$ K				$T = 333.2$ K			
0.0000	2.9865	1.0748	G	0.0000	5.8068	1.1075	G
0.2083	3.0741	1.0829	G	0.2083	5.7894	1.1195	G
0.4998	3.0346	1.0878	G	0.4998	5.8016	1.1261	G
1.0110	3.1979	1.0980	G	1.0110	5.9143	1.1351	G
1.5035	3.1701	1.1033	G	1.5035	6.1101	1.1435	G
2.0039	3.2905	1.1111	G	2.0039	6.1816	1.1488	G
2.5012	3.2846	1.1158	G	2.5012	6.4292	1.1564	G
3.0011	3.5574	1.1252	G	3.0011	6.4330	1.1596	G
4.0313	3.5498	1.1343	G	4.0313	6.6658	1.1700	G
5.0260	3.7746	1.1458	G	5.0260	7.0969	1.1780	G
5.9965	3.8851	1.1541	G	5.9965	7.2324	1.1831	G
6.8012	4.0690	1.1621	G	10.2512	8.2796	1.2019	G
7.9054	4.3615	1.1726	G + N	12.5521	8.7864	1.2082	G + N
7.1331	0.0000	1.0837	N	9.9874	0.0000	1.0696	N
7.1438	0.5003	1.0952	N	10.2803	0.5003	1.0804	N
7.2837	1.0004	1.1070	N	10.3934	1.0004	1.0905	N

7.4012	1.5002	1.1179	N	10.5769	1.5002	1.1001	N
7.5478	2.5002	1.1384	N	10.7035	2.5002	1.1181	N
7.7947	3.8016	1.1629	N	12.2471	8.2335	1.2007	N
$T = 298.2 \text{ K}$				$T = 343.2 \text{ K}$			
0.0000	3.2440	1.0797	G	0.0000	6.7132	1.1131	G
0.2083	3.3081	1.0877	G	0.2083	6.7629	1.1281	G
0.4998	3.4033	1.0940	G	0.4998	6.7818	1.1355	G
1.0110	3.5261	1.1030	G	1.0110	6.9717	1.1451	G
1.5035	3.6427	1.1105	G	1.5035	7.0249	1.1526	G
2.0039	3.6594	1.1171	G	2.0039	7.1050	1.1586	G
2.5012	3.7574	1.1236	G	2.5012	7.3399	1.1649	G
3.0011	3.8750	1.1295	G	3.0011	7.5070	1.1700	G
4.0315	3.9813	1.1400	G	4.0313	7.6377	1.1776	G
5.0261	4.1560	1.1498	G	5.0260	8.1563	1.1860	G
5.9965	4.3005	1.1580	G	5.9965	8.2807	1.1918	G
7.2514	4.4699	1.1673	G	11.2516	9.7750	1.2116	G
8.4370	4.7748	1.1774	G + N	13.9100	10.1428	1.2165	G + N
7.5263	0.0000	1.0828	N	10.6672	0.0000	1.0654	N
7.6013	0.5003	1.0945	N	11.0293	0.5003	1.0759	N
7.6949	1.0004	1.1057	N	11.1415	1.0004	1.0857	N
7.8186	1.5002	1.1164	N	11.2652	1.5002	1.0951	N
8.0010	2.5002	1.1367	N	11.4822	2.5002	1.1126	N
8.3255	4.2518	1.1686	N	13.5337	9.5347	1.2071	N
$T = 303.2 \text{ K}$				$T = 353.2 \text{ K}$			
0.0000	3.6383	1.0845	G	0.0000	7.5860	1.1151	G
0.2083	3.6853	1.0933	G	0.2083	7.7020	1.1344	G
0.4998	3.7619	1.0992	G	0.4998	7.6171	1.1423	G
1.0110	3.9085	1.1082	G	1.0110	7.8418	1.1527	G
1.5035	3.9684	1.1156	G	1.5035	7.8803	1.1597	G
2.0039	4.0745	1.1223	G	2.0039	7.9720	1.1661	G
2.5012	4.1501	1.1283	G	2.5012	8.0418	1.1706	G
3.0011	4.2345	1.1340	G	3.0011	8.1719	1.1754	G
4.0313	4.3294	1.1439	G	4.0313	8.6200	1.1862	G
5.0260	4.5984	1.1536	G	5.0260	9.2202	1.1934	G
5.9965	4.7698	1.1616	G	5.9965	9.3741	1.1993	G
7.5033	4.9890	1.1726	G	12.2521	10.9939	1.2186	G
9.1256	5.0778	1.1820	G + N	15.4101	11.8045	1.2255	G + N
7.8726	0.0000	1.0815	N	11.3751	0.0000	1.0616	N
8.0063	0.5003	1.0930	N	11.7484	0.5003	1.0718	N
8.0811	1.0004	1.1039	N	11.9680	1.0004	1.0813	N
8.2299	1.5002	1.1146	N	11.9843	1.5002	1.0903	N
8.4101	2.5002	1.1345	N	12.2678	2.5002	1.1074	N
8.8442	4.8088	1.1750	N	14.7885	10.8286	1.2121	N
$T = 313.2 \text{ K}$							

0.0000	4.3856	1.0941	G
0.2083	4.4099	1.1035	G
0.4998	4.5025	1.1095	G
1.0110	4.6889	1.1185	G
1.5035	4.6878	1.1258	G
2.0039	4.8019	1.1323	G
2.5012	4.8806	1.1381	G
3.0011	4.9639	1.1434	G
4.0313	5.1151	1.1529	G
5.0260	5.4410	1.1613	G
5.9965	5.5706	1.1683	G
8.2507	5.8821	1.1815	G
10.1500	6.3349	1.1910	G + N
8.6103	0.0000	1.0781	N
8.7706	0.5003	1.0893	N
8.8820	1.0004	1.1000	N
9.0241	1.5002	1.1102	N
9.2048	2.5002	1.1295	N
9.8912	5.7181	1.1827	N

^a Standard uncertainties u are $u(T) = 0.10$ K, $u_r(p) = 0.05$, and $u_r(m) = 0.002$.

^b Density values were calculated by the OLI Stream Analyzer 9.1 Program.

^c Solid: N-NH₄Cl(s), G-Glycine(s).

Table S5. Experimental Solubility of Glycine in Methanol–Water Mixtures at the temperature Range from 283.2 to 323.2 K and at the Pressure $p = 0.1$ MPa ^a

$w(\text{Methanol})$	$m(\text{Glycine}),$ $\text{mol} \cdot \text{kg}^{-1} \text{ solvent}$	$\rho^b,$ $\text{g} \cdot \text{mL}^{-1}$	$w(\text{Methanol})$	$m(\text{Glycine}),$ $\text{mol} \cdot \text{kg}^{-1} \text{ solvent}$	$\rho^b,$ $\text{g} \cdot \text{mL}^{-1}$
$T=283.2$ K			$T=310.0$ K		
0.1011	1.3802	1.0231	0.1011	2.7439	1.0428
0.1830	0.8680	0.9953	0.1830	1.8958	1.0110
0.3014	0.4129	0.9625	0.3014	0.9810	0.9715
0.4996	0.1463	0.9235	0.4996	0.3043	0.9242
0.7992	0.0214	0.8767	0.7992	0.0401	0.8763
1.0000	0.0035	0.8039	1.0000	0.0063	0.7849
$T=293.2$ K			$T=313.2$ K		
0.1011	1.8417	1.0331	0.1011	2.9244	1.0521
0.1830	1.1917	1.0027	0.1830	1.9900	1.0182
0.3014	0.5923	0.9667	0.3014	1.0448	0.9756
0.4996	0.1976	0.9243	0.4996	0.3347	0.9257
0.7992	0.0269	0.9040	0.7992	0.0472	0.8759
1.0000	0.0044	0.7945	1.0000	0.0071	0.7752
$T=298.2$ K			$T=323.2$ K		

0.1011	2.0890	1.0379	0.1011	3.5839	1.0614
0.1830	1.3846	1.0069	0.1830	2.5878	1.0323
0.3014	0.7010	0.9690	0.3014	1.4069	0.9825
0.4996	0.2029	0.9239	0.4996	0.4597	0.9274
0.7992	0.0295	0.8764	0.7992	0.0589	0.8751
1.0000	0.0048	0.7897	1.0000	0.0084	0.7651
$T=303.2\text{ K}$					
0.1011	2.3535	1.0428			
0.1830	1.5879	1.0110			
0.3014	0.8187	0.9715			
0.4996	0.2322	0.9242			
0.7992	0.0333	0.8763			
1.0000	0.0054	0.7849			

^a Standard uncertainties u are $u(T) = 0.10\text{ K}$, $u_r(p) = 0.05$, and $u_r(m) = 0.002$.

^b Density values were calculated by the OLI Stream Analyzer 9.1 Program.