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The importance of the metal ion and complex geometry on the interaction between a coordinated amino acid and a free water molecule

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Using quantum chemistry calculations and analysis of crystal structures from the Cambridge Structural Database (CSD), three types of hydrogen bonds, NH/O, O1/HO (hydrogen bond of a coordinated oxygen atom), and O2/HO (hydrogen bond of a non-coordinated oxygen atom) between different metal ion complexes of amino acids and a free water molecule were studied. Octahedral cobalt(III) [1] and nickel(II), square pyramidal copper(II), square planar copper(II), palladium(II), and platinum(II) complexes were investigated at M06L-GD3/def2-TZVPP level, and interaction energies were calculated using basis set superposition error (BSSE) corrected values. The NH/O hydrogen bond of a doubly positive complex has an interaction energy of -16.9 kcal/mol. For singly positive complexes, NH/O hydrogen bonds are weaker, from -8.3 to -12.1 kcal/mol strong, while for neutral complexes their values are the weakest, from -5.2 to -7.2 kcal/mol. In neutral complexes with O1/HO, interaction energies are from -2.2 to -5.1 kcal/mol, while interactions in singly negatively charged complexes are stronger, from -6.9 to 8.2 kcal/mol. Neutral complexes also have weaker O2/HO hydrogen bonds, from -3.7 to -5.0 kcal/mol, than the singly negatively charged systems, which have interaction energy values from -8.0 to -9.0 kcal/mol. Therefore, the results of quantum chemistry calculations showed that the strongest hydrogen bond is the NH/O, followed by O1/HO, and lastly, O2/HO interaction. The results also show a strong influence of the complex charge on the interaction energy. Other factors that influence the interaction energy to a smaller extent are metal oxidation number, coordination number, and metal atomic number. In the crystal structures from the CSD search, the *d* distributions for copper(II) and cobalt(III) amino acid complexes are in good agreement with the quantum chemistry results.

References

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