**Table 3.** Charge of metals after complexation with the chelating agent

|  |  |  |  |
| --- | --- | --- | --- |
| Metals | Mulliken atomic charge of metals in metal–complexes | | |
| Initial | After optimized (CA3H) | After optimized (EDTA4H) |
| Ba | +2 | +1.544 | +1.508 |
| Y | +3 | +2.104 | +1.449 |
| Zr | +4 | +2.672 | +1.911 |