

Supplementary Material for

The Elusive $[\text{Ni}(\text{H}_2\text{O})_2(\text{15-crown-5})]^{2+}$ Cation

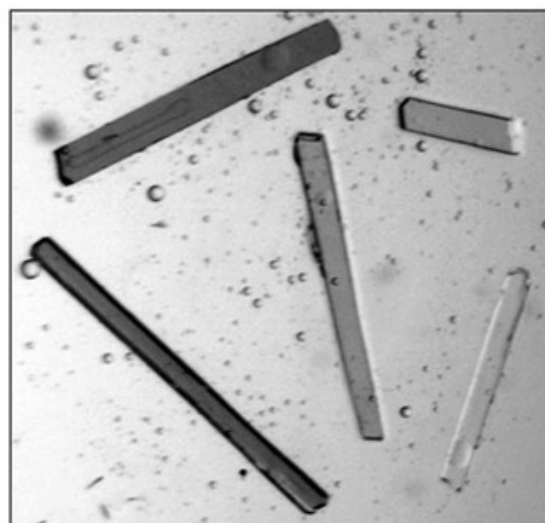
and Related Co-Crystals of Ni(II) Hydrates and 15-Crown-5

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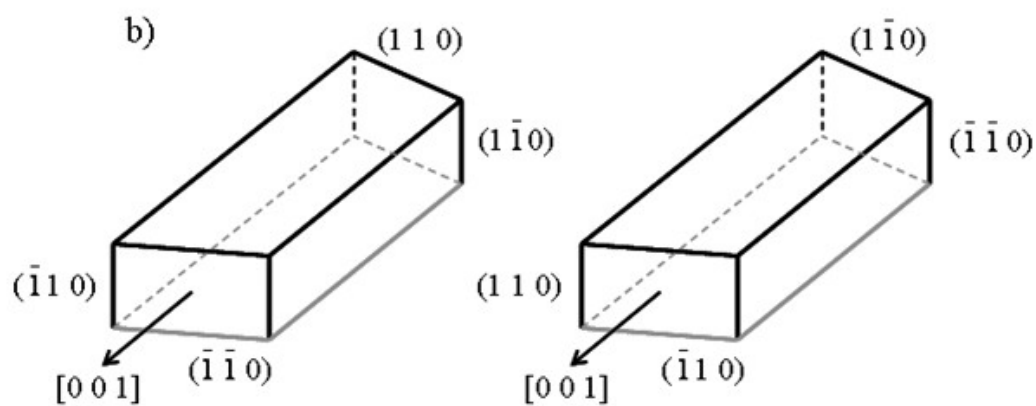
- Fig S-1. Crystals of the dihydrate (**1**).
- Fig S-2. Crystals of the first polymorph of the monohydrate (**2a**).
- Fig S-3. Crystal of the *cis/trans* compound (**4**).
- Fig S-4. Sequence of pictures taken during heating of a dihydrate crystal (**1**).
- Fig S-5. Two more pictures taken during heating of a dihydrate crystal (**1**).
- Fig S-6. DSC traces of one sample of the dihydrate (**1**) (1 of 2).
- Fig S-7. DSC traces of one sample of the dihydrate (**1**) (2 of 2).
- Fig S-8. Ellipsoid plot of the dihydrate (**1**).
- Fig S-9. Ellipsoid plot of the first polymorph of the monohydrate (**2a**).
- Fig S-10. Ellipsoid plot of the second polymorph of the monohydrate (**2a**).
- Fig S-11. Ellipsoid plot of the methanol compound (**3**).
- Fig S-12. Ellipsoid plot of the *cis/trans* compound (**4**).
- Fig S-13. Ellipsoid plot of the acetonitrile compound (**5**).
- Fig S-14. Ellipsoid plot of the target compound (**6**).

Fig. S-1

a)

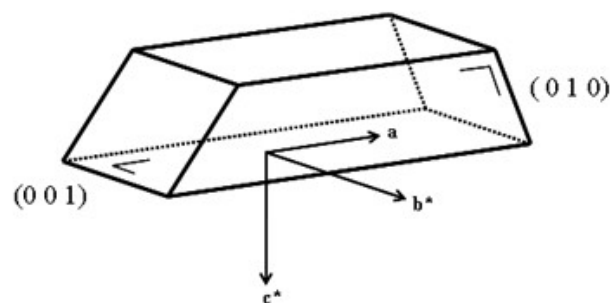
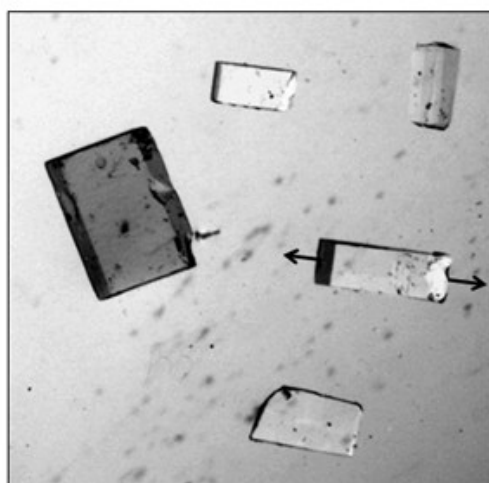


b)



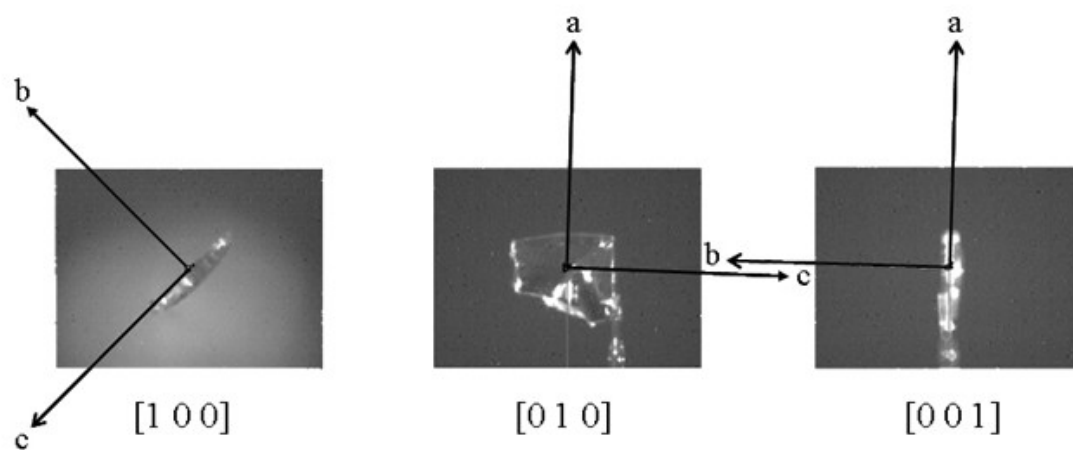
Crystals of the dihydrate (1). The morphology and directions of the crystal axes are shown.

Fig. S-2



Crystals of the first polymorph of the monohydrate (**2a**). The morphology and directions of the crystal axes are shown.

Fig. S-3



Crystal of the *cis/trans* compound (4) used for data collection,
The morphology and directions of the crystal axes are shown.

Fig. S-4

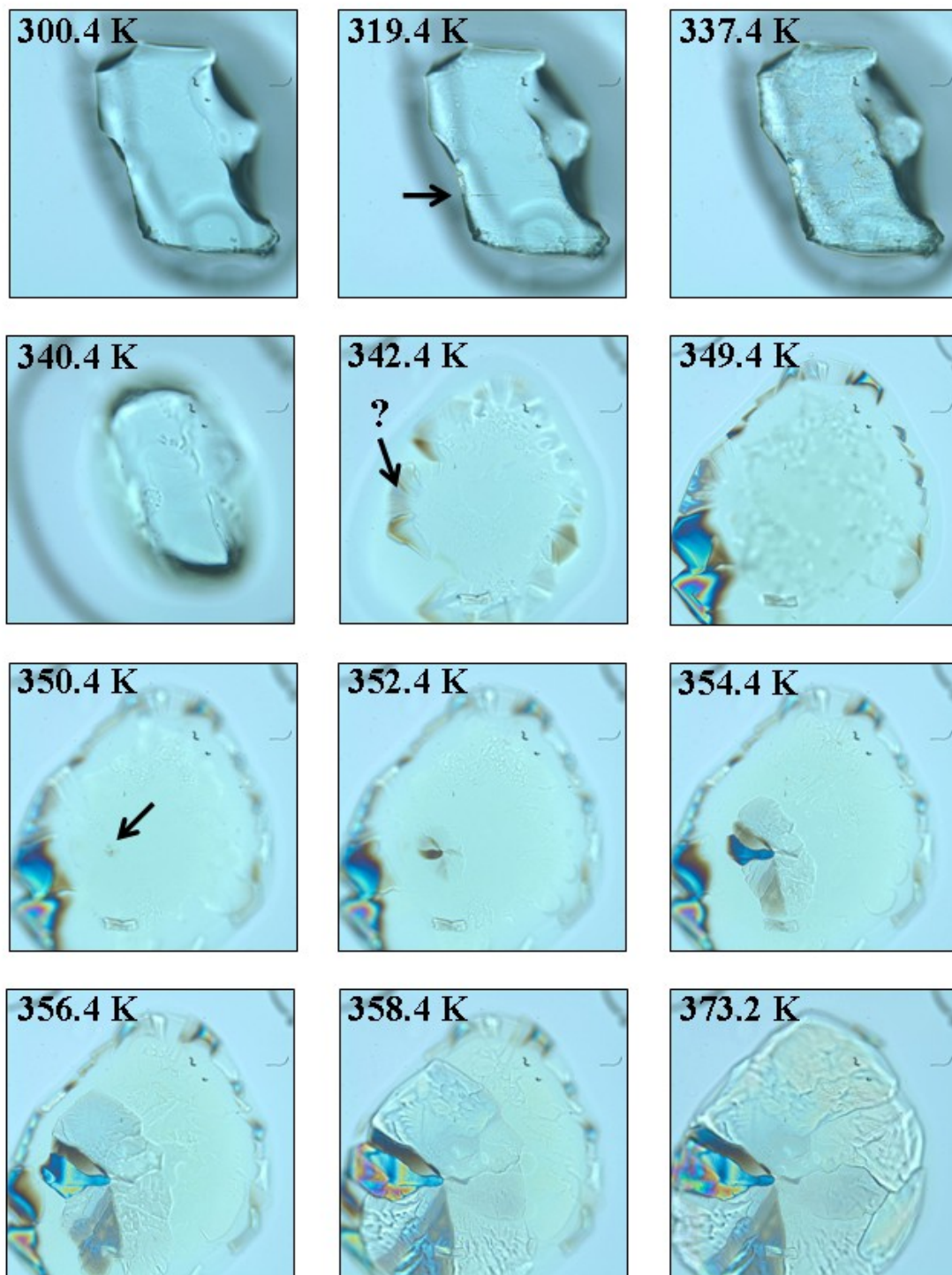


Fig. S-5

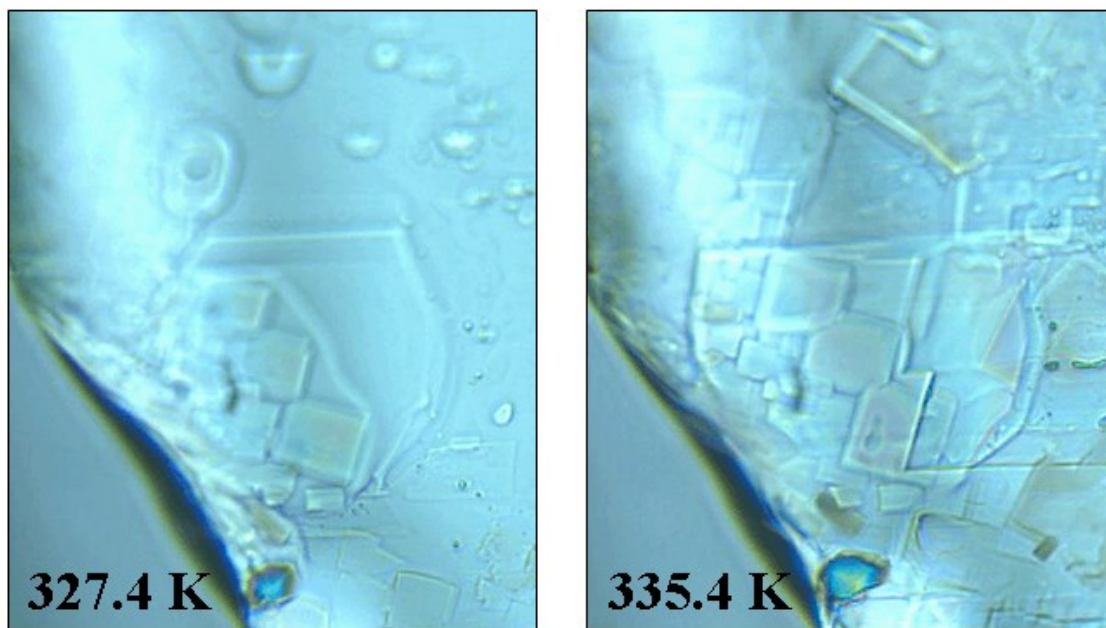
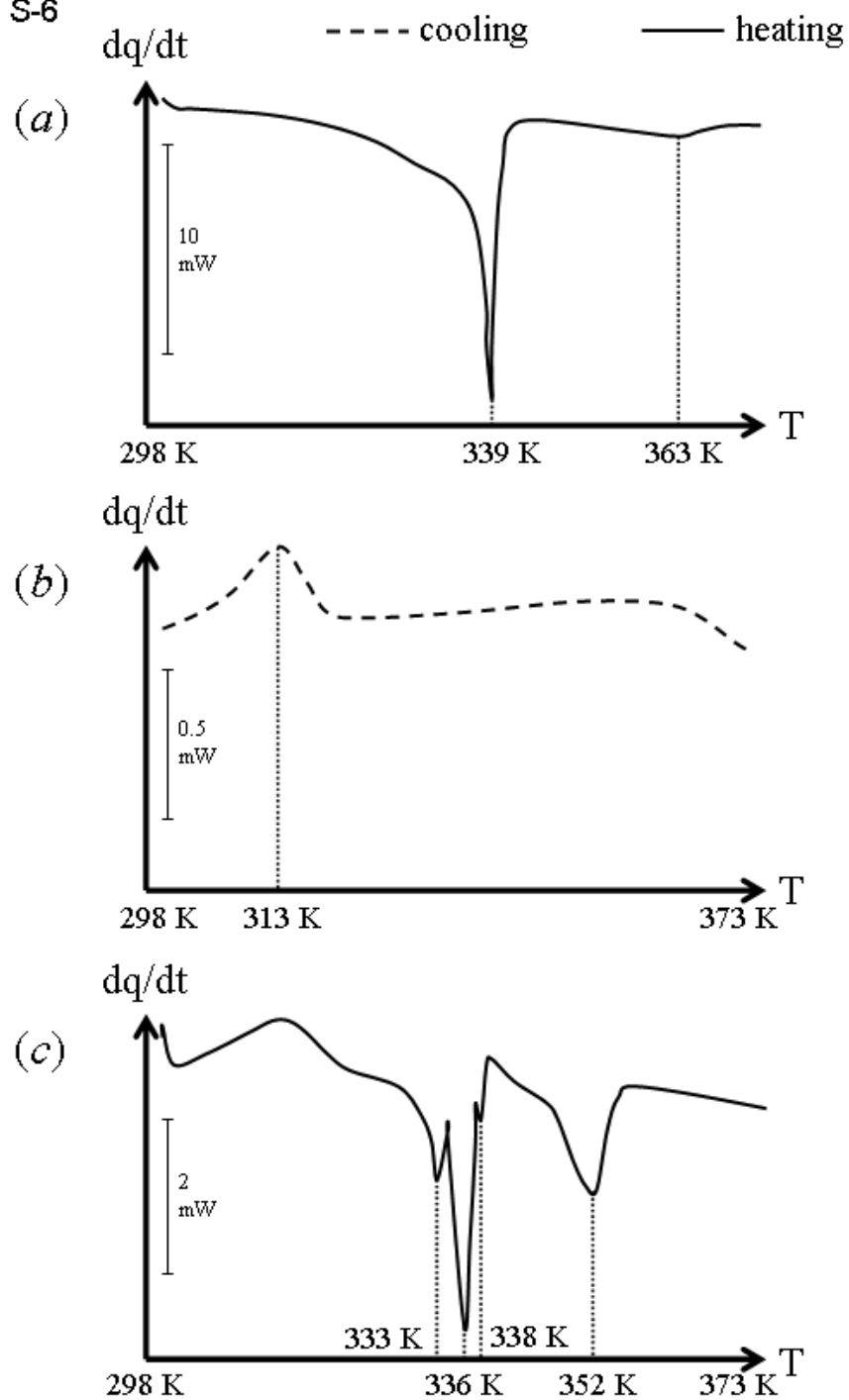
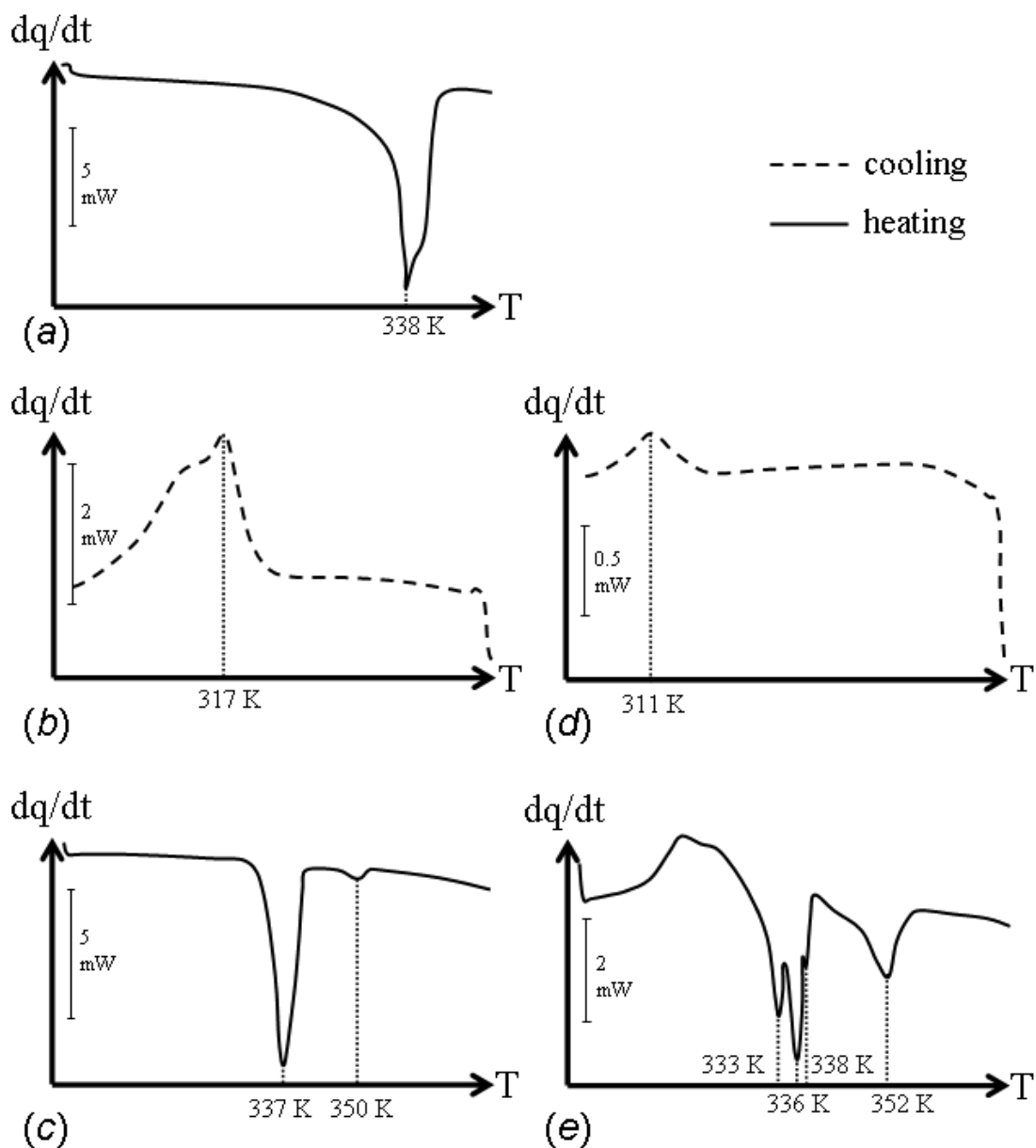


Fig. S-6



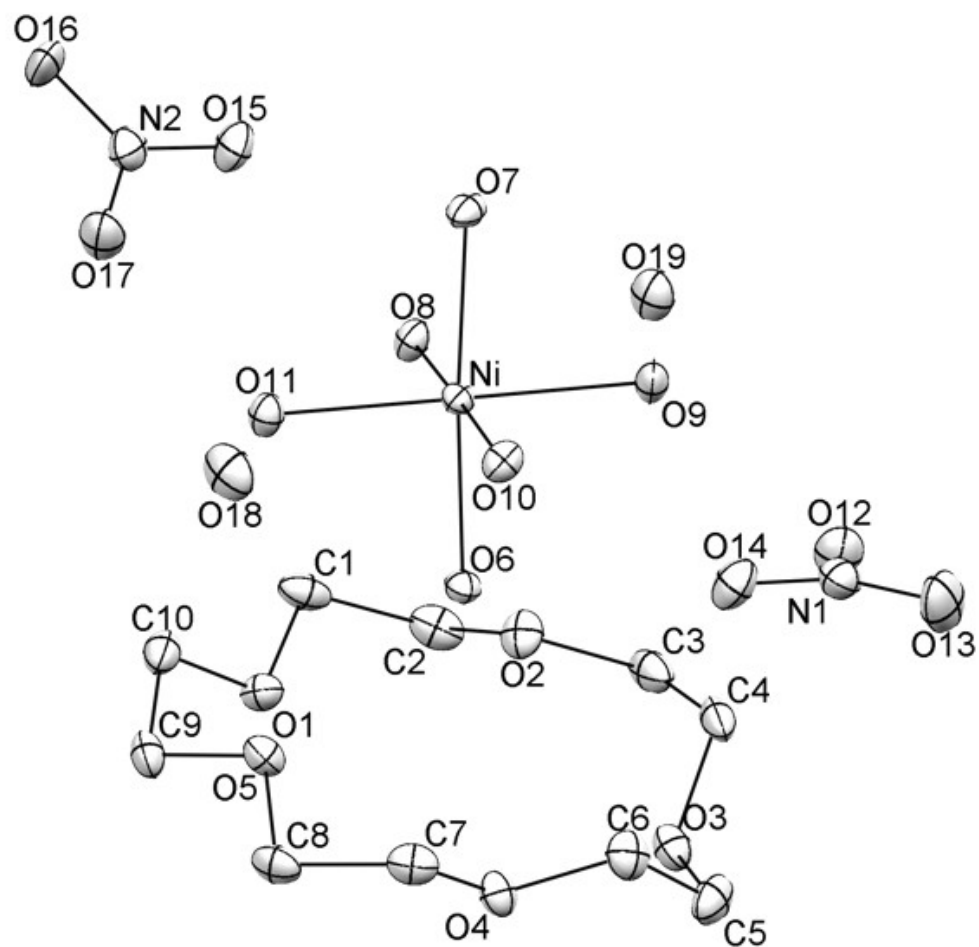
DSC traces of one sample of the dihydrate (1) made from 298 K to 373 K at 5 K/min. Traces (a), (b), and (c) were made in sequence.

Fig. S-7



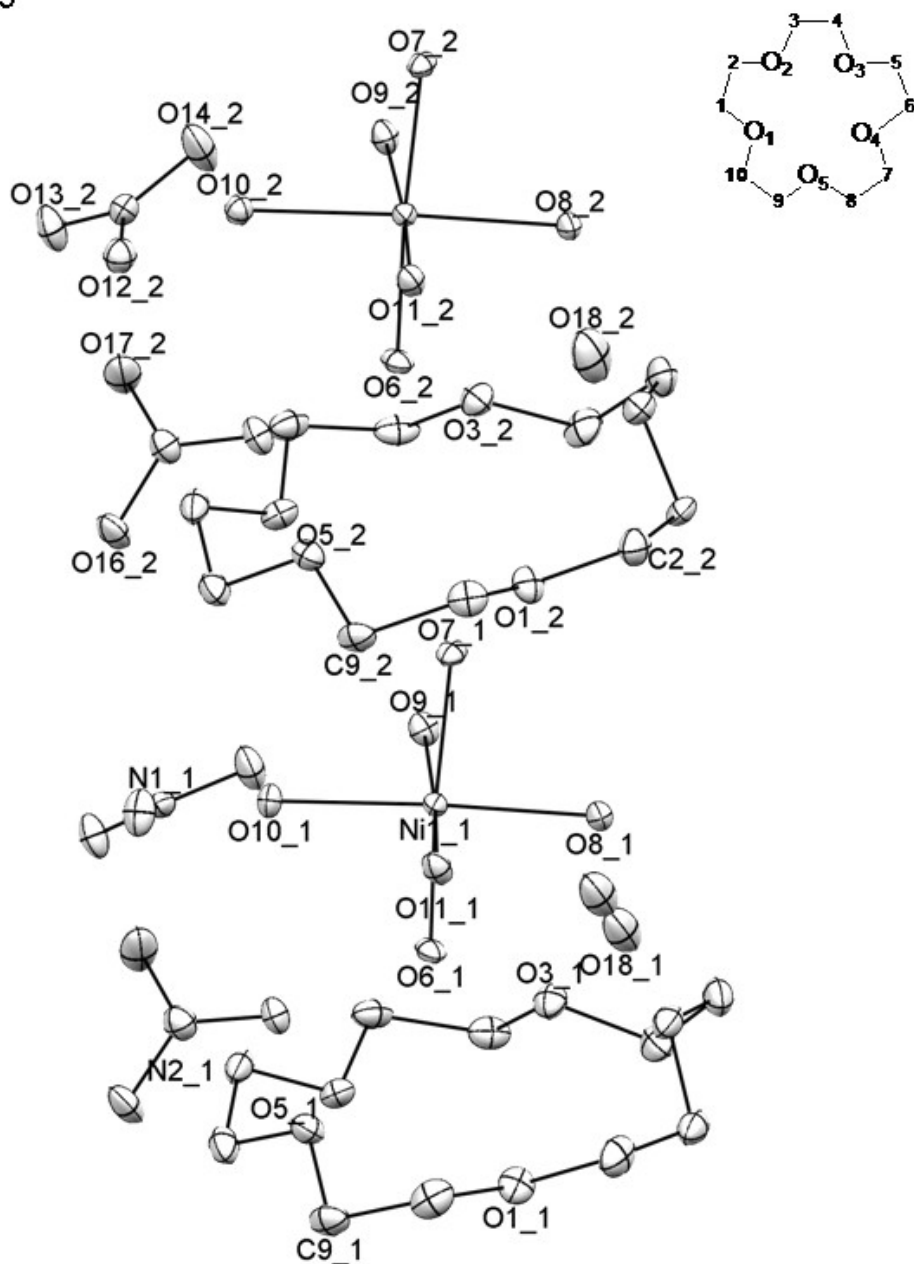
DSC traces of one sample of the dihydrate (1) made at 5 K/min and in sequence. Traces (a) and (b) had T in the range 298-348 K; traces (c), (d), and (e) had T in the range 298-373 K. Traces were made in sequence.

Fig. S-8



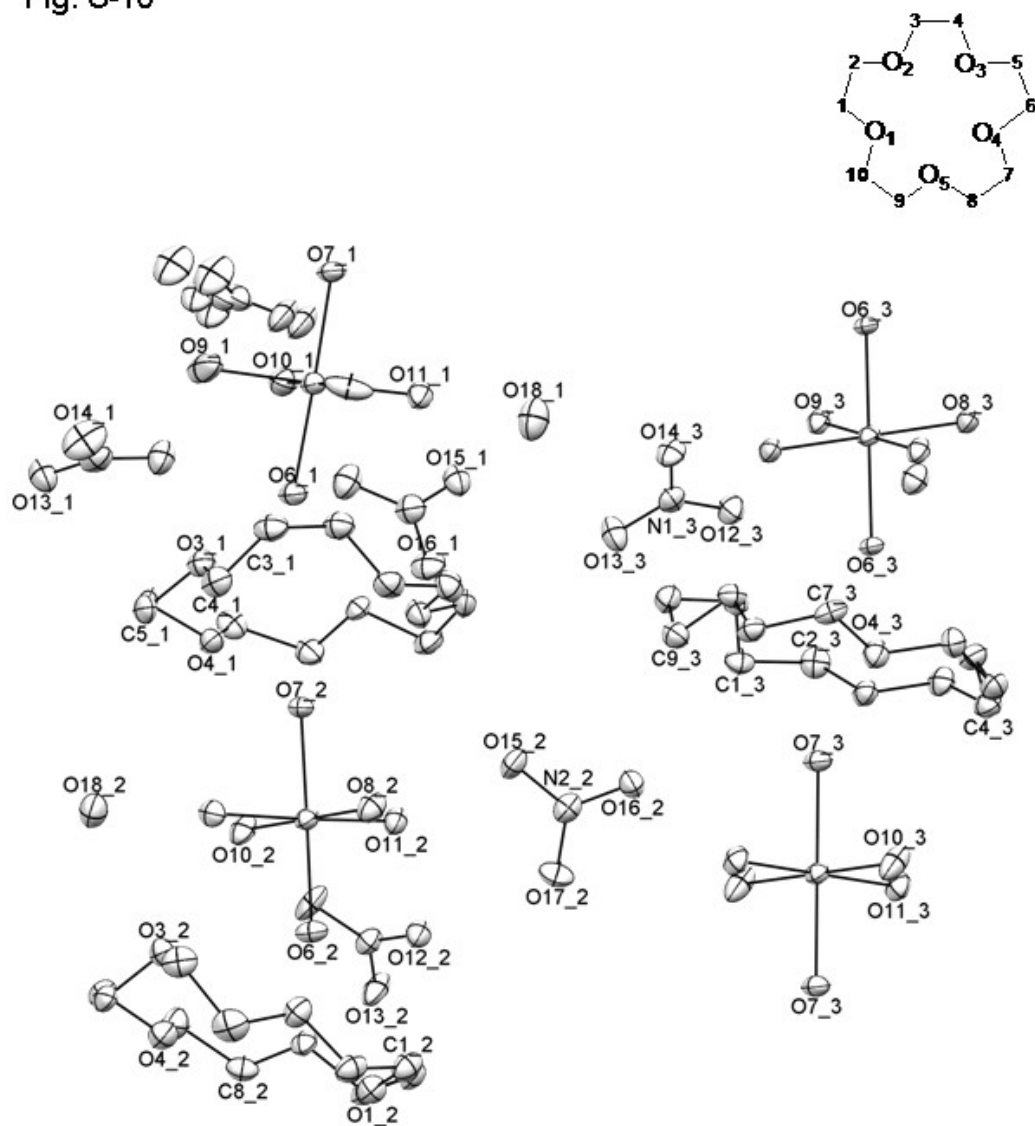
Ellipsoid plot (50% probability level) of the dihydrate (1).

Fig. S-9



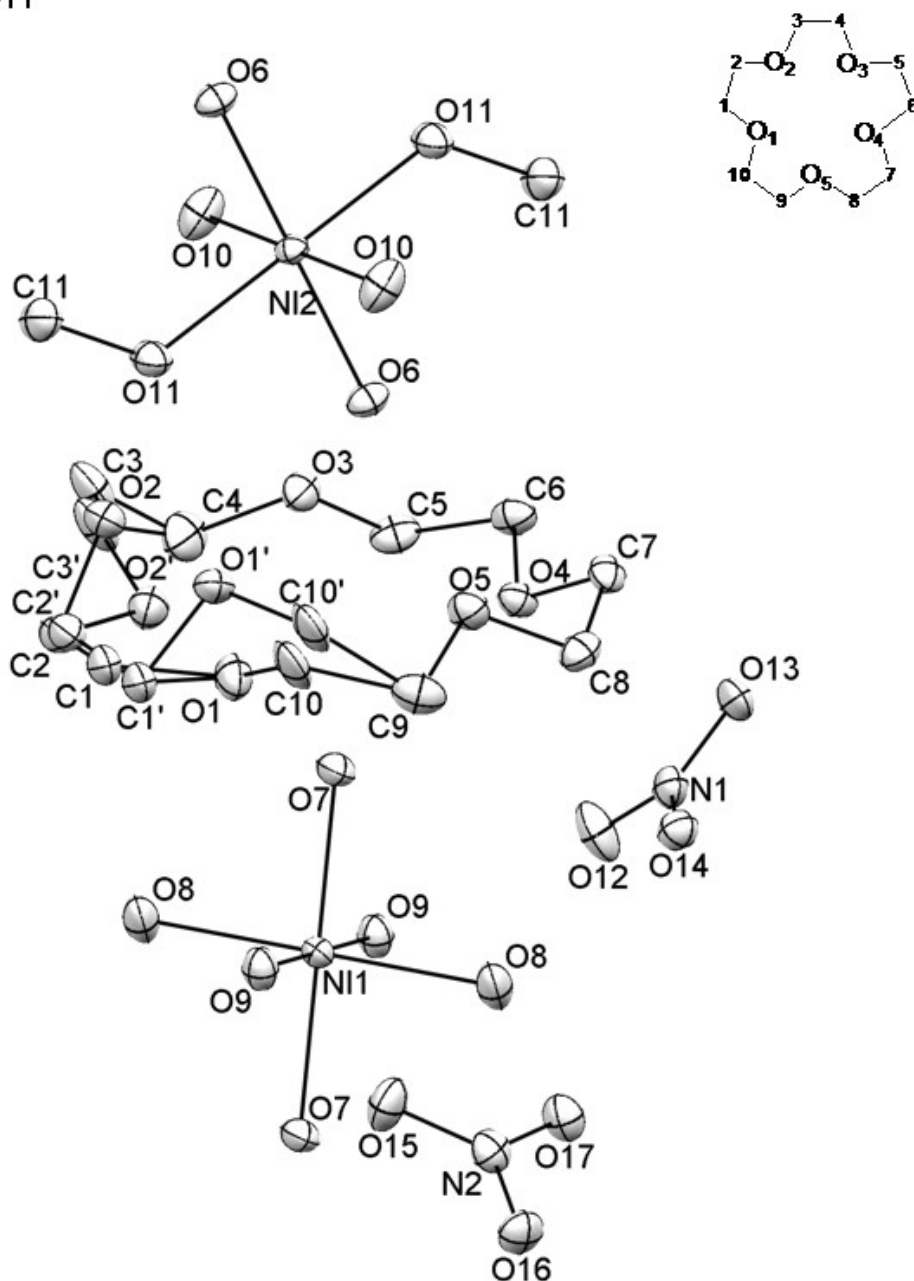
Ellipsoid plot (50% probability level) of the first polymorph of the monohydrate (2a). The numbering scheme for the atoms that are not labeled can be worked out from the information given. Both positions of the disordered water molecule containing O18_1 are shown.

Fig. S-10



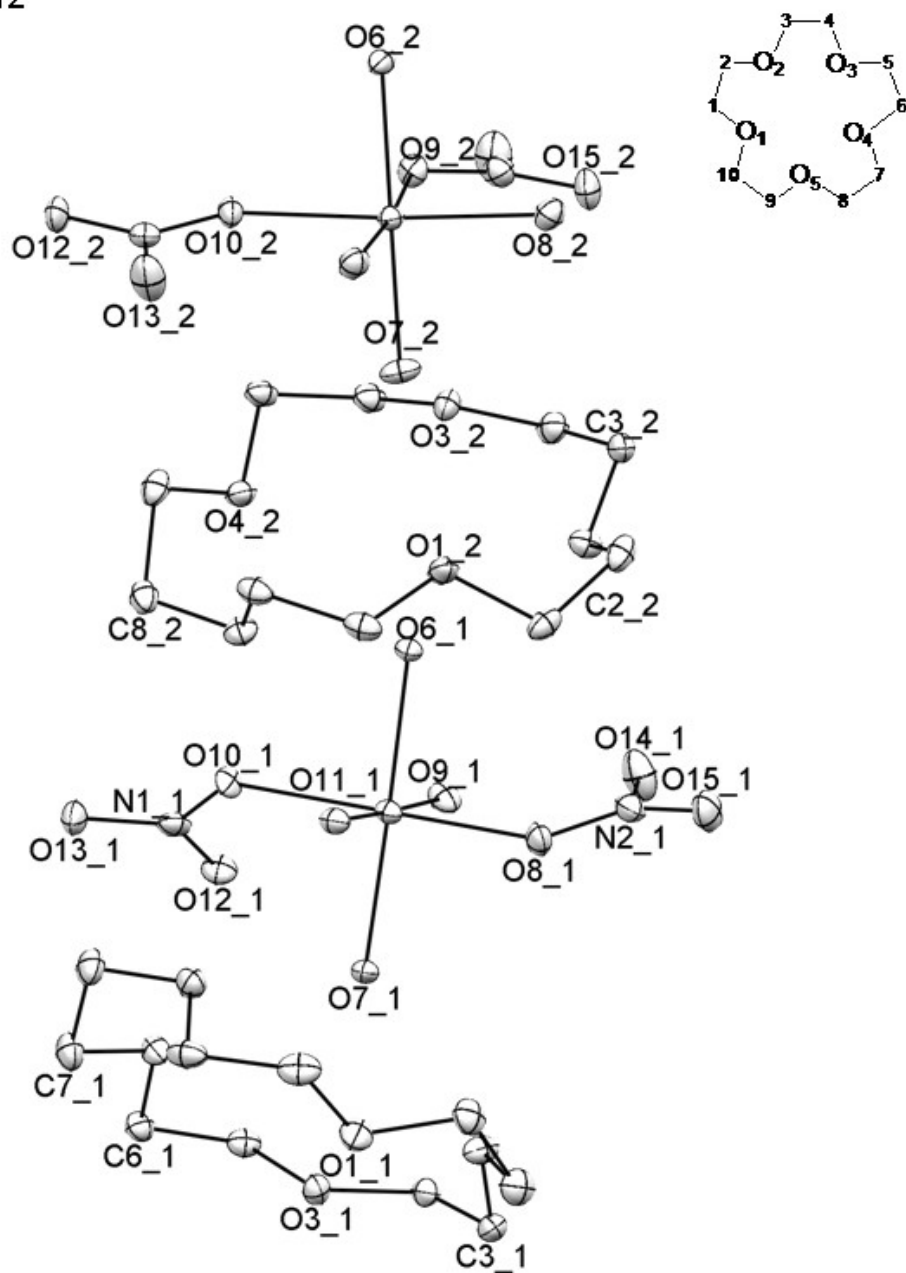
Ellipsoid plot (50% probability level) of the second polymorph of the monohydrate (**2b**). The numbering scheme for the atoms that are not labeled can be worked out from the information given.

Fig. S-11



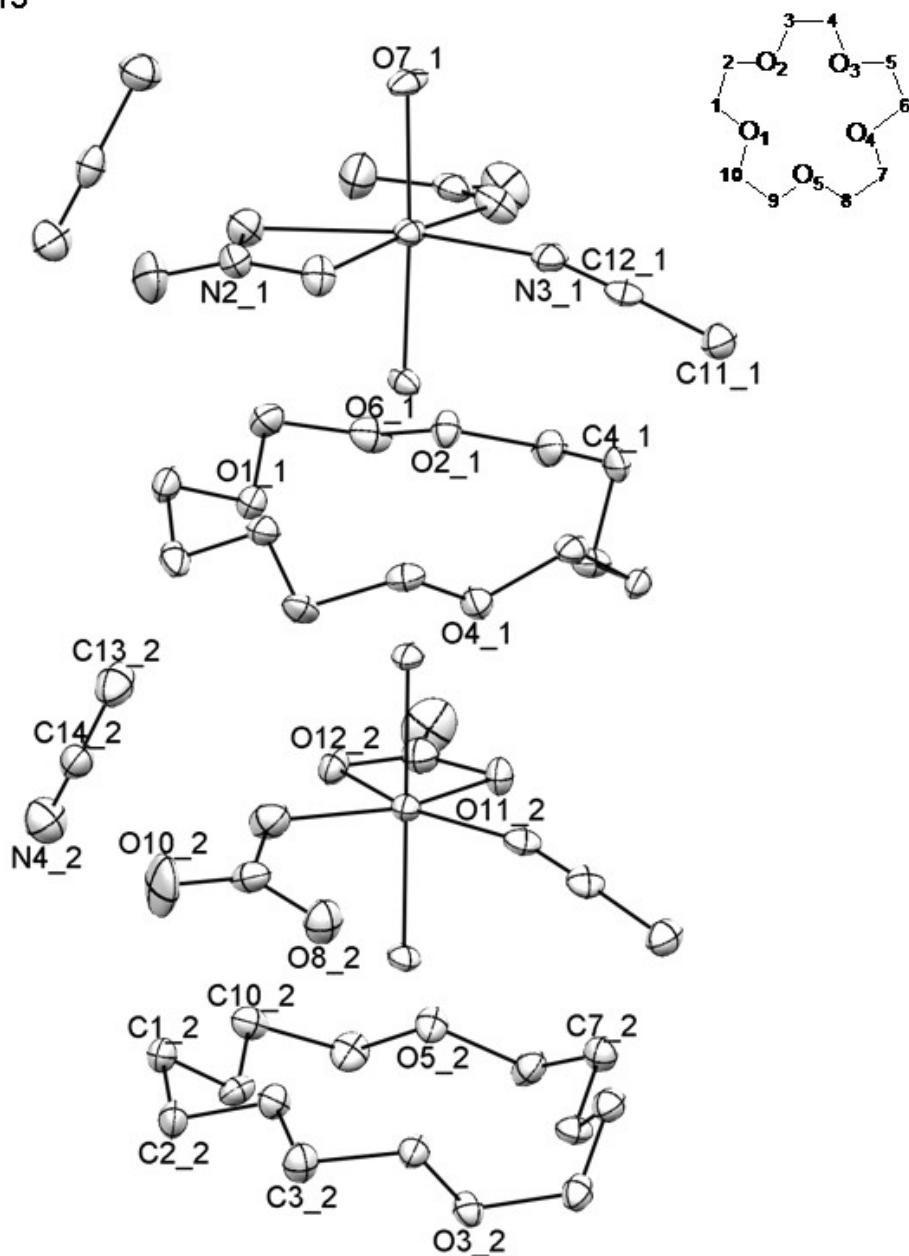
Ellipsoid plot (50% probability level) of the methanol compound (3). The numbering scheme for the atoms that are not labeled can be worked out from the information given.

Fig. S-12



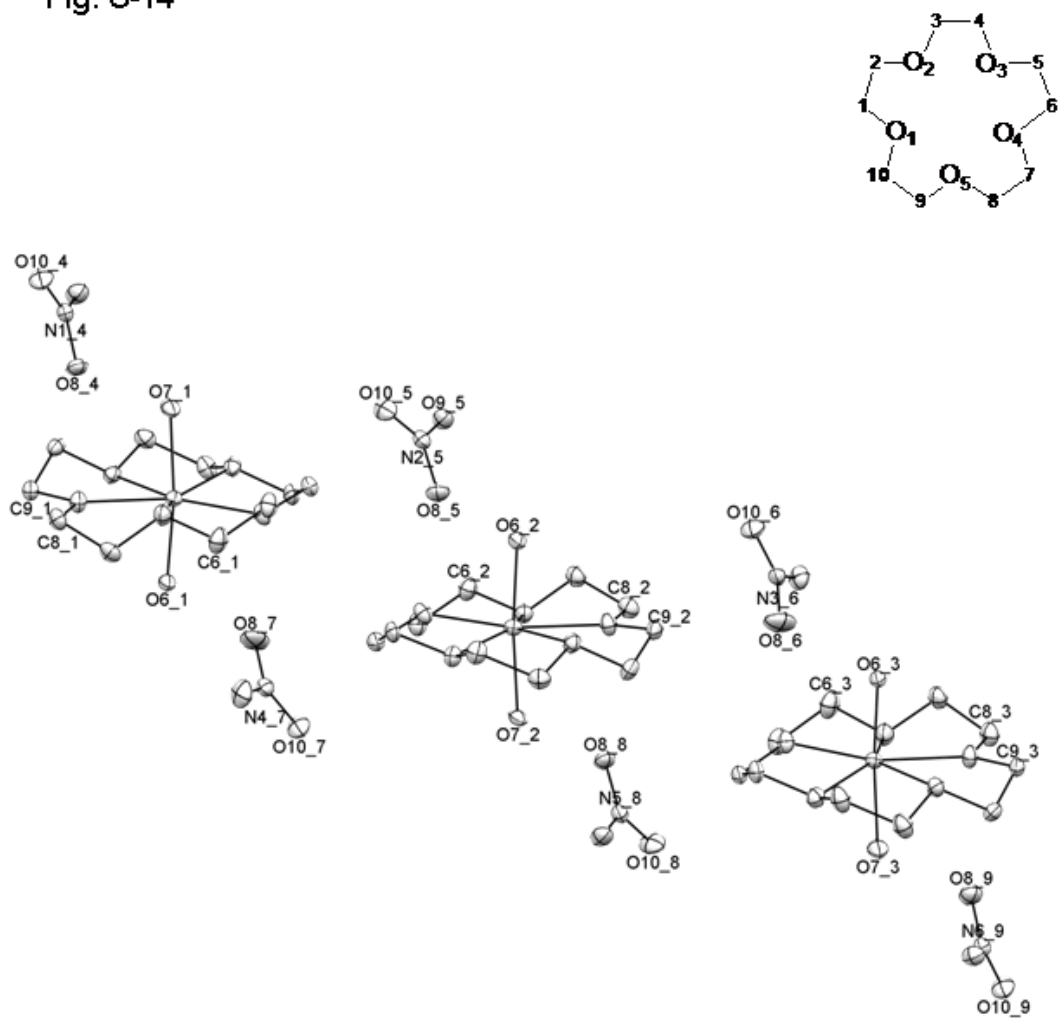
Ellipsoid plot (50% probability level) of the *cis/trans* compound (4). The numbering scheme for the atoms that are not labeled can be worked out from the information given.

Fig. S-13



Ellipsoid plot (50% probability level) of the acetonitrile compound (5). The numbering scheme for the atoms that are not labeled can be worked out from the information given.

Fig. S-14



Ellipsoid plot (50% probability level) of the target compound (6).
The numbering scheme for the atoms that are not labeled can be worked out from the information given. Only one of the two Ni positions in each cation is shown.