Supporting Information for: Quantification of Cation-Anion Interactions in Crystalline Monopotassium and Monosodium Glutamate Salts

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Table S1: Experimental 90 K atomic positions in fractional coordinates of monopotassium glutamate monohydrate. The space group is *P2₁2₁2* and the lattice parameters are *a* = 7.842 Å, *b* = 20.590 Å, *c* = 5.143 Å, and α = β = γ = 90°.

K	0.50000	0.50000	0.01328
K	0.00000	0.50000	0.88840
O	0.27724	0.55393	0.64940
O	0.90594	0.62786	0.68520
O	0.20535	0.45164	1.27420
O	0.32095	0.59184	0.24920
O	0.83222	0.71591	0.90570
N	0.22342	0.67482	0.84350
C	0.79590	0.66439	0.78960
C	0.30080	0.59922	0.48870
C	0.50090	0.69042	0.61130
C	0.60910	0.64376	0.77320
C	0.31330	0.66905	0.59020
H	0.17200	0.42040	1.36100
H	0.22700	0.48470	1.35300
H	0.60500	0.59950	0.69500
H	0.57700	0.64260	0.95600
H	0.51100	0.73370	0.68900
H	0.53900	0.69270	0.43300
H	0.10900	0.66430	0.81600
H	0.26600	0.64280	0.98300
H	0.22900	0.71670	0.91500
H	0.25700	0.69730	0.46700

Table S2: Experimental 90 K atomic positions in fractional coordinates of monosodium glutamate monohydrate. The space group is $P2_12_12_1$ and the lattice parameters are a = 5.521 Å, b = 15.130 Å, c = 17.958 Å, and $\alpha = \beta = \gamma = 90^\circ$.

Na	-0.0523	0.4244	0.1796
Na	1.067	0.4316	0.67529
O	-0.4073	0.4352	0.1037
O	0.6625	0.4915	0.2645
O	0.8914	0.3912	0.9858
O	1.4584	0.2211	0.7638
O	0.2705	0.4525	0.2556
O	1.1459	0.3518	1.0785
O	0.8763	0.348	0.5845
O	1.1186	0.3923	0.4924
O	1.4326	0.4371	0.6109
O	1.1357	0.3133	0.7586
N	1.7182	0.3225	0.8548
N	0.3011	0.3255	0.3584
C	1.4817	0.3593	0.8278
C	0.482	0.4442	0.2814
C	0.5309	0.3698	0.3366
C	1.27	0.3258	0.9518
C	0.674	0.4013	0.4044
C	1.35	0.2912	0.7793
C	1.33	0.3949	0.893
C	1.091	0.3588	1.0102
C	0.739	0.3294	0.4589
C	0.929	0.3599	0.5164
H	1.403	0.307	0.978
H	1.206	0.266	0.924
H	1.167	0.418	0.871
H	1.399	0.441	0.916
H	1.81	0.348	0.902
H	1.846	0.325	0.814
H	1.699	0.27	0.866
H	-0.29	0.418	0.058
H	-0.51	0.418	0.092
H	0.31	0.246	0.376
H	0.242	0.36	0.394
H	0.813	0.283	0.435
H	0.583	0.307	0.485
H	0.815	0.436	0.386
H	0.589	0.451	0.429
H	0.634	0.325	0.307
H	1.561	0.413	0.606
H	1.34	0.429	0.574
H	1.508	0.41	0.794
H	0.207	0.319	0.323