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Short Note

3-Methyl-1-phenyl-4-thioacetylpyrazol-5-one

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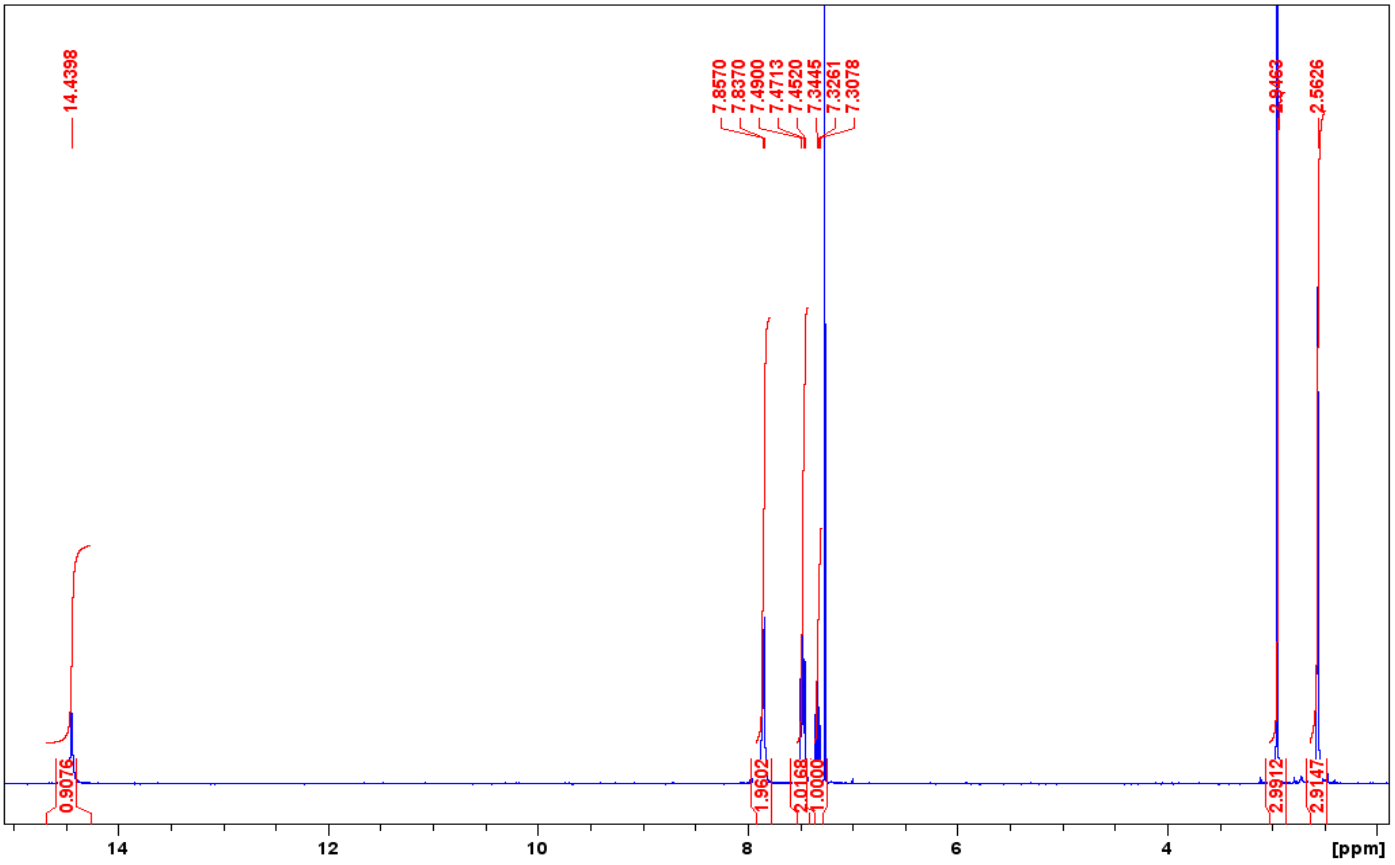
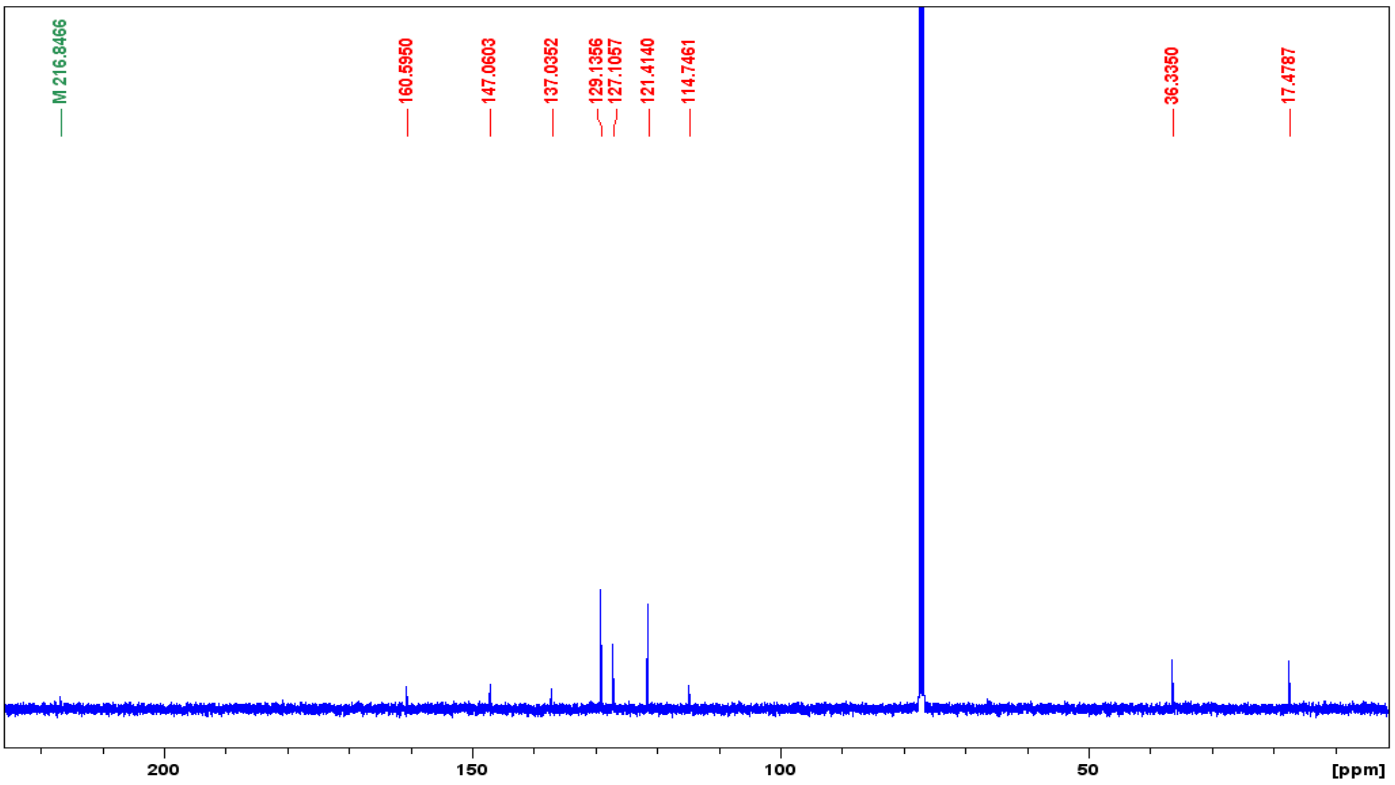
Supporting Information

Table of contents

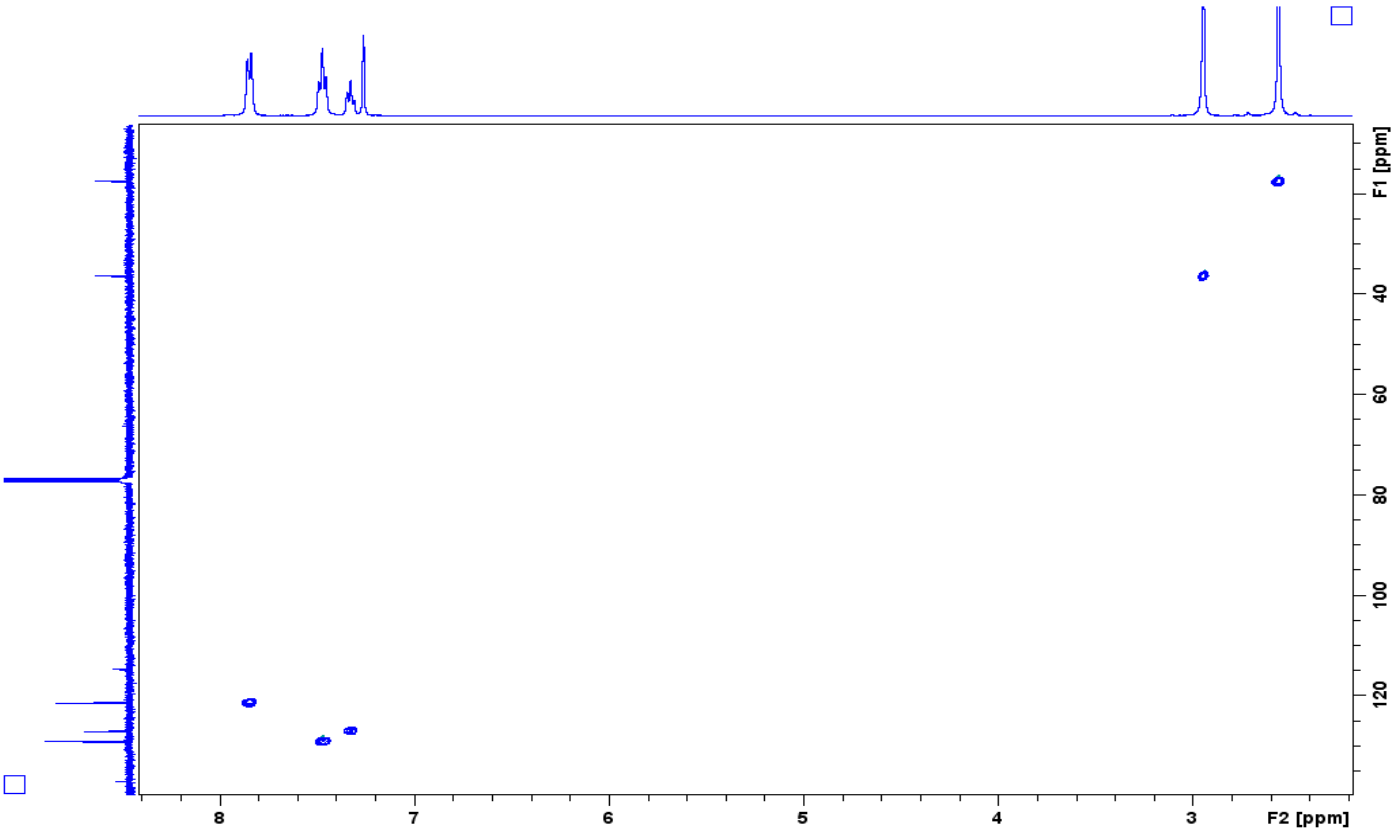
1. NMR spectra of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one



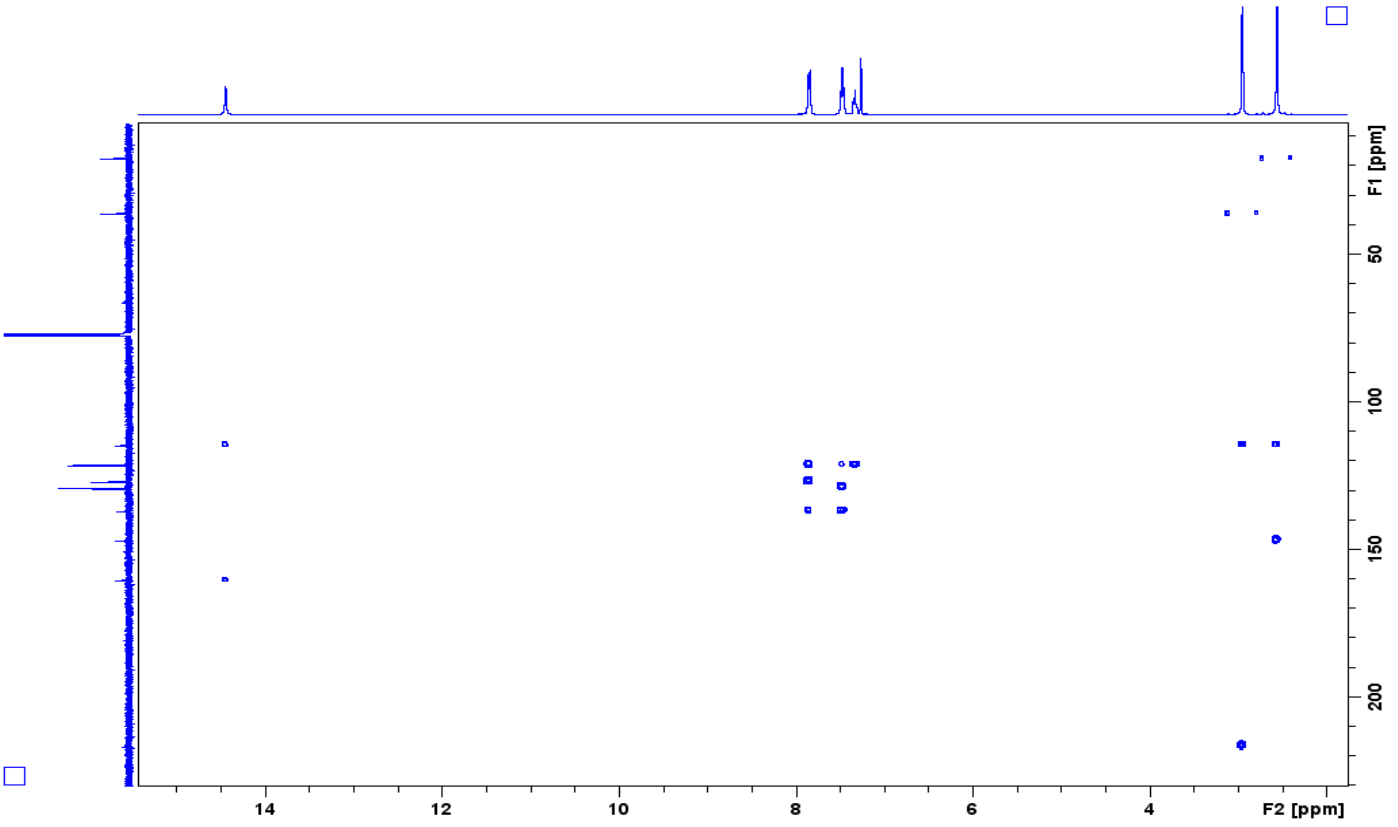
^{1}H NMR spectrum of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one in $CDCl_3$.



^{13}C NMR spectrum of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one in $CDCl_3$.

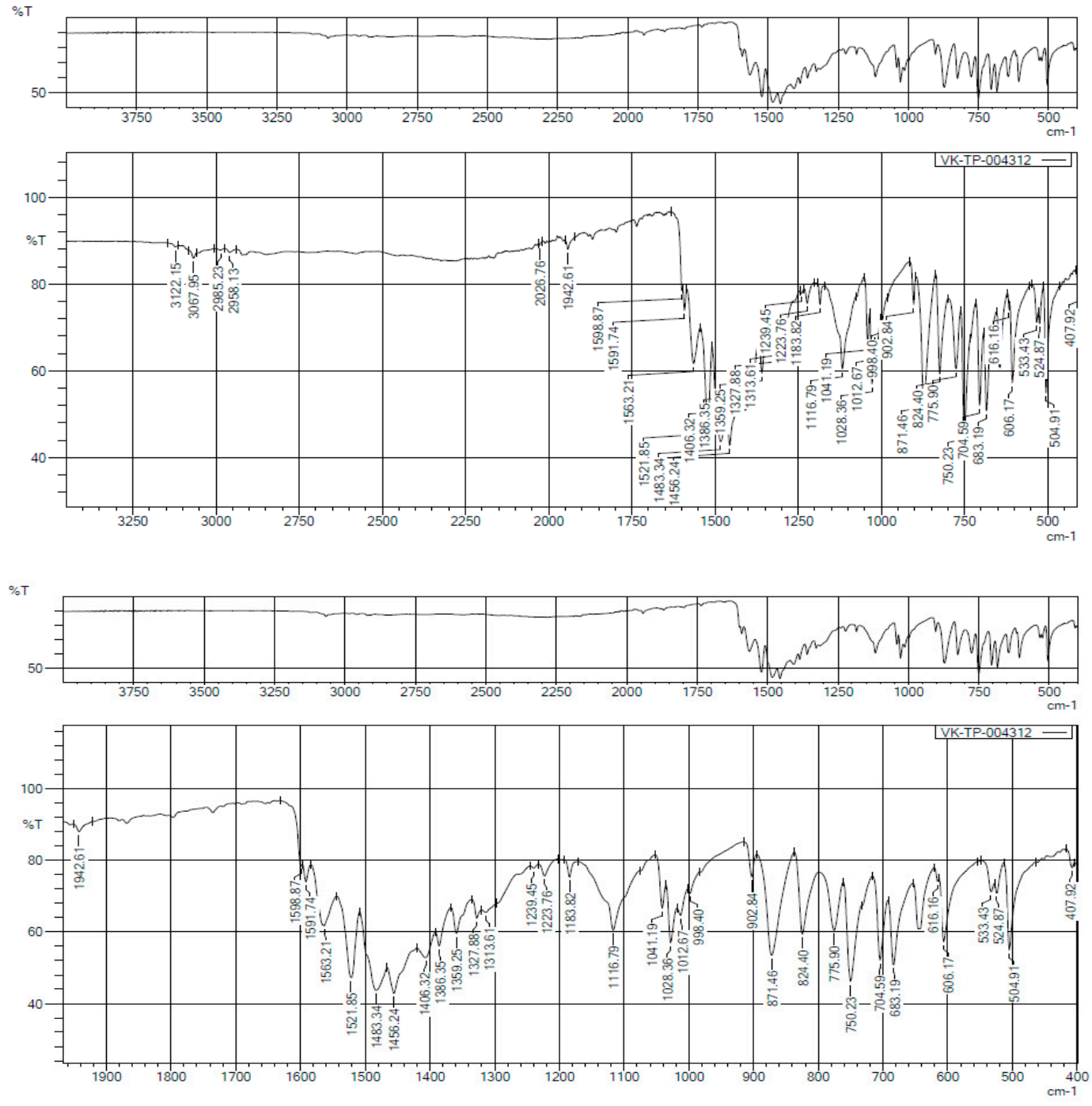


HSQC spectrum of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one in $CDCl_3$.

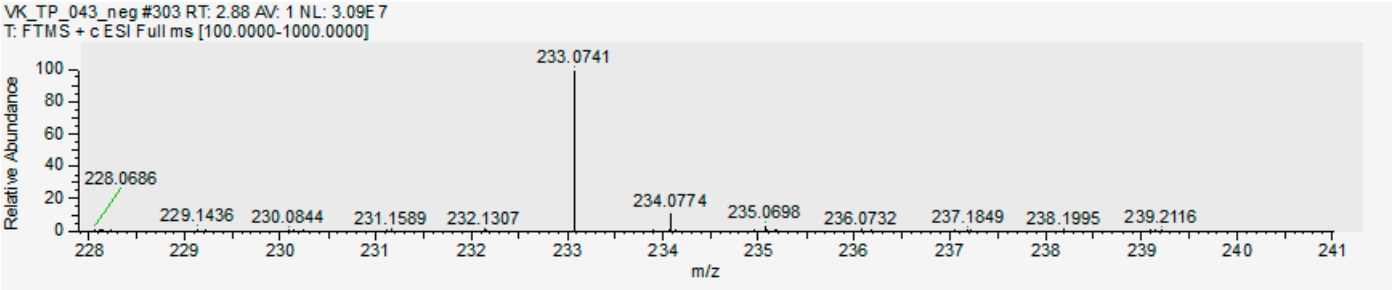


HMBC spectrum of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one in $CDCl_3$.

2. IR spectrum of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one



3. HRMS spectra of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one



4. Table S1. The most important data collection and crystallographic refinement parameters

Compound	3-methyl-1-phenyl-4-thioacetylpyrazol-5-one
Empirical formula	$C_{12}H_{12}N_2OS$
Formula weight	232.30
Temperature/K	290
Crystal system	monoclinic
Space group	C2/c
a/Å	17.9610(6)
b/Å	4.9709(2)
c/Å	26.2901(8)
α/°	90
β/°	102.3570(10)
γ/°	90
Volume/Å3	2292.86(14)
Z	8
ϱcalcg/cm3	1.346
μ/mm-1	0.261
F(000)	976.0
Crystal size/mm3	0.32 × 0.24 × 0.21
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.644 to 54.186
Index ranges	-22 ≤ h ≤ 22, -6 ≤ k ≤ 6, -32 ≤ l ≤ 33
Reflections collected	28537
Independent reflections	2518 [R_{int} = 0.0702, R*sigma* = 0.0314]
Data/restraints/parameters	2518/0/151
Goodness-of-fit on F^2	1.103
Final R indexes [I>=2σ (I)]	R1 = 0.0574, wR2 = 0.1419
Final R indexes [all data]	R1 = 0.0712, wR2 = 0.1511
Largest diff. peak/hole / e Å-3	0.21/-0.22
CCDC	2239465

5. Table S2. Observed weak interactions in the crystal structure of 3-methyl-1-phenyl-4-thioacetylpyrazol-5-one

D H A	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
C10 H10 S1[1]	0.93	2.96	3.618(3)	129.1
C10 H10 O1	0.93	2.23	2.869(3)	125.0
O1 H1 S1	0.96(4)	2.02(4)	2.914(2)	154(3)

[1]*1/2-x,3/2-y,1-z*