New Efficient Adsorbent Materials for the Removal of Cd(II) from Aqueous Solutions

Aurelia Visa 1, Bianca Maranescu 1, Lavinia Lupa 2, Luminita Crisan 1 and Ana Borota 1*

1 “Coriolan Dragulescu” Institute of Chemistry, 24 M. Viteazu Ave, Timișoara - 300223, Romania,
2 Faculty of Industrial Chemistry and Environmental Engineering, University Politehnica Timisoara, 2 Piata Victoriei, 300006, Timisoara, Romania
*Correspondence: ana_borota@acad-icht.tm.edu.ro
Received: date; Accepted: date; Published: date

Figure S1. Superposition of the crystal structure of Mg-Gly (carbon atoms in grey) over the optimized structure of Mg-Gly (carbon atoms in purple) with PM3 semiempirical method. The RMSD between them is of 1.219 for heavy atoms.
Table S1. Geometric properties of the Mg-Gly model (CS - Crystal structure; OS - Optimized structure)

| Bond | Distance | Bond Angle | Degree | Torsion Angle | Degree |
|------|----------|------------|--------|---------------|--------|
|      | CS  | OS  | Residuals | CS  | OS  | Residuals | CS  | OS  | Residuals |
| 57-O66 | 1.561 | 1.715 | -0.154 | O29-Mg56-O36 | 89.442 | 109.344 | -19.902 | C46-P25-O29-Mg56 | 66.587 | -24.389 | 90.976 |
| P57-O60 | 1.505 | 1.471 | 0.035 | Mg56-O36-P26 | 151.054 | 156.611 | -5.557 | P25-O29-Mg56-O36 | -77.663 | -2.868 | -74.795 |
| P57-C74 | 1.822 | 1.958 | -0.136 | O36-P26-C43 | 110.219 | 105.944 | 4.275 | O29-Mg56-O36-P26 | -30.074 | -10.206 | -19.868 |
| P2-O8 | 1.485 | 1.590 | -0.105 | P26-C43-N30 | 115.200 | 124.237 | -9.037 | Mg56-O36-P26-O32 | 147.757 | 118.695 | 29.062 |
| P2-O7 | 1.496 | 1.474 | 0.022 | C43-N30-C46 | 115.746 | 114.588 | 1.158 | O36-P26-O32-Mg27 | -36.196 | -123.688 | 87.492 |
| P2-O13 | 1.577 | 1.693 | -0.116 | N30-C46-P25 | 120.139 | 129.166 | -9.027 | P26-O32-Mg27-O4 | -82.983 | 24.247 | -107.230 |
| P26-O41 | 1.577 | 1.637 | -0.061 | C46-P25-O29 | 108.631 | 106.910 | 1.721 | P26-O32-Mg27-O8 | -171.513 | -56.855 | -114.658 |
| P26-O32 | 1.496 | 1.521 | -0.025 | P25-O29-Mg56 | 132.492 | 150.599 | -18.107 | P26-O32-Mg27-O33 | 12.571 | 100.428 | -87.857 |
| P26-C43 | 1.831 | 1.877 | -0.046 | O4-Mg27-O8 | 89.442 | 85.255 | 4.187 | P26-O32-Mg27-O65 | 99.401 | -167.967 | 267.368 |
| P25-O38 | 1.561 | 1.694 | -0.133 | O8-Mg27-O53 | 89.928 | 70.351 | 19.577 | O32-Mg27-O4-P1 | -178.943 | 172.126 | -351.069 |
| P25-O37 | 1.480 | 1.466 | 0.014 | O53-Mg27-O65 | 92.418 | 70.148 | 22.270 | O32-Mg27-O8-P2 | 55.192 | 35.097 | 20.095 |
| P1-O9 | 1.480 | 1.484 | -0.004 | O65-Mg27-O33 | 86.855 | 88.898 | -2.043 | Mg27-O8-P2-C15 | 23.384 | 33.866 | -10.482 |
| Bond  | Length 1 | Length 2 | Length 3 | Angle 1 | Angle 2 | Angle 3 | Bond Angle 1 | Bond Angle 2 | Bond Angle 3 |
|-------|----------|----------|----------|---------|---------|---------|-------------|-------------|-------------|
| P1-O10 | 1.561    | 1.724    | -0.163   | O33-Mg27-O32 | 89.632 | 109.699 | -20.067     | O4-Mg27-O8-P2 | -30.075     | -45.615     | 15.540     |
| P1-C18 | 1.822    | 1.959    | -0.137   | O32-Mg27-O4  | 85.465 | 84.555 | 0.910       | O32-Mg27-O65-P57 | -119.670    | 16.094      | -135.764   |
| O65-P57 | 1.505    | 1.471    | 0.035    | O4-Mg27-O53 | 89.329 | 105.720 | -16.391     | Mg27-O4-P1-C18 | 66.587      | 64.821      | 1.766      |
| O53-H55 | 0.930    | 0.971    | -0.041   | O4-Mg27-O65 | 177.264 | 167.653 | 9.611       |                        |             |             |            |
| O53-H54 | 0.929    | 0.970    | -0.041   | O4-Mg27-O33 | 95.508 | 78.936 | 16.572      |                        |             |             |            |
| O4-P1  | 1.505    | 1.556    | -0.051   | O8-Mg27-O65 | 88.486 | 103.645 | -15.159     |                        |             |             |            |
| O36-P26 | 1.485    | 1.642    | -0.157   | O8-Mg27-O33 | 168.434 | 124.678 | 43.756      |                        |             |             |            |
| O33-H35 | 0.900    | 0.959    | -0.059   | O8-Mg27-O32 | 101.199 | 121.142 | -19.943     |                        |             |             |            |
| O33-H34 | 0.821    | 0.973    | -0.152   | O53-Mg27-O33 | 80.704 | 63.954 | 16.750      |                        |             |             |            |
| O32-Mg27 | 2.033    | 1.867    | 0.167    | O53-Mg27-O32 | 168.544 | 165.792 | 2.752       |                        |             |             |            |
| N5-C15 | 1.504    | 1.493    | 0.011    | O65-Mg27-O32 | 93.183 | 97.732 | -4.549      |                        |             |             |            |
| N30-C46 | 1.511    | 1.521    | -0.010   |                        |         |         |             |                        |             |             |            |
| Mg56-O36 | 2.023    | 1.789    | 0.234    |                        |         |         |             |                        |             |             |            |
| Mg56-O29 | 2.088    | 1.804    | 0.285    |                        |         |         |             |                        |             |             |            |
| Mg27-O8  | 2.023    | 1.861    | 0.163    |                        |         |         |             |                        |             |             |            |
| Mg27-O65 | 2.018    | 1.876    | 0.143    |                        |         |         |             |                        |             |             |            |
| Mg27-O53 | 2.145    | 2.479    | -0.334   |                        |         |         |             |                        |             |             |            |
| Mg27-O4  | 2.088    | 2.500    | -0.412   |                        |         |         |             |                        |             |             |            |
| Mg27-O33 | 2.113    | 1.891    | 0.222    |                        |         |         |             |                        |             |             |            |
|     | 1.822 | 1.918 | -0.097 |
|-----|-------|-------|--------|
| C46-P25 | 1.822 | 1.918 | -0.097 |
| C43-N30 | 1.504 | 1.499 | 0.005  |
| C18-N5  | 1.511 | 1.500 | 0.012  |
| C15-P2  | 1.831 | 1.952 | -0.121 |