6	H31B	0.34214						0.34214				
7	H31C	0.34214						0.34214				
U(i,j)-Average		0.3293	0.0906	0.2335	-0.0770	0.0665	-0.0078	0.2311	0.0566	0.2568	0.3800	6.72

==========

The Displacement Factor has the Form of Exp(-T)

where

T = 8*(pi**2)*Uiso*sin(theta/lambda)**2, for Isotropic Atoms,

T = 2*(pi**2)*(U11*(h*as)**2+U22*(k*bs)**2+U33*(l*cs)**2+2*U23*k*l*bs*cs+2*U13*h*l*as*cs+2*U12*h*k*as*bs),for Anisotr. Atoms

Ueq = 1/3 Sum(i,j) (Uij*as(i)*as(j)*a(i).a(j))

U1, U2, U3 are the three Main Axes Components of Uij

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	Cl	Co	N	O
Average	0.1364	0.1454	0.2295	0.0000	0.0659	0.1007	0.1579
Minimum	0.0659	0.0771	0.0944	0.0000	0.0659	0.0671	0.0728
Maximum	0.3731	0.2994	0.4492	0.0000	0.0659	0.1504	0.3731
Ratio	5.6589	3.8845	4.7586	0.0000	1.0000	2.2402	5.1221
Number	50	33	69	0	1	10	6

:: Reflection Data are READ from File : robs003bs.hkl - (OBS-Data)

:: TRMX = 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00

:: Nr. of Eliminated Reflections (Theta Limit = 25.0 Deg) =13331