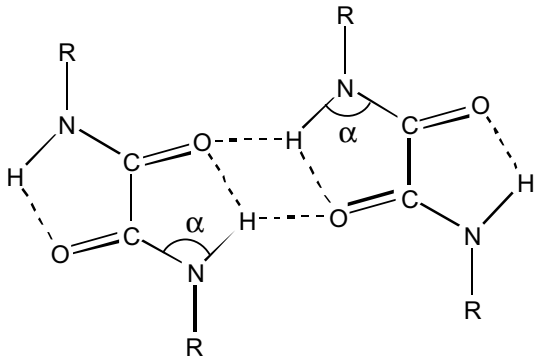
s9.m1.o5 **Structure and Properties of Alkyloxamides**.
K. Clou[a], B. Rousseau[b], H.O. Desseyn[a], A.T.H. Lenstra[b],
[a]*Department of Chemistry, University of Antwerp (RUCA), Groenenborgerlaan 171, B-2020 Antwerpen, Belgium.*
[b]*Department of Chemistry, University of Antwerp (UIA), Universiteitsplein 1, B-2610 Antwerpen, Belgium.*
Keywords: molecular interactions, hydrogen bond.

The structures of N-cyclopropyloxamide and N,N'-dicyclopropyloxamide are investigated using X-ray diffraction. The three dimensional structure of these two compounds shows a similar pattern, in which hydrofylic layers alternate with hydrophobic layers. Within the hydrophilic layers neighboring molecules are linked together by H-bonds. A typical example of the hydrogen bonding scheme is shown below.



The structure exhibits bifurcated N-H…O hydrogen bonds, in which an intramolecular N-H…O bond is combined with an intermolecular one. The weight of the intramolecular component depends strongly on the valence angle C-N-H (alpha). The value of the latter is influenced by the steric demands of the alkyl substituent R, which is supported by calculations at the B3LYP/6-31++G** level of theory. For the standard alkyl substituents we measured the difference in intramolecular character spectroscopically via:

i) diluted solution in CH_2Cl_2. Here we look at the intramolecular H-bonds, which get stronger with lower frequencies for ν(N-H).
ii) the solid state. Temperature induced shifts in ν(N-H) are indicative for the importance of the intermolecular H-bonds. The larger the frequency shift, the higher the intermolecular bond strength.

ν(N-H) in cm^{-1}				
R-group	dil. CH_2Cl_2	Crystalline State		Δν
		298K	77K	
methyl	3411	3312	3294	13
ethyl	3399	3303	3288	15
cyclopropyl	3391	3278	3271	7
isopropyl	3390	3296	3291	5
t-butyl	3377	3327	3324	3

Notes