Synthesis, crystal structure and luminescence studies of zinc(II) and cadmium(II) complexes with 6-(1H-tetrazol-5-yl)-2-naphthoic acid

Xi Chen, Biquan Zhang, Fan Yu, Min Su, Wenming Qin, Bao Li, Gui-lin Zhuang, and Tianle Zhang

Department of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, Wuhan, Hubei 430074, P.R. China

Key Laboratory of Optoelectronic Chemical Materials and Devices of Ministry of Education, School of Chemical and Environmental Engineering, Jianghan University, Wuhan 430056, PR China

Institute of Industrial Catalysis, College of Chemical Engineering, Zhejiang University of Technology, Hangzhou, 310032, P.R. China

National Center for Protein Science, 333 Haike Road, Pudong District, Shanghai, 201210, P.R. China

Figure S1. TGA curve of 1 and 2
Figure S2. Electric hysteresis loop of 1, observed for a powdered sample in the form of a pellet at room temperature.

Figure S3. XRD pattern of 1
Figure S4. XRD pattern of 2

Figure S5. HNMR spectra of free ligand

Table S1 Comparison of Coordination-bond length (unit: Å) between Experimental and Theory

<table>
<thead>
<tr>
<th>Name</th>
<th>Exp.</th>
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<th>Exp.</th>
<th>The.</th>
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</thead>
<tbody>
<tr>
<td>Compound 1</td>
<td>Zn-O1</td>
<td>1.951</td>
<td>Zn-O1</td>
<td>1.968</td>
<td>2.011</td>
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<td></td>
<td>Zn-N1</td>
<td>1.978</td>
<td>Zn-N2</td>
<td>1.993</td>
<td>2.017</td>
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</table>
The dihedral angles between the naphthyl group and the tetrazolyl group

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<tbody>
<tr>
<td>Compound 2</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Cd-O1</td>
<td>2.336</td>
<td>2.232</td>
<td>Cd-O2</td>
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<tr>
<td>Cd-O3</td>
<td>2.361</td>
<td>2.478</td>
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<tr>
<td>Cd-N2</td>
<td>2.368</td>
<td>2.451</td>
<td>Cd-N3</td>
</tr>
</tbody>
</table>

The dihedral angles between the naphthyl group and the tetrazolyl group

- 29.6°
- 30.2°

- 87.6°
- 88.55°

**Computational Details**

Geometry optimization and electronic structure calculations were carried out using the VASP program [3-4]. Projector-augmented wave (PAW) [5] method, featuring the accuracy of augmented plane-wave methods as well as the efficiency of the pseudopotential approach, was explicitly used. Generalized gradient approximation (GGA) of Perdew Burke Ernzerhof (PBE) [6] was used to describe Exchange-correlation effects. Furthermore, long dispersion interaction was corrected by one non-local correlation vdW-DF [7] based on opt88 functional. The 3d and 4s electrons of Zn and Cd, 2s and 2p electrons of C, N and O, and 1s electrons of H were explicitly treated as valence electrons. The electron wave function is expanded in plane waves up to a cutoff energy of 450 eV. For the Brillouin zone integration, we use the K-points grid of 4×2×2 for 1 (Zn) and 4×8×4 for 2 (Cd). And both cutoff energy and K-point grid was verified to be enough to exactly calculate the energy of Brillouin zone. The optimization convergence in Hellmann-Feynman force was set to $2.0 \times 10^{-2}$ eV/Å, and the SCF energy convergence was set to $1.0 \times 10^{-6}$. Band structure and Partial Density of State (PDOS) were also identified. Moreover, frontier molecular orbits analysis at Gamma point was also plot by using DMol3 program [8-9] with the exchange-correction functional of GGA-PBE[6] and DNP basic set[9].

**Reference**


