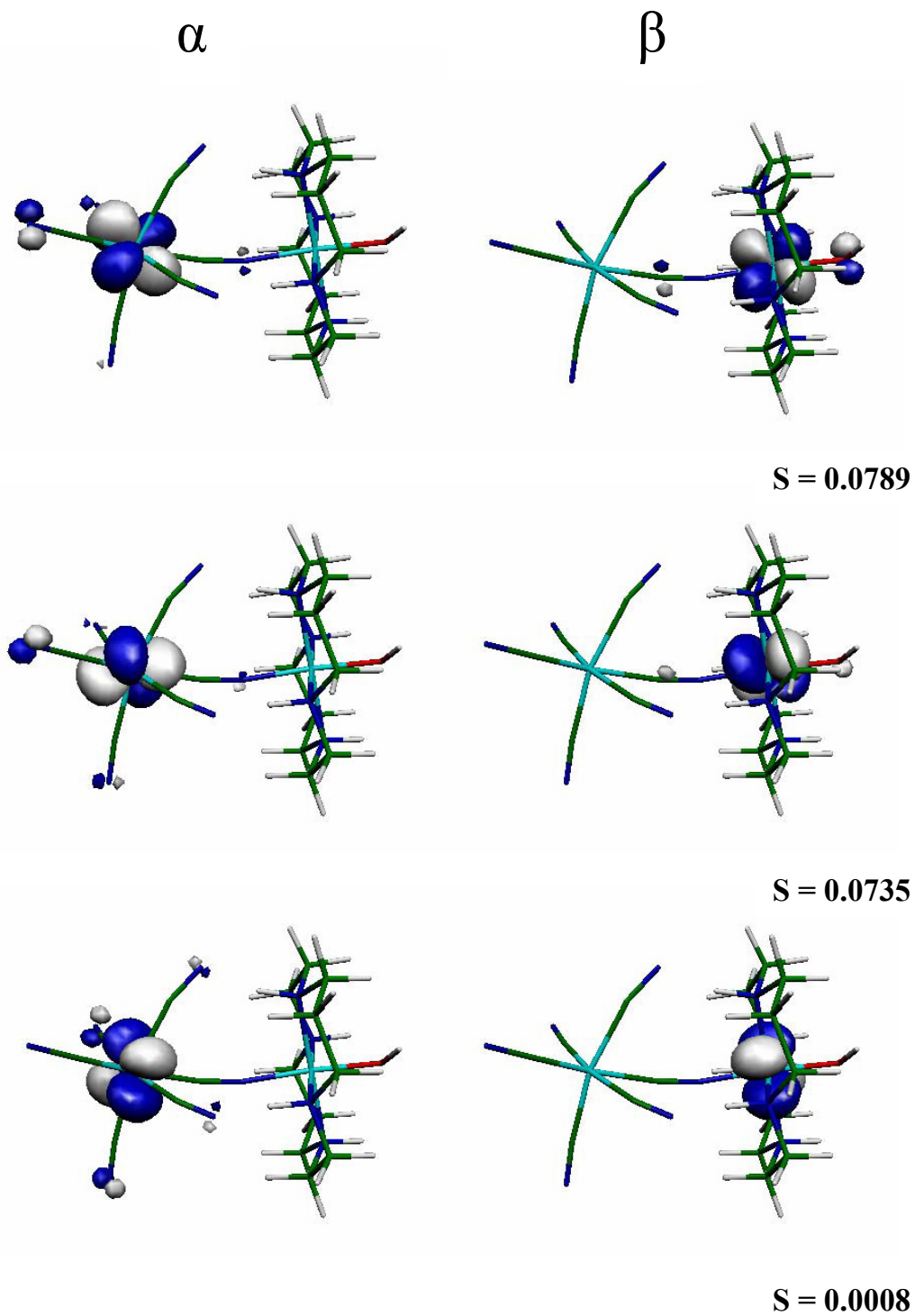


**Figure 3** – Packing structure of the crystal **1**, showing its layered structure and the H-bonding.



**Figure 6.** Magnetic orbitals for compounds **1** at the BS-B3LYP level of theory, as obtained from the corresponding orbital transformation (see text).