Synthesis, Crystal Structure and Magnetic Behaviour of Dimeric and Polymeric Gadolinium Trifluoroacetate Complexes

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Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70th birthday

The gadolinium(III) trifluoroacetates ((CH₃)₂NH₂)[Gd(CF₃COO)₄] (**1**), ((CH₃)₃NH)[Gd(CF₃COO)₄(H₂O)] (**2**), Gd(CF₃COO)₃(H₂O)₃ (**3**) as well as Gd₂(CF₃COO)₆(H₂O)₂(phen)₃ · C₂H₅OH (**4**) (phen = 1,10-phenanthroline) were synthesized and structurally characterized by X-ray crystallography. These compounds crystallize in the space group $P\overline{1}$ (No. 2, Z = 2) (**1**, **2** and **4**) and $P 2_1/c$ (No. 14, Z = 4) (**3**), respectively, with the following lattice constants **1**: a = 884.9(2), b = 1024.9(2), c = 1173.1(2) pm, $\alpha = 105.77(2)$, $\beta = 99.51(2)$, $\gamma = 107.93(2)^{\circ}$; **2**: a = 965.1(1), b = 1028.6(1), c = 1271.3(2) pm, $\alpha = 111.83(2)$, $\beta = 111.33(2)$, $\gamma = 90.44(2)^{\circ}$; **3**: a = 919.6(2), b = 1890.6(4), c = 978.7(2) pm, $\beta = 113.94(2)^{\circ}$; **4**: a = 1286.7(8), b = 1639.3(8), c = 1712.2(9) pm, $\alpha = 62.57(6)$, $\beta = 84.13(5)$, $\gamma = 68.28(5)^{\circ}$. The compounds consist of Gd³⁺ ions which are bridged by carboxylate groups either to chains (**1** and **2**) or to dimers (**3** and **4**). In addition to the Gd³⁺ dimers, compound (**4**) also contains monomeric Gd³⁺ units. The magnetic behaviour of **2** and **3** was investigated in a temperature range of 1.77 to 300 K. The magnetic data for these compounds indicate weak antiferromagnetic interactions.

Key words: Trifluoroacetates, Gadolinium Carboxylates, Synthesis, Crystal Structure, Magnetic Behaviour