THERMAL AND ELECTROCHEMICAL BEHAVIOR OF ACIDIC PYROPHOSPHATE (NH4)2Zn(H2P2O7)2.2H2O

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**Supplemental Materials**



Figure S 1: Infrared Spectrum of (NH4)2Zn(H2P2O7)2.2H2O at 460°C, amorphous phase.



Figure S 2: X-ray powder diffractogram of the (NH4)2Zn(H2P2O7)2.2H2O at 460°C, amorphous.

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Figure S 3: Infrared spectrum of Zn2P4O12 after heating the (NH4)2Zn(H2P2O7)2.2H2O at 910°

Figure S 4: Nyquist diagram for mild steel with selected concentrations of (NH4)2Zn(H2P2O7)2.2H2O



**Figure S 5**: Equivalent circuit model used to fit the impedance spectra



Figure S 6: Langmuir adsorption isotherm in 1.0M HCl solution containing different concentrations of (NH4)2Zn(H2P2O7)2.2H2O



Figure S 7: Arrhenius plots for mild steel corrosion in 1.0 M HCl in the absence and in presence of (NH4)2Zn(H2P2O7)2.2H2O

**Table S 1:** Potentiodynamic polarization parameters for mild steel in 1.0 M HCl with and without different concentrations of (NH4)2Zn (H2P2O7)2.2H2O at 298K.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Medium** | **Conc.****M** | **-Ecorr mV/SCE** | **icorr****µA cm-2** | **-βc****mV dec-1** | **βa****mV dec-1** | ***η*PP****%** |
| **HCl 1.0M** | -- | 470 | 714 | 145 | 121 | - |
| **Inh** | 10-3 | 595 | 50 | 97 | 90 | 93.0 |
| 10-4 | 596 | 80 | 91 | 86 | 88.7 |
| 10-5 | 598 | 102 | 102 | 85 | 85.7 |
| 10-6 | 575 | 109 | 98 | 83 | 84.7 |

Table S 2: AC impedance parameters for mild steel in 1.0 M HCl solution with respect to the concentration of (NH4)2Zn (H2P2O7)2.2H2O

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Conc.****(M)** | **Rs****(Ω cm2)** | **Rct****(Ω cm2)** | **Cdl****(µF.cm-2 )** | **ndl** | **Q****(µF.Sn-1)** | **Ɵ** | ***ƞ*imp****%** |
| **HCl 1.0M** | -- | 1.9 | 23.4 | 190 | 0.897 | 470 | - | - |
| Inh | 10-3 | 1.6 | 305.5 | 73.7 | 0.853 | 128 | 0.923 | 92.3 |
| 10-4 | 1.4 | 202.8 | 90.8 | 0.854 | 162 | 0.884 | 88.4 |
| 10-5 | 0.9 | 157.9 | 93.9 | 0.827 | 194 | 0.851 | 85.1 |
| 10-6 | 1.3 | 147.1 | 101.2 | 0.865 | 178 | 0.841 | 84.1 |

Table S 3: Polarization parameters for mild steel in 1 M HCl with 10-3 M of (NH4)2Zn(H2P2O7)2.2H2O at various temperatures

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compounds | TemperatureK | -EcorrmV/SCE | icorrµA cm-2 | -βcmV dec-1 | βamV dec-1 | *η*PP% |
| Blank | 298 | 470 | 714 | 145 | 121 | - |
| 308 | 491 | 950 | 154 | 112 | - |
| 318 | 475 | 1340 | 151 | 126 | - |
| 328 | 465 | 2080 | 159 | 108 | - |
| inh | 298 | 595 | 50 | 97 | 90 | 93.0 |
| 308 | 497 | 92 | 115 | 96 | 90.3 |
| 318 | 495 | 175 | 107 | 112 | 86.9 |
| 328 | 499 | 332 | 100 | 105 | 84.0 |

Table S 4: Corrosion kinetic parameters of mild steel dissolution in 1M HCl in the absence and in the presence of 10−3M of (NH4)2Zn (H2P2O7)2.2H2O

|  |  |  |  |
| --- | --- | --- | --- |
| Conc | Ea (kJ/mol) | ΔHa(kJ/mol) | ΔSa(kJ/mol.K) |
| Blank | 28.7 | 26.1 | -102.8 |
| inh | 51.3 | 48.7 | -49.0 |

Table S 5: Crystal Structure and Data Refinement Parameters

|  |  |  |
| --- | --- | --- |
| **Compound** | **This work** | **Literature** [10] |
| Empirical Formula | (NH4)2Zn(H2P2O7)2.2H2O |
| Formula Weight | [489.4](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_chemical_formula_weight) | [489.4](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_chemical_formula_weight) |
| Crystal System / Space Group | [Triclinic](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_symmetry_cell_setting), Pī  | [Triclinic](file:///C%3A%5CUsers%5CDELL%5CDesktop%5CArticle%202%20r%C3%A9vis%C3%A9%5C1506_A1%20_symmetry_cell_setting), Pī |
| a / Å | [7.0144 (3)](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_length_a) | 7.0026(2) |
| b / Å | [7.2891 (3](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_length_b)) | 7.3297(2) |
| c / Å | [7.7721 (4)](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_length_c) | 7.7885(3 |
| α / ° | [80.436 (4)](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_angle_alpha) | 81.229(1) |
| β / ° | [70.594 (4)](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_angle_beta) | 71.064(1) |
| γ / ° | [88.654 (4)](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_angle_gamma) | 88.172(1) |
| V / Å3 | [369.38 (3)](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_volume) | 373.64(2) |
| Z | [1](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_formula_units_Z) | 1 |
| D calc (g/cm3) | 2.2001 | 2.175 |
| μ (mm-1) | 2.19 | 2.160 |
| Crystal size (mm) | [0.64](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_exptl_crystal_size_max) × [0.54](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_exptl_crystal_size_mid) × [0.38](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_exptl_crystal_size_min) | 0.19×0.31×0.40 |
| Color / Shape | Colourless /Prism | Colourless/Prism |
| Temp (K) | [120](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_cell_measurement_temperature) | 293 |
| Theta range for collection | 3.41° to 29.49° | 2.81° to 30.00° |
| Reflections collected | 5646 | 5328 |
| Independent reflections | [1839](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_reflns_number_total) | 2055 |
| Data/restraints/parameters | [1839](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_reflns_number_total)/8/130 | 2055/6/135 |
| Goodness of fit on F2 | 1.48 | 1.240 |
| Final R indices [I > 2σ(I)] | R1=0.0228, wR2=0.0784 | R1 =0.0447, wR2 =0.1336 |
| R indices (all data) | R1= 0.0245, wR2= 0.0794 | R1 = 0.0480, wR2=0.1360 |
| Largest difference peak/hole | [0.43](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_refine_diff_density_max) and [-0.39](file:///C%3A%5CUsers%5CDELL%5CDownloads%5C1506_A1%20_refine_diff_density_min) e Å−3 | 1.295 and -1.168 e Å−3 |