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**Fig. S1.** Various isotherm plots for the adsorption of EDTP, DITP and DPTP on the surface of C1018 carbon steel determined by electrochemical impedance spectroscopy.

|  |  |
| --- | --- |
|  | **Fukui function** |
| **Electrophilic (***fk*-) | **Nucleophilic (***fk*+) |
| **EDTP** |  |  |
| **DITP** |  |  |
| **DPTP** |  |  |

**Fig. S2**. Visualization of Fukui functions of EDTP, DITP and DPTP.

**Table S1**

Fukui Indices for EDTP, DITP and DPTP determined by using BLYP/DNP.

|  |  |  |  |
| --- | --- | --- | --- |
| **Inhibitor** | **Atom** | **Mulliken Population Analysis** | **Hirshfeld population analysis** |
| ***f*k-** | ***f*k+** | ***f*k-** | ***f*k+** |
|  **EDTP** | C(1) | **0.046** | 0.006 | **0.059** | 0.017 |
| C(2 | 0.017 | 0.004 | 0.038 | 0.011 |
| C(3) | 0.019 | 0.018 | 0.037 | 0.019 |
| C(4) | **0.058** | -0.023 | **0.076** | -0.016 |
| C(5) | 0.040 | 0.009 | 0.051 | 0.013 |
| C(6) | 0.020 | -0.012 | 0.037 | -0.007 |
| C(7) | -0.007 | -0.013 | 0.007 | 0.007 |
| N(8) | 0.012 | 0.003 | 0.018 | 0.015 |
| C(9) | -0.008 | 0.012 | 0.007 | 0.032 |
| N(10) | 0.009 | 0.010 | 0.012 | 0.037 |
| C(11) | -0.007 | 0.039 | 0.003 | 0.054 |
| C(12) | 0.011 | **0.131** | 0.014 | **0.114** |
| C(13) | -0.006 | -0.031 | 0.007 | 0.028 |
| C(14) | 0.006 | **0.099** | 0.002 | **0.083** |
| O(15) | 0.002  | **0.107** | 0.004 | **0.105** |
| O(16) | 0.006 | 0.018 | 0.007 | 0.029 |
| C(17) | -0.010 | -0.031 | 0.003 | 0.011 |
| N(18) | **0.090** | 0.007 | **0.108** | 0.012 |
| C(19) | -0.040 | -0.014 | 0.026 | 0.006 |
| C(20) | -0.039 | -0.012 | 0.026 | 0.006 |
| N(21) | **0.060** | **0.086** | **0.053** | **0.081** |
| C(22) | -0.005 | -0.014 | 0.004 | 0.008 |
|  **DITP** | C(1) | 0.047 | 0.007 | **0.059** | 0.016 |
| C(2 | 0.017 | -0.001 | 0.039 | 0.006 |
| C(3) | 0.018 | 0.016 | 0.037 | 0.017 |
| C(4) | **0.061** | -0.023 | **0.078** | -0.019 |
| C(5) | 0.042 | 0.006 | **0.054** | 0.011 |
| C(6) | 0.018 | -0.011 | 0.038 | -0.009 |
| C(7) | -0.008 | -0.014 | 0.007 | 0.005 |
| N(8) | 0.017 | 0.011 | 0.020 | 0.013 |
| C(9) | -0.013 | 0.017 | 0.005 | 0.027 |
| N(10) | 0.004 | 0.017 | 0.009 | 0.041 |
| C(11) | -0.011 | 0.023  | 0.002 | 0.046 |
| C(12) | 0.009 | **0.130** | 0.012 | **0.113** |
| C(13) | -0.008 | -0.031 | 0.007 | 0.027 |
| C(14) | 0.004 | **0.109**  | 0.005 | **0.105** |
| O(15) | 0.010 | **0.135** | 0.011 | **0.137** |
| N(16) | **0.091** | 0.006 | **0.109** | 0.012 |
| C(17) | -0.039 | -0.013 | 0.026 | 0.006 |
| C(18) | -0.040 | -0.012 | 0.026 | 0.006 |
| N(19) | **0.056** | **0.082** | 0.048 | **0.078** |
| C(20) | -0.007 | -0.029 | 0.006 | 0.023 |
| **DPTP** | C(1) | 0.045 | 0.007 | 0.057 | 0.016 |
| C(2 | 0.015 | 0.009 | 0.035 | 0.013 |
| C(3) | 0.017 | 0.012  | 0.034 | 0.015 |
| C(4) | **0.052** | -0.024 | **0.068** | -0.012 |
| C(5) | 0.036 | 0.012 | 0.046 | 0.014 |
| C(6) | 0.018 | -0.011 | 0.034 | -0.004 |
| C(7) | -0.003 | -0.008 | 0.007 | 0.006 |
| N(8) | 0.007 | 0.006  | 0.017 | 0.010 |
| C(9) | 0.000 | 0.011 | 0.012 | 0.020 |
| N(10) | 0.016 | 0.009 | 0.019 | 0.026 |
| C(11) | -0.002 | 0.018 | 0.009 | 0.031 |
| C(12) | 0.012 | **0.083** | 0.018 | **0.074** |
| C(13) | -0.008 | -0.022 | 0.008 | 0.018 |
| C(14) | -0.008 | **0.092** | -0.005 | **0.077** |
| O(15) | 0.008 | **0.089** | 0.007 | **0.088** |
| N(16) | **0.084** | 0.007 | **0.100** | 0.010 |
| C(17) | -0.036 | -0.012 | 0.024 | 0.005 |
| C(18) | -0.036 | -0.010  | 0.024 | 0.005 |
| N(19) | **0.070** | 0.063  | **0.065** | 0.059 |
| N(20) | 0.004 | -0.002 | 0.002 | 0.021 |
| C(21) | -0.009 | 0.014 | -0.007 | 0.017 |
| C(22) | -0.001 | 0.016 | 0.002 | 0.028 |
| C(23) | -0.002 | 0.014 | 0.001 | 0.022 |
| C(24) | 0.002 | 0.006 | 0.009 | 0.030 |
| C(25) | 0.001 | 0.009  | 0.008 | 0.030 |
| C(26) | 0.008 | 0.043 | 0.015 | 0.055 |