**Table 2.** Binding energies (*E*b)of EDTA4H complexes. Numbers in bold represent the most stable metal complexes.

|  |  |  |  |
| --- | --- | --- | --- |
| Positions | *E*b (eV) | | |
| Ba–EDTA4H | Y–EDTA4H | Zr–EDTA4H |
| P1 | –26.66 | –29.62 | –32.31 |
| P2 | **–26.67** | –29.62 | –32.31 |
| P3 | –25.71 | –27.34 | –28.99 |
| P4 | –17.08 | –27.33 | –28.96 |
| P5 | –26.56 | **–33.12** | **–37.33** |