



STRUCTURAL  
CHEMISTRY

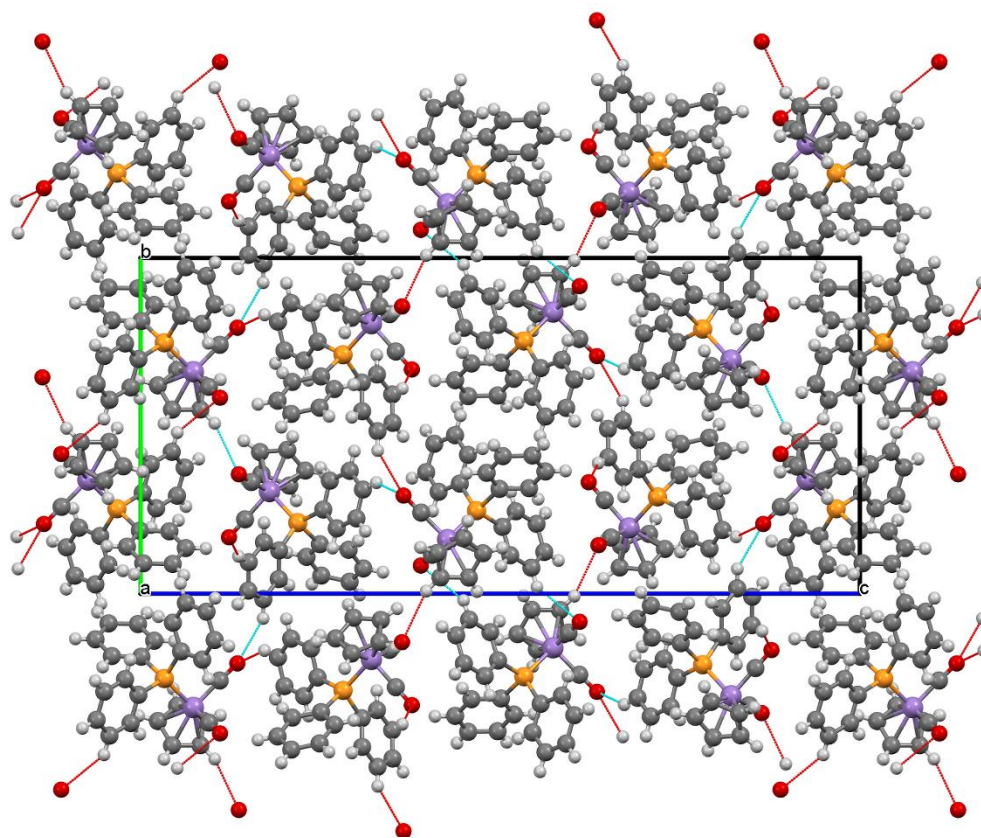
**Volume 77 (2021)**

**Supporting information for article:**

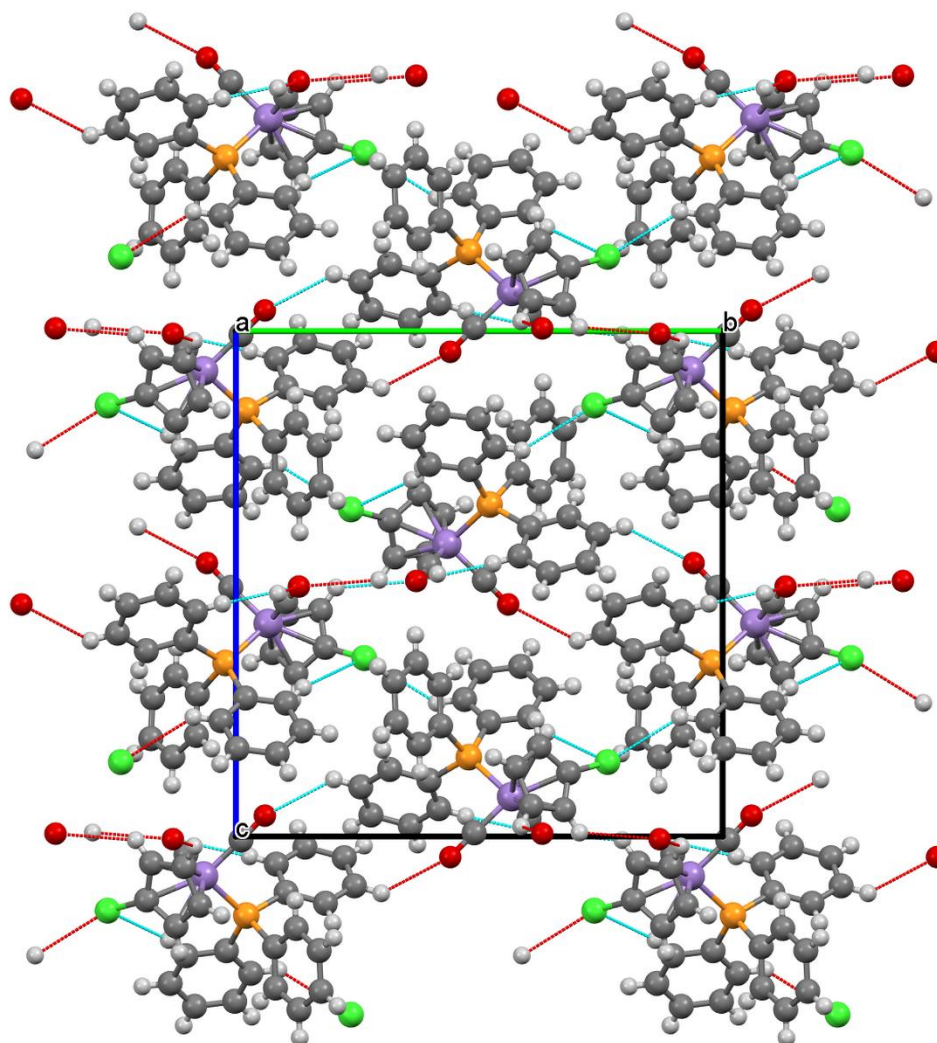
**Crystal and molecular structures of some phosphane-substituted cymantrenes [(C<sub>5</sub>H<sub>4</sub>X)Mn(CO)LL'] (X = H or Cl, L = CO, L' = PPh<sub>3</sub> or PCy<sub>3</sub>, and LL' = Ph<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PPh<sub>2</sub>)**

**Karlheinz Sünkel and Christian Klein-Hessling**

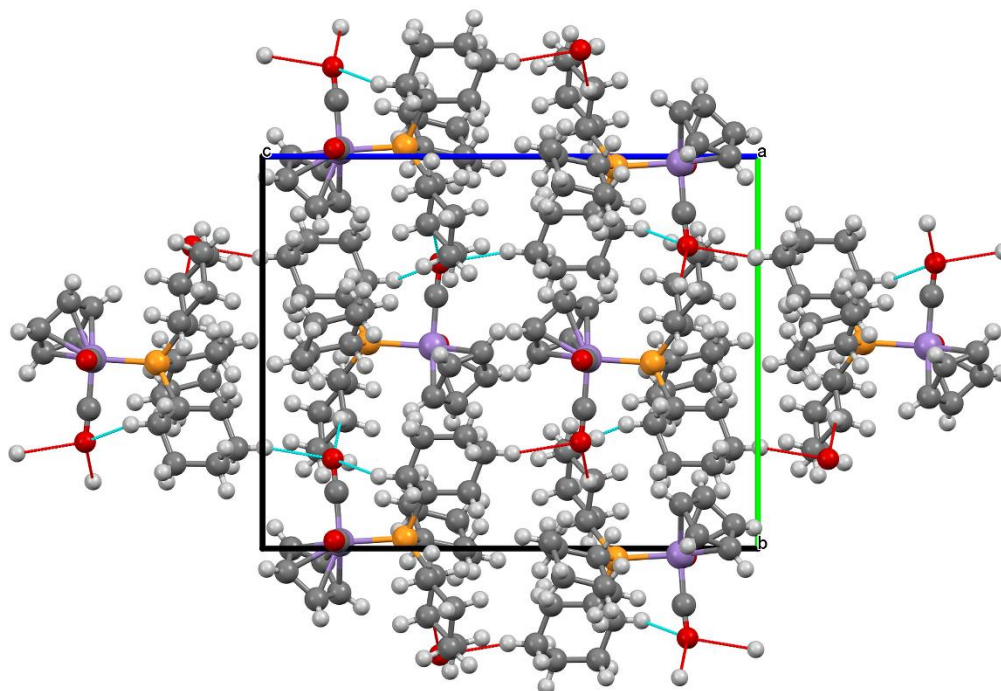
## S1. Packing Diagrams



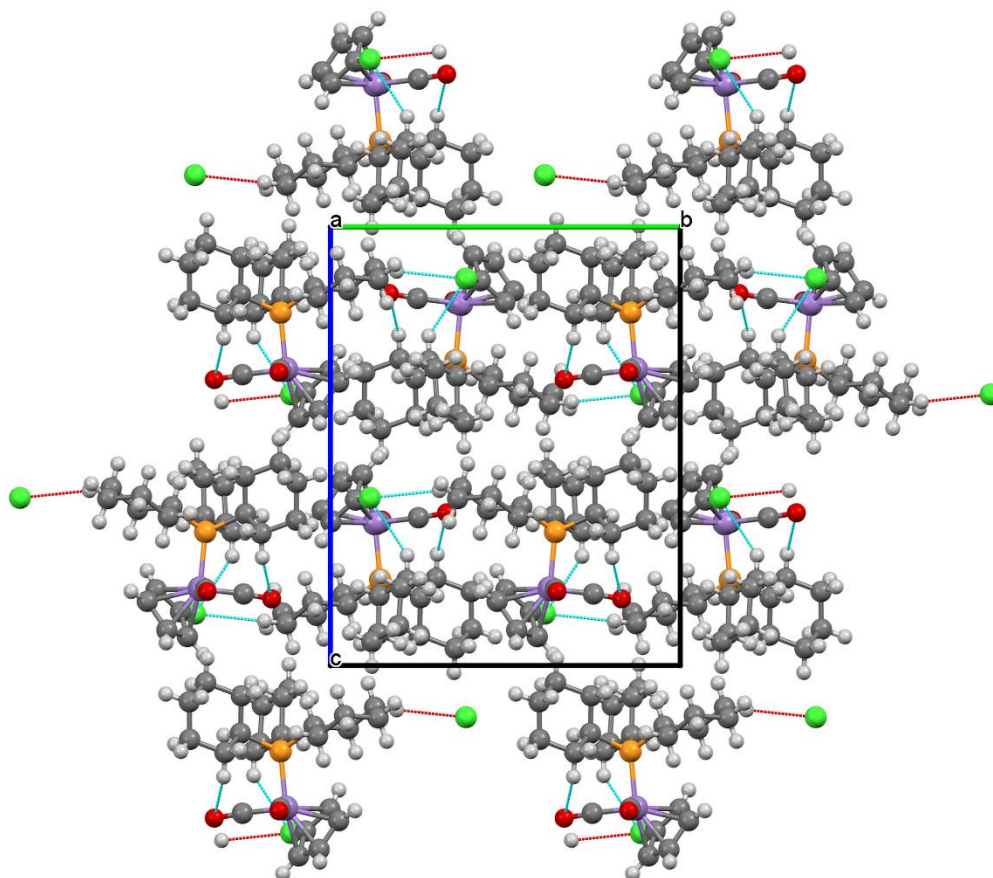
**Figure S1** Packing diagram (MERCURY) of compound **1a** watched along the *a* axis. Red and blue lines show C–H...O hydrogen bonds (colour coding as defined by mercury; red are “hanging contacts” and blue are “not-hanging contacts”).



**Figure S2** Packing diagram (MERCURY) of compound **1b** watched along the *a* axis. Red and blue lines show C–H...Cl and C–H...O hydrogen bonds (colour coding as defined by mercury; red are “hanging contacts” and blue are “not-hanging contacts”)

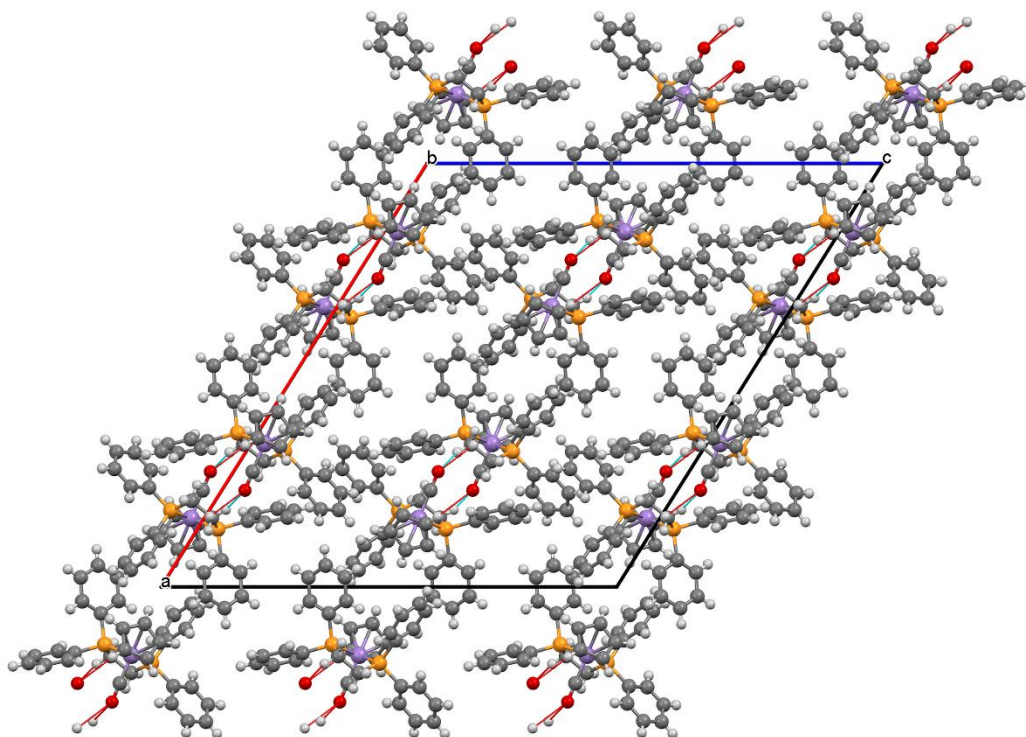


**Figure S3** Packing diagram (MERCURY) of compound **2a** watched along the *a* axis. Red and blue lines show C–H...O hydrogen bonds (colour coding as defined by mercury; red are “hanging contacts” and blue are “not-hanging contacts”)

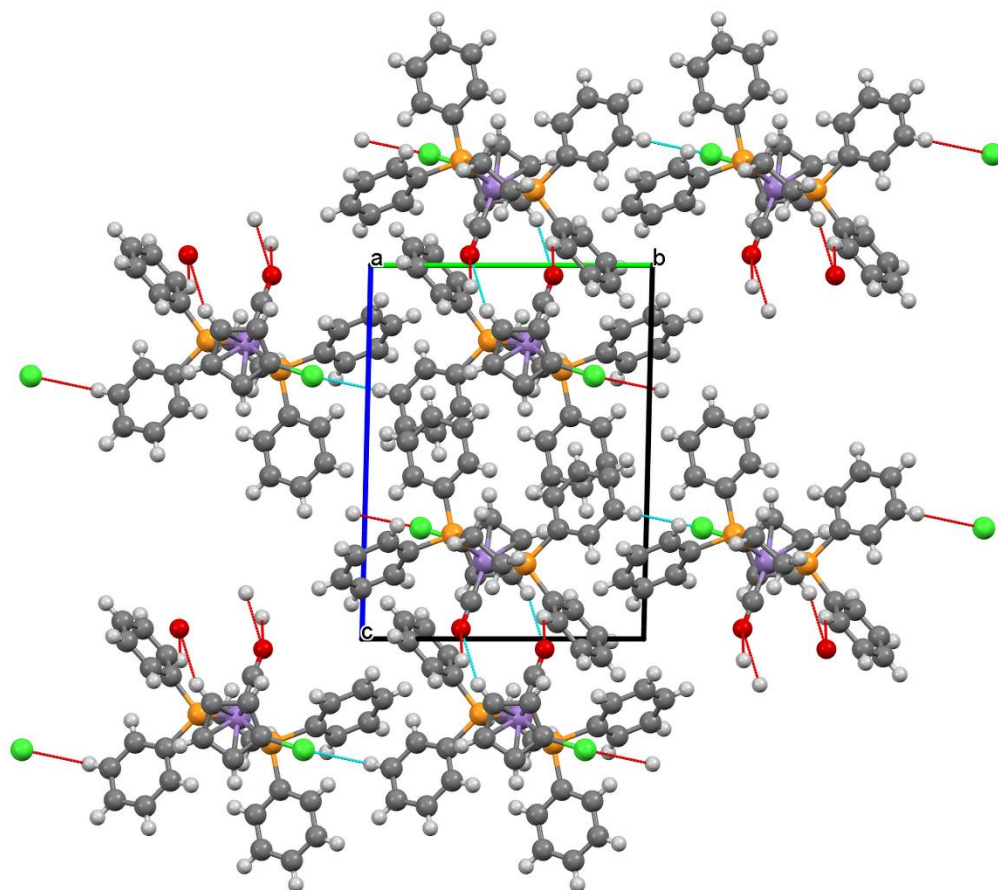


**Figure S4** Packing diagram (MERCURY) of compound **2b** watched along the *a* axis. Red and blue lines show C–H...O and C–H...Cl hydrogen bridges (colour coding as defined by mercury; red are “hanging contacts” and blue are “not-hanging contacts”)





**Figure S5** Packing diagram (MERCURY) of compound **3a** watched along the *b* axis. Red and blue lines show C–H...O hydrogen bonds (colour coding as defined by mercury; red are “hanging contacts” and blue are “not-hanging contacts”)



**Figure S6** Packing diagram (MERCURY) of compound **3b** watched along the *a* axis. Red and blue lines show C–H...O and C–H...Cl hydrogen bonds (colour coding as defined by mercury; red are “hanging contacts” and blue are “not-hanging contacts”)

**Table S1** Hydrogen bonds

Compound	Atom Pair	Distance [Å]	Symmetry code
<b>1a</b>	H103...O11	2.577	x-1, y, z
	O12...H23	2.677	1-x, -y, 1-z
	H105...O22	2.528	1-x, 1-y, 1-z
	H124...O22	2.616	x- ½, ½ -y, ½ +z
	O21...H205	2.686	2-x, -y, 1-z
<b>1b</b>	H16...Cl1	2.649	x, y, z
	Cl1...H12	2.999	1-x, y- ½, ½-z
	H26...O1	2.746	x, y, z
	O1...H4	2.761	x-1,y,z
	O1...H5	2.750	x- ½, ½-y, 1-z
	H23...O2	2.770	x- ½, 1.5-y, 1-z
<b>2a</b>	H36B...O1	2.538	x, y, z
	H22A...O1	2.584	1.5-x, y- ½, ½ -z
	H33B...O1	2.626	x- ½, 1.5-y, z- ½
<b>2b</b>	H12A...Cl1	2.835	x, y, z
	H36A...O1	2.694	x, y, z
	Cl1...H23B	2.821	1-x, y- ½, ½ -z
<b>3a</b>	O1...H3	2.647	½ -x, ½ -y, 1-z
	O1...H12A	2.713	½ -x, 1.5-y, 1-z
<b>3b</b>	Cl1...H215	2.887	x, y-1, z
	H202...O1	2.651	1-x, 1-y, 2-z
	H4...O1	2.355	2-x, 1-y, 2-z