Mn^{2+} luminescence of $Gd(Zn,Mg)B_5O_{10}$ pentaborate under high pressure

Supplement for:
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Supplement

Among the six nearest Gd-Mg distances in $GdMg_{0.95-x}Zn_xMn_{0.05}B_5O_{10}$, the two longest ones gradually increase with increasing Zn content, x, the two intermediate distances slightly decrease, whereas the two shortest ones remain unchanged in the limit of error. They are presented in Fig. S1.

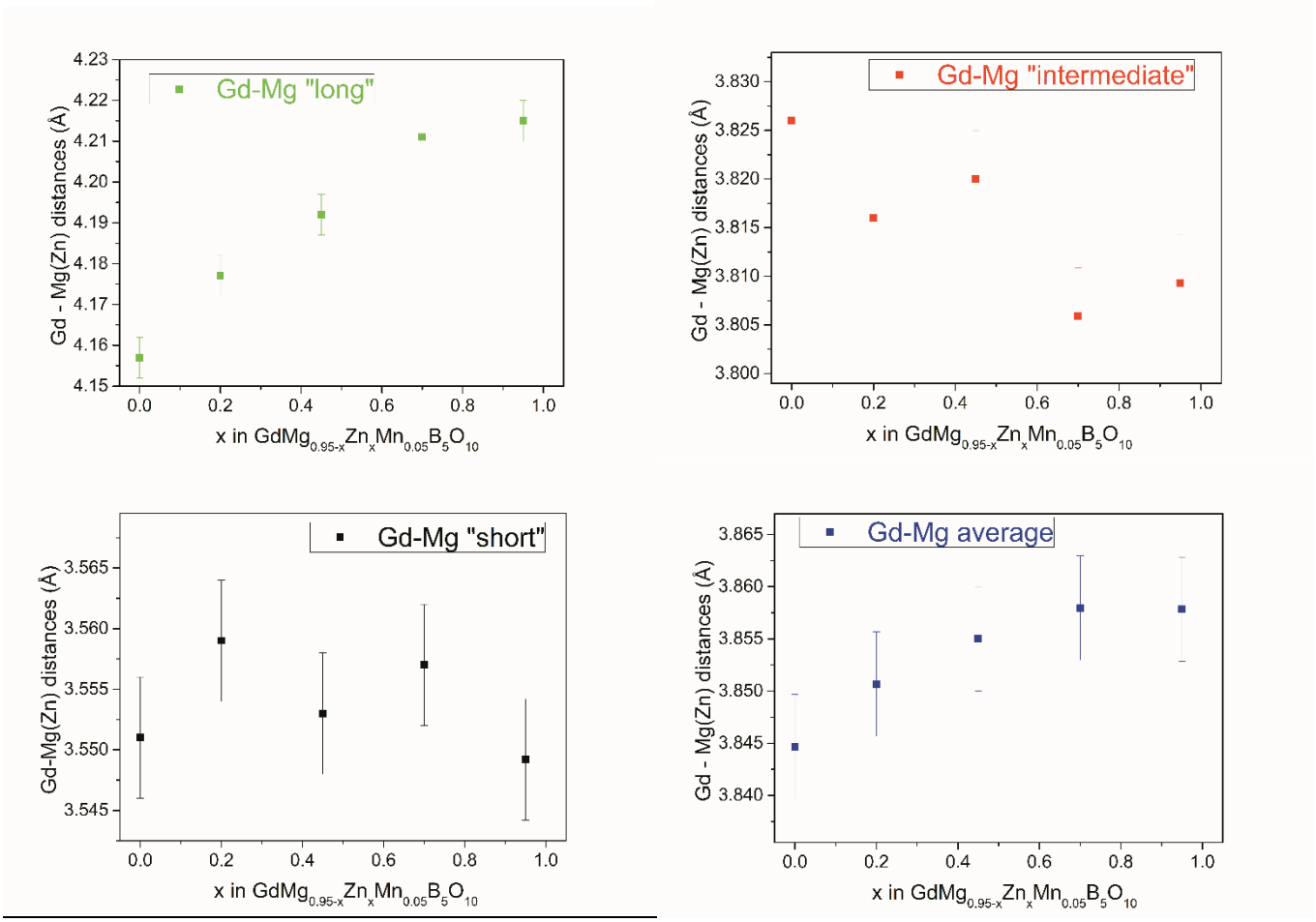

Fig. S1. Concentration dependence of the Gd-Mg(Zn) distances vs. Zn content in the $GdMg_{0.95-x}ZnxMn_{0.05}B_5O_{10}$ series.

Among the six M-O bonds within the distorted MO_6 octahedra a considerable increase is observed for the longest one, while the shortest M-O bond length noticeably decreases with x (see Fig. S2).

A

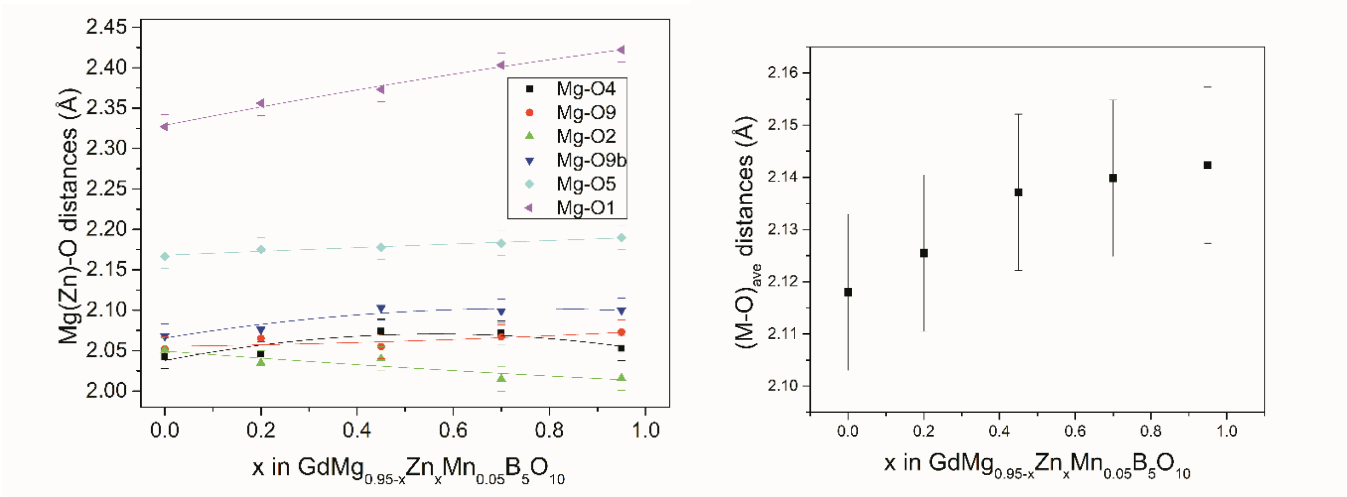

Fig. S2. Concentration dependence of the individual (left) and averaged (right) Mg(Zn)-O distances vs Zn content in the $GdMg_{0.95-x}Zn_xMn_{0.05}B_5O_{10}$ series as derived from the X-ray synchrotron powder diffraction data.

An increase is also observed for the shortest Mg(Zn)-Mg(Zn) distances (see Fig. S3).

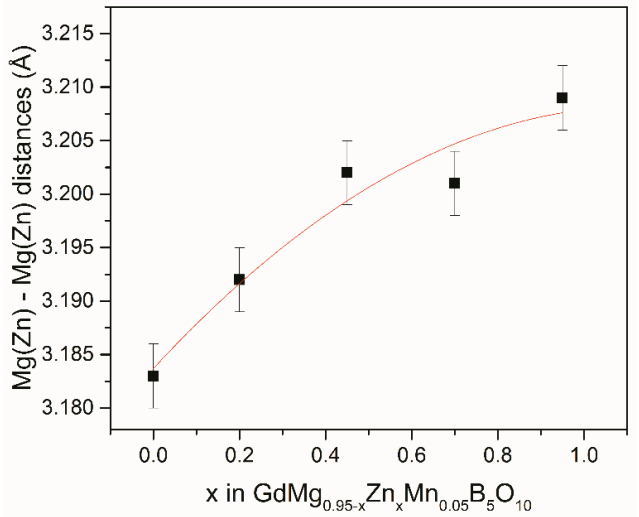

Fig. S3. Concentration dependence of the shortest Mg(Zn)- Mg(Zn) distances vs. Zn content in the $GdMg_{0.95-x}ZnxMn_{0.05}B_5O_{10}$ series

In contrast to the abovementioned distances, the majority of individual Gd-O bond lengths in the $GdMg_{0.95-x}Zn_xMn_{0.05}B_5O_{10}$ structures and the average Gd-O distance calculated for CN 10 gradually decrease with increasing Zn content (see Fig. S4).

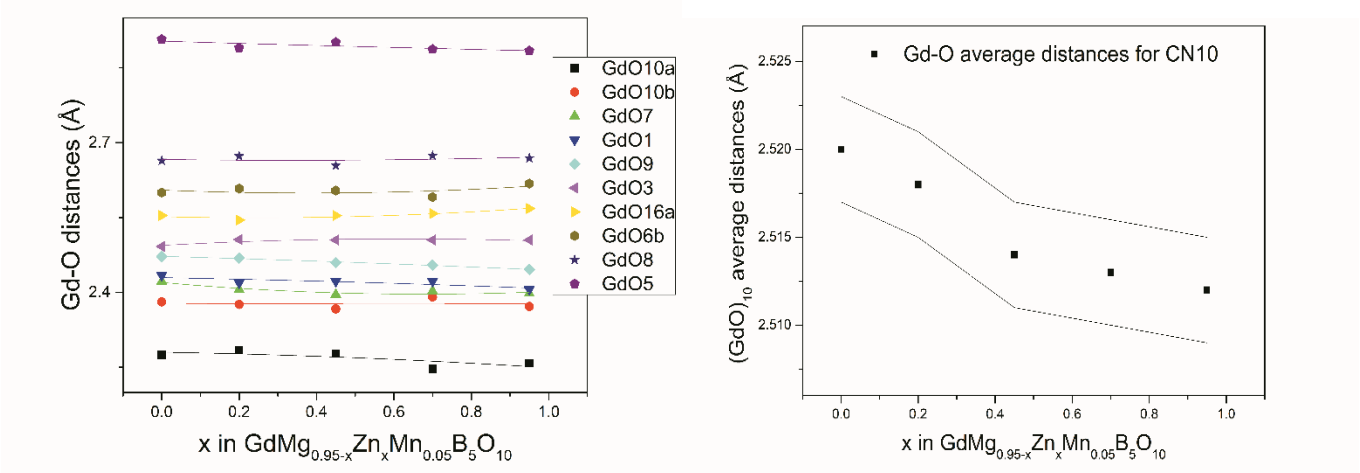

Fig. S4. Concentration dependence of the individual (left) and averaged (right) Gd-O distances vs. Zn content in the $GdMg_{0.95-x}Zn_xMn_{0.05}B_5O_{10}$ series as derived from the X-ray synchrotron powder diffraction data

1. Partial density of states (PDOS) of $GdMg_{1-x}Zn_xB_5O_{10}$ crystals calculated per unit cell.

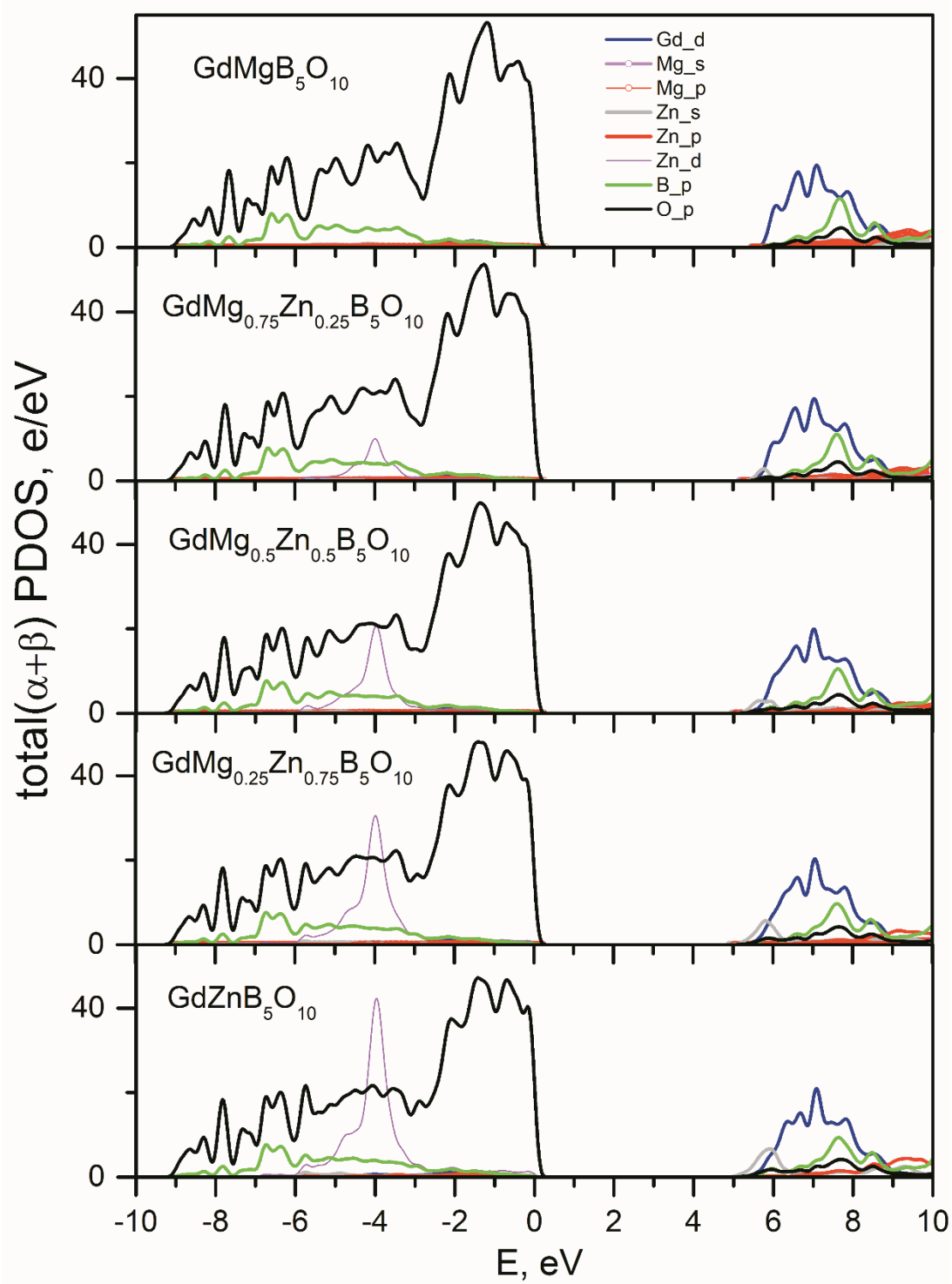

Fig. S5. PDOS of $GdMg_{1-x}Zn_xB_5O_{10}$ crystals calculated per unit cell.

Fig. S5 shows increasing contribution of Zn states with increasing Zn content of the material.