MS35-P17 | Crystallographic Evidence for Aggregation Patterns of Two Cyclic Triimidazole Phosphors in Zn(II) and Cd(II) Complexes

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Design of materials with ligand-centered emission from a highly emissive ligand with the use of optically inactive metal ions Zn(II) and Cd(II) allows tuning the ligands stacking and influences on the lifetime, quantum yield and stability of emitters. Generally, d^{10} metal complexes show no emission originating from MLCT/LMCT excited states, since these ions are in a stable oxidation state. Otherwise, d^{10} metals have flexible coordination numbers, providing the diversity of coordination arrays. Furthermore, these metals compete with platinum group compounds in view of their low cost and availability. Depending on the ligand structure and the nature of the metal core, bright luminescent materials can be prepared and used in LEDs. Under consideration are complexes obtained from Zn/Cd perchlorates, tetrafluoroborates, nitrates, and acetates by successive substitution aqua ligands in the metals' coordination cores by the photophysically active triimidazo[1,2-*a*:1',2'-*c*:1'',2''-*e*][1,3,5] triazine (L_1), which displays crystallization-induced and mechanochromic emission due to H-aggregation, and its positional isomer, triimidazo[1,2-*a*:1',2'-*c*:1'',5''-*e*][1,3,5]triazine (L_2). The reactions resulted in coordination of one, two or six phosphor molecules to the metal centers. Ligands' association patterns represent the stacking dimers in salt-cocrystals $[M(H_2O)_6](An)_2(L_1)_2$ (M=Zn, Cd, An=$[BF_4]^-$, $[ClO_4]^-$, $[NO_3]^-$); infinite stacks in the mononuclear complexes $[Zn(H_2O)_3(L_1)(NO_3)](NO_3)$, $[Cd(L_1)_2(H_2O)_2(NO_3)_2]$, $[Cd(L_2)_2(NO_3)_2(H_2O)]$, $[Zn(L_2)_2(CH_3COO)_2]$, $[Cd(L_2)_2(CH_3COO)_2(Im)]\cdot H_2O$ with either one or two ligand molecules coordinated to the metals, and stacking layers in the salt-cocrystal $[Zn_3(CH_3COO)_6(H_2O)_2](L_1)_2$, where the ligands arrangement similar to that in pure phase. The reported complexes give examples of isomorphs, polymorphs, and isostructural compounds.

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