

Supporting Information

Bifunctional Fe(II) spin crossover-complexes based on ω -(1*H*-tetrazol-1-yl) carboxylic acids

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- Fe-N bond lengths for **4, 6, 7, 9**
 - DSC / TGA data for **1, 2, 3**

Table S1. Bond-lengths for $[\text{Fe}(\text{2COOHTz})_6](\text{BF}_4)_2 \cdot 2 \text{ MeCN}$ (**4**) in HS and LS state

	4 , HS [Å]	4 , LS [Å]
Fe-N ₄	2.176	1.987

Table S2. Bond-lengths for $[\text{Fe}(\text{4COOHTz})_6](\text{BF}_4)_2 \cdot \text{Et}_2\text{O}$ (**6**) in HS and LS state

	6 , HS [Å]	6 , LS [Å]
Fe-N ₄	2.165	1.969
Fe-N _{4A}	2.182	1.979
Fe-N _{4B}	2.185	1.981

Table S3. Bond-lengths for $[\text{Fe}(\text{2COOHTz})_6](\text{ClO}_4)_2 \cdot 2 \text{ MeCN}$ (**7**) in HS and LS state

	7 , HS [Å]	7 , LS [Å]
Fe-N ₄	2.184	2.004

Table S4. Bond-lengths for $[\text{Fe}(\text{4COOHTz})_6](\text{ClO}_4)_2 \cdot \text{Et}_2\text{O}$ (**9**) in HS and LS state

	9 , HS [Å]	9 , LS [Å]
Fe ₁ -N ₄	2.181	1.984
Fe ₁ -N _{4A}	2.176	1.987
Fe ₁ -N _{4B}	2.173	1.992
Fe ₂ -N _{4C}	2.174	1.987
Fe ₂ -N _{4D}	2.185	1.997
Fe ₂ -N _{4E}	2.176	1.984

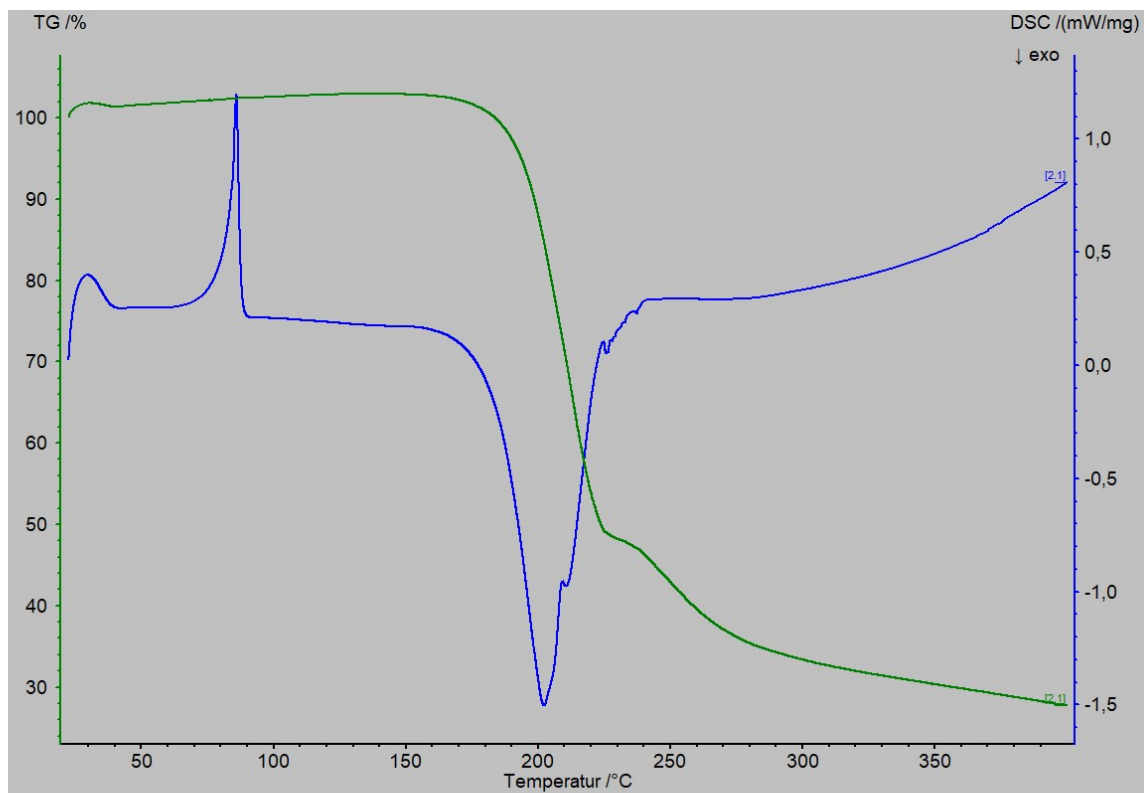


Figure S1. DSC / TGA analysis for 2COOHTz (1)

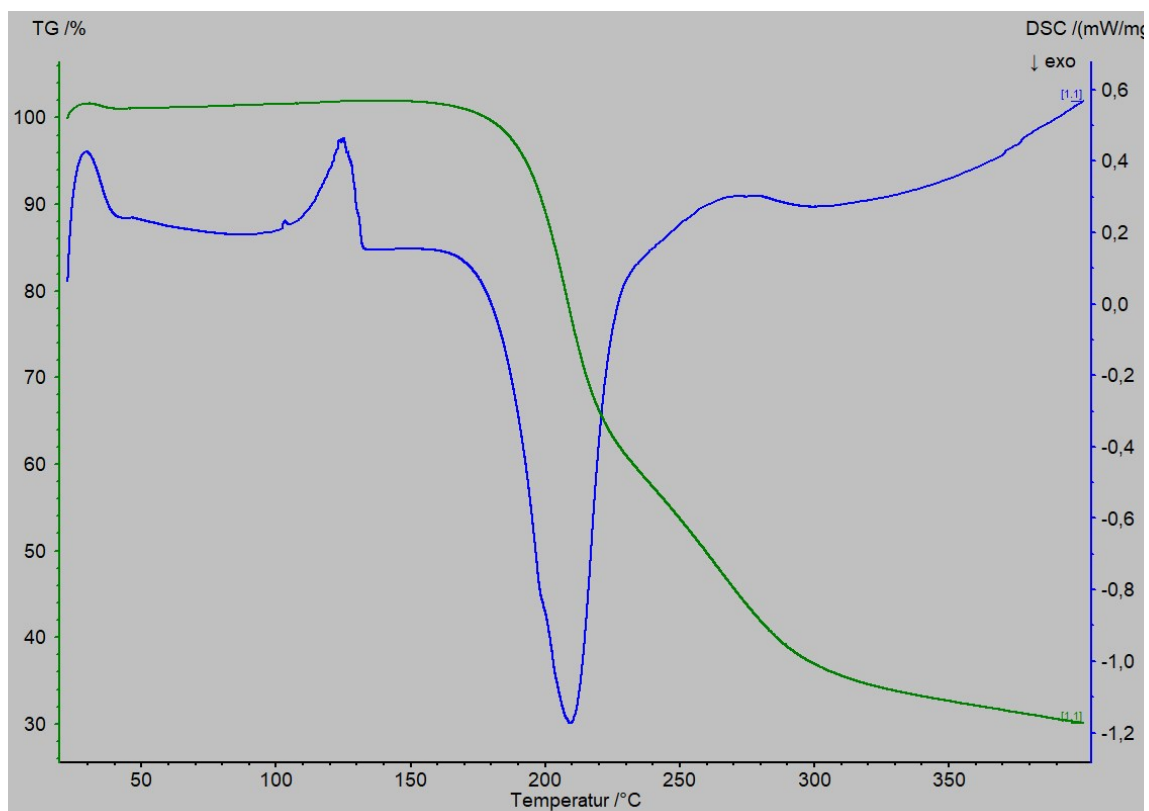


Figure S2. DSC / TGA analysis for 3COOHTz (2)

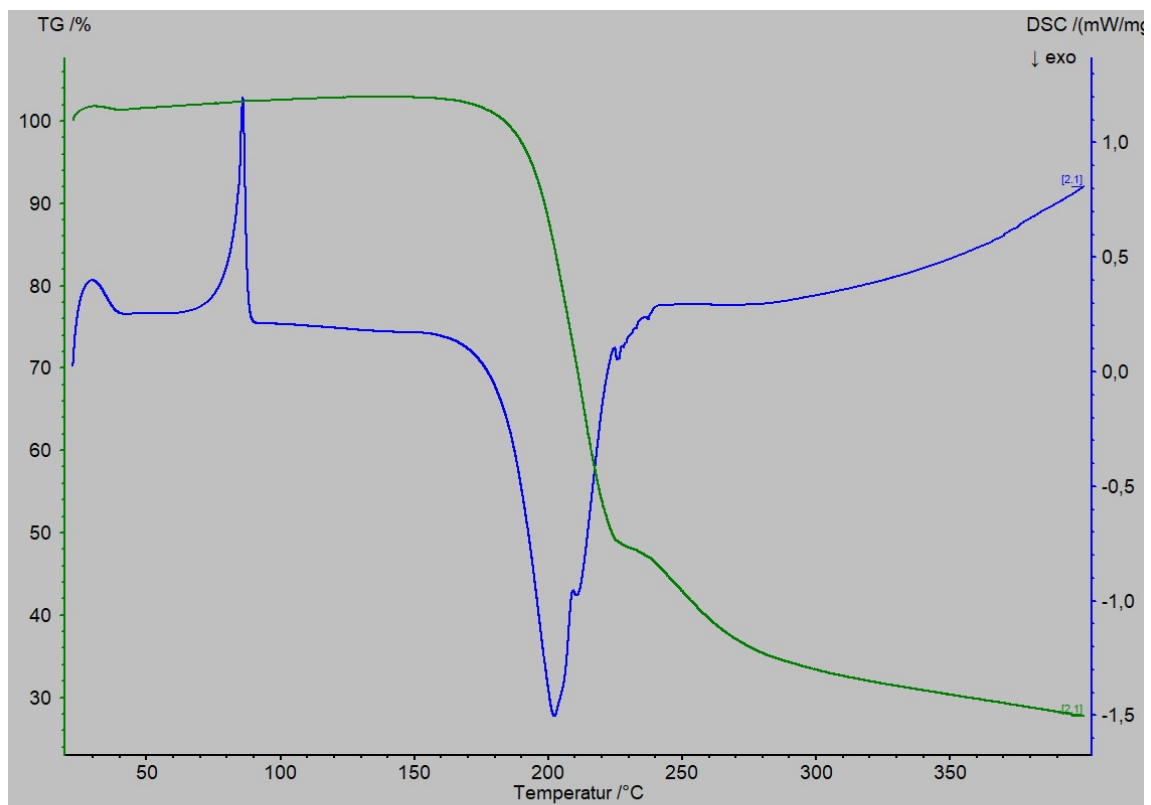


Figure S3. DSC / TGA analysis for 4COHTz (**3**)