Supporting Information

Di(1H-tetrazol-5-yl)methanone oxime and 5,5'-(hydrazonomethylene)bis(1H-tetrazole) and their salts: a family of highly useful new tetrazoles and energetic materials

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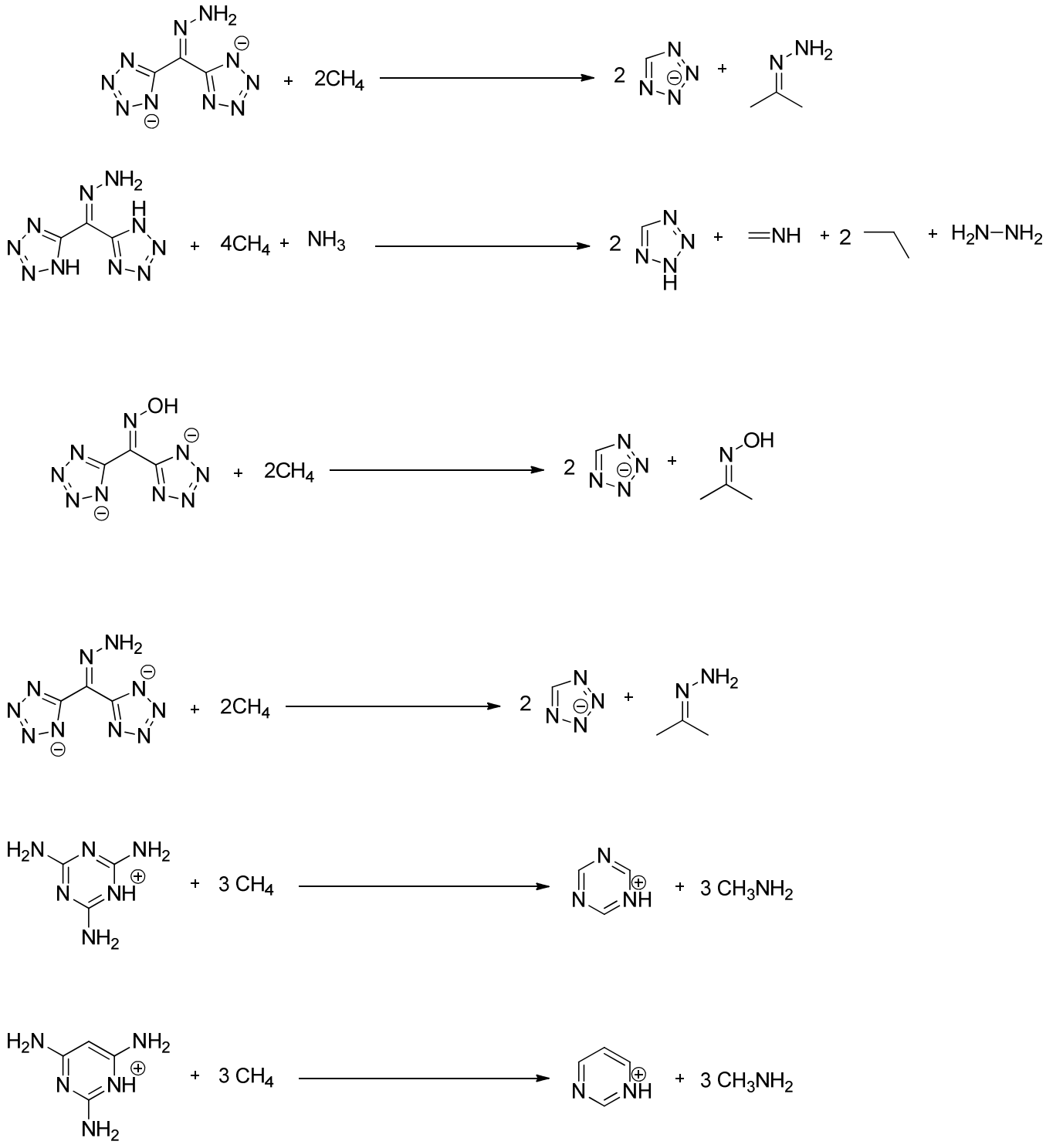
Computational data

All *ab* initio calculations were carried out by using the Gaussian 03 (Revision D.01) suite of programs. The geometric optimization of the structures and frequency analyses were accomplished by using the B3LYP with the 6-31+G** basis set, and single-point energies were calculated at the MP2/6-311++G** level. Atomization energies were calculated by the G2 method. All of the optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies. The remaining task is to determine the heats of formation of these new energetic compounds, which are computed by using the method of isodesmic reactions (Scheme S1).



Scheme S1. Isodesmic reactions

Table 1 *Ab initio* computational values

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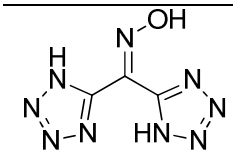
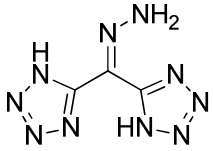
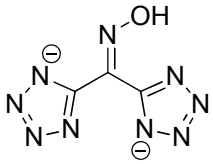
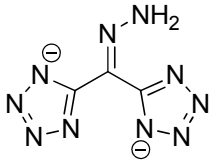
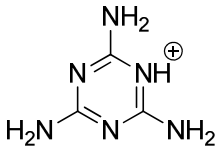
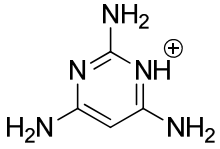
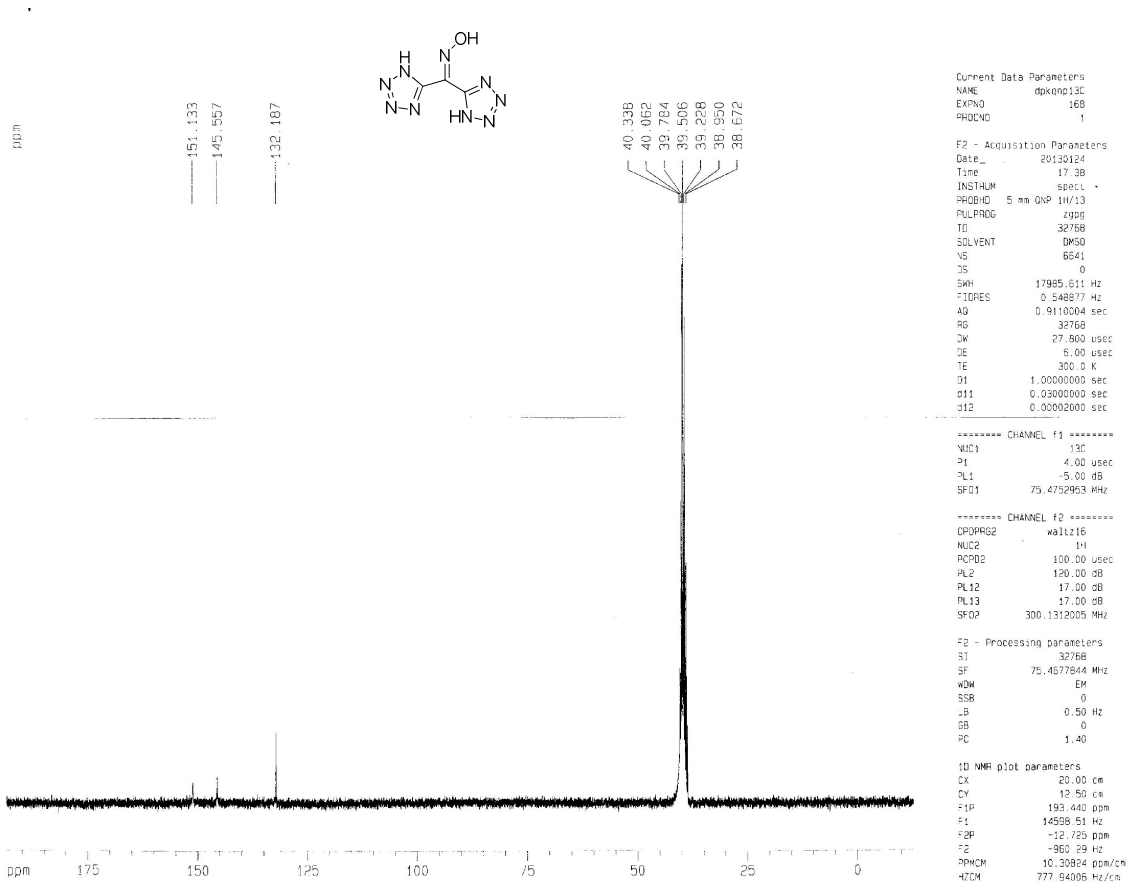
	-682.28432	0.0965424	0.010916	674.5243486
	-662.45924	0.10931232	0.010815	730.5033453
	-681.18548	0.07139328	0.010259	545.2200254
	-661.32701	0.08389344	0.01054	720.4415699
	-445.65669	0.123912	0.009482	650.9953919
	-429.60242	0.13405	0.010309	654.2531447

[a] Total energy calculated by B3LYP/6-31+G**//MP2/6-311++G** method (Hartree/Particle); [b] zero-point correction (Hartree/Particle); [c] thermal correction to enthalpy (Hartree/Particle); [d] heat of formation (kJ/mol).

NMR Spectra



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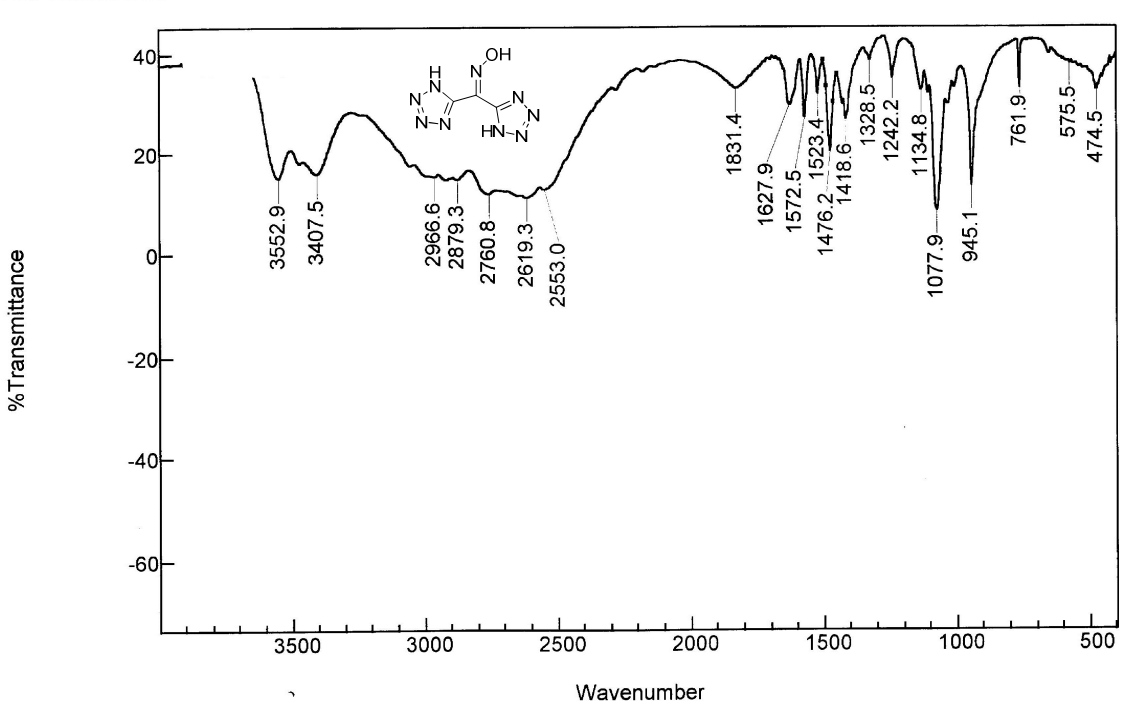

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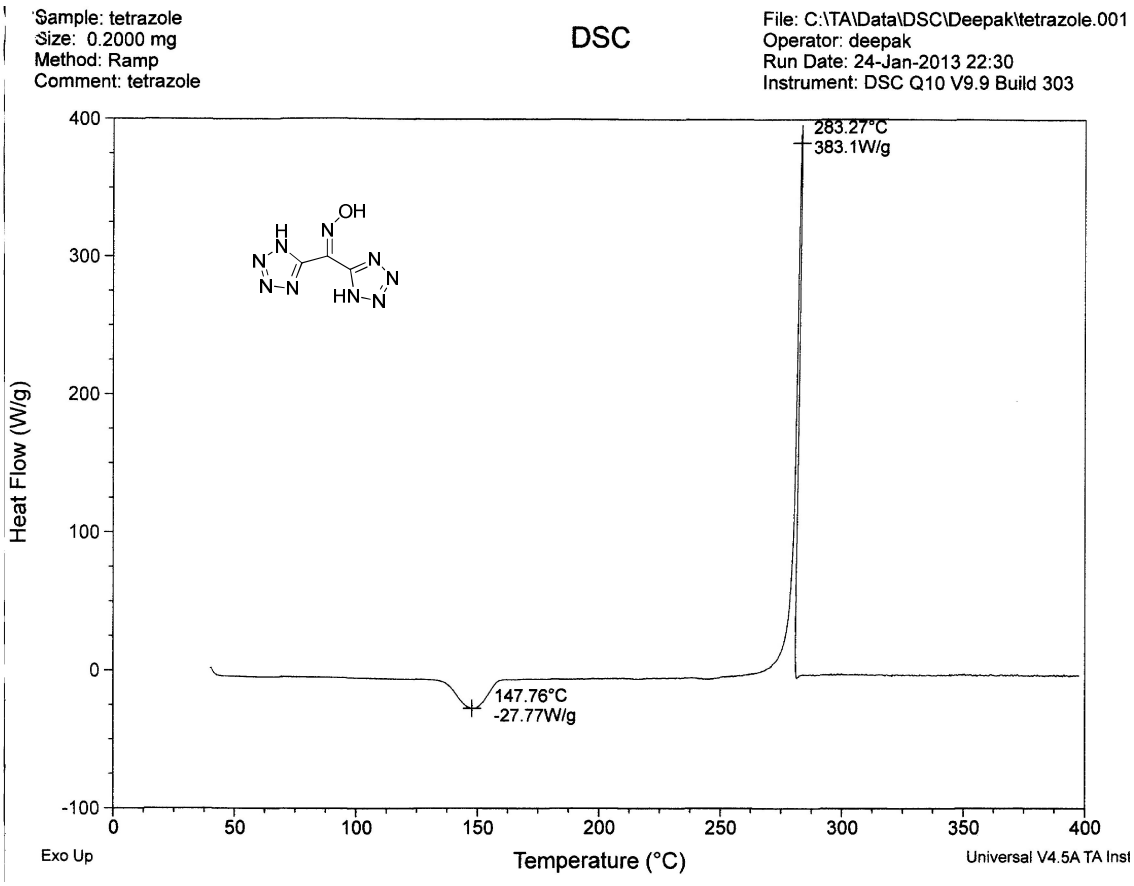

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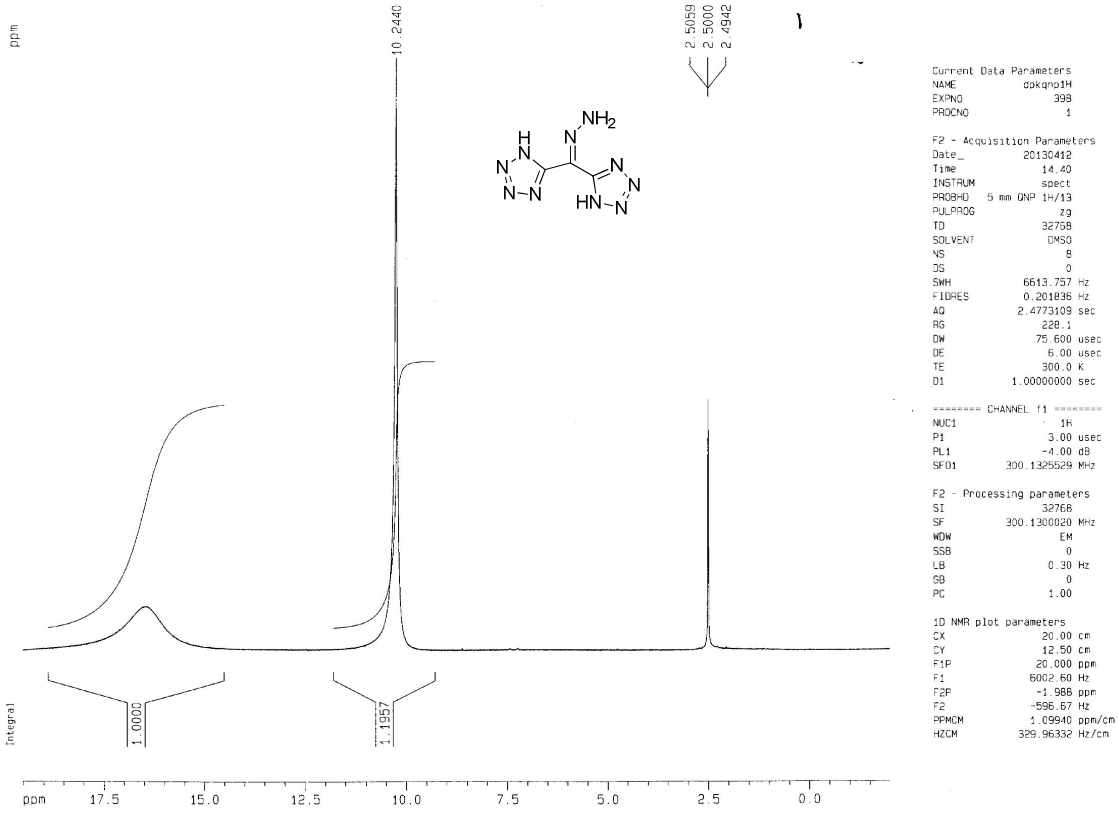

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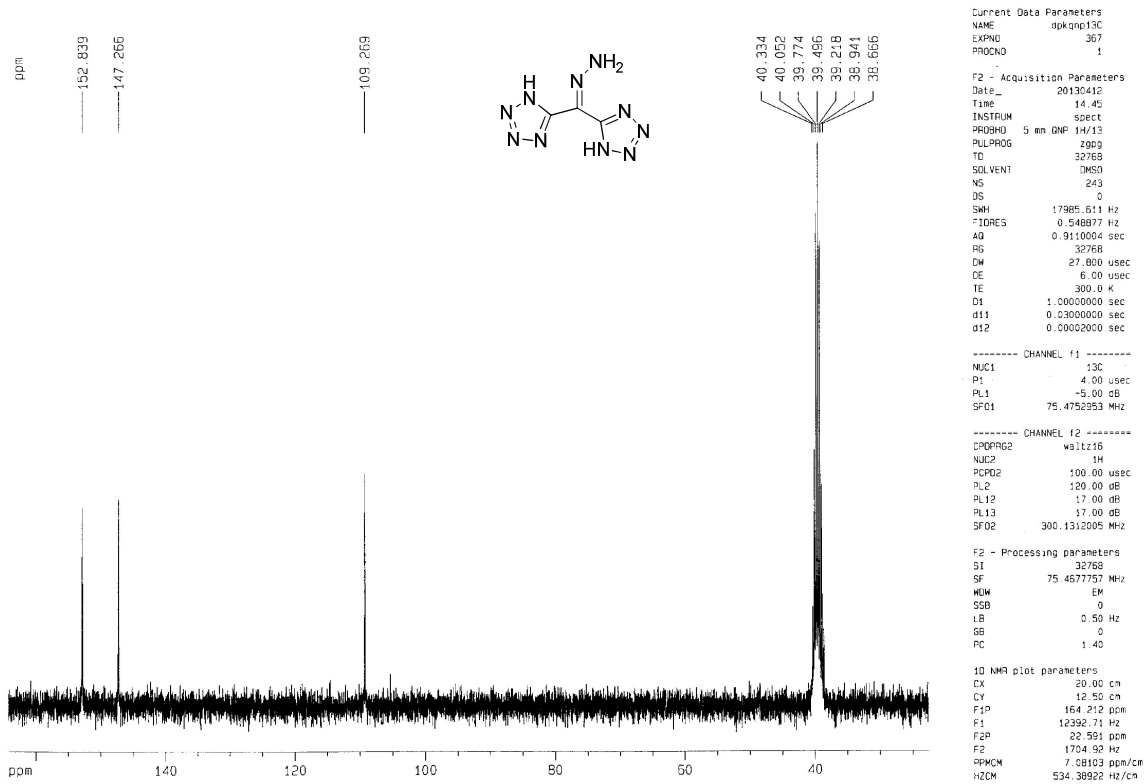

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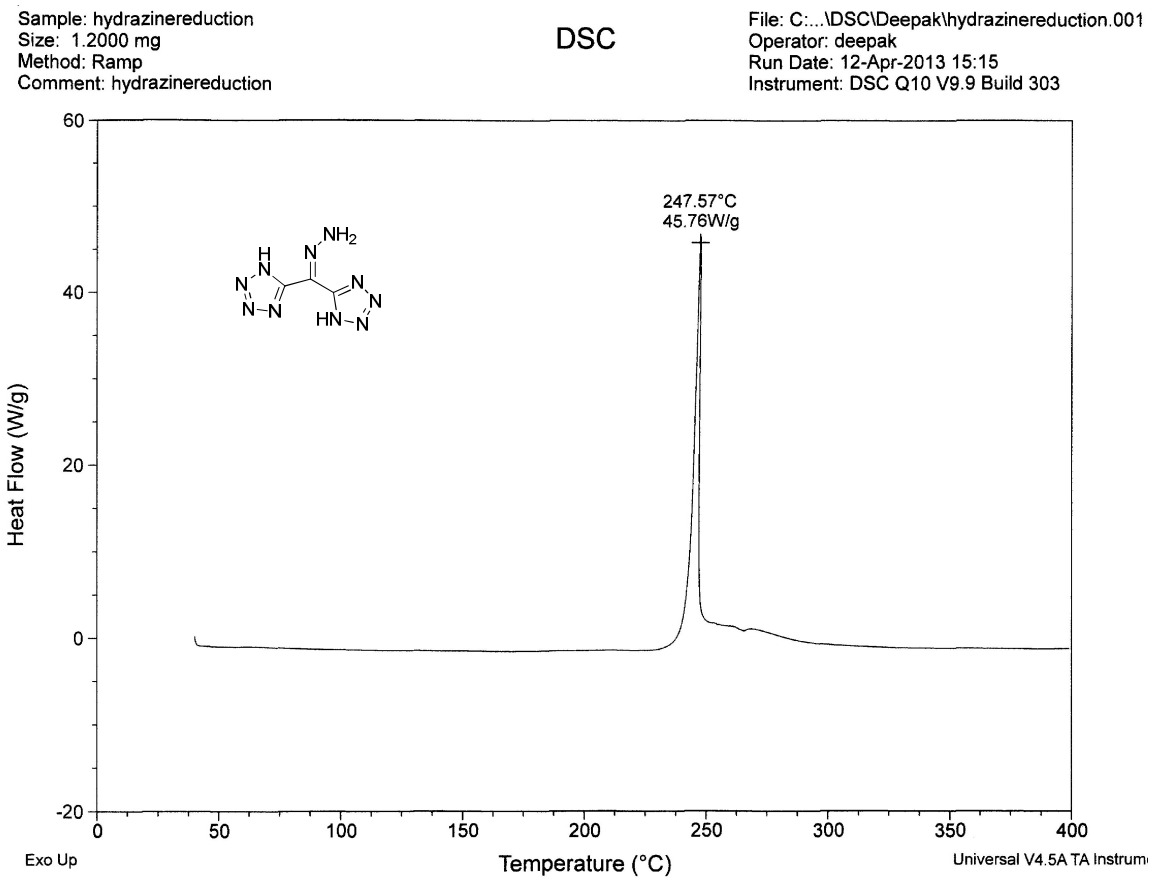

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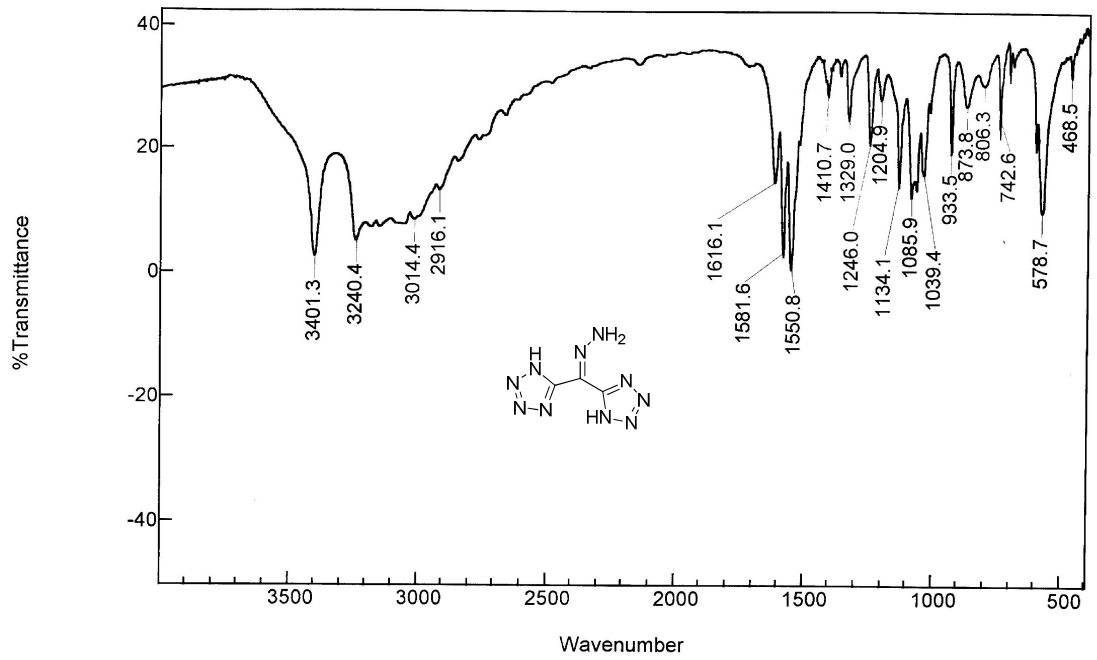

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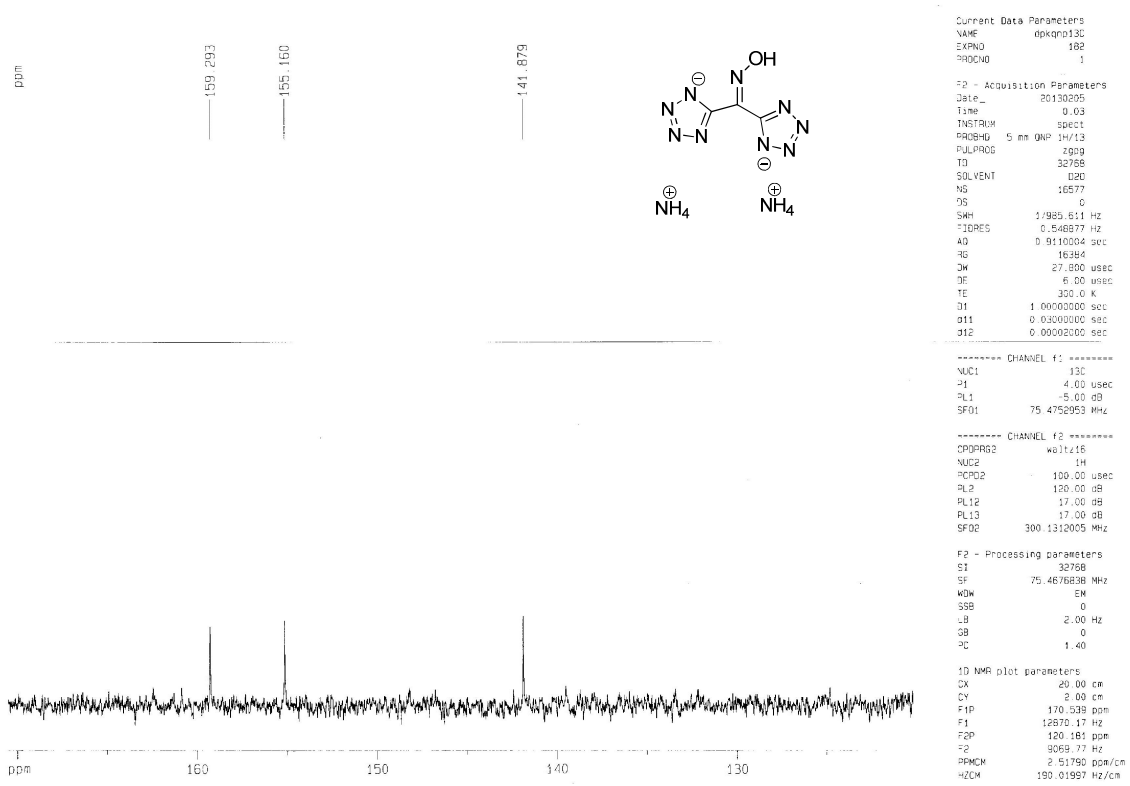

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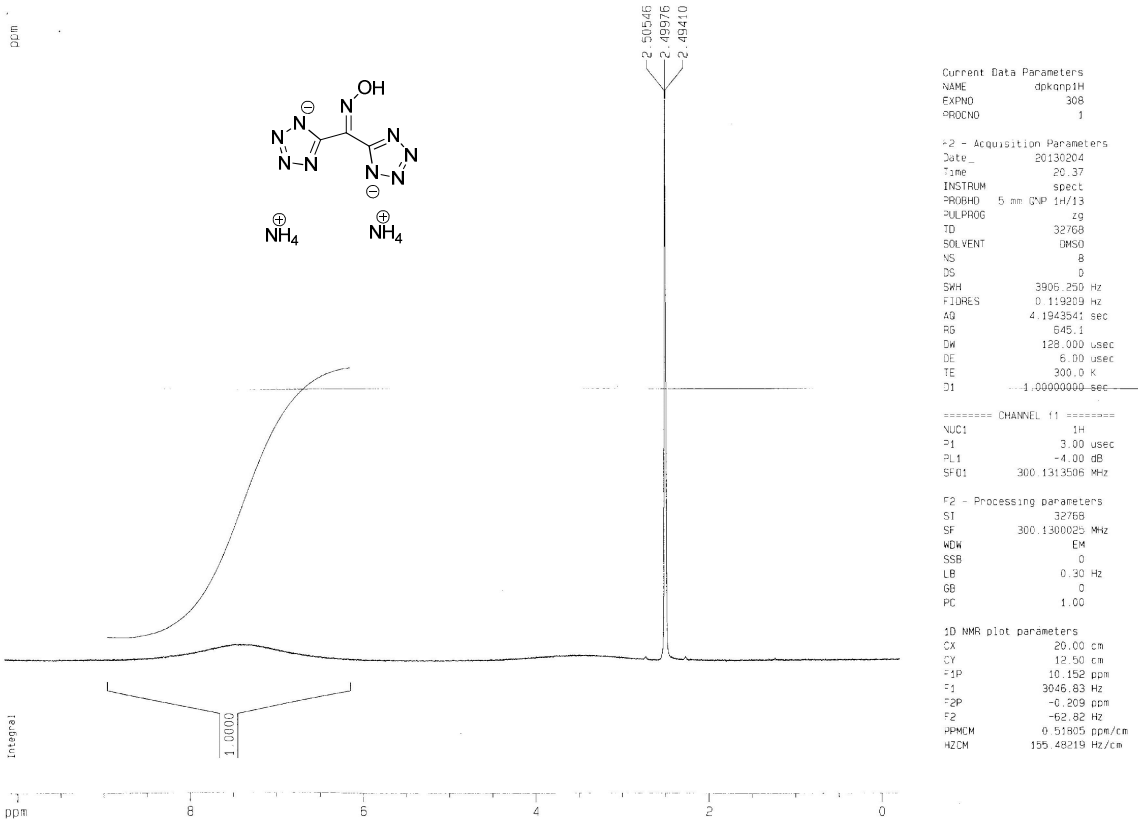

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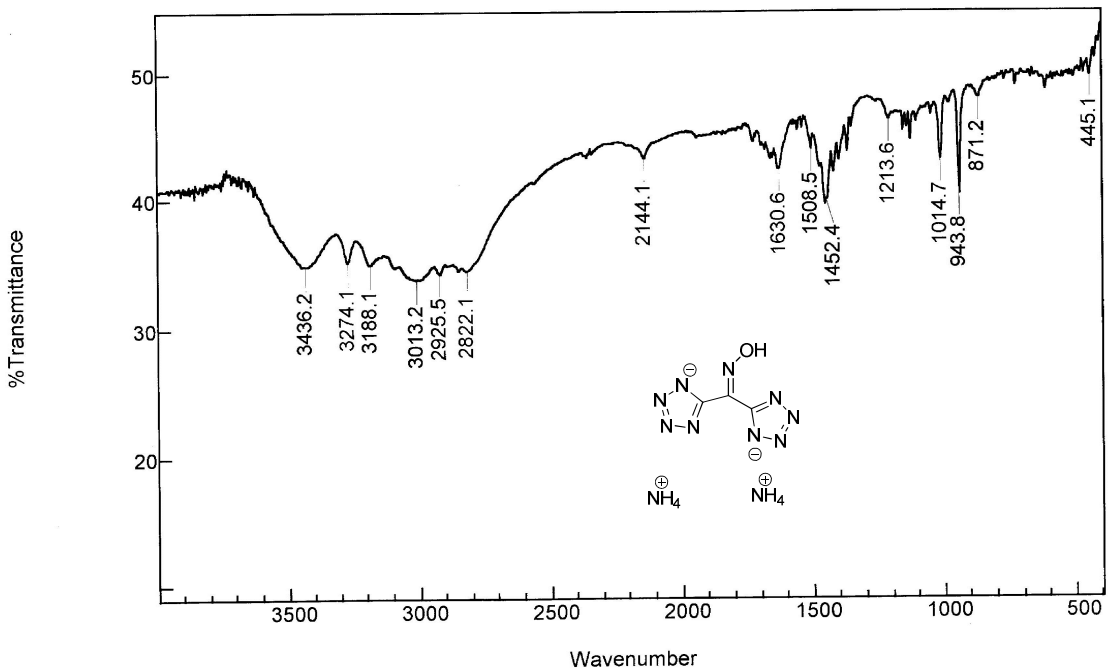

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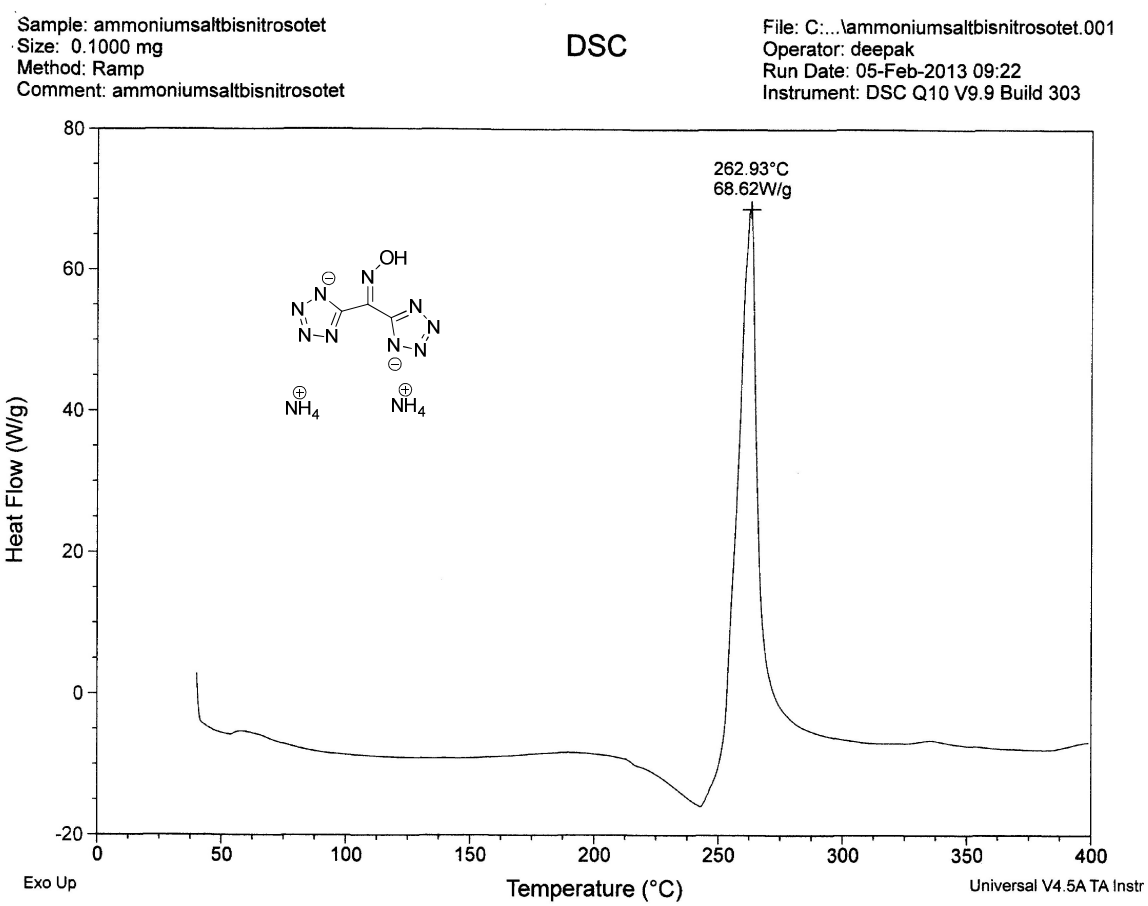
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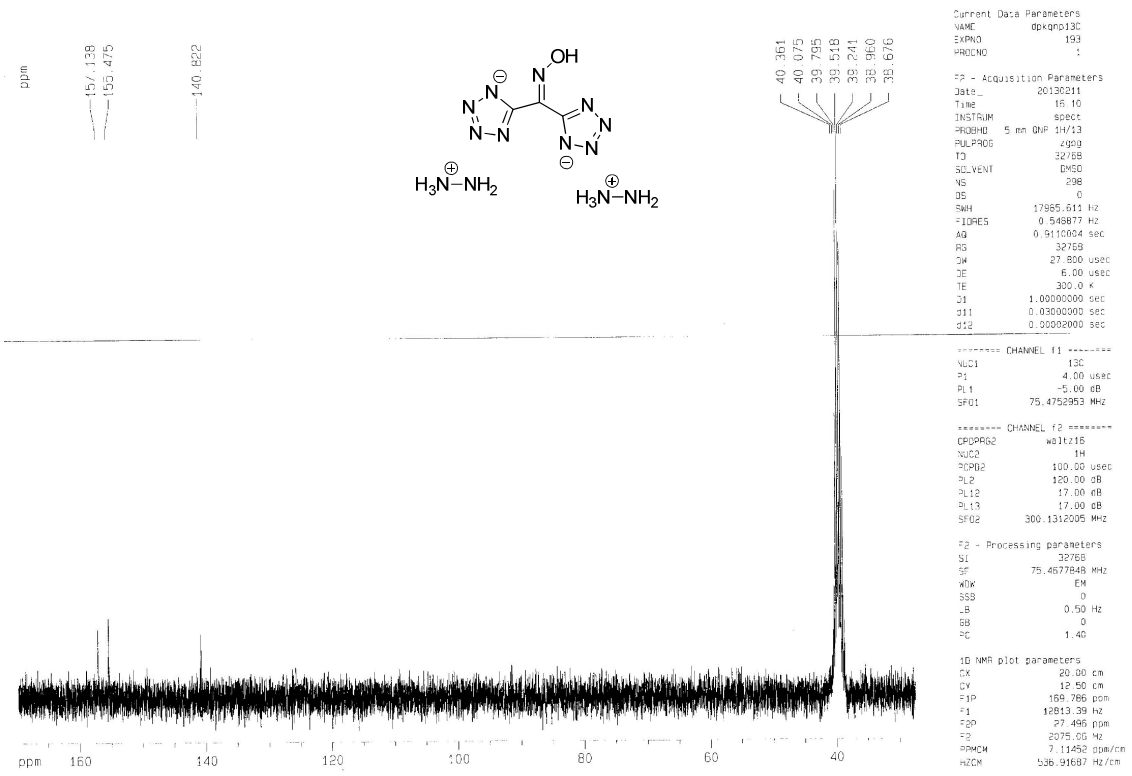

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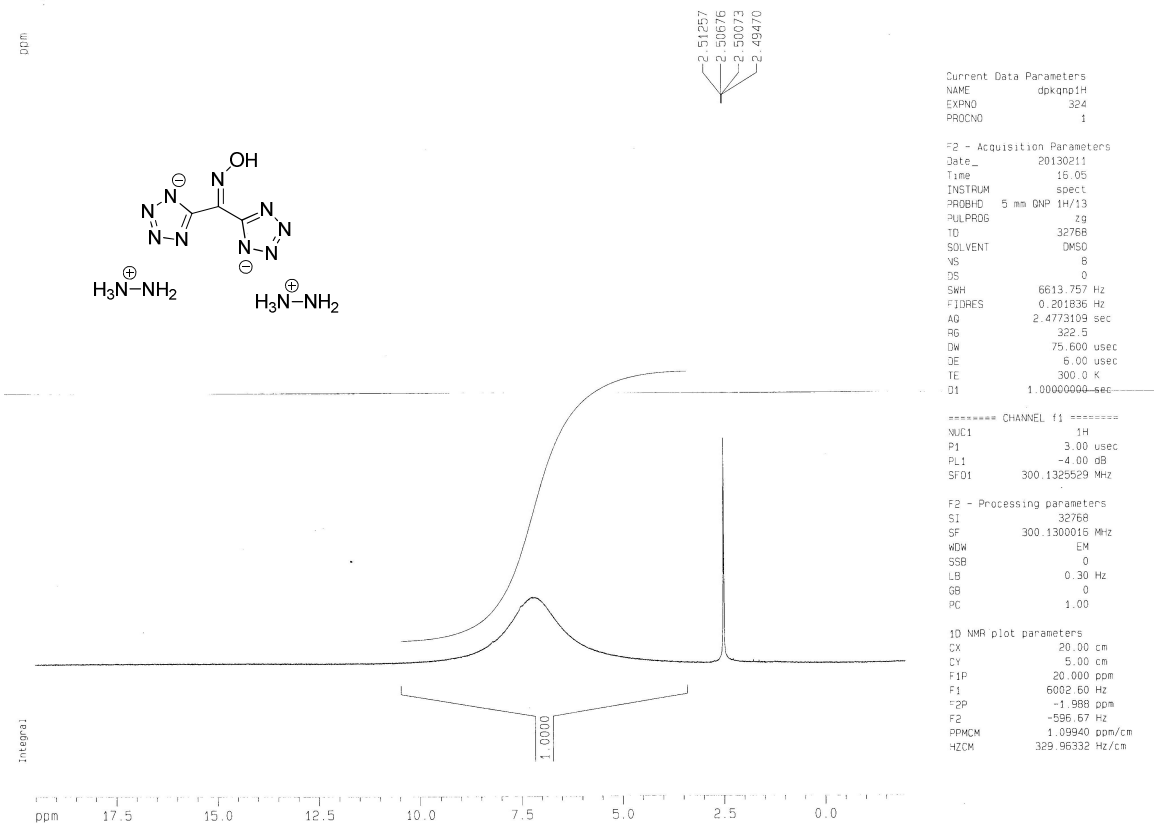

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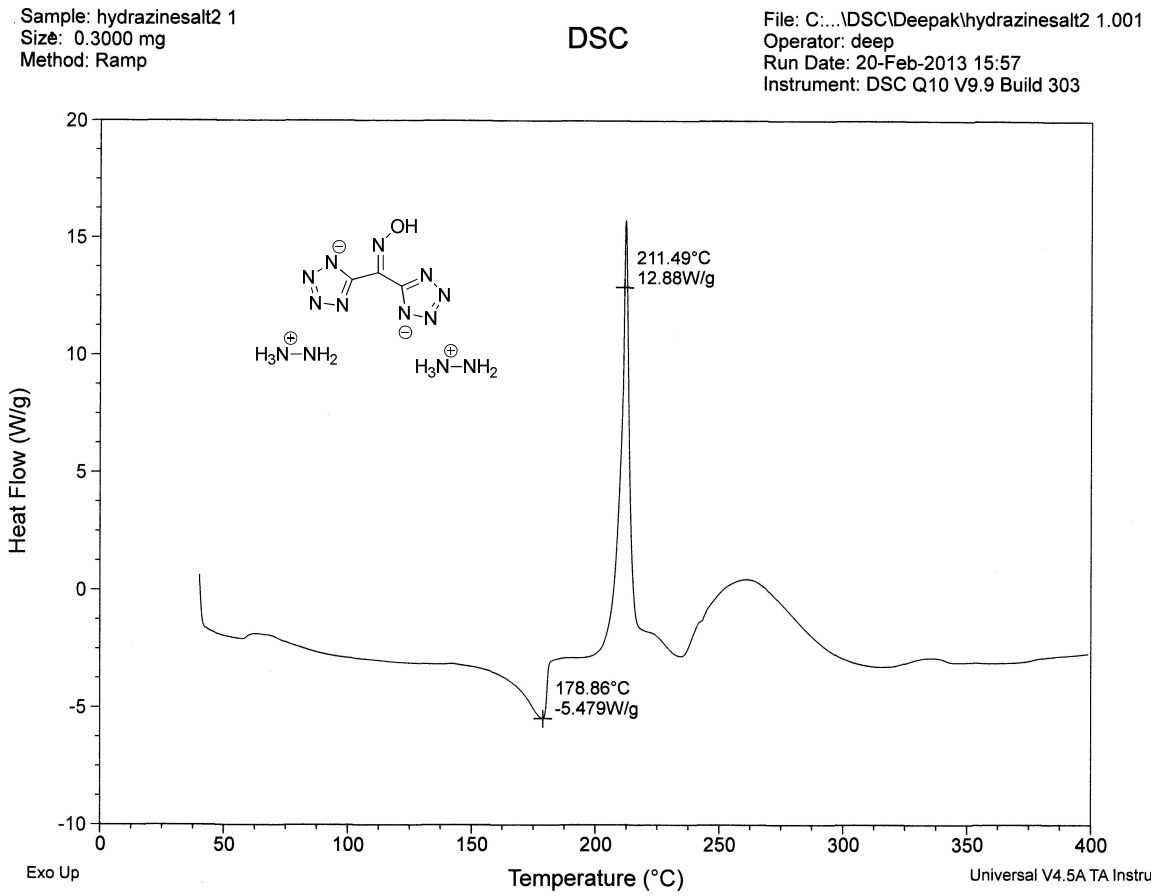

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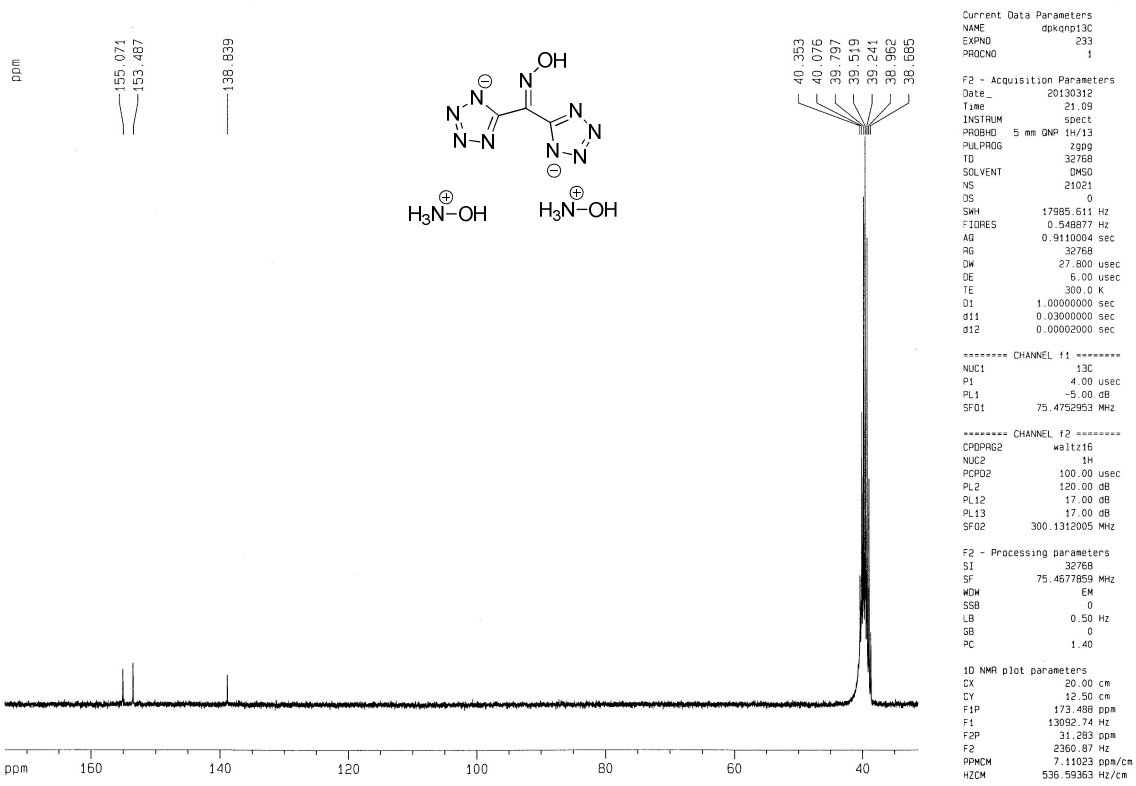

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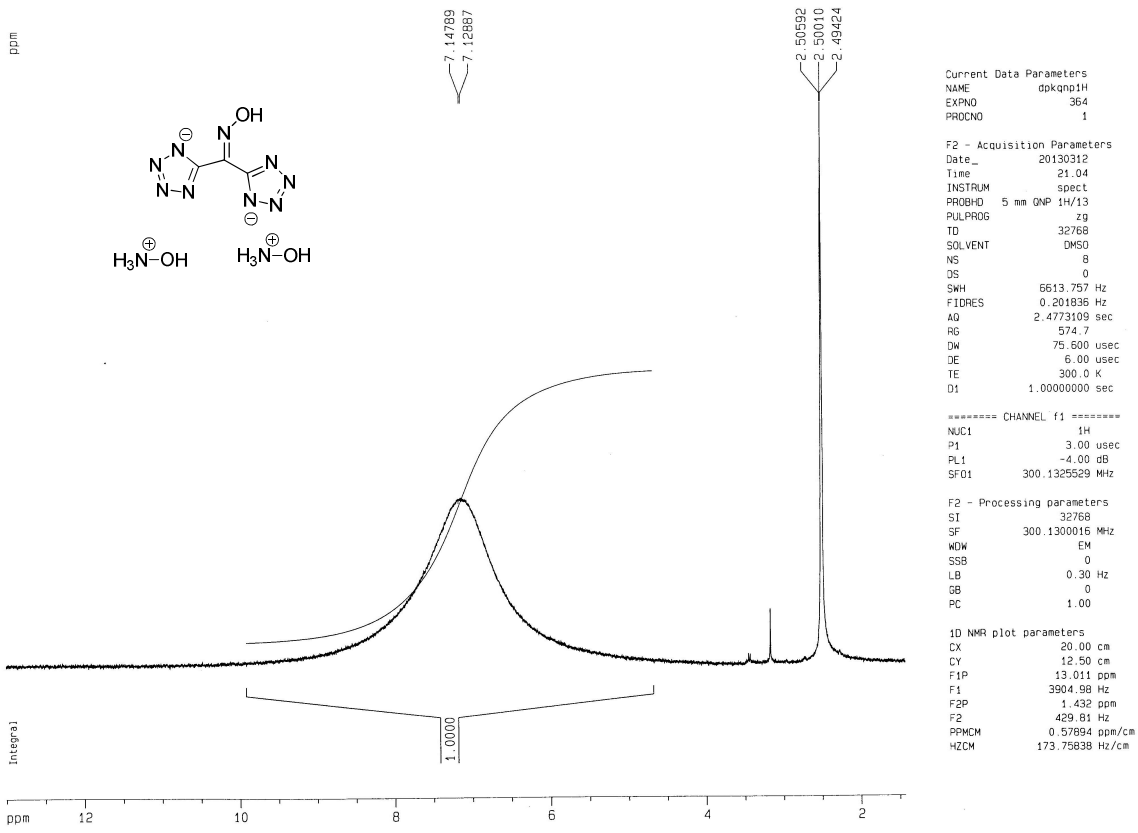

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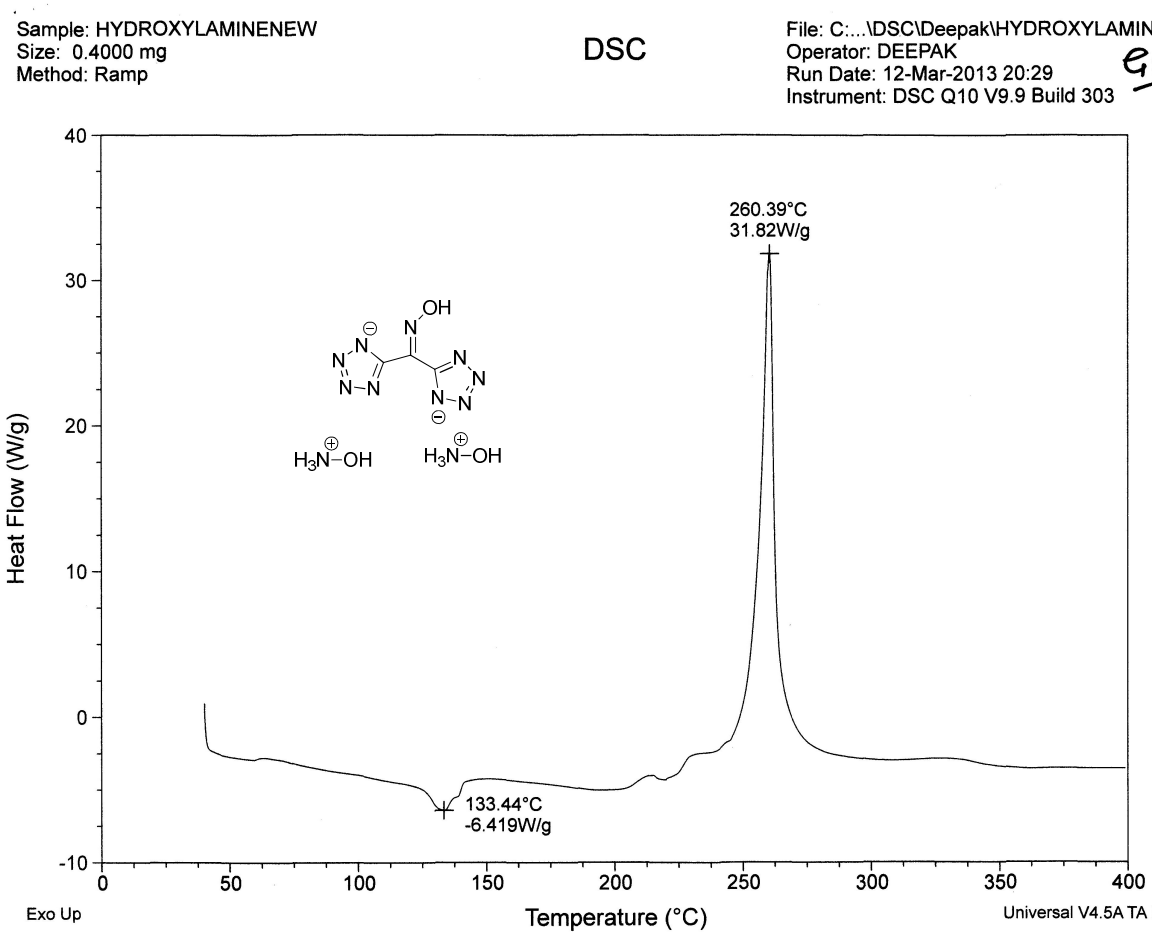

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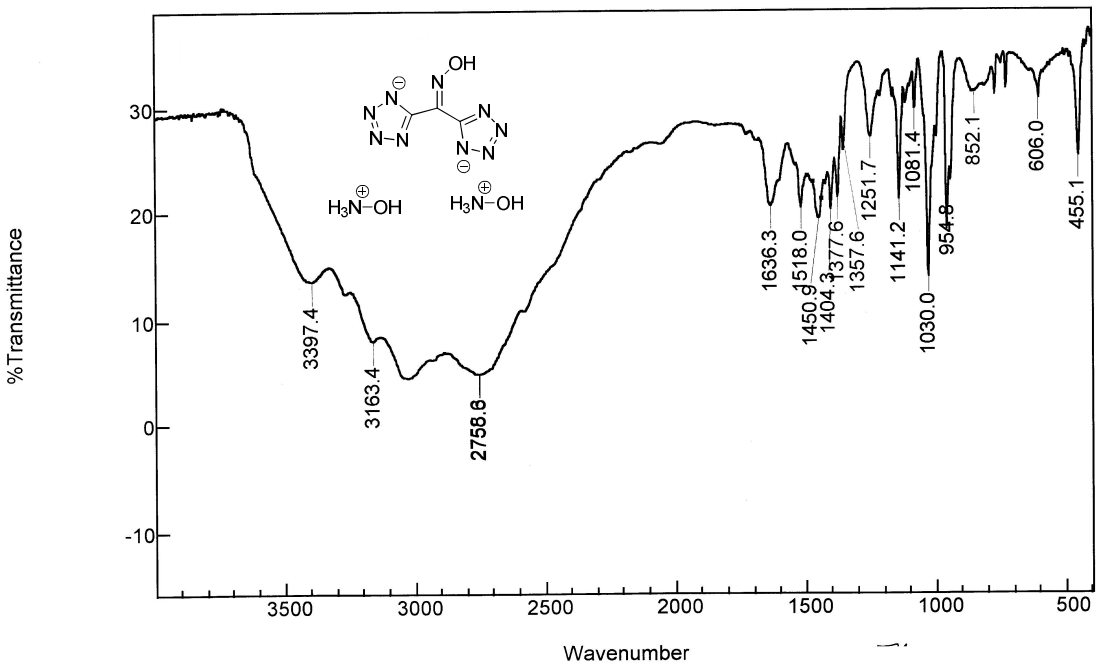

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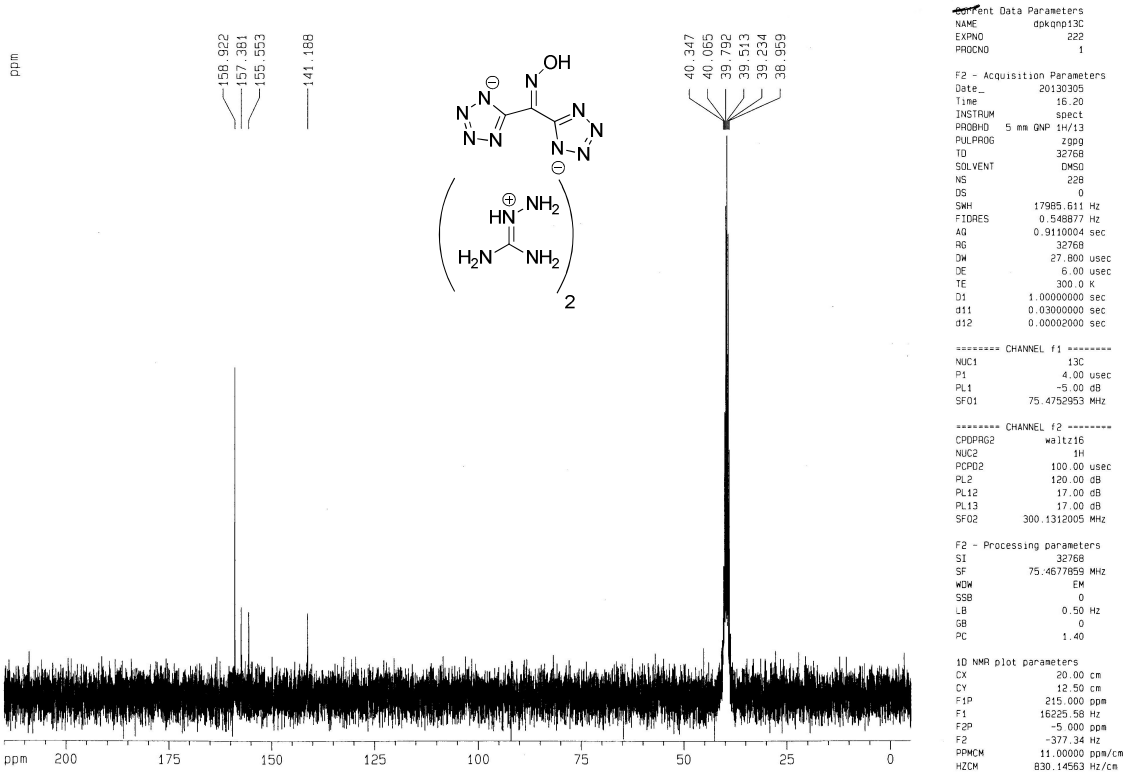

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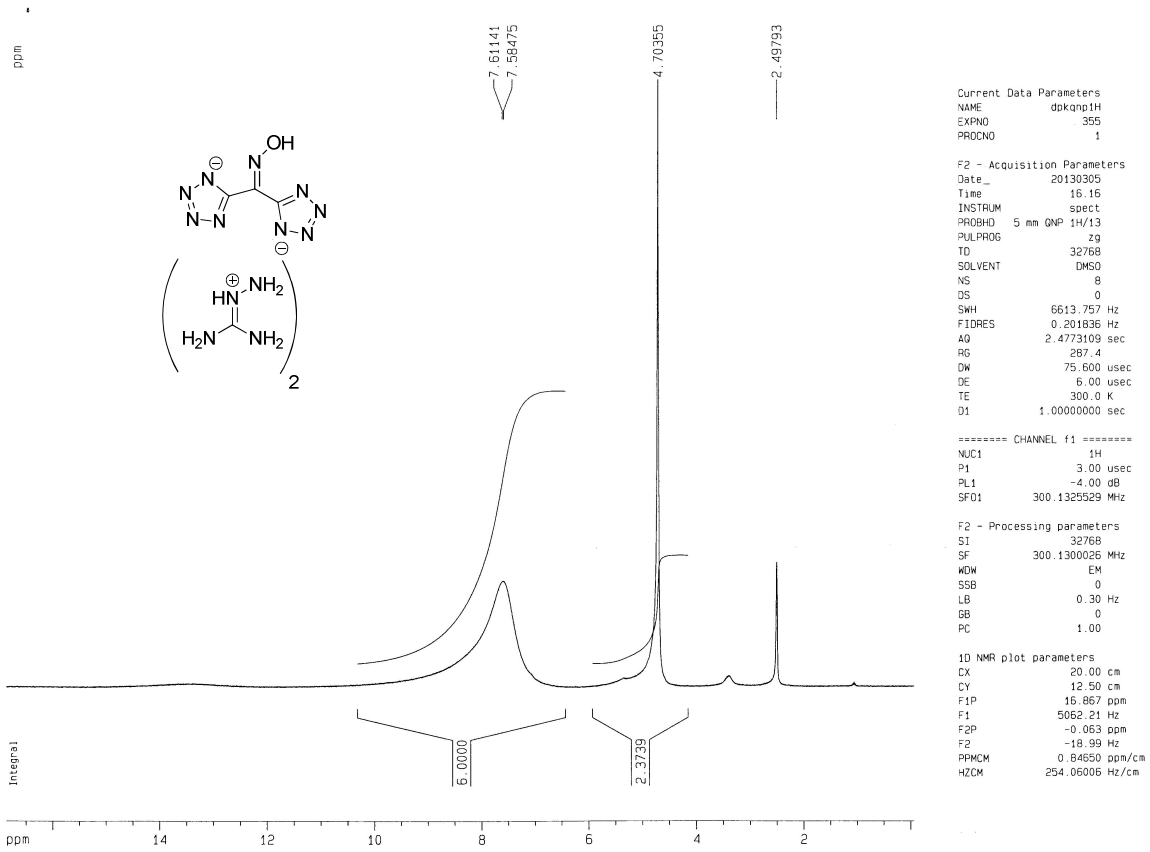

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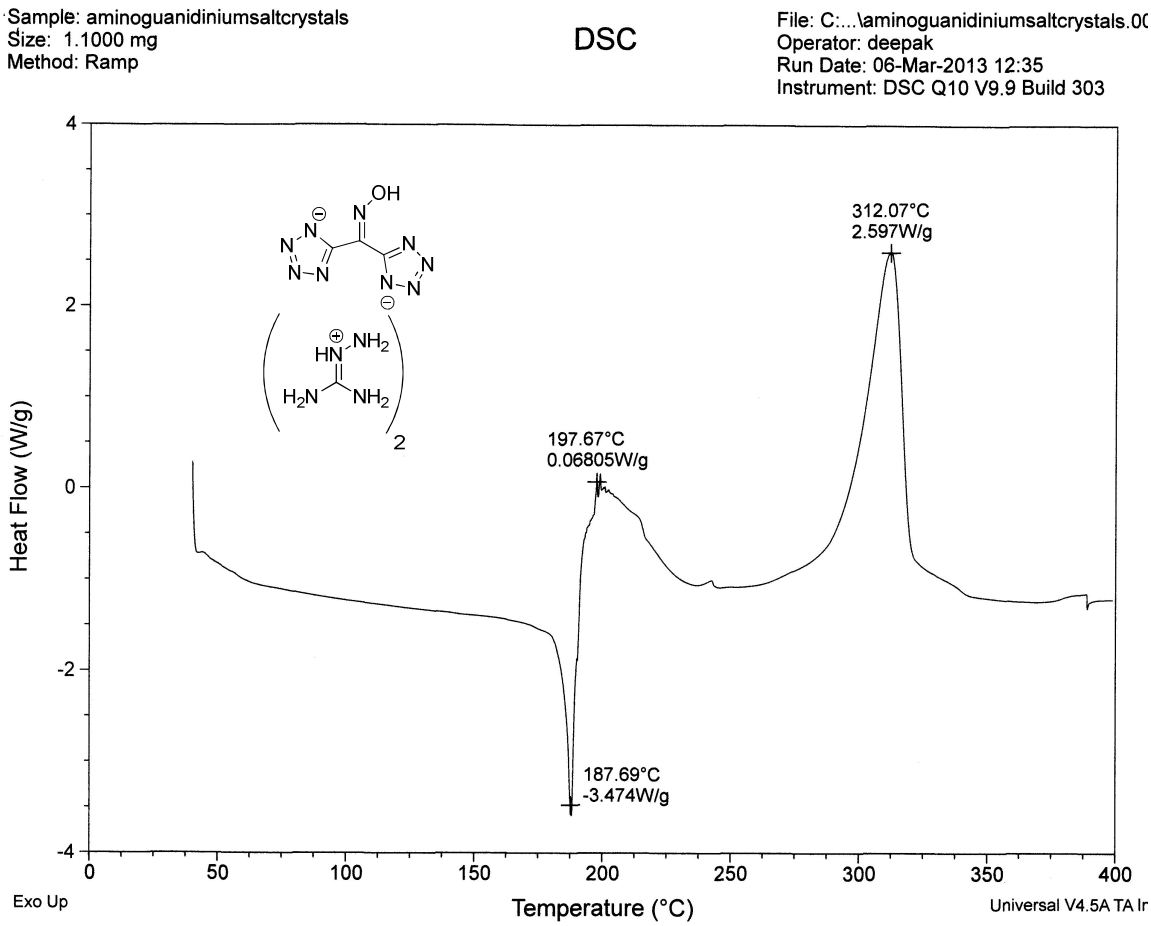

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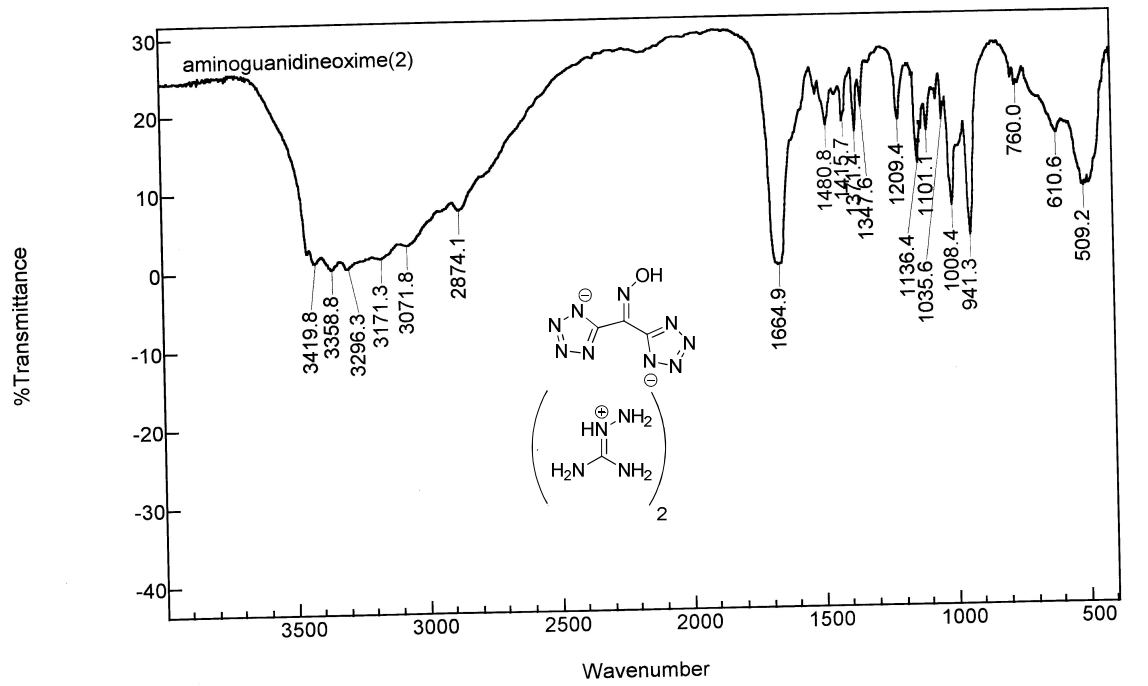

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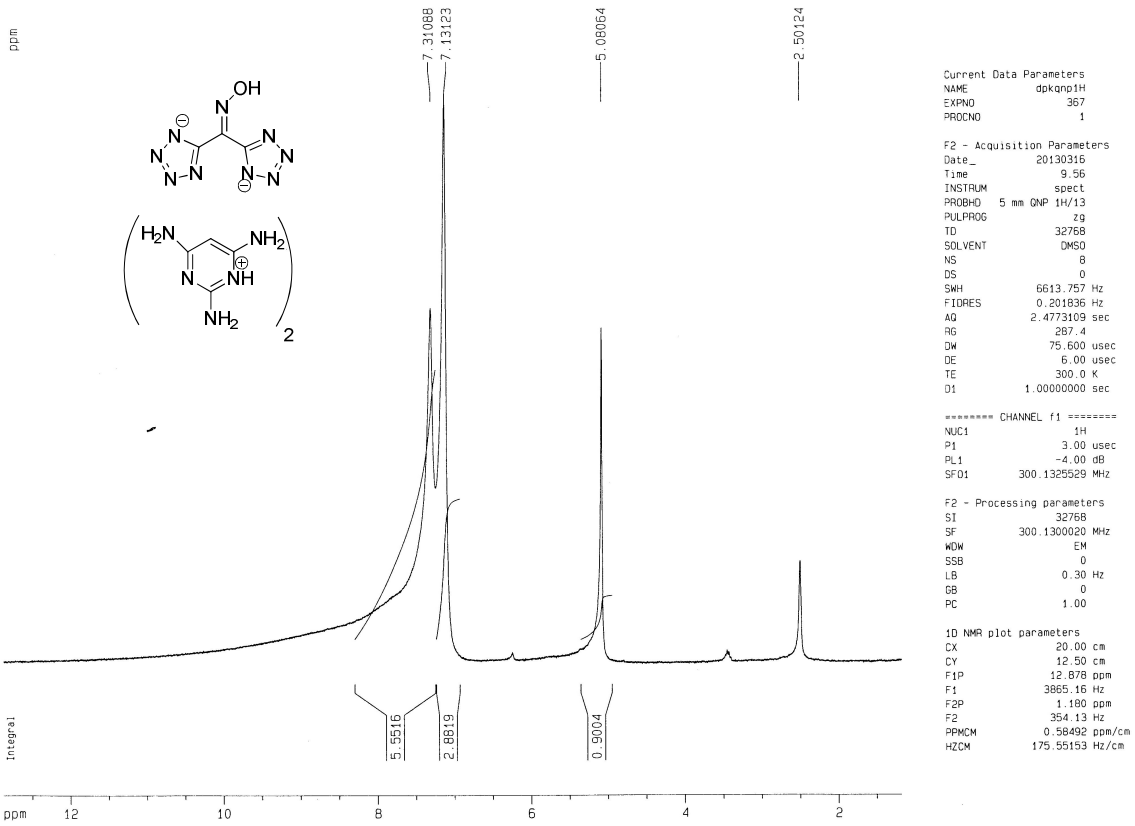

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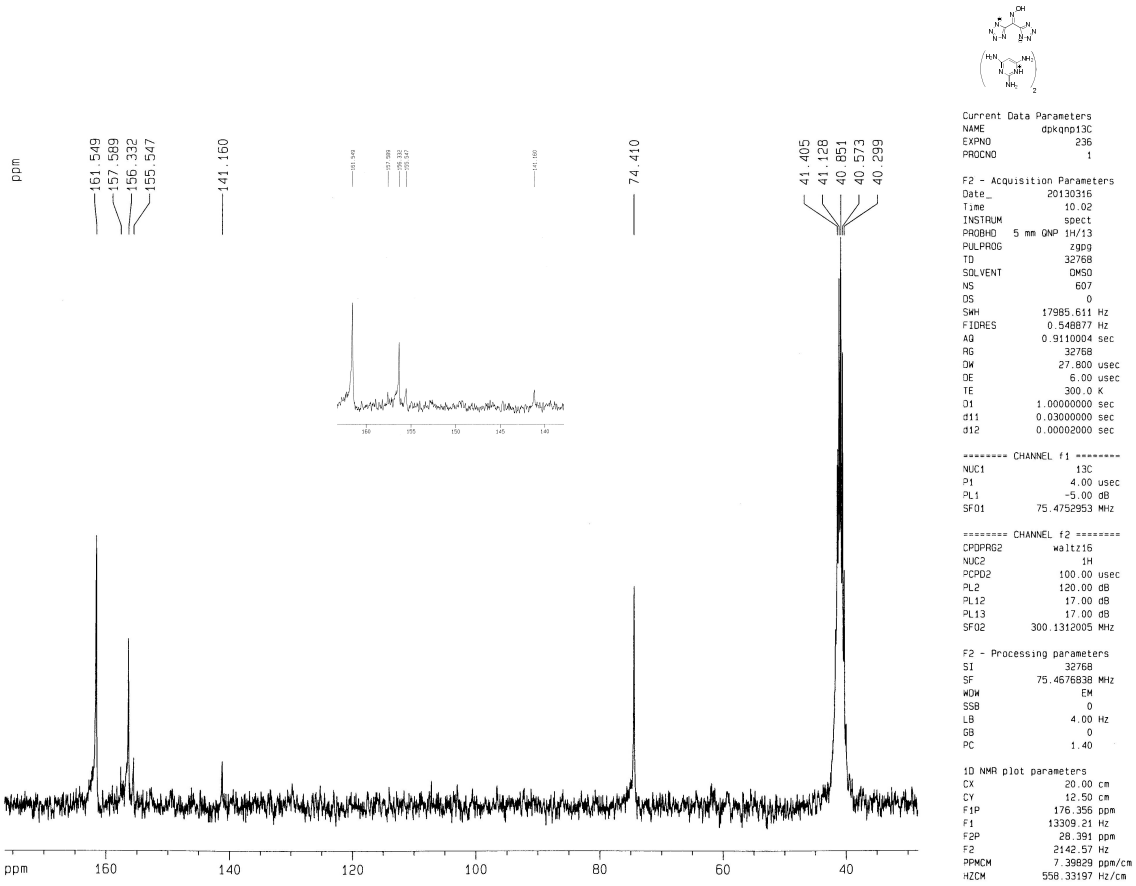

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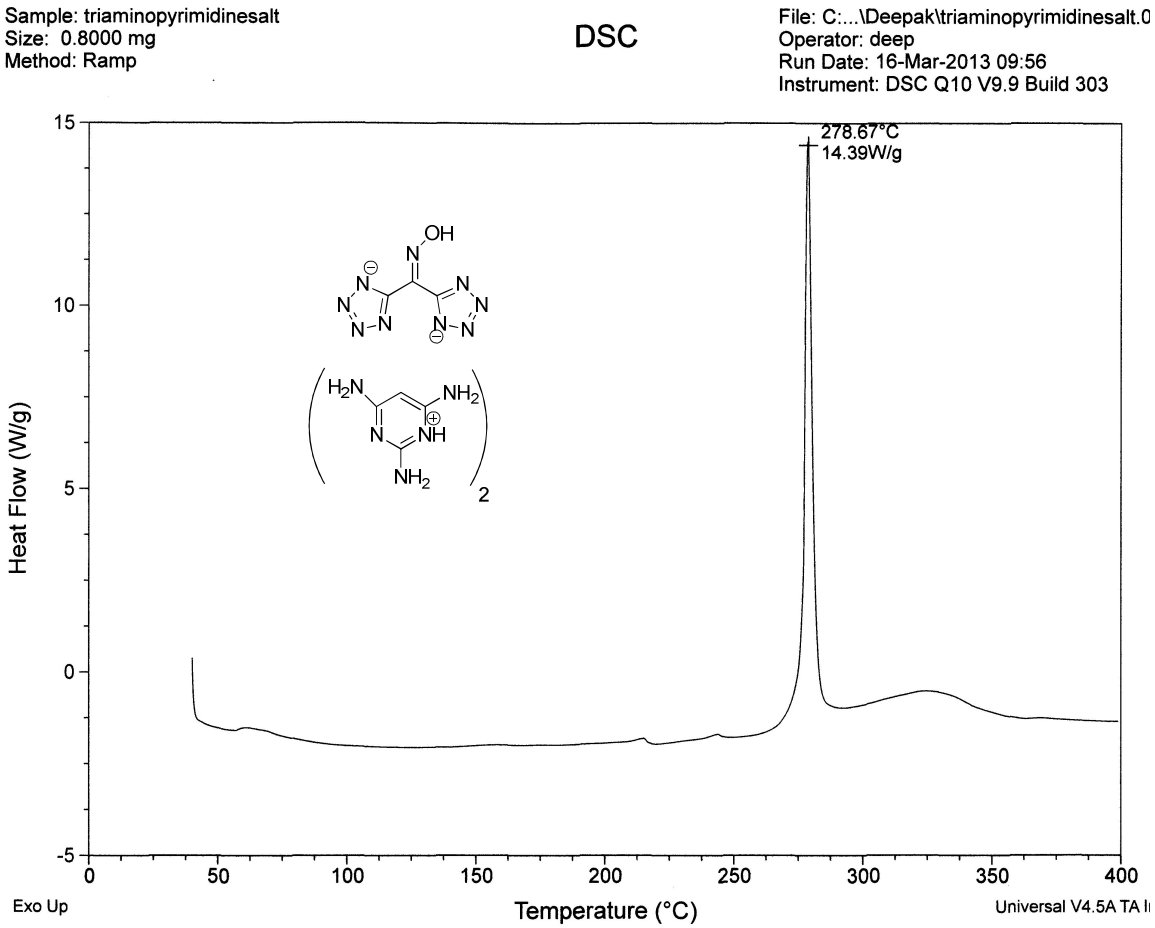

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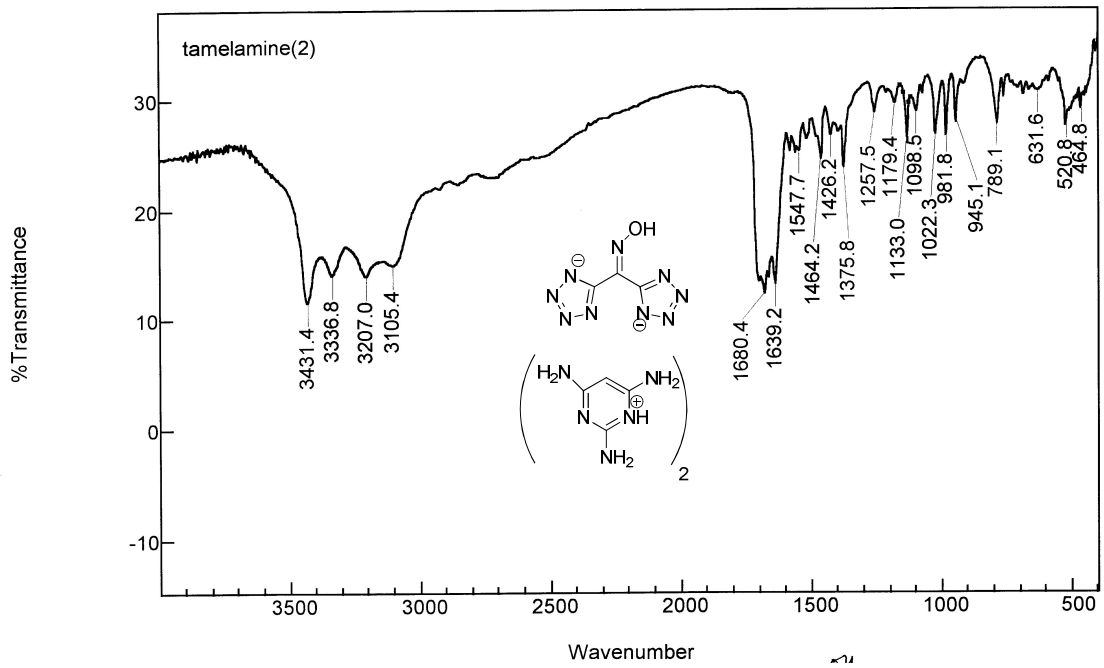

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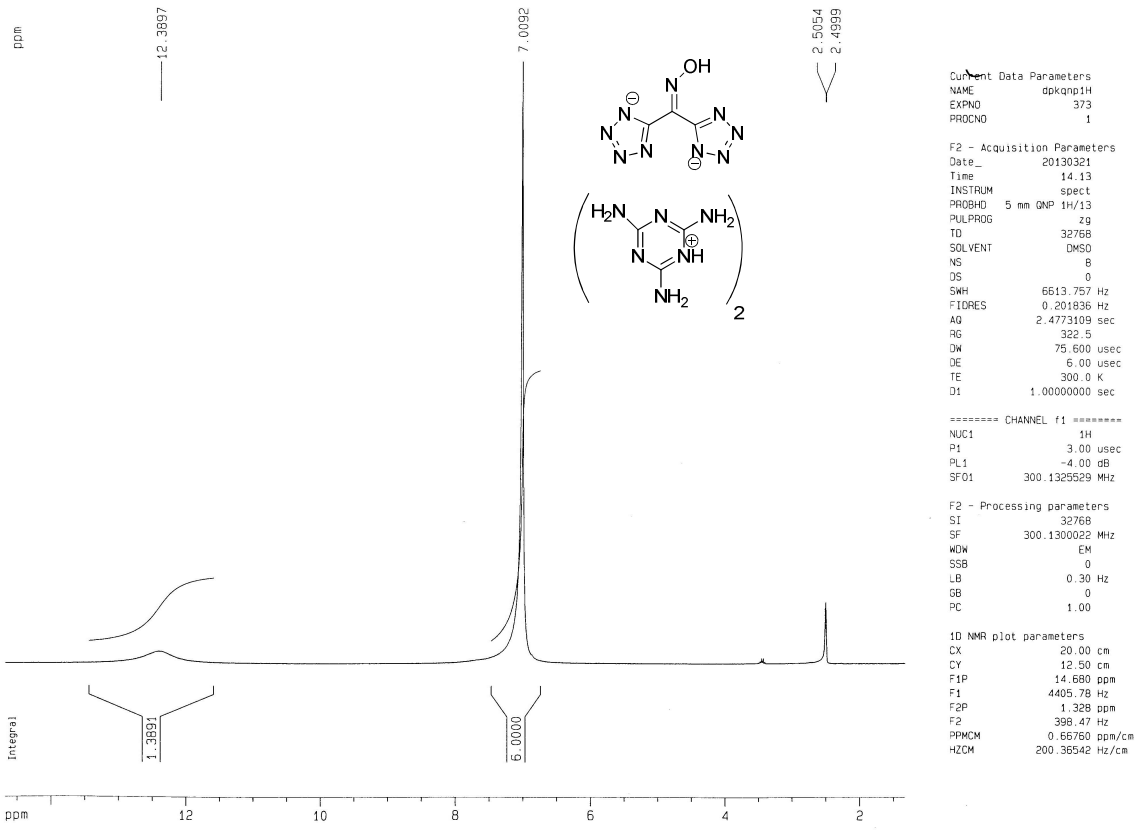

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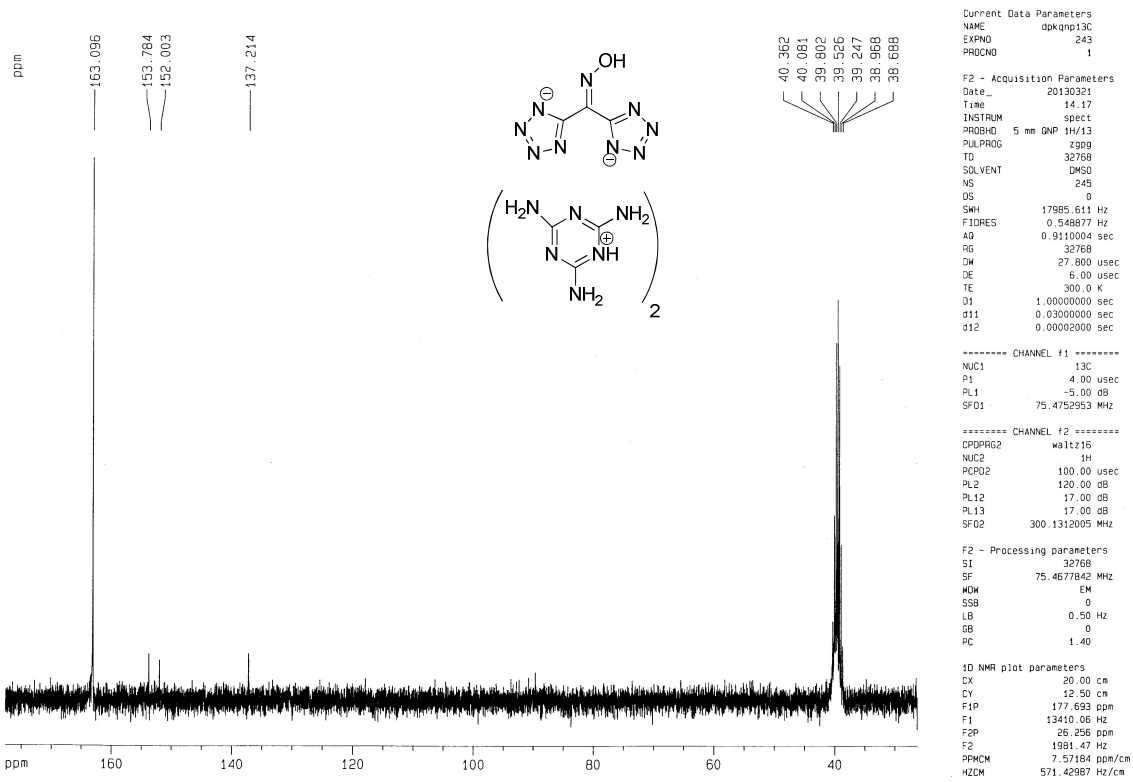

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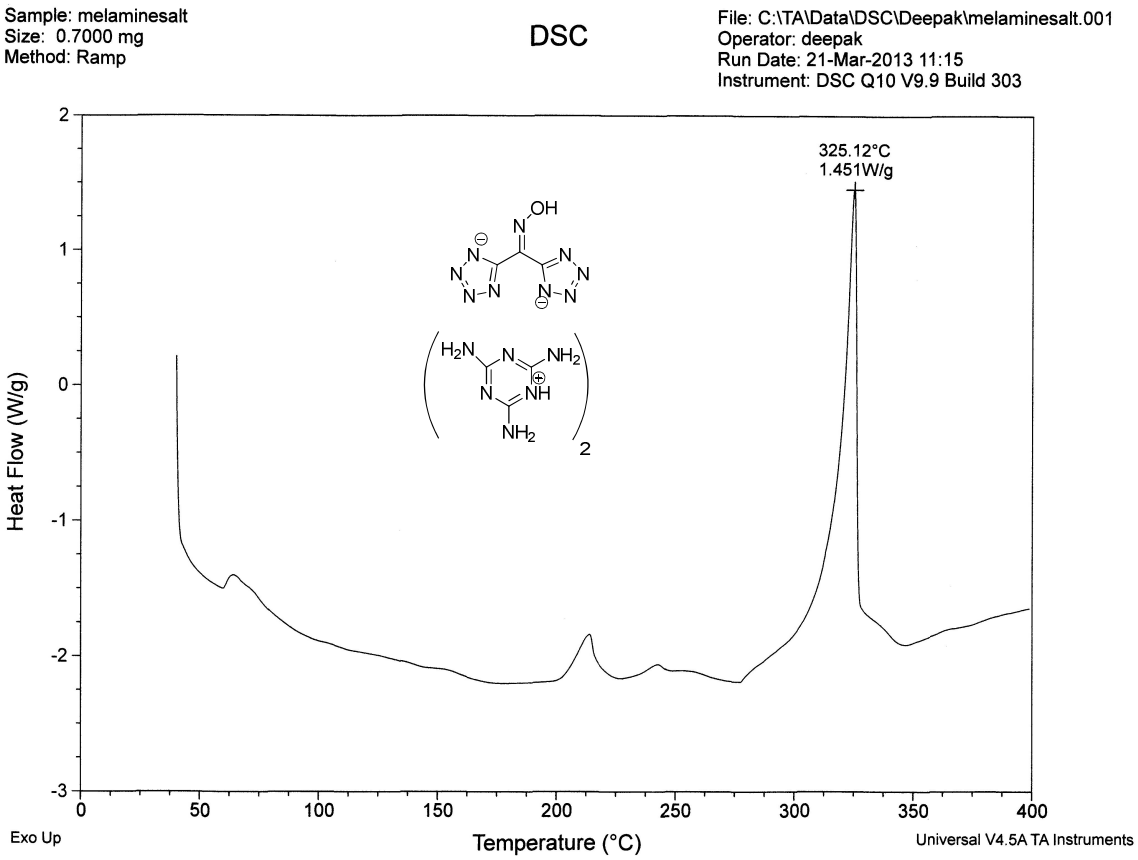
Fig : ^{13}C NMR of **8**



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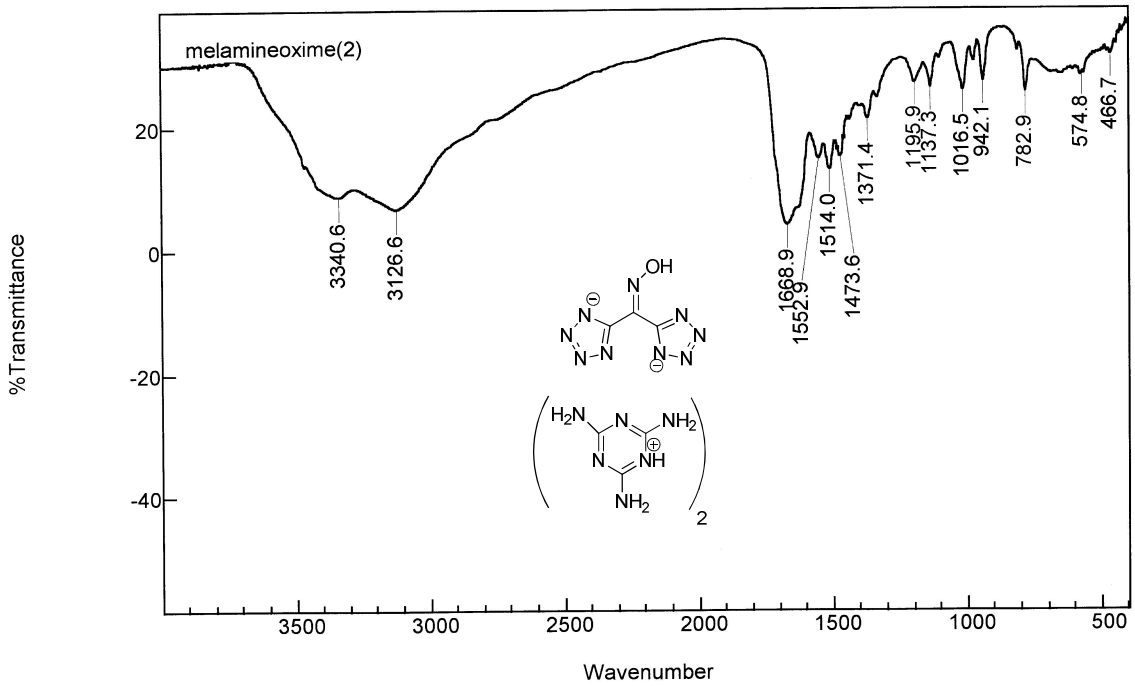

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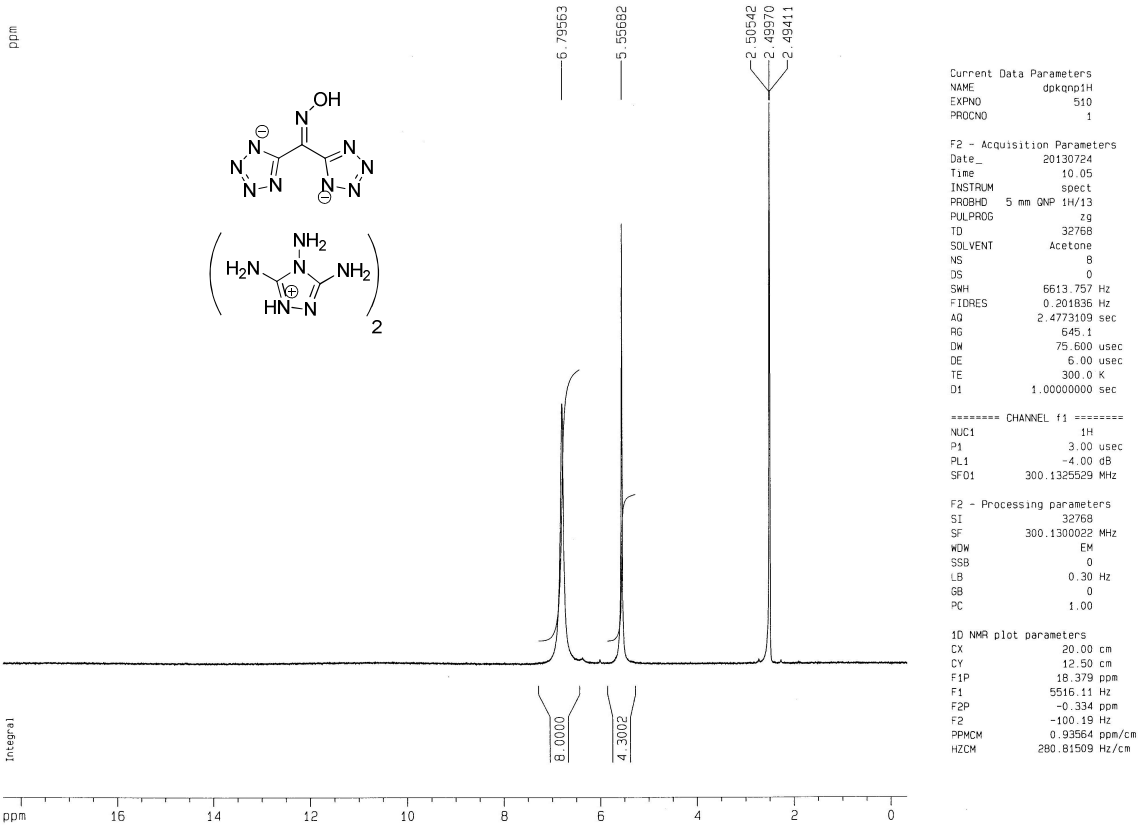

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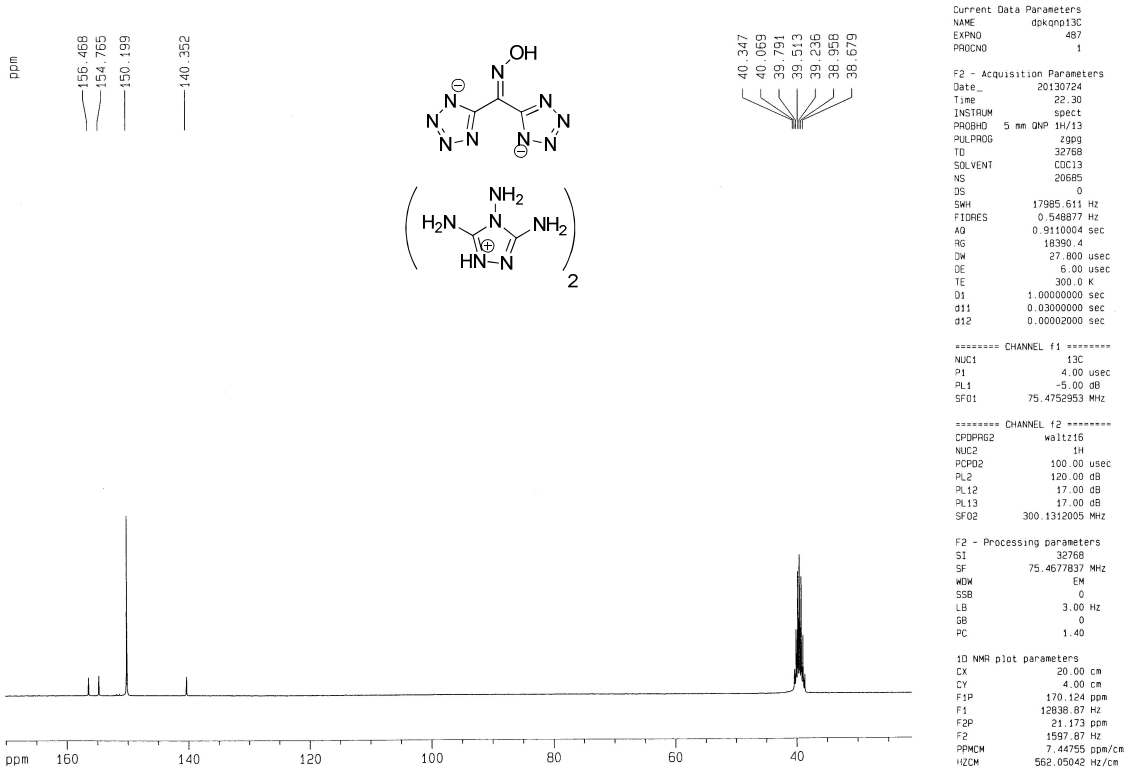


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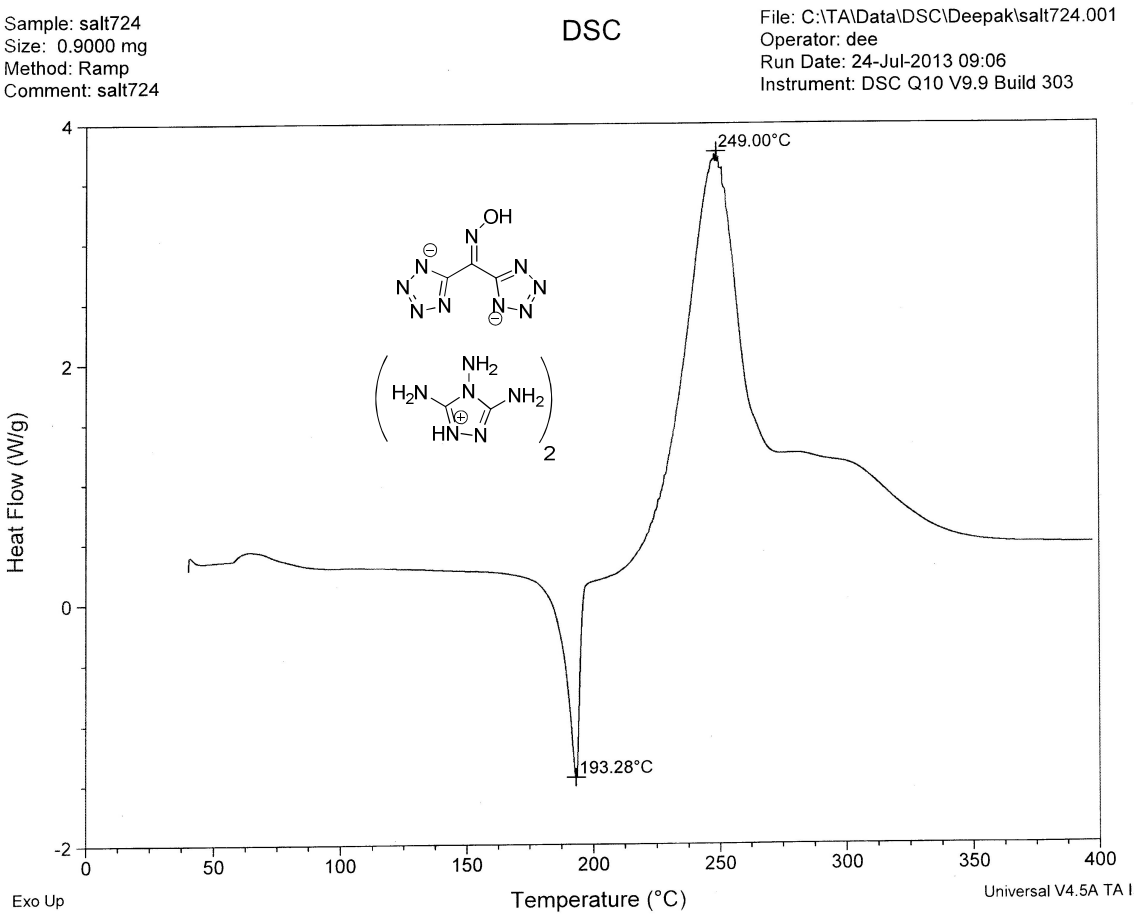

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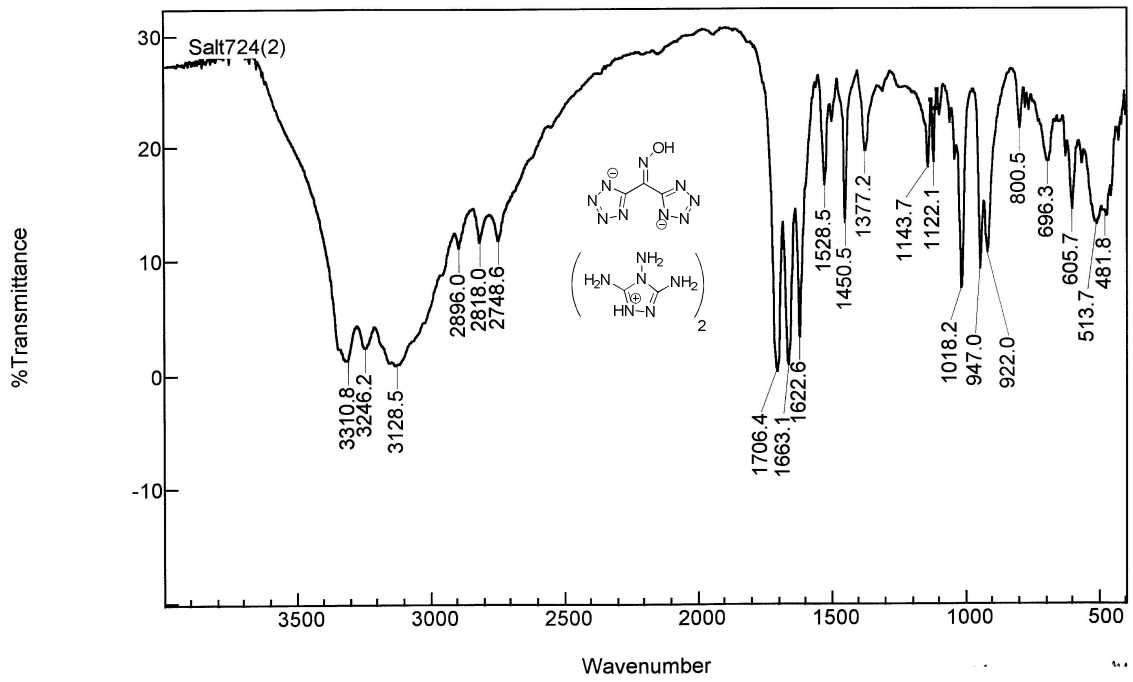

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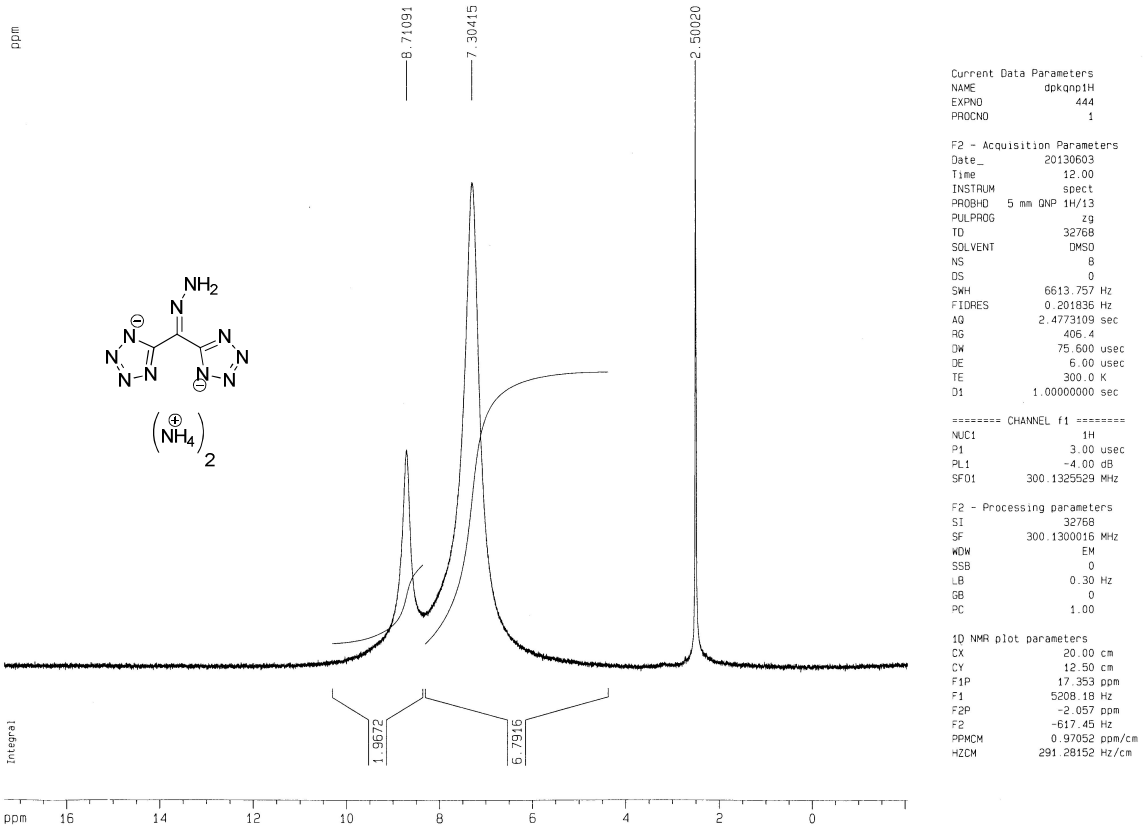

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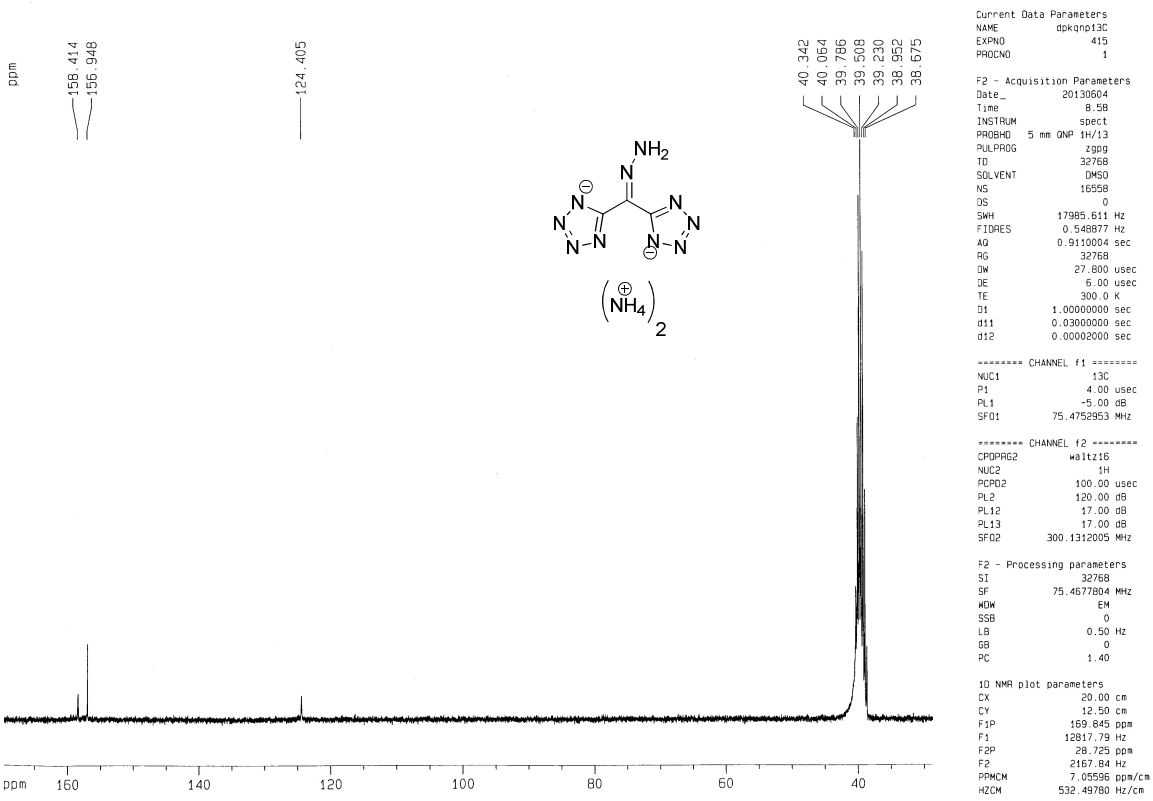

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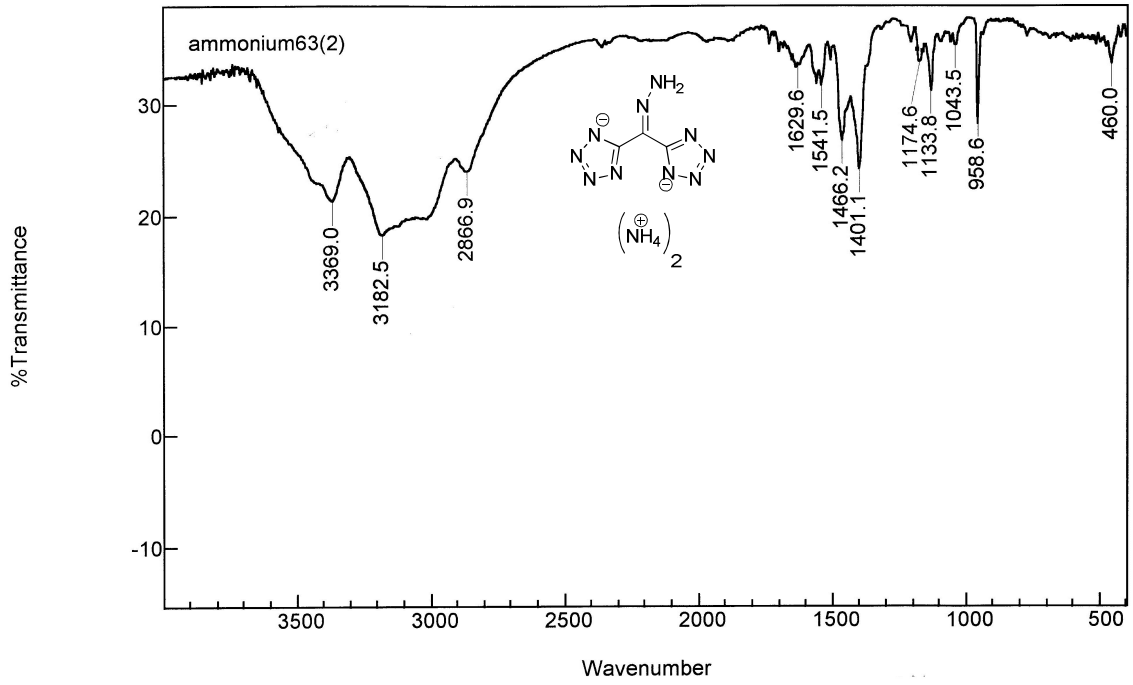

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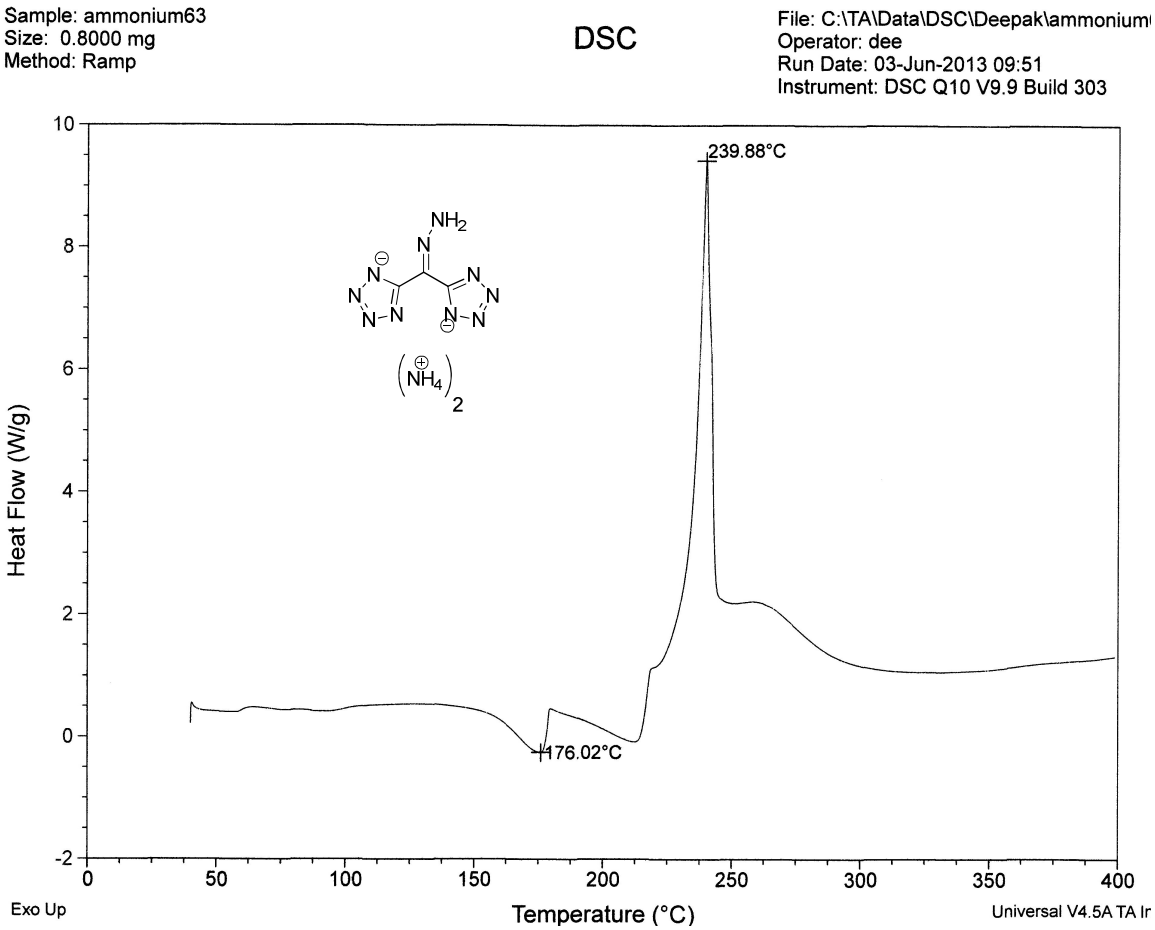

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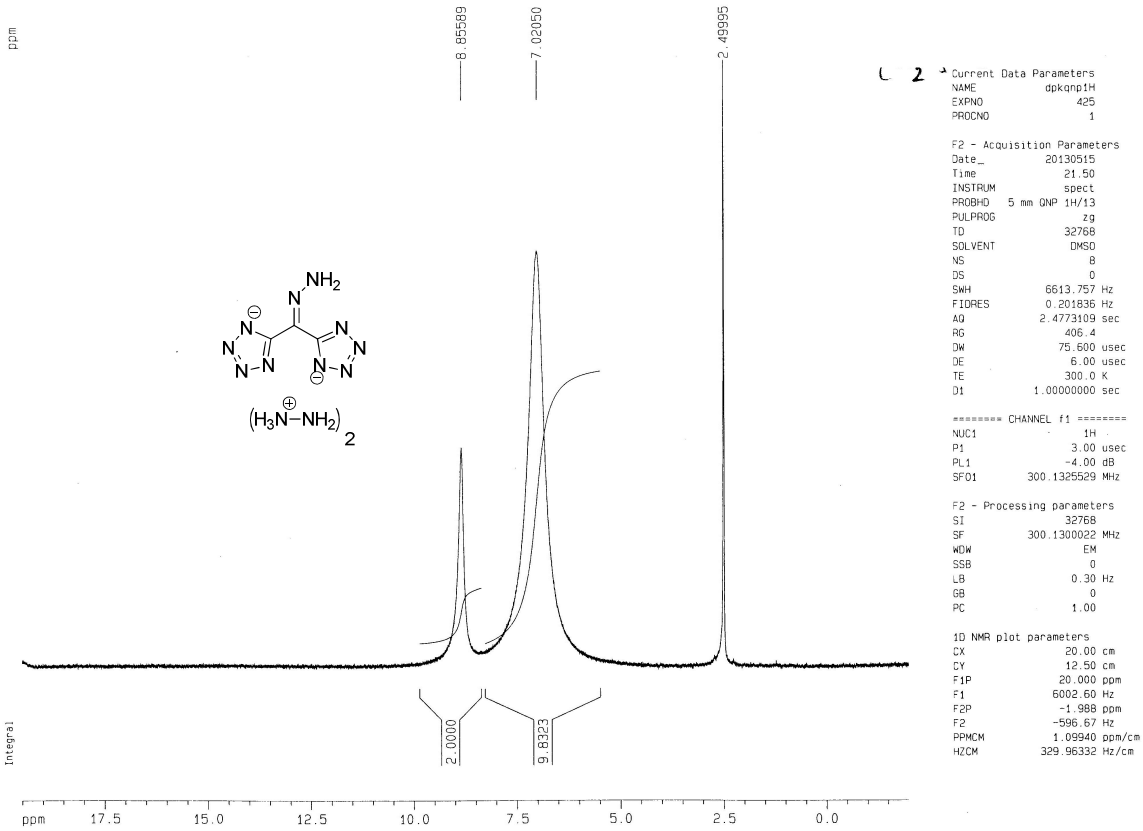


Fig : ^{1}H NMR of **11**

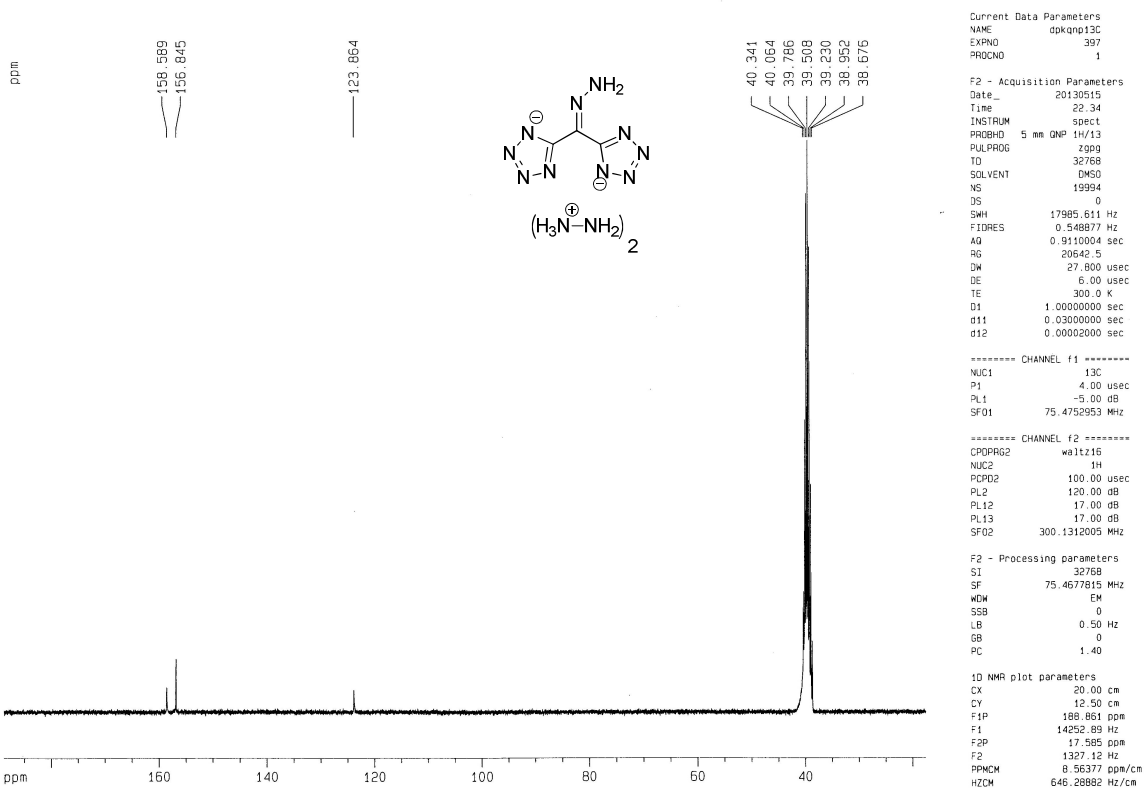


Fig : ^{13}C NMR of **11**

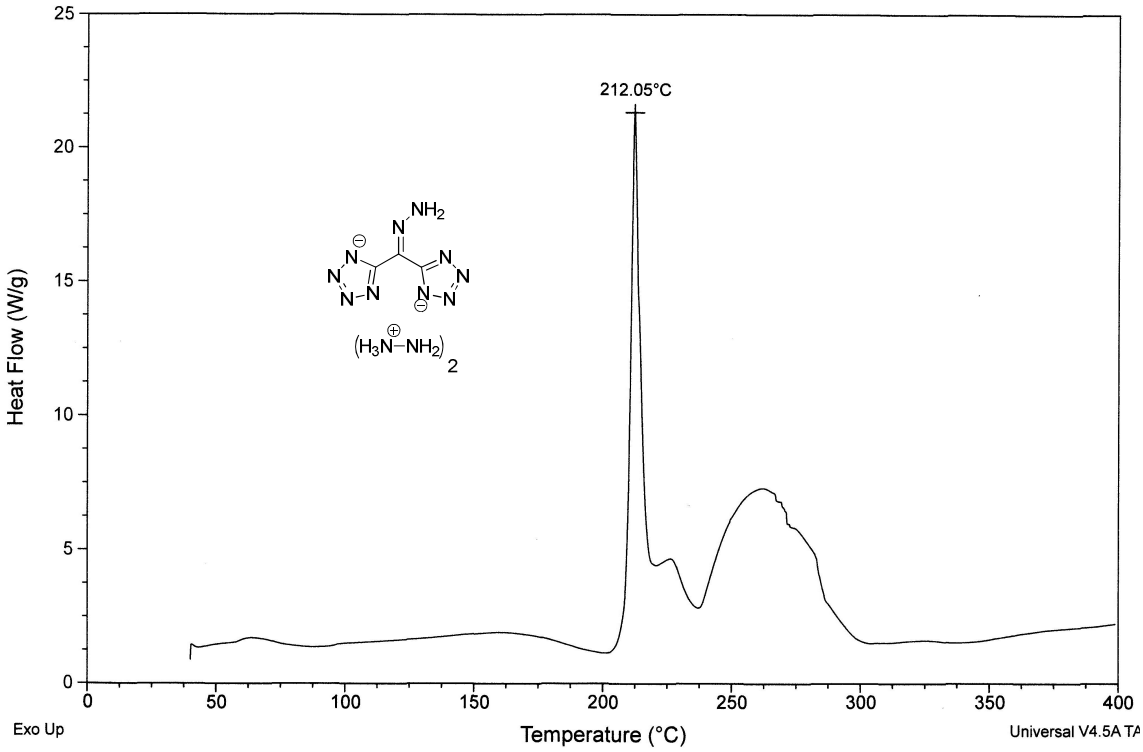


Fig : DSC of **11**

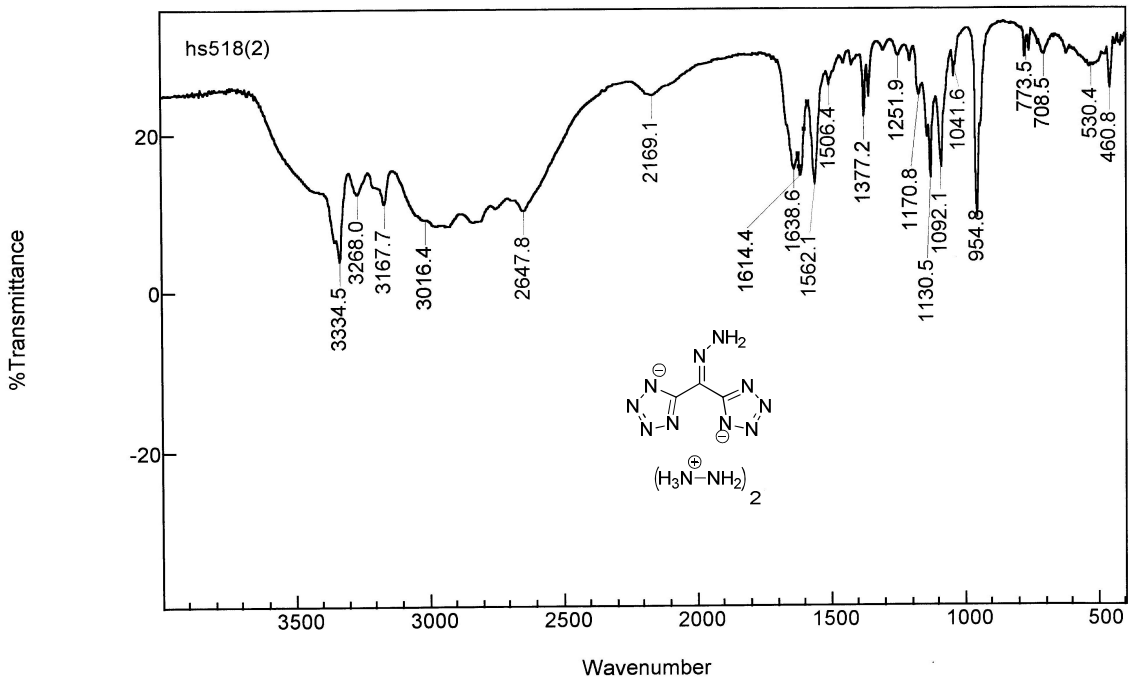


Fig : IR of **11**

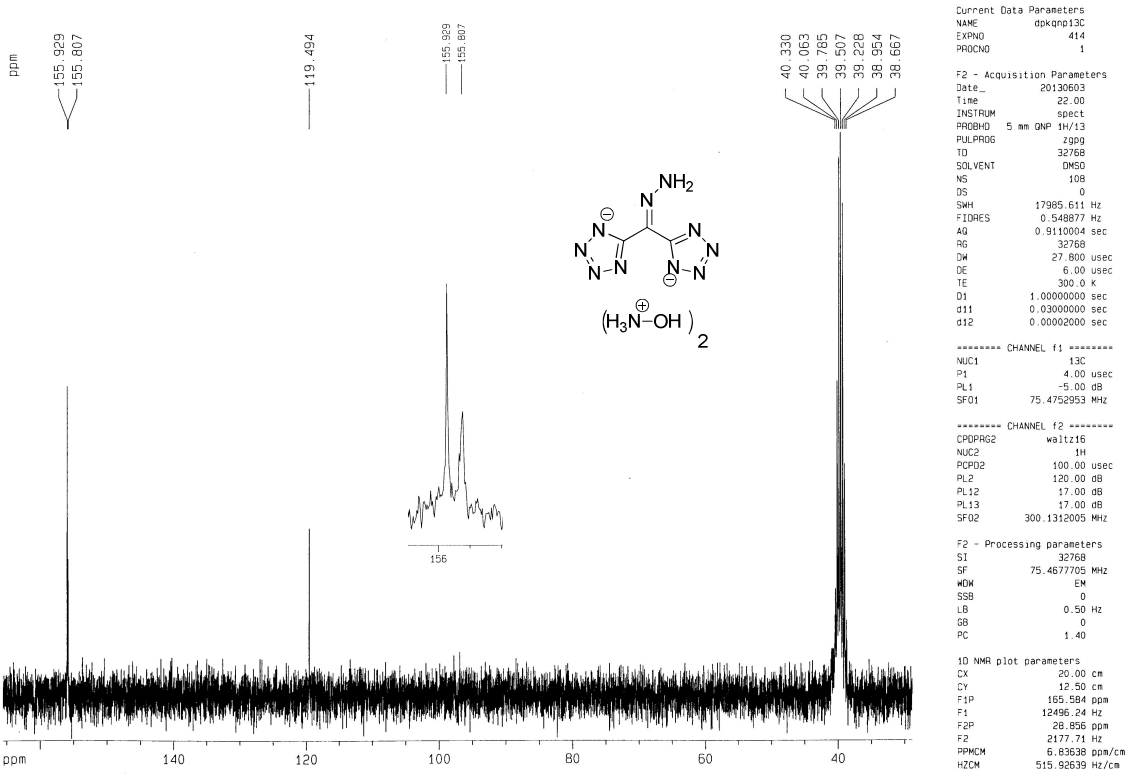


Fig : ^{13}C NMR of **12**

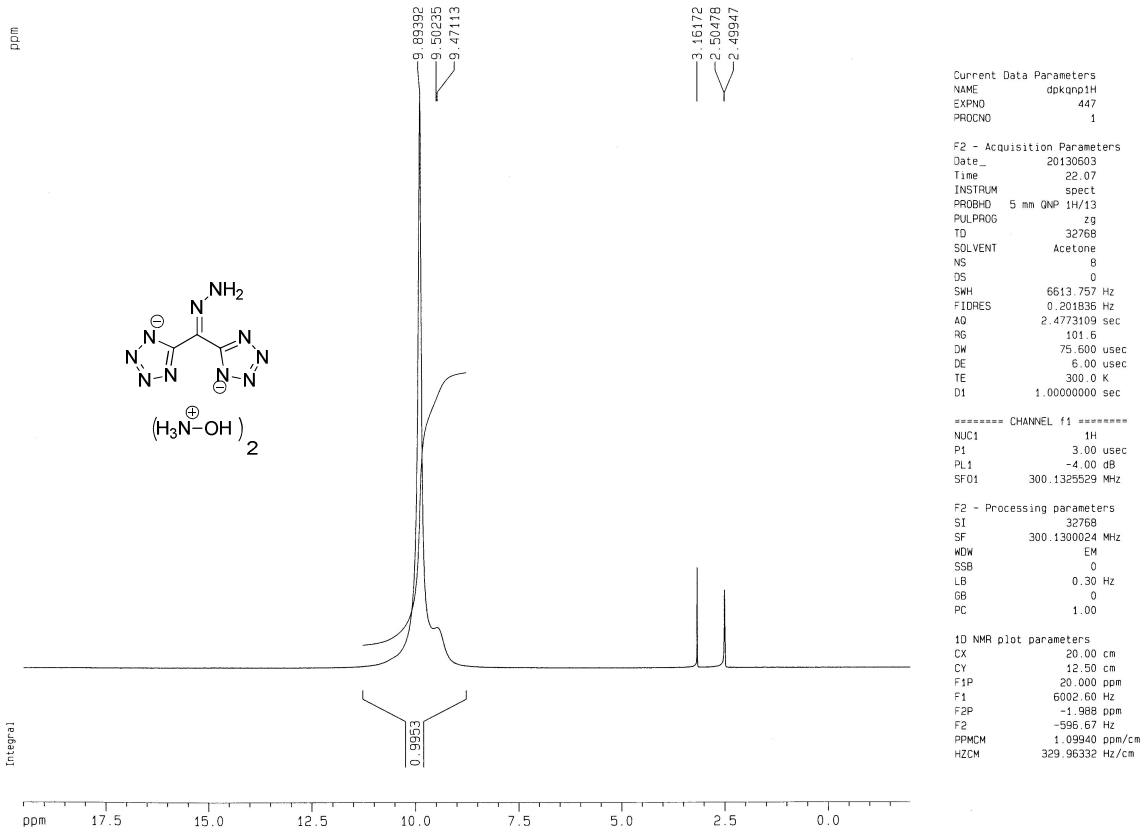


Fig : ^{1}H NMR of **12**

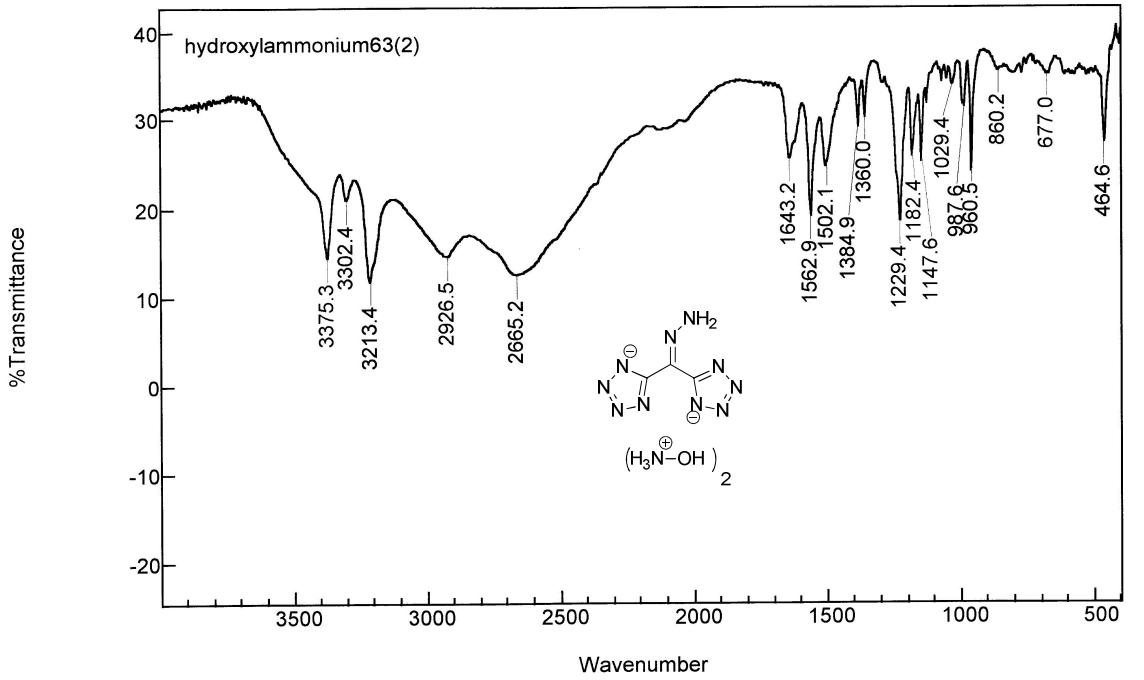
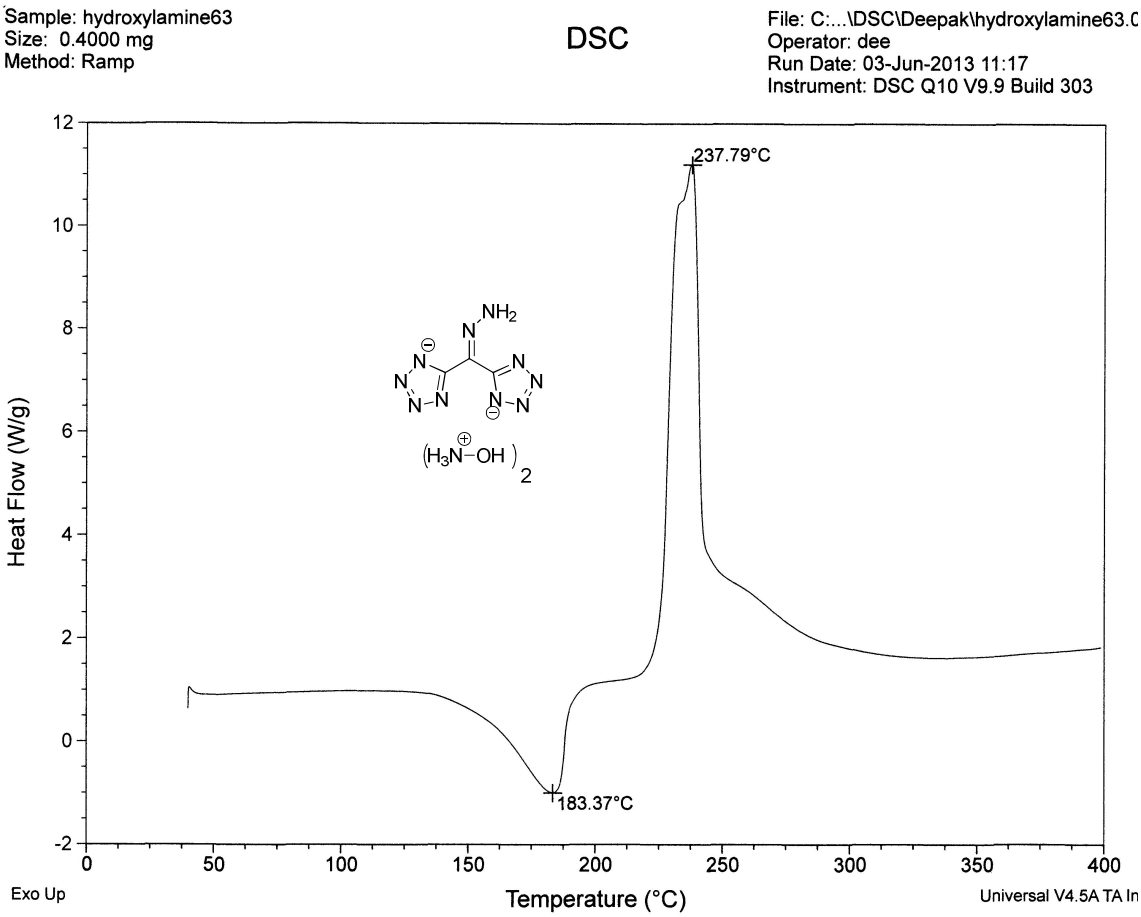


Fig : IR of **12**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Size: 0.4000 mg
Method: Ramp
DSC
File: C:...\DSC\Deepak\hydroxylamine63.0
Operator: dee
Run Date: 03-Jun-2013 11:17
Instrument: DSC Q10 V9.9 Build 303
237.79°C
183.37°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA In

Fig : DSC of **12**

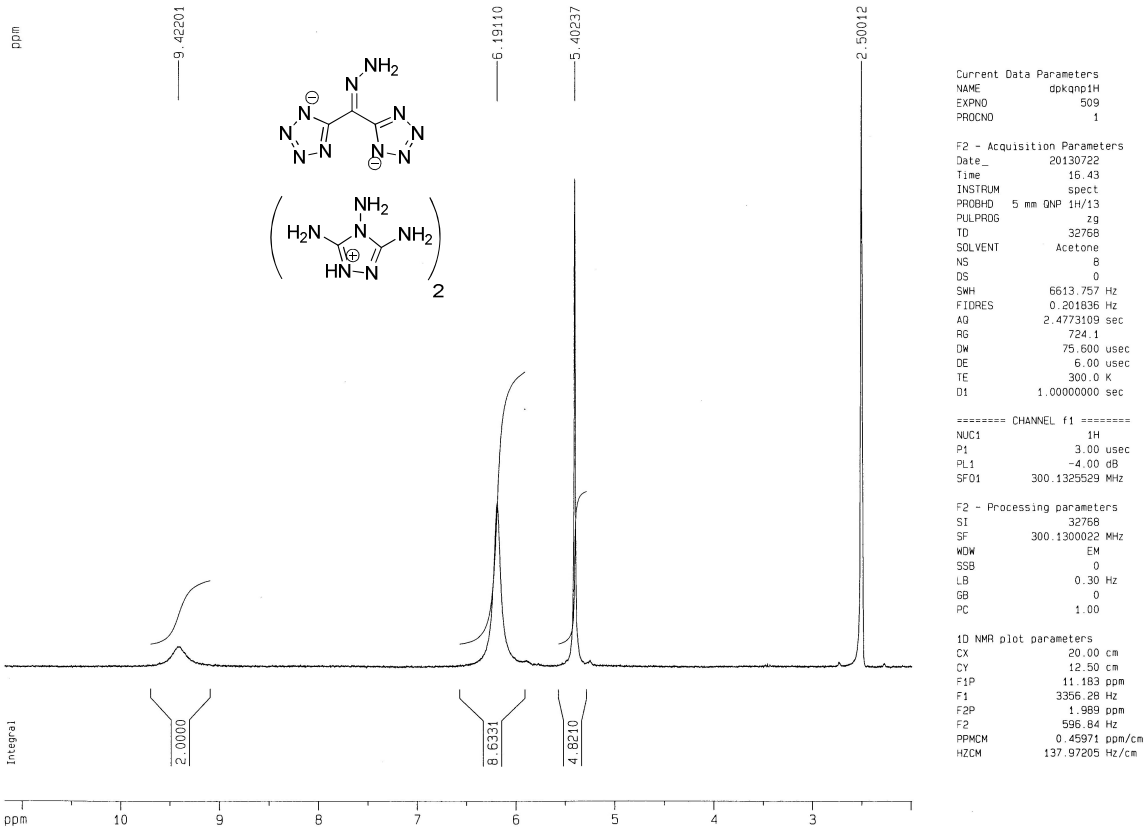

Fig : ^{1}H NMR of **13**

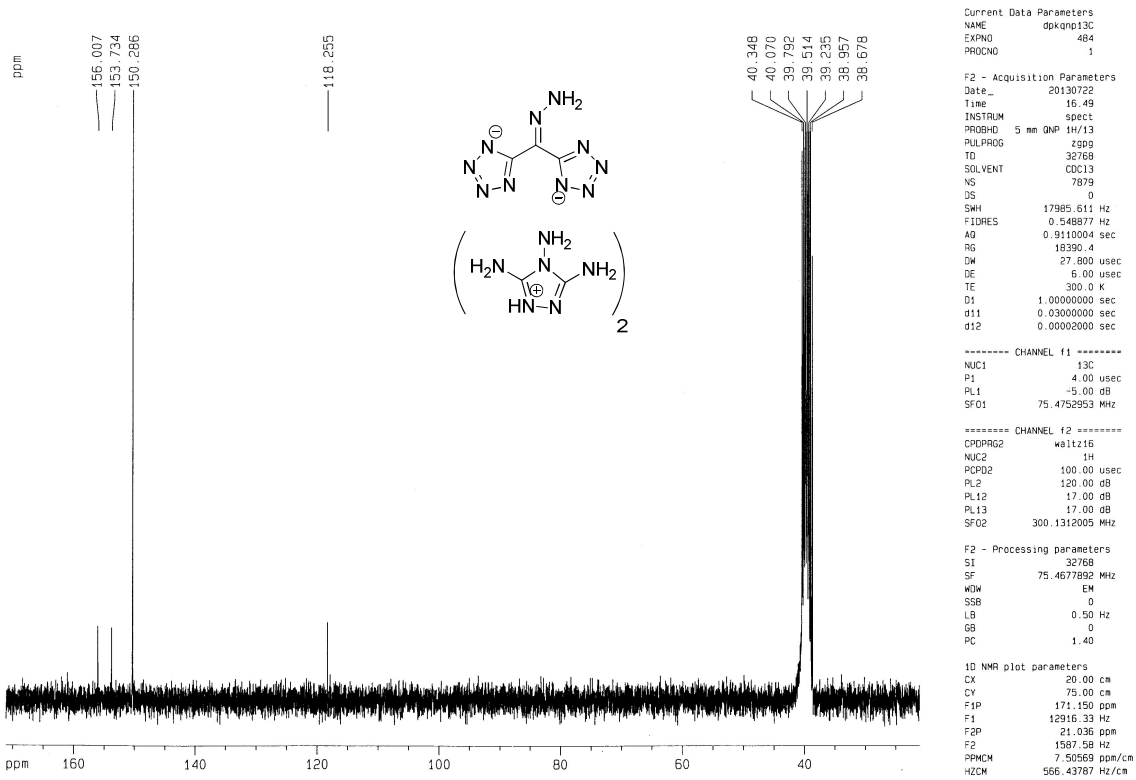

Fig : ^{13}C NMR of **13**

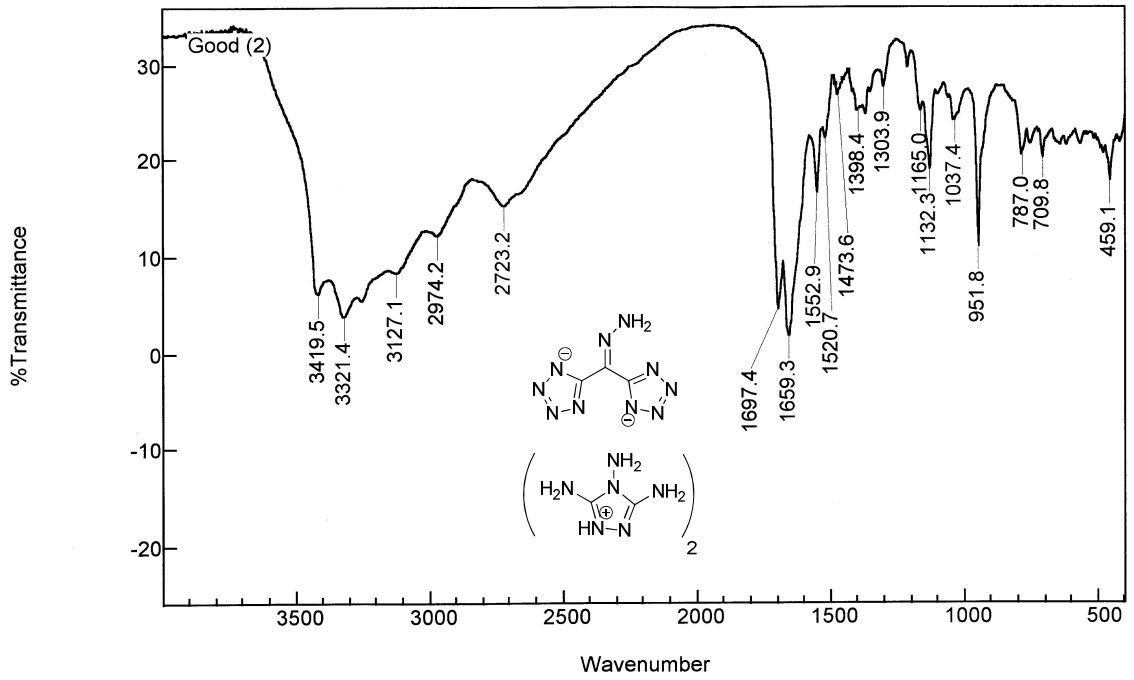

Fig : IR of **13**

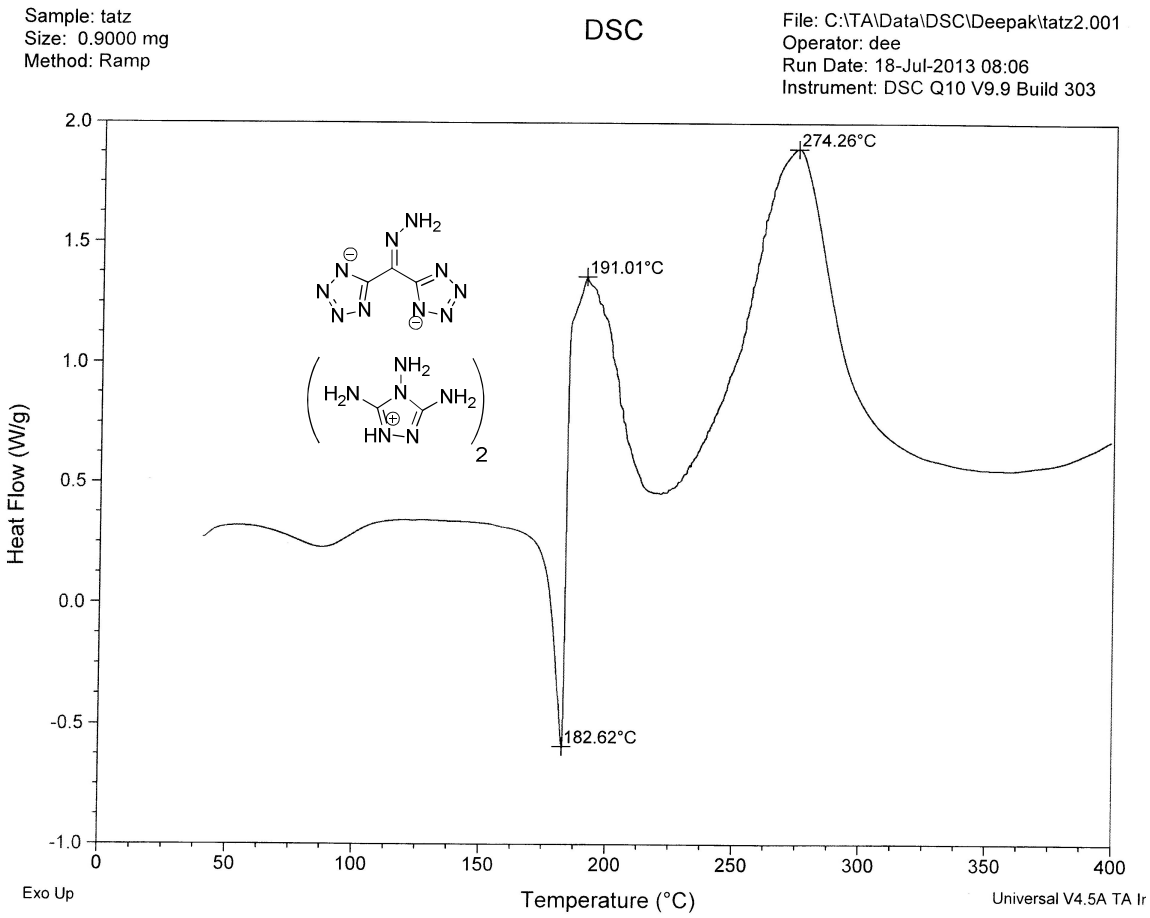
Sample: tatz
Size: 0.9000 mg
Method: Ramp
DSC
File: C:\TA\Data\DSC\Deepak\tatz2.001
Operator: dee
Run Date: 18-Jul-2013 08:06
Instrument: DSC Q10 V9.9 Build 303
274.26°C
191.01°C
182.62°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA Ir

Fig : DSC of **13**