**Supplementary Material**

**Removal of Phenol from Aqueous Solution by Adsorption onto Hematite (**α**-Fe2O3): Mechanism Exploration from both Experimental and Theoretical Studies**

**Younes Dehmani1, Awad A. Alrashdi2, Hassane Lgaz3,\*, Taibi Lamhasni4, Sadik Abouarnadasse1, Ill-Min Chung3,\***

1Laboratory of Chemistry and Biology Applied to the Environment, Moulay Ismail University, Faculty of Sciences of Meknes, Meknes, Morocco.

2Chemistry Department, Umm Al-Qura University, Al-Qunfudah University College, Saudi Arabia.

3Department of Crop Science, College of Sanghur Life Science, Konkuk University, Seoul 05029, South Korea.

4Institut National des Sciences de l’Archéologie et du Patrimoine (INSAP), BP 6828, Madinat al Irfane, avenue Allal El Fassi, Angle rues 5 et 7, Rabat-Instituts, Morocco.

\*Corresponding author:

Email: [hlgaz@konkuk.ac.kr](mailto:hlgaz@konkuk.ac.kr) (Hassane Lgaz), [imcim@konkuk.ac.kr](mailto:imcim@konkuk.ac.kr) (Ill-Min Chung).

**Table S1.** Equations of kinetic and adsorption models.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Model** | **Equation** | **Reference** |
| Kinetic models | Pseudo-first order |  | (Lagergren, 1898) |
| Pseudo-second order |  | (Ho and McKay, 1999) |
| Isotherms models | Langmuir |  | (Banerjee et al., 2019) |
| Freundlich |  | (Banerjee et al., 2019) |

**Table S2.** NBO data of the Phenol-α-Fe2O3 complex in aqueous solution calculated at the CPCM/B3LYP with LANL2DZ basis set for Fe atoms and 6–311++G(d,p) basis set for other atoms.

|  |  |  |
| --- | --- | --- |
| Donor NBO (i) | Acceptor NBO (j) | E2 (kJ/mol) |
| BD ( 1)Fe 1 - O 3 | RY\*( 3) C 9 | 22.3844 |
|  | RY\*( 2) C 10 | 10.0416 |
|  | RY\*( 1) C 11 | 10.8784 |
| CR ( 1)Fe 1 | LP ( 1) C 9 | 35.9824 |
| CR ( 1)Fe 5 | LP ( 1) C 11 | 28.11648 |
| LP ( 2)Fe 1 | LP ( 1) C 9 | 16.02472 |
| LP\*( 3)Fe 1 | RY\*( 1) C 6 | 24.14168 |
|  | RY\*( 2) C 6 | 18.49328 |
|  | RY\*( 1) C 7 | 19.99952 |
|  | RY\*( 2) C 7 | 89.5376 |
|  | RY\*( 1) C 8 | 17.3636 |
|  | RY\*( 2) C 8 | 162.7576 |
|  | RY\*( 3) C 8 | 13.97456 |
|  | RY\*( 2) C 9 | 61.00272 |
|  | RY\*( 3) C 9 | 116.35704 |
|  | RY\*( 1) C 10 | 29.7064 |
|  | RY\*( 2) C 10 | 91.58776 |
|  | RY\*( 3) C 10 | 90.83464 |
|  | RY\*( 1) C 11 | 41.29608 |
|  | RY\*( 1) O 17 | 16.48496 |
|  | BD\*( 1) C 11 - H 16 | 9.74872 |
| LP\*( 4)Fe 1 | RY\*( 3) C 9 | 17.1544 |
| LP\*( 5)Fe 1 | RY\*( 2) C 6 | 10.29264 |
|  | RY\*( 2) C 7 | 23.93248 |
|  | RY\*( 3) C 7 | 10.37632 |
|  | RY\*( 2) C 8 | 10.83656 |
|  | RY\*( 3) C 9 | 10.96208 |
|  | RY\*( 2) C 10 | 25.89896 |
|  | RY\*( 3) C 11 | 11.9244 |
|  | BD\*( 1) C 9 - C 10 | 36.73552 |
| LP\*( 5)Fe 5 | RY\*( 1) C 6 | 66.35824 |
|  | RY\*( 1) C 7 | 9.49768 |
|  | RY\*( 2) C 7 | 246.14472 |
|  | RY\*( 1) C 8 | 15.56448 |
|  | RY\*( 2) C 8 | 62.76 |
|  | RY\*( 1) C 9 | 11.38048 |
|  | RY\*( 3) C 9 | 24.35088 |
|  | RY\*( 2) C 10 | 122.04728 |
|  | RY\*( 1) C 11 | 52.80208 |
|  | RY\*( 3) C 11 | 123.2188 |
|  | RY\*( 1) O 17 | 17.86568 |
|  | BD\*( 1) C 9 - H 15 | 21.88232 |
|  | BD\*( 1) C 11 - H 16 | 50.16616 |
| BD\*( 1)Fe 1 - O 3 | RY\*( 3) C 9 | 23.17936 |
|  | RY\*( 2) C 10 | 11.33864 |
| BD\*( 1)Fe 1 - O 4 | RY\*( 3) C 9 | 17.5728 |
| BD ( 1) C 6 - C 11 | LP\*( 6)Fe 5 | 12.17544 |
| BD ( 1) C 8 - C 9 | LP\*( 3)Fe 1 | 14.2256 |
|  | LP\*( 5)Fe 1 | 13.93272 |
| BD ( 1) C 9 - C 10 | LP\*( 3)Fe 1 | 8.82824 |
|  | LP\*( 5)Fe 1 | 10.62736 |
| BD ( 1) C 9 - H 15 | LP\*( 3)Fe 1 | 37.53048 |
|  | LP\*( 5)Fe 1 | 12.67752 |
| BD ( 1) C 10 - C 11 | LP\*( 4)Fe 5 | 11.96624 |
|  | LP\*( 6)Fe 5 | 15.60632 |
| BD ( 1) C 11 - H 16 | LP\*( 4)Fe 5 | 13.72352 |
|  | LP\*( 5)Fe 5 | 10.6692 |
|  | LP\*( 6)Fe 5 | 17.19624 |
| CR ( 1) C 9 | LP\*( 3)Fe 1 | 17.90752 |
|  | LP\*( 5)Fe 1 | 11.506 |
| CR ( 1) C 11 | LP\*( 6)Fe 5 | 15.81552 |
| LP\*( 1) C 8 | BD\*( 2)Fe 1 - O 4 | 12.7612 |
|  | BD\*( 3)Fe 1 - O 4 | 9.16296 |
| LP ( 1) C 9 | LP\*( 3)Fe 1 | 201.83616 |
|  | LP\*( 5)Fe 1 | 65.43776 |
|  | RY\*( 14)Fe 1 | 10.54368 |
|  | RY\*( 21)Fe 1 | 10.41816 |
|  | RY\*( 35)Fe 1 | 9.74872 |
|  | BD\*( 2)Fe 1 - O 4 | 65.0612 |
|  | BD\*( 3)Fe 1 - O 4 | 33.84856 |
| LP ( 1) C 11 | LP\*( 4)Fe 5 | 553.29216 |
|  | LP\*( 5)Fe 5 | 80.16544 |
|  | LP\*( 6)Fe 5 | 70.66776 |
|  | LP\*( 7)Fe 5 | 10.83656 |
|  | RY\*( 17)Fe 5 | 10.83656 |
|  | RY\*( 18)Fe 5 | 9.03744 |
|  | RY\*( 24)Fe 5 | 13.09592 |