**Table 1.** Binding energies (*E*b) of CA3H complexes. Numbers in bold represent the most stable metal complexes.

|  |  |  |  |
| --- | --- | --- | --- |
| Positions | *E*b (eV) | | |
| Ba–CA3H | Y–CA3H | Zr–CA3H |
| P1 | –18.92 | –21.65 | –24.23 |
| P2 | **–19.39** | –21.65 | –24.23 |
| P3 | –19.01 | –21.72 | **–25.69** |
| P4 | –18.92 | **–21.82** | –24.89 |
| P5 | –18.92 | **–21.82** | –24.89 |