Crystal structures of Pigment Red 170 and derivatives, 
determined from X-ray powder diagrams

(Kristallstrukturen von Pigment Red 170 und Derivaten, 
bestimmt aus Röntgen-Pulverdiagrammen)

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1. Comparison of X-ray powder diagrams for $\alpha$-1a and $\alpha$-1b, showing the isotopy of both compounds.

All diagrams were measured in transmission geometry on a STOE-STADI-P-Diffractometer 
equipped with a curved Ge(111) primay monochromator and a linear position sensitive 
detector. Cu-K$_{\alpha 1}$ radiation ($\lambda=1.540598$ Å)
2. Crystal structures of $\alpha$-1a to $\alpha$-1f:

a) Structure of $\alpha$-1a (R=H)

b) Structure of $\alpha$-1b (R=CH$_3$)
c) Structure of $\alpha$-1c (R=F)

d) Structure of $\alpha$-1d (R=Cl)
e) Structure of α-1e (R=Br)

f) Structure of α-1f (R=NO₂)
g) Comparison of $\alpha\mathrm{-}1a$ to $\alpha\mathrm{-}1f$
h) Comparison of \( \alpha \)-1a to \( \alpha \)-1f, structures marked by colours:

R = H: grey
R = F: green
R = Cl: red
R = Br: brown
R = NO\(_2\): blue
R = Me: violet
i) View of the crystal structure of α-1a showing the helical hydrogen-bridge topology between the CONH$_2$ groups
3) Rietveld-Plots of $\alpha$-1c to $\alpha$-1f:

Experimental powder diagrams shown in black, simulated diagrams in red, background curves in green, difference curves in blue

c) $\alpha$-1c (R=F)

d) $\alpha$-1d (R=Cl)

e) $\alpha$-1e (R=Br)
4) Rietveld-Plot of $\gamma$-1a:

Experimental powder diagram shown in black, simulated diagram in red, background curve in green, difference curve in blue

f) $\alpha$-1f (R=NO$_2$)