

3.7.5 Crystallographic description of the Complexes C17

The reaction between $\text{MoO}_2(\text{acac})_2$ and Schiff base containing furyl substituent leads to a water-coordinated derivative in which 4,4'-bipyridine interacts indirectly, through the water molecule, in an outer-sphere coordination mode. The Mo(VI) atom in the co-crystal, $\text{MoO}_2(\text{H}_2\text{O})(\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_4) \cdot 0.5\text{C}_{10}\text{H}_{10}\text{N}_2$, is *O,N,O'*-chelated by the deprotonated Schiff base and coordinated by the terminal oxo oxygen atom and water O atoms in an octahedral geometry (fig. 39). The five-membered chelate ring is planar [r.m.s. deviation 0.019 Å] but the six-membered chelate ring is puckered [r.m.s. deviation 0.108 Å]. Two mononuclear molecules are linked across a center-of-inversion by an $\text{O}-\text{H}_{\text{water}} \cdots \text{O}$ hydrogen bond while the adjacent dinuclear units are linked by an $\text{O}-\text{H}_{\text{water}} \cdots \text{N}_{4,4'\text{-bipyridine}}$ hydrogen bond to generate a linear chain structure (table 33). The 4,4'-bipyridine molecule is disordered over two positions in a 1:1 ratio.

Table 33. Hydrogen bonds in **C17** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O1w-H11...N3	0.83 (1)	1.86 (1)	2.689 (3)	174 (3)
O1w-H12...N1#	0.84 (1)	1.97 (1)	2.794 (2)	167 (3)

Symmetry code#: -x+2, -y+1, -z+1

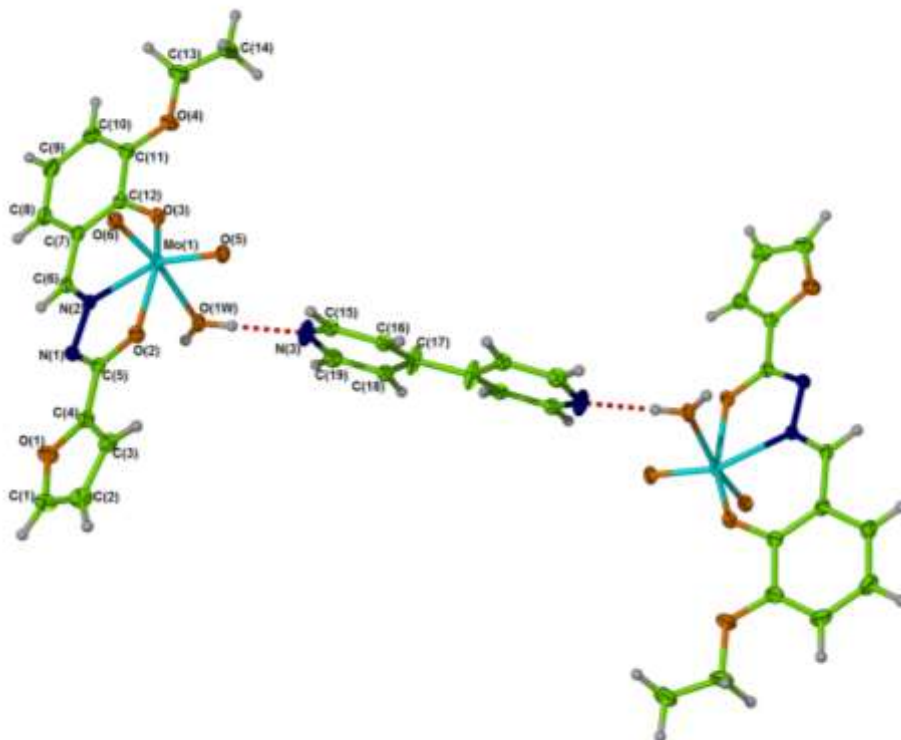


Figure 39: Ellipsoidal plot of C17 with 50% level of probability. The atomic coordinates were given in the Appendix on page 244.

3.7.6 Crystallographic description of the Binuclear and Polynuclear Complexes

The molecular structures and the atom-numbering scheme for **C18–C23** (Figs. 40 – 46) show that in **C18** and **C19**, the Schiff base ligands also behave as tridentate ligands, and reacted with the dioxomolybdenum cation to form six coordinated molybdenum(VI), in which the bidentate ligand, 4,4'-bipyridine or 4,4'-bipyridine *N,N'*-dioxide(**D-D**) formed a bridge between the two molybdenum atoms. In the case of **C20–C23**, the two molybdenum atoms are not bridged directly by a bidentate ligand, but are coordinated at each end to the O,N,O donor atoms of the symmetrical hexadentate Schiff base ligand. The reaction of the bidentate ligand, 4,4'-bipyridine and symmetrical hexadentate Schiff base ligand with $\text{MoO}_2(\text{acac})_2$ yielded a polynuclear Mo(VI), **C24**. All the complexes possess two equivalent halves with a center of inversion except for **C18**, in which the two halves of the dinuclear complex are not crystallographically equivalent but their structural dimension is closely related.

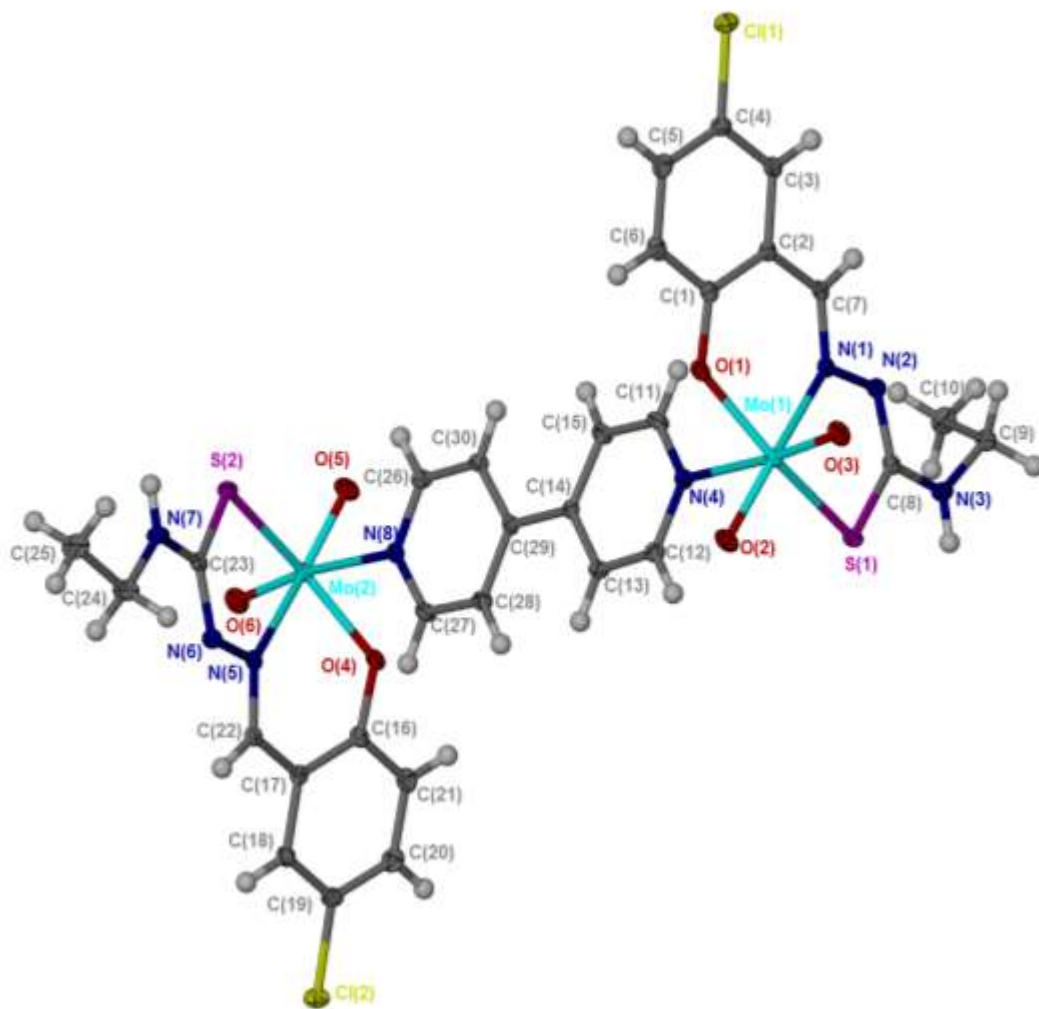


Figure 40: Ellipsoidal plot of C18 with 50% level of probability. The atomic coordinates were given in the Appendix on page 245.

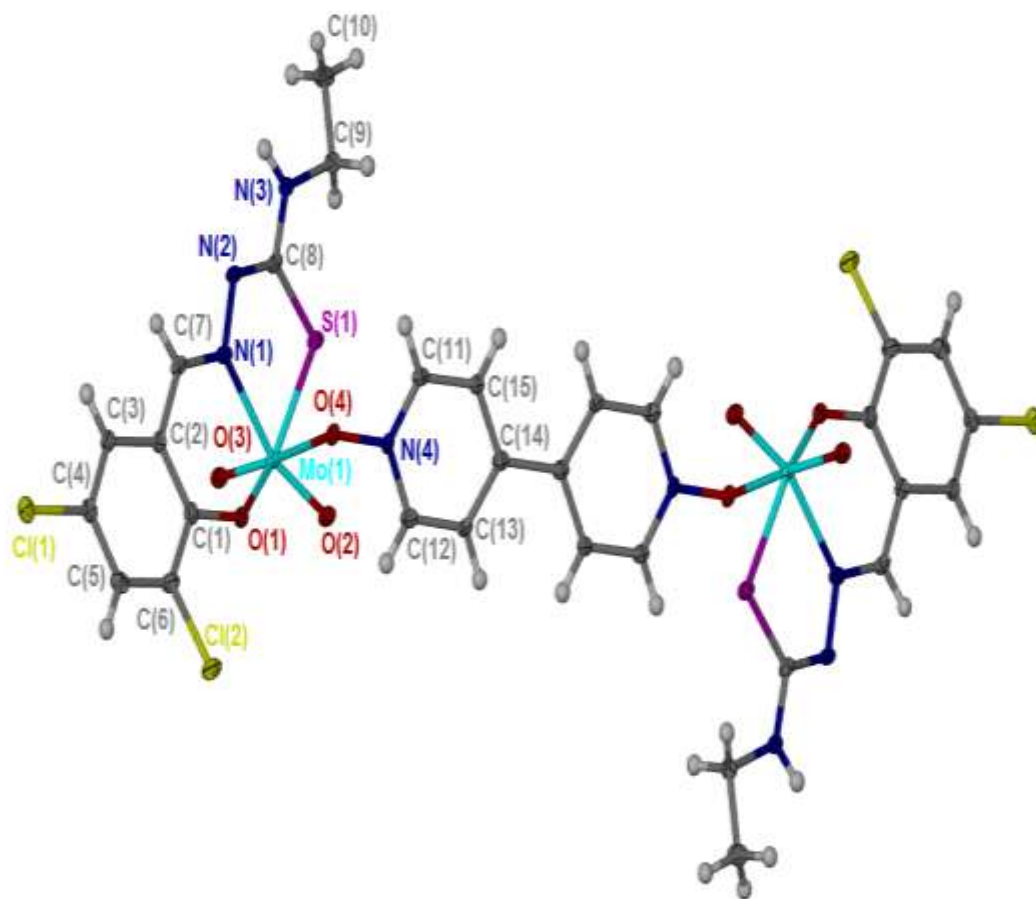


Figure 41: Ellipsoidal plot of C19 with 50% level of probability. The atomic coordinates were given in the Appendix on page 246.

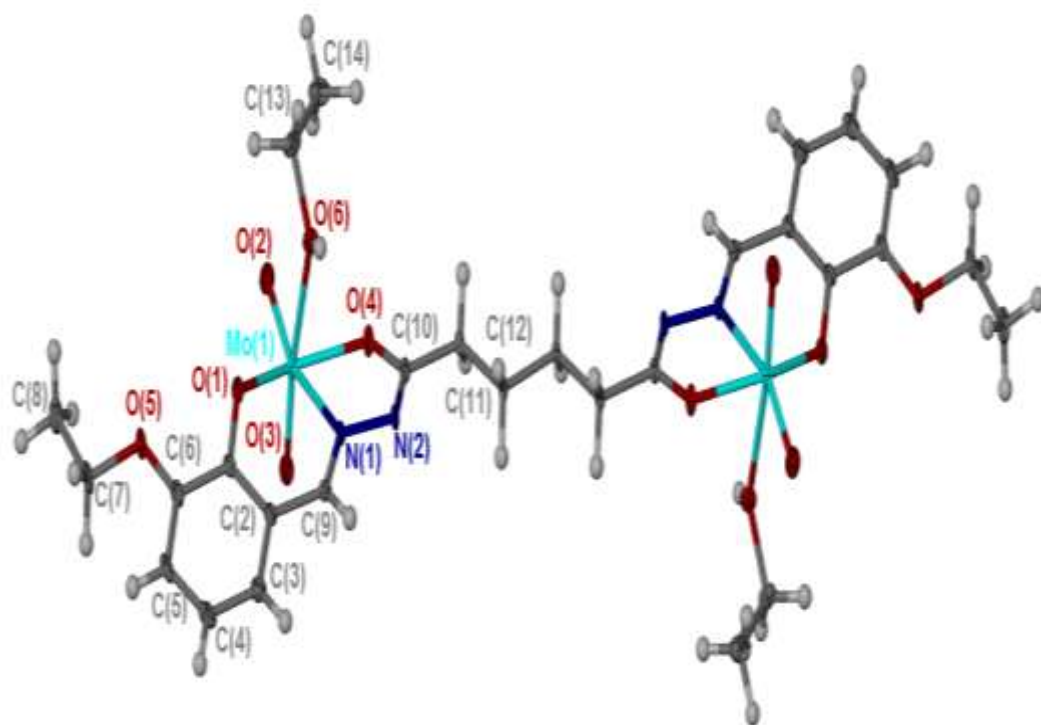


Figure 42: Ellipsoidal plot of C20 with 50% level of probability. The atomic coordinates were given in the Appendix on page 247.

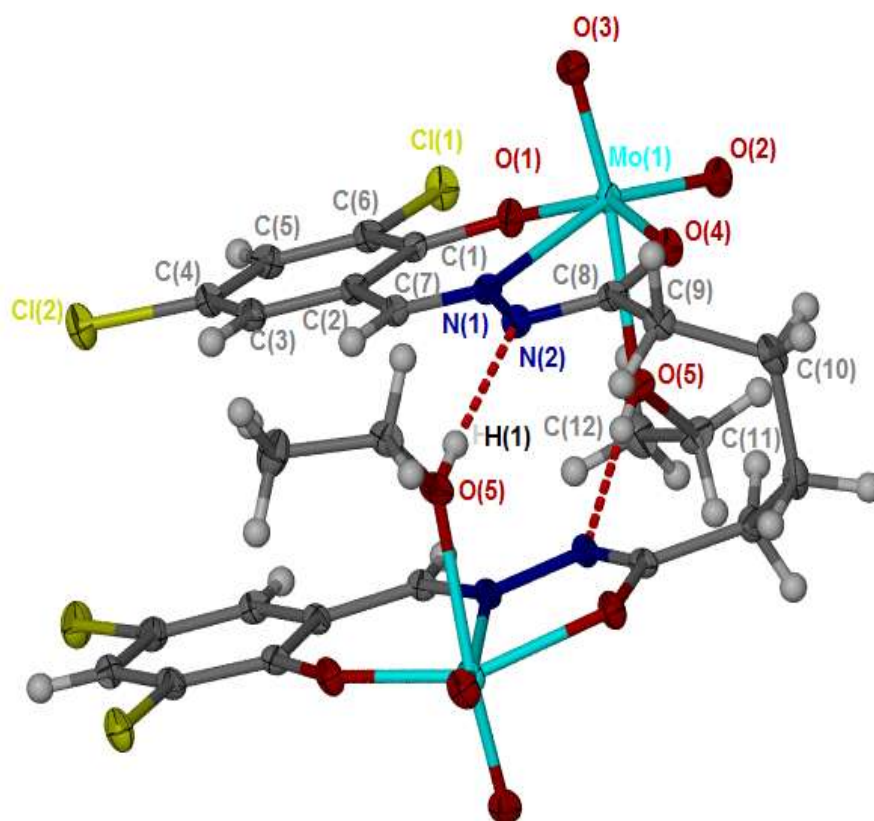


Figure 43: Ellipsoidal plot of C21 with 50% level of probability. The atomic coordination were given in the Appendix on page 248.

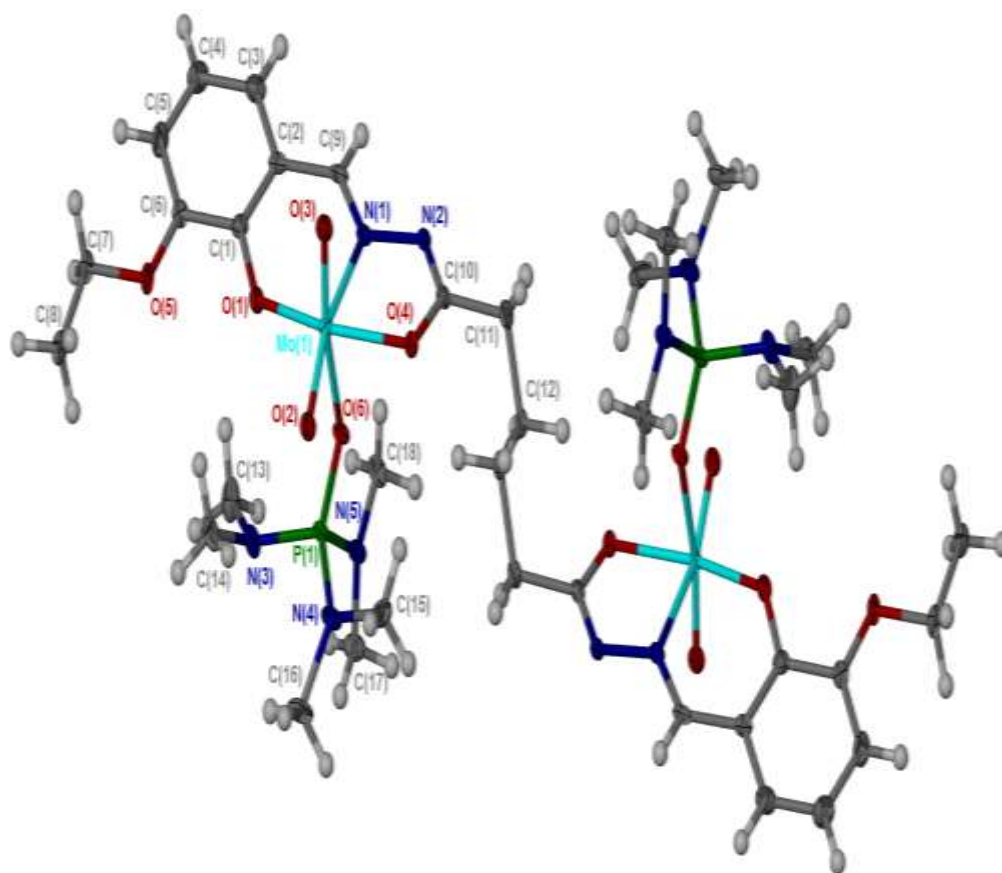


Figure 44: Ellipsoidal plot of C22 with 50% level of probability. The atomic coordinates were given in the Appendix on page 249.

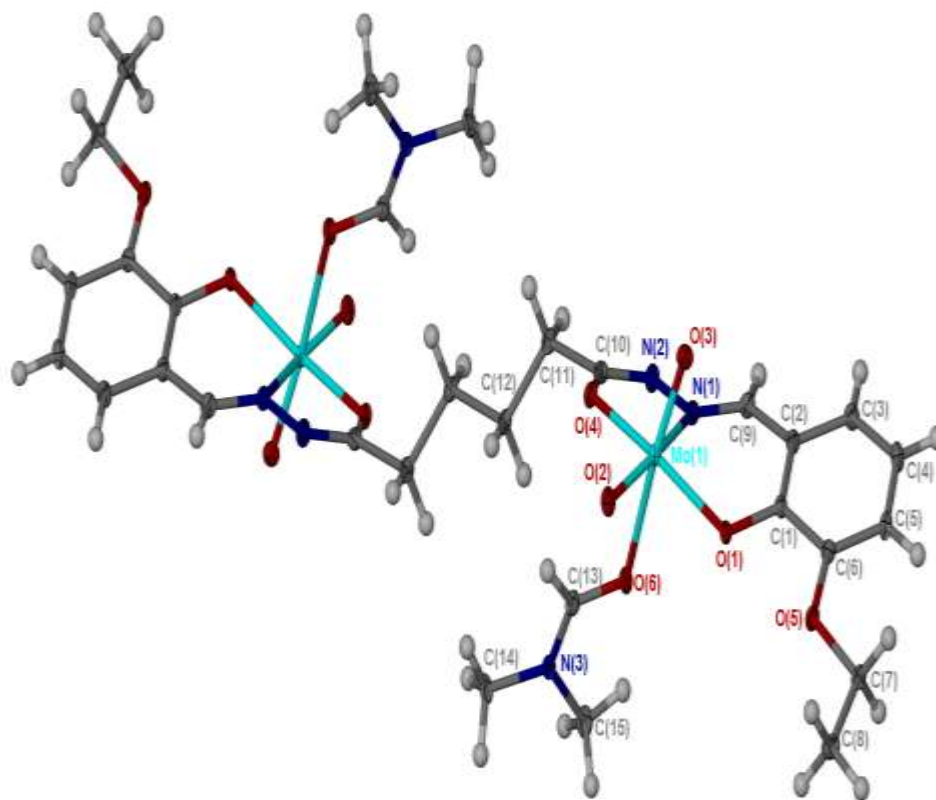


Figure 46: Ellipsoidal plot of C23 with 50% level of probability. The atomic coordinates were given in the Appendix on page 250.

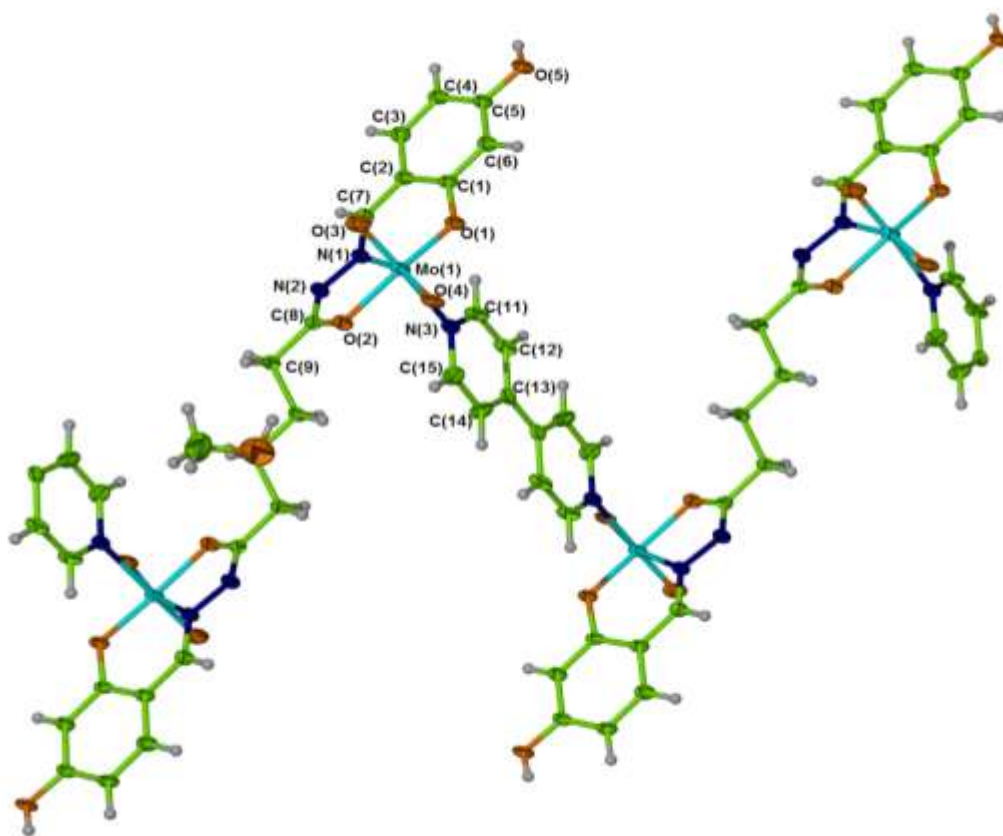


Figure 46: Ellipsoidal plot of C24 with 50% level of probability. The atomic coordinates were given in the Appendix on page 251.