

a (Å) 9.558
 c (Å) 8.981
 tetragonal I4 structure

Angstroms	x	y	z
Ni	0.000	0.000	0.108
Cl (1)	0.000	0.000	2.507
Cl (2)	0.000	0.000	-2.408
S	0.272	2.430	-0.179
C	1.477	3.126	0.851
N (1)	1.881	4.368	0.557
N (2)	1.979	2.478	1.890
H (1)	1.548	4.714	0.003
H (2)	2.527	4.504	-0.009
H (3)	2.565	2.832	-0.028
H (4)	1.707	1.696	-0.025

unitless	x/a	y/b	z/c
Ni	0.0000	0.0000	0.0120
Cl (1)	0.0000	0.0000	0.2791
Cl (2)	0.0000	0.0000	-0.2681
S	0.0285	0.2542	-0.0199
C	0.1545	0.3271	0.0948
N (1)	0.1968	0.4570	0.0620
N (2)	0.2071	0.2593	0.2104
H (1)	0.1620	0.4932	0.0258
H (2)	0.2644	0.4712	-0.0777
H (3)	0.2684	0.2963	-0.2512
H (4)	0.1786	0.1774	-0.2250

A. Lopez-Castro and M. Truter, J. Chem. Soc. (London) pg 1309 yr 1963.
 Hydrogen positions from S. C. Abrahamas, Acta Cryst. B55, 494 (1999) Table 4