**Table 5.** Mulliken charges of the most stable metal–EDTA4H complexes

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Complexes** |  |  | **Atom Charges** | | | | | | |
|  | **O1** | **O2** | **O3** | **O4** | **O5** | **O6** | **O7** | **O8** | **N9** |
| Ba–EDTA4H | –0.640 | –0.650 | –0.643 | –0.650 | –0.629 | –0.619 | –0.627 | –0.618 | –0.359 |
| Y–EDTA4H | –0.535 | –0.542 | –0.536 | –0.542 | –0.623 | –0.627 | –0.623 | –0.627 | –0.501 |
| Zr–EDTA4H | –0.471 | –0.483 | –0.471 | –0.483 | –0.650 | –0.653 | –0.650 | –0.653 | –0.532 |
|  |  |  |  |  |  |  |  |  |  |
|  | **C11** | **C12** | **C13** | **C14** | **C15** | **C16** | **C17** | **C18** | **C19** |
| Ba–EDTA4H | –0.138 | –0.137 | –0.208 | –0.224 | –0.206 | –0.224 | 0.532 | 0.449 | 0.526 |
| Y–EDTA4H | –0.145 | –0.145 | –0.246 | –0.239 | –0.246 | –0.239 | 0.561 | 0.572 | 0.561 |
| Zr–EDTA4H | –0.156 | –0.156 | –0.266 | –0.246 | –0.266 | –0.246 | 0.593 | 0.603 | 0.593 |
|  |  |  |  |  |  |  |  |  |  |
|  | **H21** | **H22** | **H23** | **H24** | **H25** | **H26** | **H27** | **H28** |  |
| Ba–EDTA4H | 0.113 | 0.143 | 0.106 | 0.151 | 0.095 | 0.159 | 0.092 | 0.129 |  |
| Y–EDTA4H | 0.173 | 0.183 | 0.173 | 0.183 | 0.171 | 0.205 | 0.170 | 0.199 |  |
| Zr–EDTA4H | 0.210 | 0.205 | 0.210 | 0.205 | 0.214 | 0.239 | 0.209 | 0.229 |  |
|  |  |  |  |  |  |  |  |  |  |
|  | **H29** | **H30** | **H31** | **H32** | **H29** | **H30** | **H31** |  |  |
| Ba–EDTA4H | 0.095 | 0.160 | 0.093 | 0.130 | 0.095 | 0.160 | 0.093 |  |  |
| Y–EDTA4H | 0.171 | 0.205 | 0.170 | 0.199 | 0.171 | 0.205 | 0.170 |  |  |
| Zr–EDTA4H | 0.214 | 0.239 | 0.209 | 0.229 | 0.214 | 0.239 | 0.209 |  |  |