Electronic Supplementary Information for Dalton Transactions

Supplementary Information for:

Self-assembly of Zn(salphen) complexes: Steric regulation, stability studies and crystallographic analysis revealing an unexpected dimeric 3,3´-*t*-Bu-substituted Zn(salphen) complex

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Contents:

Crystallographic comments

Complex 2:

The unit cell of this compound contains a CH_3CN molecule and one of the benzene rings at the main molecule is showing some disorder. The completeness of the data is 95 %. The structure has an R1 value of 4.0 %.

Complex 5:

The unit cell contains two half independent molecules of the complex. The unit cell contains also three independent molecules of CH_3CN. Some of the tert-butyl groups are disordered. The completeness of the data is 91 %. The structure has an R1 value of 4.42%.

Complex 6:

The unit cell of this compound contains one molecule of CH_3CN and non relevant disorder was observed. The completeness of the data is 91 %. The structure has an R1 value of 2.67 %.

Complex 9:

The structure contains three molecules of CH_3CN and one of the tert-butyl groups is disordered in two positions. The structure has an R1 value of 8.28 %.

Complex 11:

The structure is a solvate of 2,6-lutidine (2,6-dimethylpyridine). The 2,6-lutidine molecule is disordered in two overlaid positions (50:50) which are related through a C2-operation. The structure has an R1 value of 4.76 %.

The residual electron density near the Zn atom is a residual artifact due to the presence of a second crystal that was not enough intense to perform a combined data reduction and absorption. This is also shown in the unusually large second term of the weighting scheme: 5.9979

Complex 18:

The unit cell does not contain solvent molecules and only diminutive disorder was observed. The completeness of the data is of 94 %. This structure has an R1 value of 3.22 %.

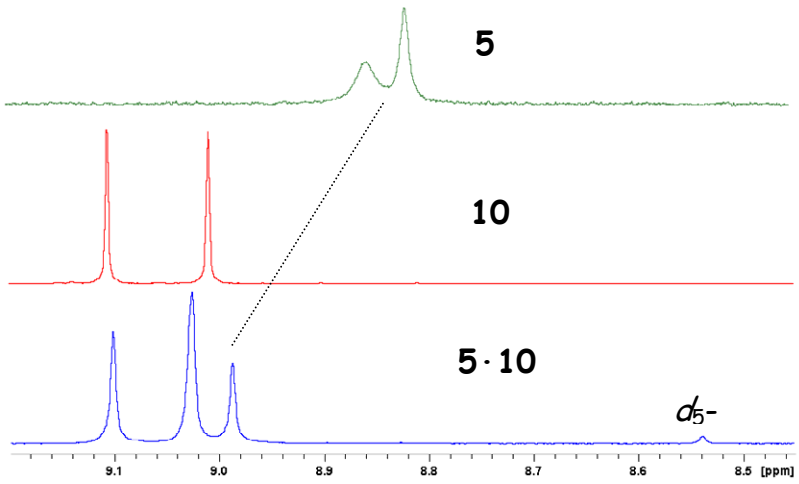
Complex 19:

The unit cell of this compound contains one molecule of CH_3CN and non relevant disorder was observed. The completeness of the data is 87 %. The crystal measured was a twin (crystal ratio of 51:49) and for the absorption correction TWINABS was used

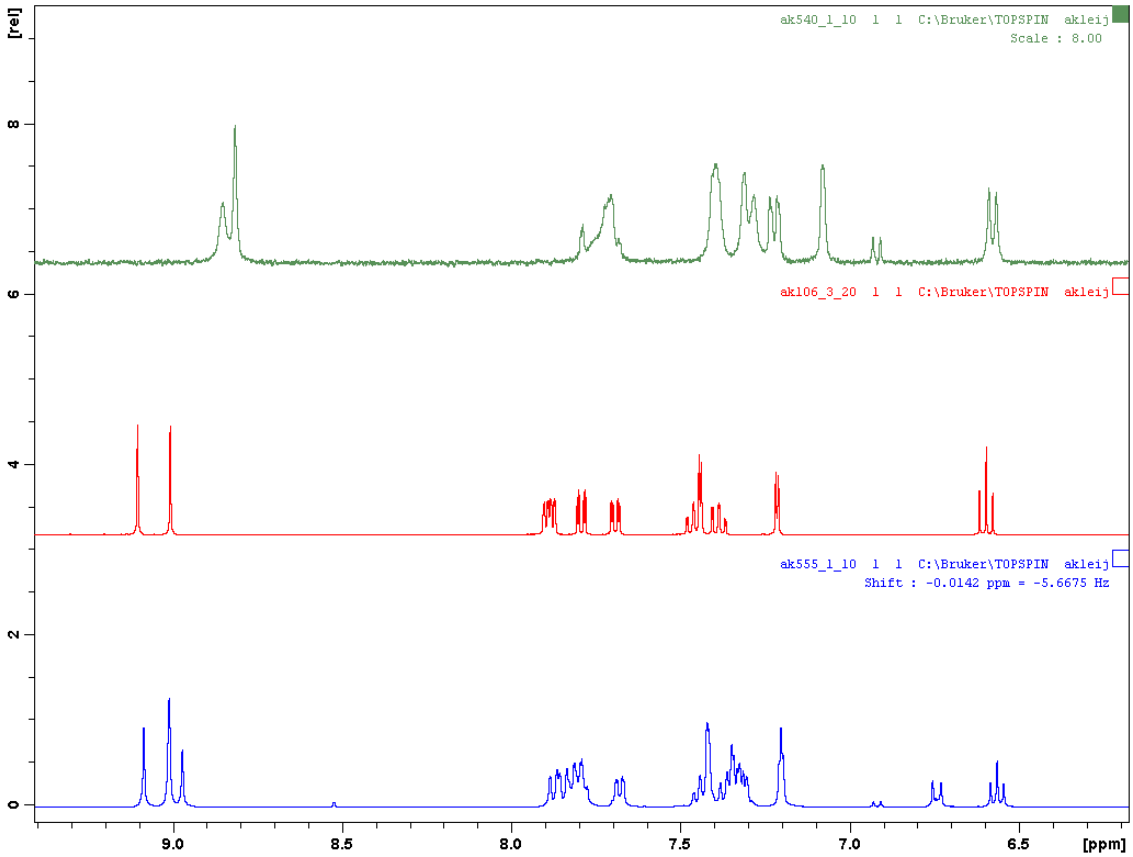
(TWINABS Version 2008/4 Bruker AXS; Blessing, Acta Cryst. (1995) A51 33-38). The structure has a R1 value of 5.7 %.

^{1}H NMR comparison between dimers $(\mathbf{5})_2$ and $(\mathbf{10})_2$ and hetero-dimeric assembly **5·10**

Imine region of the ^{1}H NMR (d_6-acetone) spectra of the respective species:

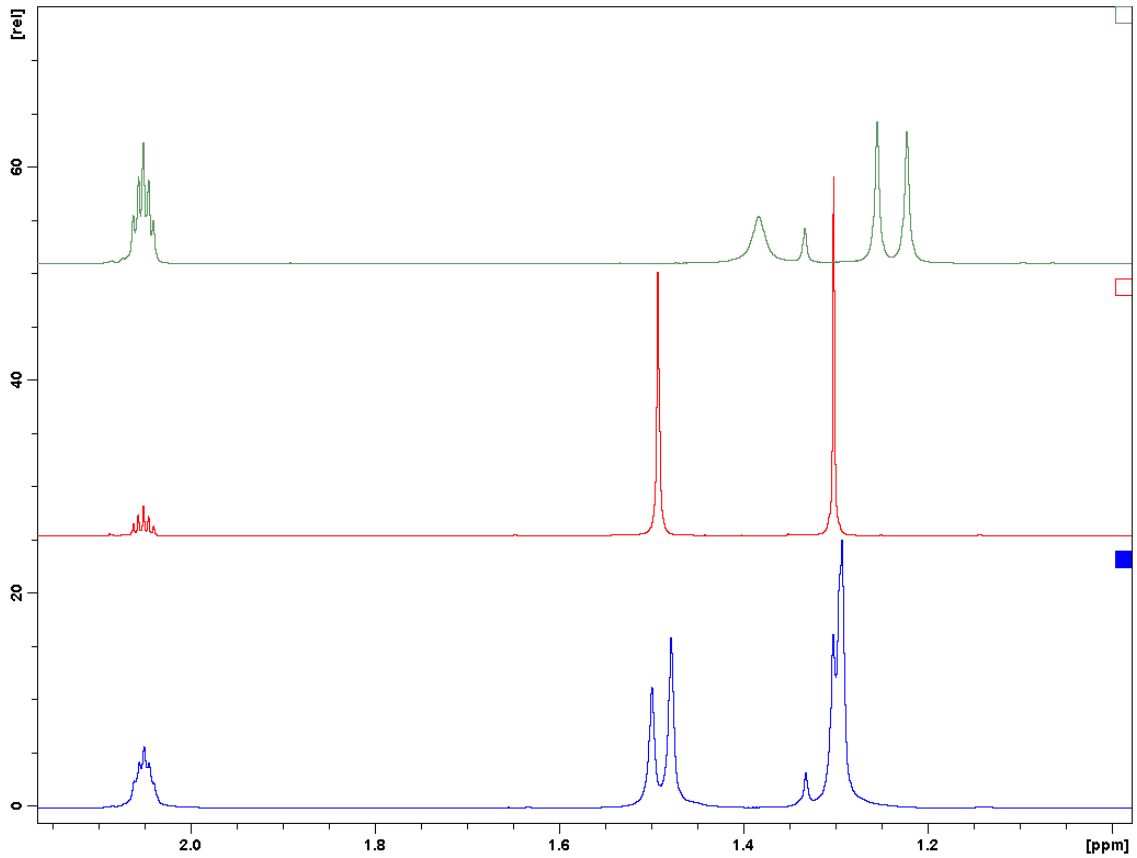


Full aromatic region:



In GREEN: complex **5**, in RED: complex **10**, and in BLUE hetero-complex **5·10**.

t-Bu region:



In GREEN: complex **5**, in RED: complex **10**, and in BLUE hetero-complex **5·10**.

MALDI-TOF mass spectrometric analysis of **5·10**.

Calcd masses (molecular ions) of the DIMERS:

See**:** **http://winter.group.shef.ac.uk/chemputer/isotopes.html**

For $(\mathbf{5})_2$: *m/z* = 1096 (100%)
For $(\mathbf{10})_2$: *m/z* = 1074 (100%)
For **5·10**: *m/z* = 1085 (100%)