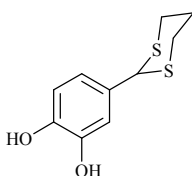


### Electronic Supplementary information

#### **Adsorption of cadmium (II) and copper (II) onto magnetic organozeolite modified with 2-(3,4-Dihydroxyphenyl)-1,3-dithiane from soil and water samples by flame atomic absorption spectrometry using artificial neural network**

Mahboube Shirani<sup>a</sup>, Ali Akbari<sup>a</sup>, Mohsen Hassani<sup>b</sup>

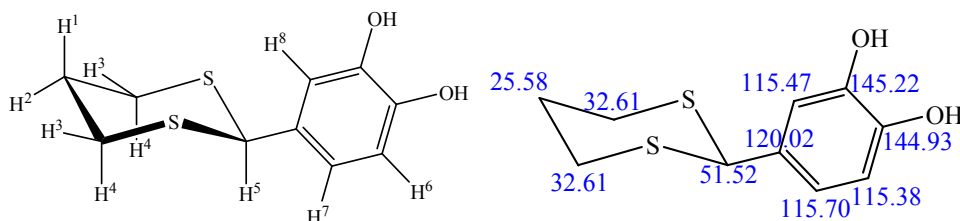
#### **Preparation of 2-(3,4-Dihydroxyphenyl)-1,3-dithiane (DHPDT)**



A mixture of 2, 3-dihydroxy Benz aldehyde (10 mmol), 1, 3-Ethanedithiol (12 mmol) and 37%  $\text{BF}_3 \cdot \text{SiO}_2$  (0.3 g) was ground in a pestle at an ambient temperature. The progress of reaction was monitored by TLC. After the completion of the reaction, the products were dissolved in ethanol, filtered, and the solvent was evaporated. The obtained solid was recrystallized in chloroform (yield= 91%).

The spectroscopic data of IR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR are as bellow:

FT- IR:  $\nu_{\text{max}}$  (KBr) = 3479, 3306, 2929, 2891, 1622, 1607, 1620, 1454, 1428, 1408, 1352, 1299, 1275, 1248, 1183, 1112, 961, 907, 873, 816, 797, 763, 706, 677, 582, 436  $\text{cm}^{-1}$ .

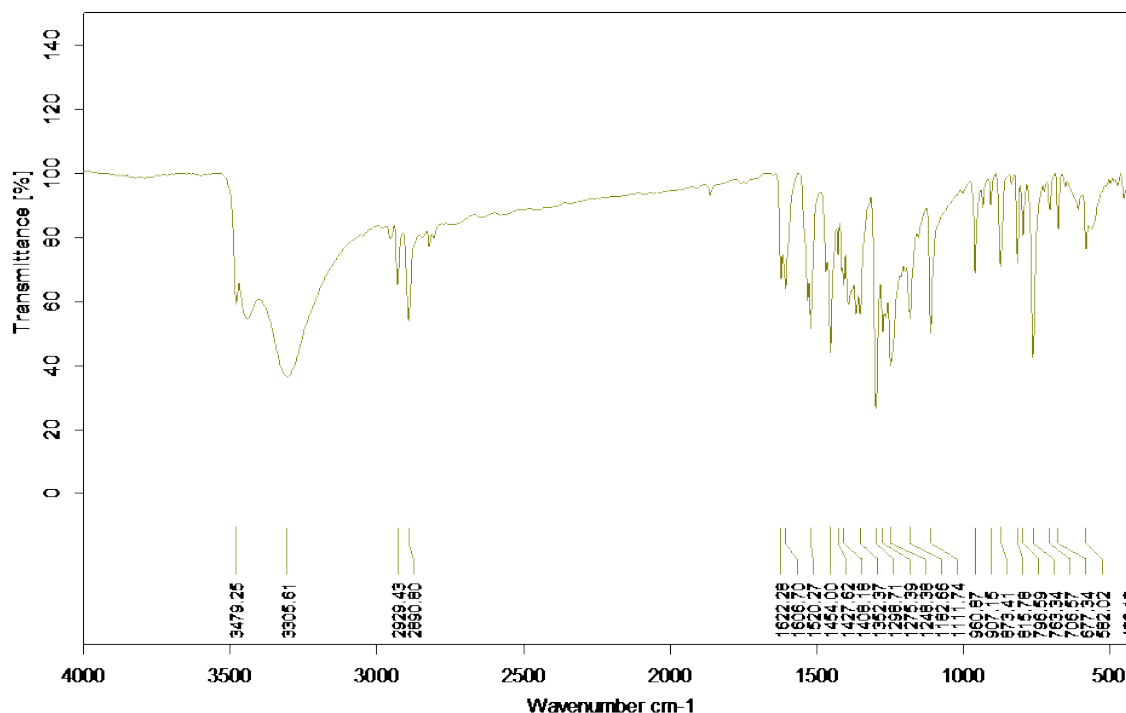


$^1\text{H}$ -NMR (500 MHz,  $\text{CDCl}_3/\text{DMSO}$ )  $\delta$ = 1.88 (m, 1 H,  $\text{H}^1$ ), 2.13 (m, 1 H,  $\text{H}^2$ ), 2.87 (m, 2 H,  $\text{H}^3$ ), 3.03 (m, 2 H,  $\text{H}^4$ ), 5.05 (s, 1 H,  $\text{H}^5$ ), 6.82 (d,  $J$  = 8.15 Hz, 1 H,  $\text{H}^6$ ), 6.84 (dd,  $J$  = 8.15 Hz and  $J$  = 1.86 Hz, 1 H,  $\text{H}^7$ ), 7.14 (d,  $J$  = 1.86 Hz, 1 H,  $\text{H}^8$ ) ppm.

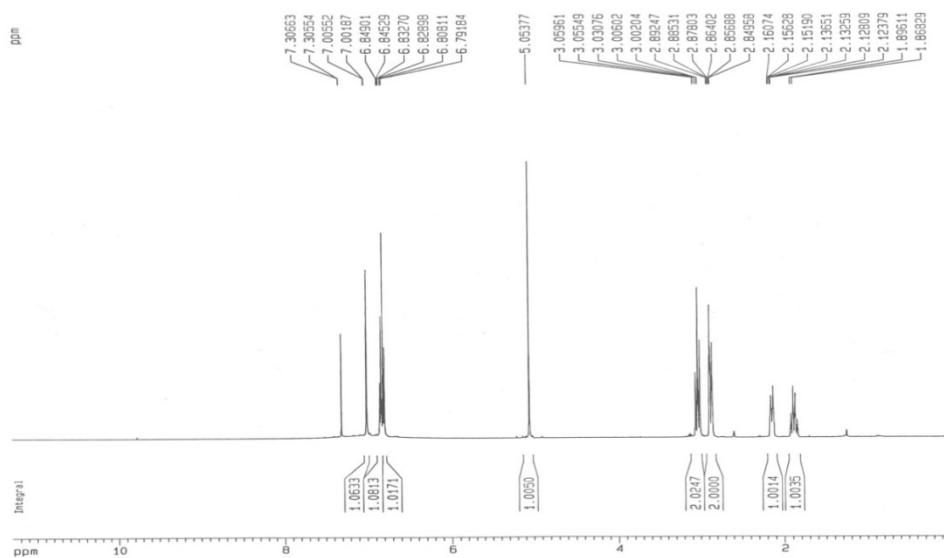
$^{13}\text{C}$ -NMR (125 MHz,  $\text{CDCl}_3/\text{DMSO}$ )  $\delta$ = 25.58, 32.61, 51.52, 115.47, 115.38, 115.70, 120.02, 144.93, 145.22 ppm.

One case of long-range coupling in phenyl system occurs through a rigid arrangement of bond in form of a **w** ( $4J$ ) with hydrogen coupling the end position. Two possible types of overlap have been suggested to explain this type of coupling [ $J$ =1.86 Hz,  $\text{H}^7$ - $\text{H}^8$ ].

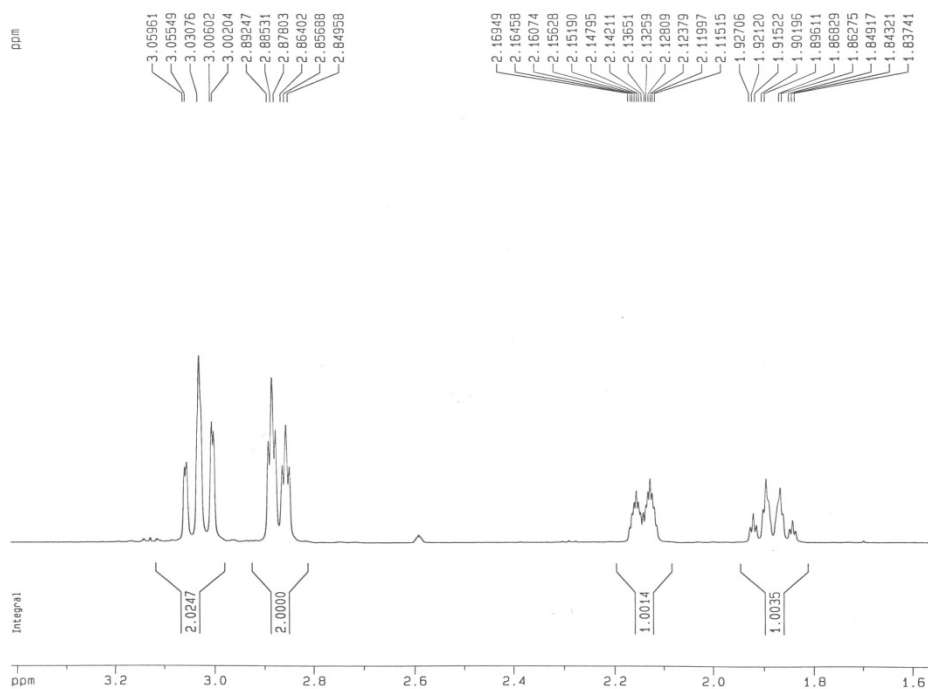
The H atoms on the six-membered 1,3-dithiane ring are non-equivalent. H 1, 3 is *cis* to the phenyl group and *trans* to the hydrogen ( $\text{H}^5$ ) group, while H 2, 4 is the reverse. Since they are in different chemical environments, they are non-equivalent and exhibit geminal coupling. The geminal coupling constant is small but discernable in the spectrum as the signals for both H 1, 3 and H 2, 4 are doublets. The H atoms group are *cis* to the phenyl group, labeled as “1, 3”, appears at a higher chemical shift compared to the other H atoms group are *trans* to the phenyl group.



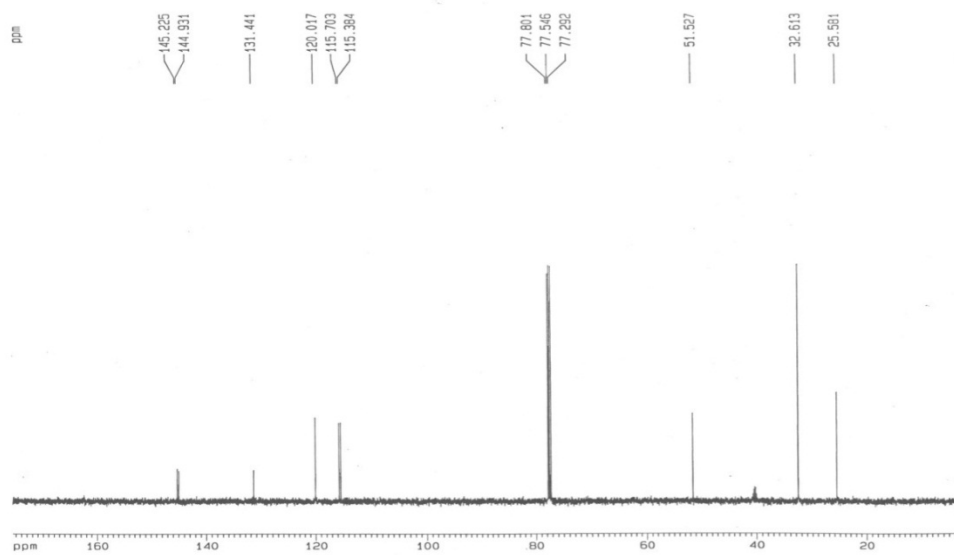
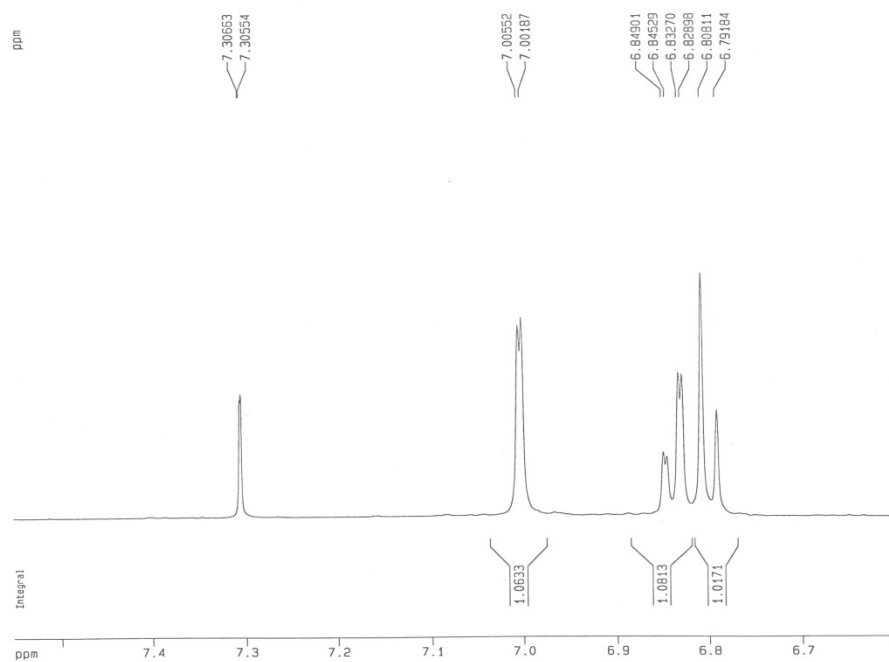
FT- IR:  $\nu_{\text{max}}$  (KBr) 2-(3,4-Dihydroxyphenyl)-1,3-dithiane

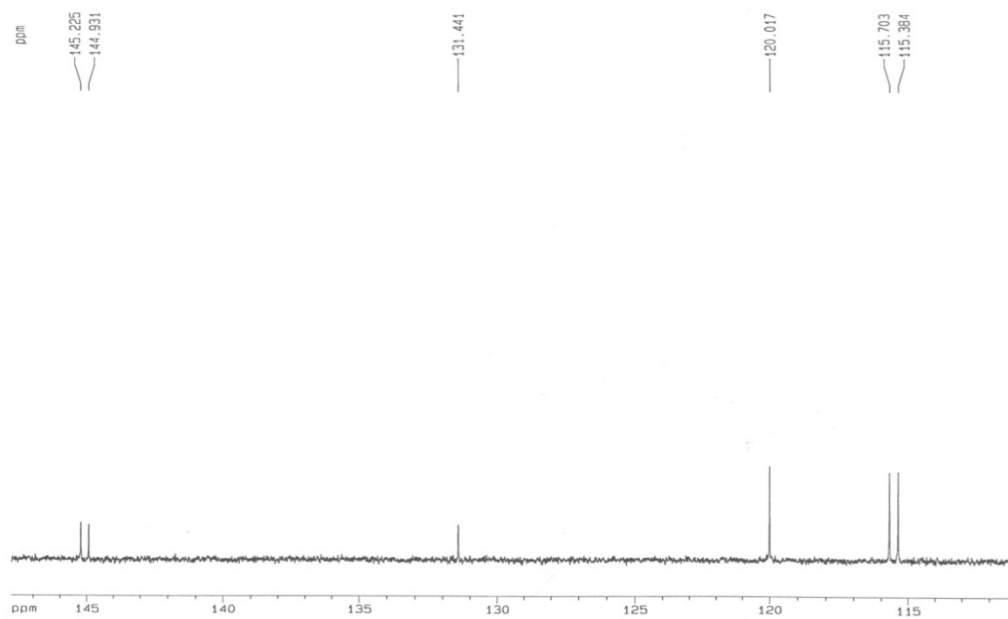


<sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>): 2-(3,4-Dihydroxyphenyl)-1,3-dithiane

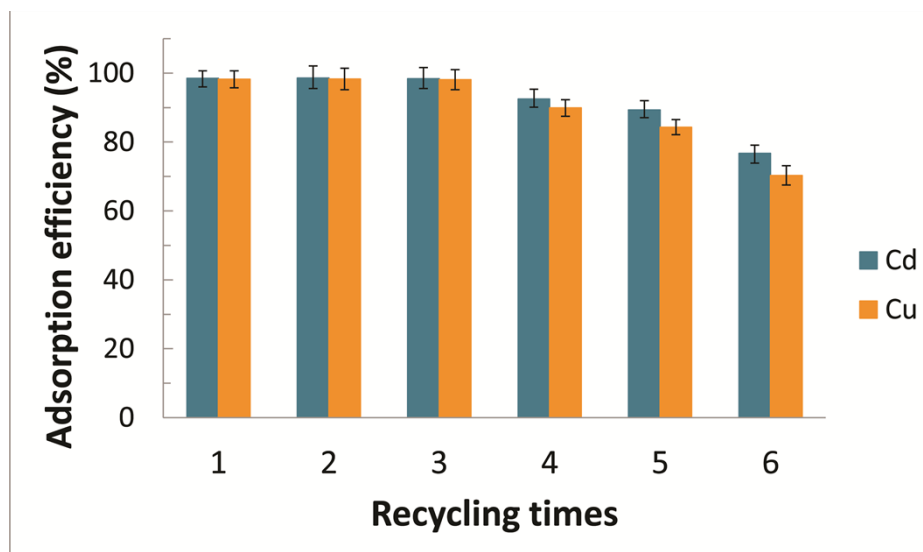


<sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>): 2-(3,4-Dihydroxyphenyl)-1,3-dithiane

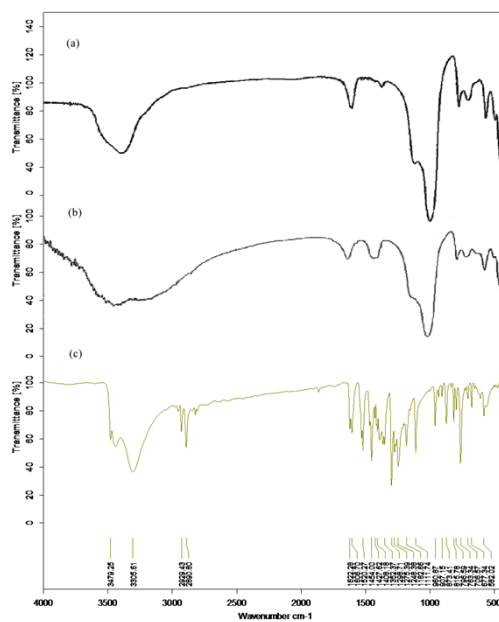




<sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>): 2-(3,4-Dihydroxyphenyl)-1,3-dithiane



The effect of recycling times on adsorption efficiency of the sorbent at the optimum conditions



The FT-IR spectrum of zeolite (a), magnetic zeolite (b), and magnetic organozeolite (c)