**Lead/Rare Earth-free Green-Light-Emitting Crystal of Molecular-based Hybrid Compound: [(C5H13ClN)2][MnCl4] with Large Crystal Size**

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**Fig. S1** Infrared spectrum of compound **1**. Description: the IR spectrum of **1** definitely shows the existence of typical strong stretching vibration peaks (C-Cl at 600-800 cm-1, C-N at 1000-1200 cm-1, N-H/C-H at 2800-3200 cm-1), which could seem as the indirect proof to the crystalline structure we have acquired.

**单分子 - 副本**

**Fig. S2** Schematic presentations of the positions of Mn and N atoms at 293 K, while other atoms had been omitted for clarity.

**Table S1 Selected structural data under 293 K**

|  |  |  |  |
| --- | --- | --- | --- |
| *Bond lengths / nm and bond angles / °* | | | |
| Cl1-Mn | 0.236 (2) | Cl2-Mn | 0.238 (2) |
| Cl3-Mn | 0.238 (2) | Cl4-Mn | 0.238 (2) |
| C1-N1 | 0.153 (13) | C2-N1 | 0.151 (10) |
| C3-C4 | 0.144 (12) | C3-N1 | 0.147 (11) |
| C4-C5 | 0.154 (10) | C4-Cl5 | 0.180 (8) |
| C6-N2 | 0.149 (11) | C7-N2 | 0.146 (10) |
| C8-N2 | 0.149 (10) | C8-C9 | 0.150 (13) |
| C9-C10 | 0.155 (10) | C9-Cl6 | 0.179 (8) |
|  | | | |
| Cl1-Mn-Cl2 | 115.79 (8) | Cl1-Mn-Cl4 | 102.82 (8) |
| Cl2-Mn-Cl4 | 112.35 (8) | Cl1-Mn-Cl3 | 109.95 (8) |
| Cl2-Mn-Cl3 | 103.76 (8) | Cl4-Mn-Cl3 | 112.45 (8) |
| C4-C3-N1 | 116.0 (7) | C3-C4-C5 | 111.8 (7) |
| C3-C4-Cl5 | 110.7 (6) | C5-C4-Cl5 | 109.6 (6) |
| N2-C8-C9 | 115.2 (7) | C8-C9-C10 | 109.4 (8) |
| C8-C9-Cl6 | 108.0 (6) | C10-C9-Cl6 | 111.8 (6) |
| C3-N1-C1 | 116.5 (7) | C3-N1-C2 | 108.6 (7) |
| C1-N1-C2 | 112.9 (7) | C7-N2-C8 | 115.8 (6) |
| C7-N2-C6 | 109.7 (7) | C8-N2-C6 | 107.1 (6) |

[Hydrogen-bond geometry (](xc2%20_geom_hbond_atom_site_label_D)*[nm](xc2%20_geom_hbond_atom_site_label_D)*[,](xc2%20_geom_hbond_atom_site_label_D) *[°](xc2%20_geom_hbond_atom_site_label_D)*[)](xc2%20_geom_hbond_atom_site_label_D)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *D—H···A* | *D—H* | *H···A* | *D···A* | *D—H···A* |
| N1—H1D···Cl2 | 0.091 | 0.247 | 0.324 (7) | 143 |
| N1—H1D···Cl5 | 0.091 | 0.264 | 0.310 (7) | 112 |
| N2—H2D···Cl6 | 0.091 | 0.268 | 0.313 (7) | 112 |
| N2—H2D···Cl4i | 0.091 | 0.243 | 0.321 (6) | 143 |

Symmetry transformations used to generate equivalent atoms: i −x+2, −y+1, −z+1.