Additional file 2: Charges of oxygen and iron atoms in the formed complex.

|  |  |
| --- | --- |
| **charge** | **Atom-Number** |
| -0.673 | Oxygen-37 |
| -0.675 | Oxygen-38 |
| -0.600 | Oxygen-39 |
| -0.648 | Oxygen-40 |
| -0.733 | Oxygen-41 |
| -0.675 | Oxygen-42 |
| 2.150 | Iron-47 |