**Table 4.** Mulliken charges of the most stable metal–CA3H complexes

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Complexes** | **Atom Charges** | | | | | | |
|  | **C1** | **C2** | **C3** | **C4** | **C6** | **C7** |  |
| Ba–CA3H | 0.259 | –0.367 | –0.389 | 0.511 | 0.515 | 0.495 |  |
| Y–CA3H | 0.215 | –0.398 | –0.389 | 0.621 | 0.587 | 0.490 |  |
| Zr–CA3H | 0.181 | –0.398 | –0.407 | 0.666 | 0.627 | 0.534 |  |
|  |  |  |  |  |  |  |  |
|  | **O5** | **O8** | **O9** | **O10** | **O11** | **O12** | **O13** |
| Ba–CA3H | –0.780 | –0.597 | –0.675 | –0.593 | –0.669 | –0.632 | –0.601 |
| Y–CA3H | –0.739 | –0.523 | –0.688 | –0.511 | –0.682 | –0.631 | –0.598 |
| Zr–CA3H | –0.745 | –0.453 | –0.723 | –0.421 | –0.713 | –0.590 | –0.563 |
|  |  |  |  |  |  |  |  |
|  | **H14** | **H15** | **H16** | **H17** | **H18** |  |  |
| Ba–CA3H | 0.150 | 0.123 | 0.136 | 0.132 | 0.438 |  |  |
| Y–CA3H | 0.189 | 0.188 | 0.135 | 0.162 | 0.471 |  |  |
| Zr–CA3H | 0.228 | 0.232 | 0.177 | 0.193 | 0.504 |  |  |