Electronic Supplementary Information (ESI):

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

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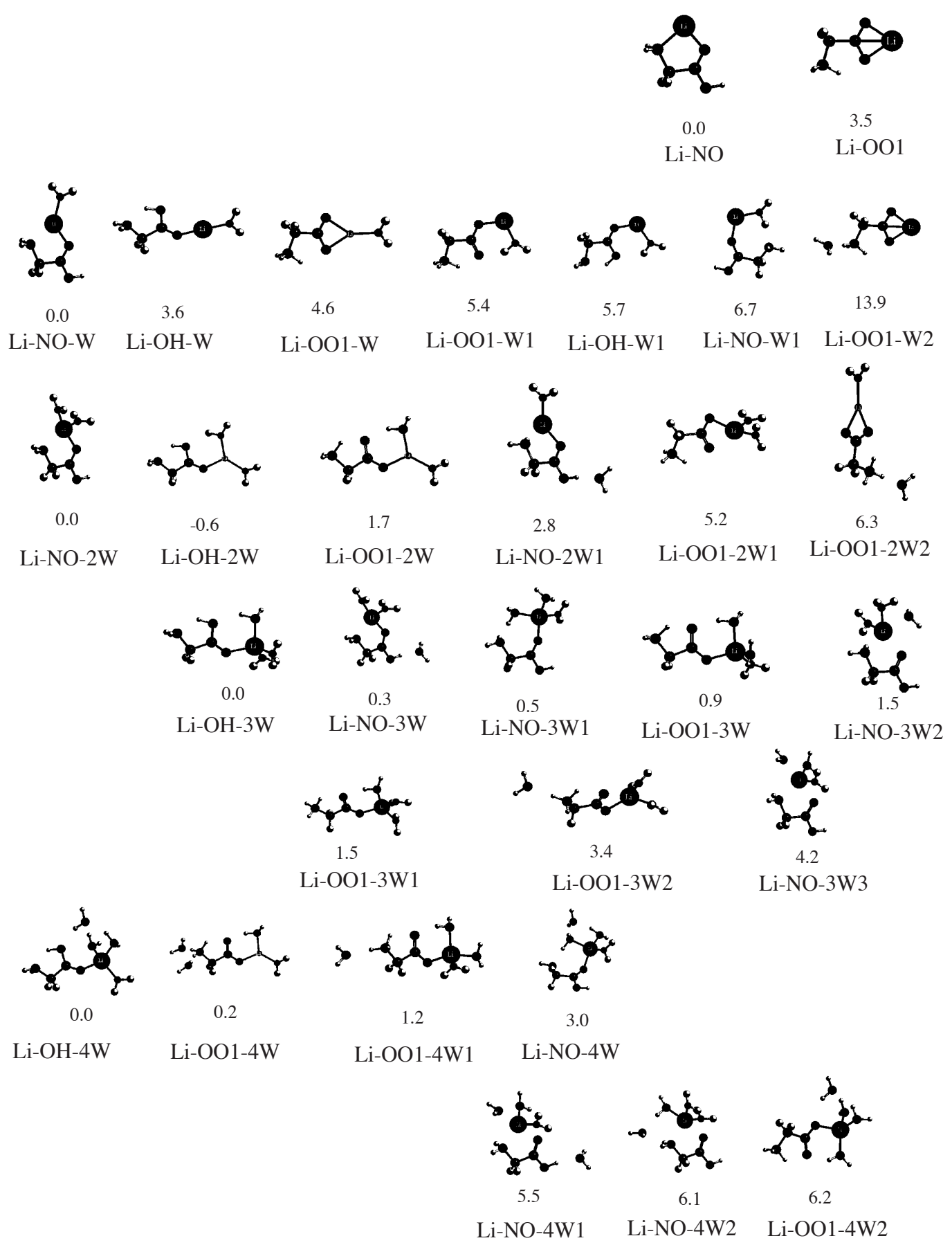

Fig. S1 HF/6-31G*-optimized geometries of NO/OO/OH-mode glycine-Li^+ complexes and their (mono-tetra)hydrates. The relative energies (in kcal mol^{-1}) under each complex are obtained at the B3LYP/6-311+G*//HF/6-31G* level with the ZPVE corrections, respectively.

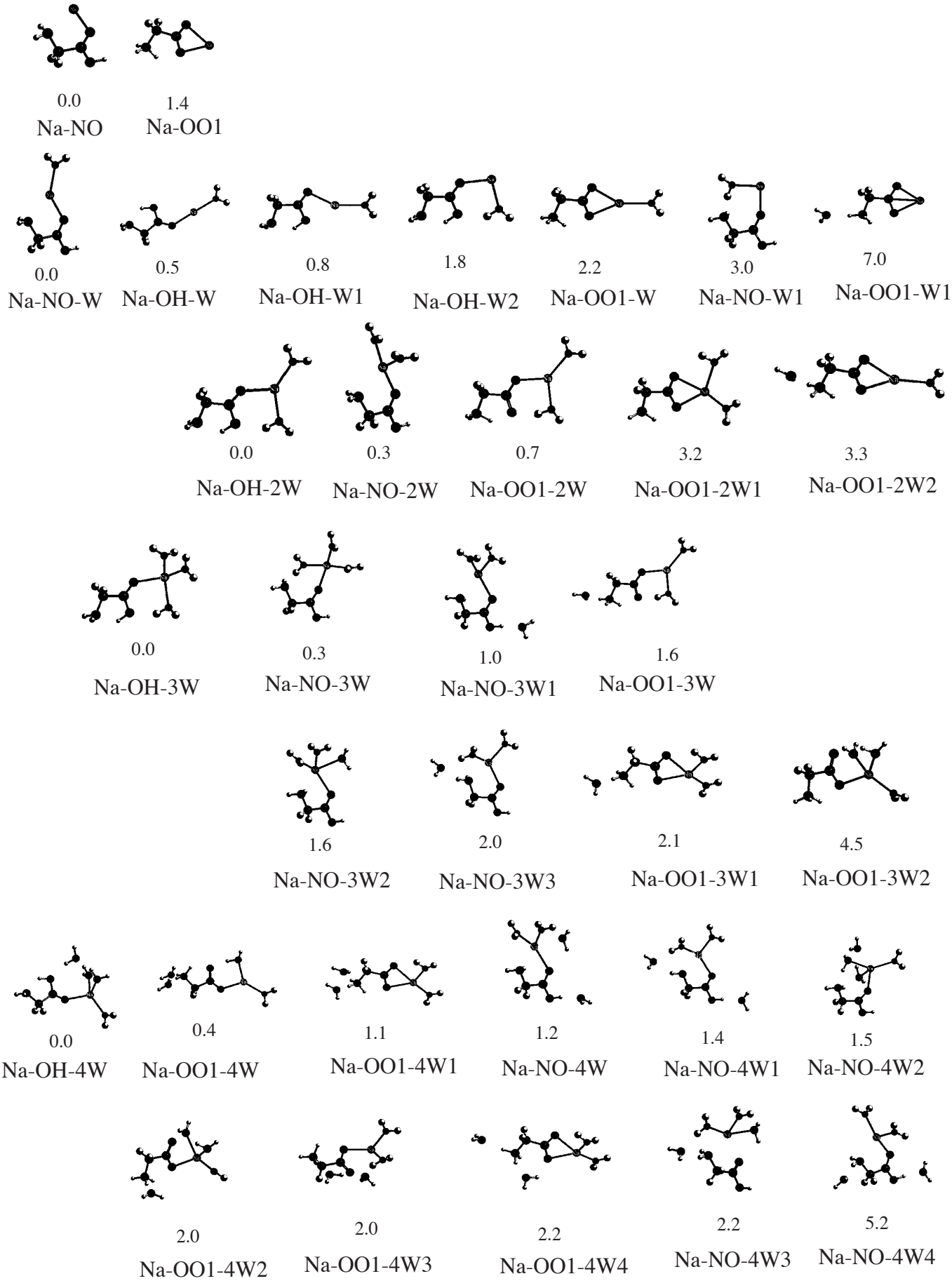

Fig. S2. HF/6-31G*-optimized geometries of NO/OO/OH-mode glycine-Na^+ complexes and their (mono-tetra)hydrates. The relative energies (in kcal mol^{-1}) under each complex are obtained at the B3LYP/6-311+G* //HF/6-31G* level with the ZPVE corrections.

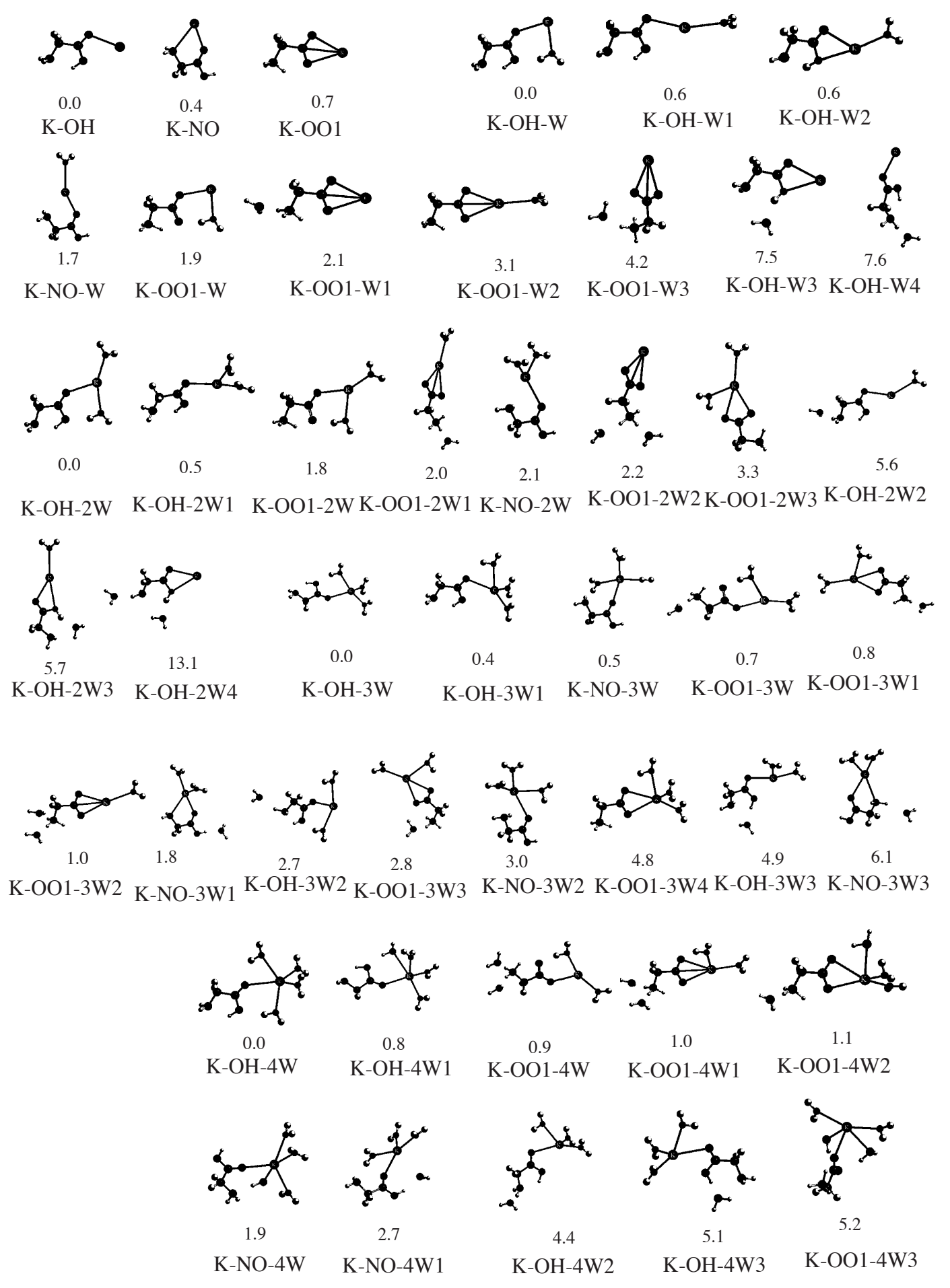

Fig. S3 HF/6-31G*-optimized geometries of OH/NO/OO-mode glycine-K^+ complexes and their (mono-tetra)hydrates. The relative energies (in kcal mol^{-1}) under each complex are obtained at the B3LYP/6-311+G* //HF/6-31G* level with the ZPVE corrections.

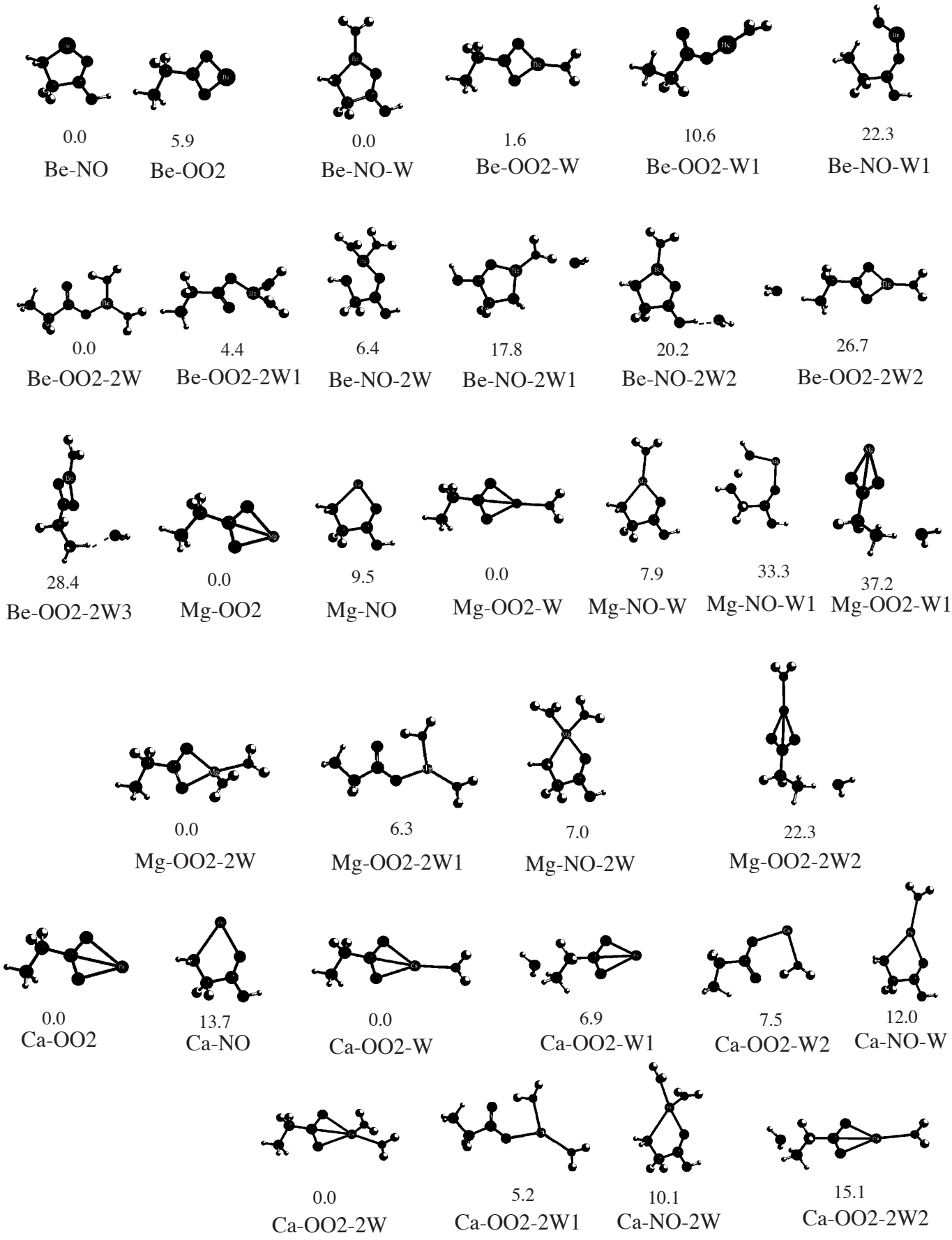

Fig. S4 HF/6-31G*-optimized geometries of NO/OO-mode glycine-Be^{2+}/Mg^{2+}/Ca^{2+} complexes and their (mono-di)hydrates. The relative energies (in kcal mol^{-1}) under each complex are obtained at the B3LYP/6-311+G* //HF/6-31G* level with the ZPVE corrections.

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

Complexes	Li^+	Na^+	K^+	Be^{2+}	Mg^{2+}	Ca^{2+}
M-NO/OO/OH	0.94/0.94/0.96	0.95/0.94/0.96	0.97/0.97/0.98	1.76/1.76/-	1.82/1.80/-	1.92/1.91/-
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	0.84/0.87/0.88	0.90/0.92/0.92	0.94/0.95/0.96	1.67/1.68/-	1.74/1.75/-	1.87/1.86/-
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	0.83/0.86/0.83	0.89/0.91/0.89	0.93/0.95/0.92			