Table S2. Electronic configurations of Mg2+ and Fe2+ in the RNA2- -Mg2+(H2O)4 and RNA2- -Fe2+(H2O)4 complexes as revealed by the NBO at the (U)B3LYP/6-31G(d,p) level of theory.

|  |  |  |
| --- | --- | --- |
| Complex | Charge | Electronic configuration |
| RNA2- -Mg2+(H2O)4 | 1.705 | [core]3s(0.26)3p(0.02)3d(0.01)4p(0.01) |
| RNA2- -Fe2+(H2O)4 (Total) | 1.562 | [core]4s(0.29)3d(6.11)4p(0.02)5p(0.01) |
| RNA2- -Fe2+(H2O)4 (Alpha) | -1.139 | [core]4s(0.15)3d(4.98)4p(0.01) |
| RNA2- -Fe2+(H2O)4 (Beta) | 2.702 | [core]4s(0.14)3d(1.14)4p(0.01) |