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Table 1. Fractional crystallographic coordinates for all atoms of **12c** and as substitute for the isotropic temperature factor the parameter U_{eq} [pm^2] defined as one third of the trace of the orthogonalized U_{ij} tensor (Table 2). For the hydrogen atoms the truely refined U value has been determined. Standard deviations are given in parentheses.

	x/a	y/b	z/c	U_{eq}
C(1)	0.15322(7)	0.08672(9)	0.56765(8)	270(2)
C(2)	0.10758(8)	0.1294(1)	0.44499(9)	314(2)
C(3)	0.13002(8)	0.0277(1)	0.37809(8)	333(2)
C(4)	0.23981(8)	-0.0131(1)	0.44318(8)	308(2)
C(5)	0.27251(7)	-0.04253(9)	0.56570(8)	260(2)
C(6)	0.11770(9)	0.1725(1)	0.6314(1)	370(3)
C(7)	0.37510(8)	-0.1064(1)	0.6275(1)	355(2)
C(8)	0.37640(9)	0.1569(1)	0.7951(1)	397(3)
N(1)	0.26233(6)	0.08076(8)	0.61678(6)	251(2)
O(1)	0.12418(5)	-0.05072(7)	0.57358(6)	311(2)
O(2)	0.20245(5)	-0.13545(7)	0.57192(6)	301(2)
O(3)	0.30513(5)	0.05459(7)	0.73561(5)	315(2)
H(2a)	0.135(1)	0.218(1)	0.445(1)	367(32)
H(2b)	0.036(1)	0.138(1)	0.415(1)	374(32)
H(3a)	0.113(1)	0.065(1)	0.305(1)	423(34)
H(3b)	0.088(1)	-0.055(1)	0.364(1)	372(32)
H(4a)	0.284(1)	0.058(1)	0.442(1)	344(31)
H(4b)	0.254(1)	-0.094(1)	0.413(1)	370(32)
H(6a)	0.137(1)	0.264(2)	0.631(1)	498(38)
H(6b)	0.148(1)	0.146(2)	0.710(1)	536(41)
H(6c)	0.046(1)	0.167(2)	0.595(1)	553(41)
H(7a)	0.424(1)	-0.046(1)	0.623(1)	448(36)
H(7b)	0.396(1)	-0.124(1)	0.706(1)	476(38)
H(7c)	0.374(1)	-0.191(2)	0.592(1)	507(39)
H(8a)	0.343(1)	0.245(1)	0.781(1)	440(36)
H(8b)	0.429(1)	0.159(1)	0.775(1)	471(37)
H(8c)	0.405(1)	0.131(1)	0.874(1)	517(40)

Table 2. Anisotropic thermal parameters U_{ij} [pm^2] and their standard deviations for **12c**. The temperature factor corresponds to the expression $\exp[-2\pi^2(U_{11}h^2a^{*2} + \ldots + 2U_{23}klb^*c^*)]$.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	286(5)	247(5)	291(5)	-32(4)	155(4)	10(4)
C(2)	328(5)	290(5)	294(5)	14(4)	132(4)	49(4)
C(3)	374(6)	353(6)	225(5)	-24(4)	114(4)	12(4)
C(4)	350(5)	341(5)	260(5)	-50(4)	171(4)	-39(4)
C(5)	268(5)	248(5)	258(5)	-56(3)	126(4)	-29(3)
C(6)	406(6)	371(6)	415(6)	13(5)	267(5)	-10(5)
C(7)	287(5)	369(6)	358(6)	12(4)	123(4)	-31(5)
C(8)	386(6)	491(7)	308(5)	-145(5)	168(5)	-146(5)
N(1)	282(4)	270(4)	206(4)	-44(3)	124(3)	-14(3)
O(1)	288(3)	278(4)	396(4)	-32(3)	193(3)	33(3)
O(2)	311(4)	232(3)	365(4)	-32(3)	173(3)	3(3)
O(3)	358(4)	360(4)	202(3)	-87(3)	120(3)	-27(3)

Table 3. Interatomic distances [pm] and angles [°] of **12c**. Standard deviations are given in units of the last significant digit. Since the molecule contains a non-crystallographic mirror plane all 'symmetry-related' figures have been arranged pairwise in neighbouring columns.

C(1)-C(2)	153.1(1)	C(5)-C(4)	153.0(1)
C(1)-C(6)	151.1(1)	C(5)-C(7)	151.2(1)
C(1)-N(1)	146.5(1)	C(5)-N(1)	146.7(1)
C(1)-O(1)	146.1(1)	C(5)-O(2)	145.8(1)
C(2)-C(3)	152.3(2)	C(4)-C(3)	152.1(1)
N(1)-O(3)	145.1(1)		
O(1)-O(2)	148.2(1)		
O(3)-C(8)	142.4(1)		

N(1)-C(1)-C(2)	108.13(8)	N(1)-C(5)-C(4)	108.15(8)
N(1)-C(1)-C(6)	114.67(8)	N(1)-C(5)-C(7)	114.63(8)
N(1)-C(1)-O(1)	104.34(7)	N(1)-C(5)-O(2)	104.47(7)
C(2)-C(1)-C(6)	112.49(9)	C(4)-C(5)-C(7)	112.31(8)
C(2)-C(1)-O(1)	109.81(8)	C(4)-C(5)-O(2)	109.94(7)
C(6)-C(1)-O(1)	107.04(8)	C(7)-C(5)-O(2)	107.01(8)
C(1)-C(2)-C(3)	111.30(8)	C(5)-C(4)-C(3)	111.10(8)
C(2)-C(3)-C(4)	110.05(8)		
C(1)-N(1)-O(3)	107.46(7)	C(5)-N(1)-O(3)	106.97(7)
C(1)-N(1)-C(5)	100.62(7)		
C(1)-O(1)-O(2)	105.33(6)	C(5)-O(2)-O(1)	105.43(7)
N(1)-O(3)-C(8)	107.79(8)		

C(1)-O(1)-O(2)-C(5)	0.27(9)

C(2)-H(2a)	98(1)	C(4)-H(4a)	99(1)
C(2)-H(2b)	98(1)	C(4)-H(4b)	98(1)
C(3)-H(3a)	98(1)		
C(3)-H(3b)	101(1)		
C(6)-H(6a)	97(2)	C(7)-H(7a)	99(1)
C(6)-H(6b)	97(2)	C(7)-H(7b)	98(2)
C(6)-H(6c)	97(2)	C(7)-H(7c)	97(2)
C(8)-H(8a)	99(1)	C(8)-H(8b)	97(2)
C(8)-H(8c)	98(2)		

cont'nd

Table 3. Interatomic distances [pm] and angles [°] of **12c**.

continued

H(2a)-C(2)-C(1)	107(1)	H(4a)-C(4)-C(5)	108(1)
H(2a)-C(2)-C(3)	112(1)	H(4a)-C(4)-C(3)	111(1)
H(2a)-C(2)-H(2b)	109(1)	H(4a)-C(4)-H(4b)	107(1)
H(2b)-C(2)-C(1)	107(1)	H(4b)-C(4)-C(5)	107(1)
H(2b)-C(2)-C(3)	111(1)	H(4b)-C(4)-C(3)	112(1)
H(3a)-C(3)-C(2)	110(1)	H(3a)-C(3)-C(4)	111(1)
H(3b)-C(3)-C(2)	110(1)	H(3b)-C(3)-C(4)	108(1)
H(3a)-C(3)-H(3b)	107(1)		
H(6a)-C(6)-C(1)	109(1)	H(7a)-C(7)-C(5)	109(1)
H(6a)-C(6)-H(6b)	107(1)	H(7a)-C(7)-H(7b)	109(1)
H(6a)-C(6)-H(6c)	110(1)	H(7a)-C(7)-H(7c)	109(1)
H(6b)-C(6)-C(1)	112(1)	H(7b)-C(7)-C(5)	112(1)
H(6b)-C(6)-H(6c)	111(1)	H(7b)-C(7)-H(7c)	108(1)
H(6c)-C(6)-C(1)	109(1)	H(7c)-C(7)-C(5)	110(1)
H(8a)-C(8)-O(3)	111(1)	H(8b)-C(8)-O(3)	111(1)
H(8a)-C(8)-H(8c)	111(1)	H(8b)-C(8)-H(8c)	110(1)
H(8a)-C(8)-H(8b)	110(1)		
H(8c)-C(8)-O(3)	104(1)		