Electronic Supplementary Information (ESI):

The Regulation Roles of Metal ions (M^{+/2+} =Li⁺, Na⁺, K⁺, Be²⁺, Mg²⁺, and Ca²⁺) and Water Molecules in Stabilizing the Zwitterionic Form of Glycine Derivatives

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Fig. S1 HF/6-31G*-optimized geometries of NO/OO/OH-mode glycine-Li⁺ complexes and their (mono-tetra)hydrates. The relative energies (in kcal mol⁻¹) under each complex are obtained at the B3LYP/6-311+G*//HF/6-31G* level with the ZPVE corrections, respectively.



 2.0
 2.0
 2.2
 2.2
 5.2

 Na-OO1-4W2
 Na-OO1-4W3
 Na-OO1-4W4
 Na-NO-4W3
 Na-NO-4W4

Fig. S2. HF/6-31G*-optimized geometries of NO/OO/OH-mode glycine-Na⁺ complexes and their (mono-tetra)hydrates. The relative energies (in kcal mol⁻¹) under each complex are obtained at the B3LYP/6-311+G* //HF/6-31G* level with the ZPVE corrections.



Fig. S3 HF/6-31G*-optimized geometries of OH/NO/OO-mode glycine-K⁺ complexes and their (mono-tetra)hydrates. The relative energies (in kcal mol⁻¹) under each complex are obtained at the B3LYP/6-311+G* //HF/6-31G* level with the ZPVE corrections.



0.0 5.9 Be-NO Be-OO2



0.0

Be-NO-W



1.6 Be-OO2-W





10.6 Be-OO2-W1

22.3 Be-NO-W1



Be-OO2-2W



6.4 Be-NO-2W

17.8 Be-NO-2W1



20.2

Be-NO-2W2

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26.7 Be-OO2-2W2





Be-OO2-2W3

0.0 Mg-OO2



0.0 Mg-OO2-W



ets ety

7.9 33.3 37.2 Mg-NO-W Mg-NO-W1 Mg-OO2-W1



0.0 Mg-OO2-2W

13.7

Ca-NO



6.3 Mg-OO2-2W1





22.3 Mg-OO2-2W2



0.0 Ca-OO2



0.0 Ca-OO2-W

0.0

Ca-OO2-2W



10.1

Ca-NO-2W



Ca-NO-W

7.5 Ca-OO2-W2



15.1 Ca-OO2-2W2

Fig. S4 HF/6-31G*-optimized geometries of NO/OO-mode glycine-Be²⁺/Mg²⁺/Ca²⁺ complexes and their (mono-di)hydrates. The relative energies (in kcal mol⁻¹) under each complex are obtained at the B3LYP/6-311+G* //HF/6-31G* level with the ZPVE corrections.

5.2

Ca-OO2-2W1

Be²⁺ K^+ Ca²⁺ Complexes Li⁺ Mg²⁺ Na^+ M-NO/OO/OH 0.94/0.94/0.96 0.95/0.94/0.96 0.97/0.97/0.98 1.82/1.80/-1.92/1.91/-1.76/1.76/-M-NO/OO/OH-W 0.88/0.89/0.92 0.92/0.92/0.94 0.96/0.97/0.97 1.68/1.68/-1.78/1.77/-1.90/1.89/-M-NO/OO/OH-2W 0.90/0.92/0.92 0.94/0.95/0.96 1.67/1.68/-1.74/1.75/-1.87/1.86/-0.84/0.87/0.88 M-NO/OO/OH-3W 0.84/0.82/0.83 0.90/0.91/0.90 0.94/0.95/0.94 M-NO/OO/OH-4W 0.89/0.91/0.89 0.93/0.95/0.92 0.83/0.86/0.83

Table S1 B3LYP/6-31(d,p)-optimized NBO charge populations over each metal ion in these different complexes