Structural properties and thermal behavior of novel interaction product 4-amino-5-(furan-2-yl)-4H-1,2,4-triazole-3-thione with molecular iodine

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**Supplemental Materials**

**Table S 1**: Crystal data and structure refinement for C6H6N4OS∙I2

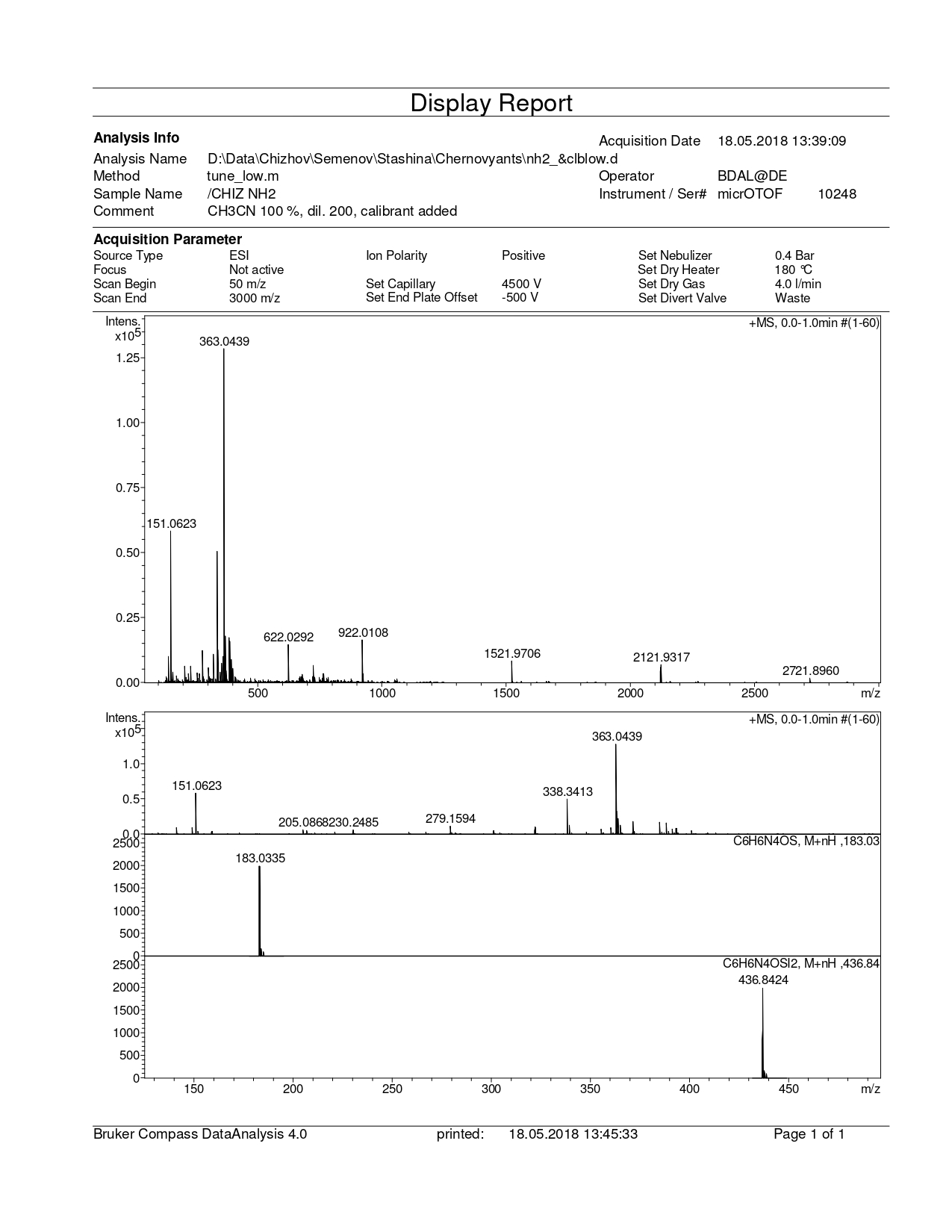
|  |  |
| --- | --- |
| **Compound** | **1** |
| Empirical Formula | C6H6I2N4OS |
| Formula Weight | 436.01 |
| Crystal System / Space Group | Monoclinic/ P21 |
| a / Å | 10.4679(6) |
| b / Å | 4.6885(3) |
| c / Å | 11.6913(8) |
| α / ° | 90 |
| β / ° | 92.903(6) |
| γ / ° | 90 |
| V / Å3 | 573.06(7) |
| Z | 2 |
| D calc (g/cm3) | 2.527 |
| μ (mm-1) | 44.641 |
| Crystal size (mm) | 0.1 × 0.05 × 0.05 |
| Color / Shape | Dark-brown/ needle-like |
| Temp (K) | 100(2) |
| Theta range for collection | 7.572 to 144.99 |
| Reflections collected | 4909 |
| Independent reflections | 2259 [Rint = 0.0628, Rsigma = 0.0762] |
| Data/restraints/parameters | 2259/1/128 |
| Goodness of fit on F2 | 1.048 |
| Final R indices [I > 2σ(I)] | R1 = 0.0423, wR2 = 0.0989 |
| R indices (all data) | R1 = 0.0458, wR2 = 0.1020 |
| Largest difference peak/hole | 1.13/-0.99 |

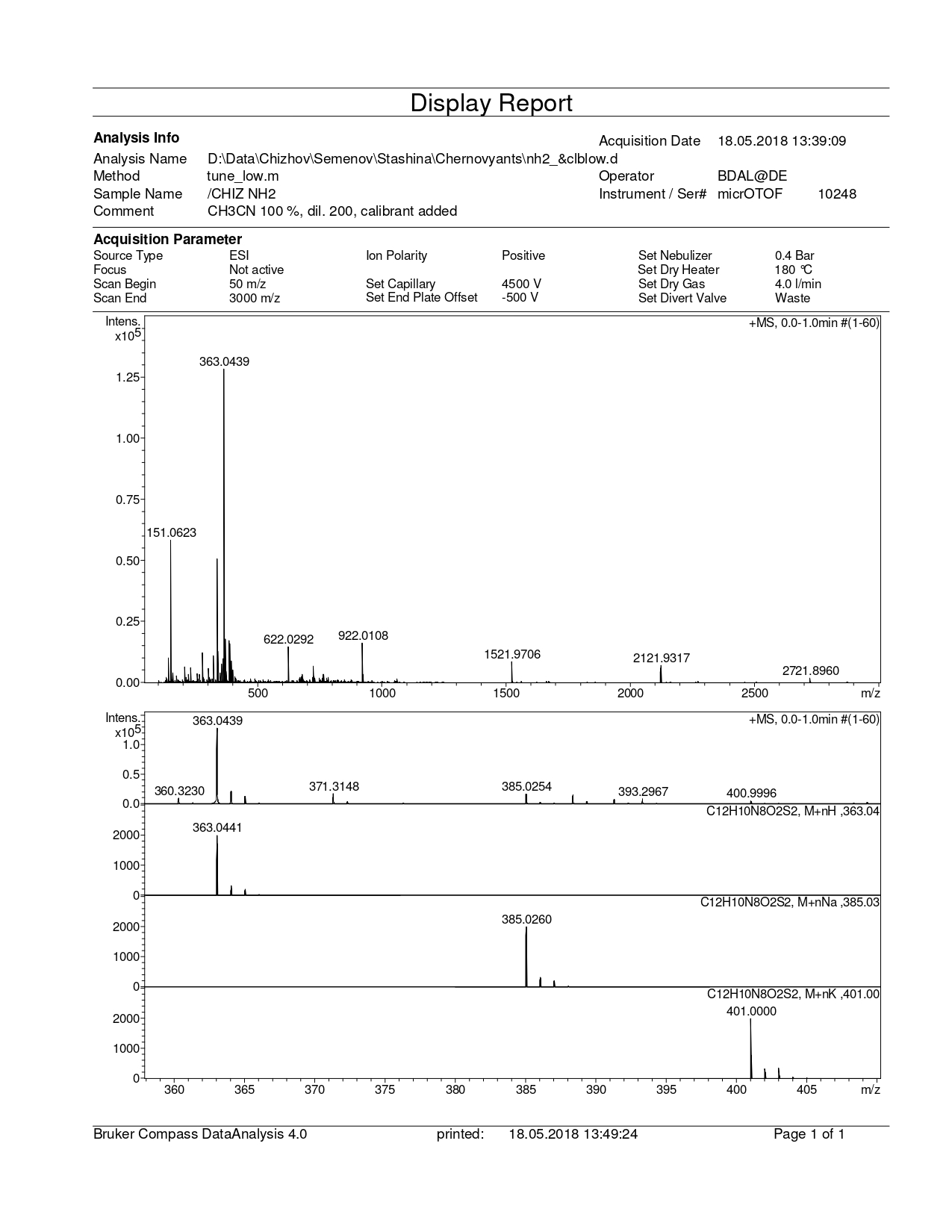
|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Table S 2**:Bond Lengths for C6H6N4OS∙I2 | | | | | | |
| **Atom** | **Atom** | **Length/Å** |  | **Atom** | **Atom** | **Length/Å** |
| I1 | I2 | 2.82(11) |  | N4 | C5 | 1.30(16) |
| I1 | S1 | 2.80(3) |  | C5 | C2 | 1.45(2) |
| S1 | C10 | 1.69(14) |  | O6 | C7 | 1.37(17) |
| N1 | N3 | 1.40(13) |  | O6 | C2 | 1.37(16) |
| N1 | C10 | 1.37(18) |  | C7 | C8 | 1.36(2) |
| N1 | C5 | 1.36(18) |  | C8 | C1 | 1.42(2) |
| C10 | N2 | 1.33(17) |  | C1 | C2 | 1.35(19) |
| N2 | N4 | 1.37(16) |  |  |  |  |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Table S 3:** Bond Angles for C6H6N4OS∙I2 | | | | | | | | |
| **Atom** | **Atom** | **Atom** | **Angle/˚** |  | **Atom** | **Atom** | **Atom** | **Angle/˚** |
| S1 | I1 | I2 | 171.74(8) |  | N1 | C5 | C2 | 125.3(11) |
| C10 | S1 | I1 | 97.4(5) |  | N4 | C5 | N1 | 111.1(12) |
| C10 | N1 | N3 | 126.9(11) |  | N4 | C5 | C2 | 123.5(12) |
| C5 | N1 | N3 | 124.8(12) |  | C7 | O6 | C2 | 106.5(11) |
| C5 | N1 | C10 | 108.1(10) |  | C8 | C7 | O6 | 110.3(12) |
| N1 | C10 | S1 | 126.6(10) |  | C7 | C8 | C1 | 106.2(12) |
| N2 | C10 | S1 | 130.1(11) |  | C2 | C1 | C8 | 106.9(13) |
| N2 | C10 | N1 | 103.2(11) |  | O6 | C2 | C5 | 113.9(11) |
| C10 | N2 | N4 | 113.8(10) |  | C1 | C2 | C5 | 136.0(13) |
| C5 | N4 | N2 | 103.6(11) |  | C1 | C2 | O6 | 110.1(13) |

**Table S 4:** Bond lengths and torsion angles(Å, °)

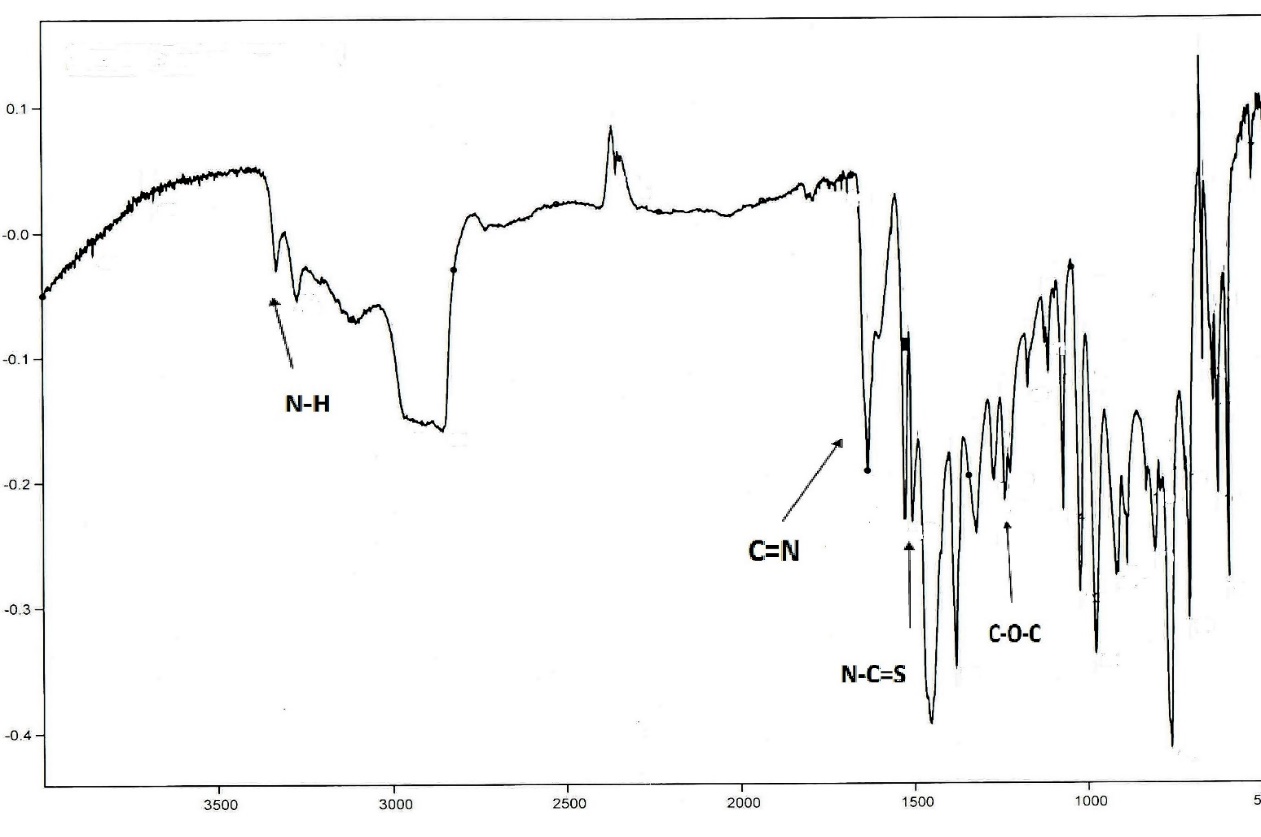
|  |
| --- |
| Bond lengths (Å)  I(1)-I(2) - 2.8182(11)  I(1)-S(1) - 2.798(3)  S(1)-C(10) - 1.687(14) |
| Torsion angles (°)  I(2)-I(1)-S(1)-C(10): -102.3(7)  I(1)-S(1)-C(10)-N(1): 134(1)  I(1)-S(1)-C(10)-N(2): -45(1) |
| Bond angles (°)  I(2)-I(1)-S(1): 2.0583(6)  I(1)-S(1)-C(10): 171.74(8) |



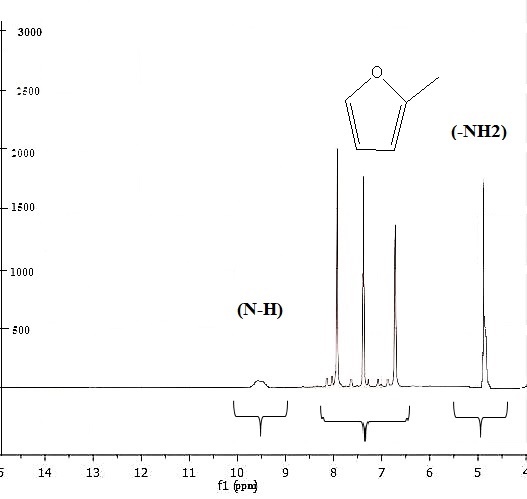


**Figure S 1:** Mass-spectra of C6H6N4OS∙I2

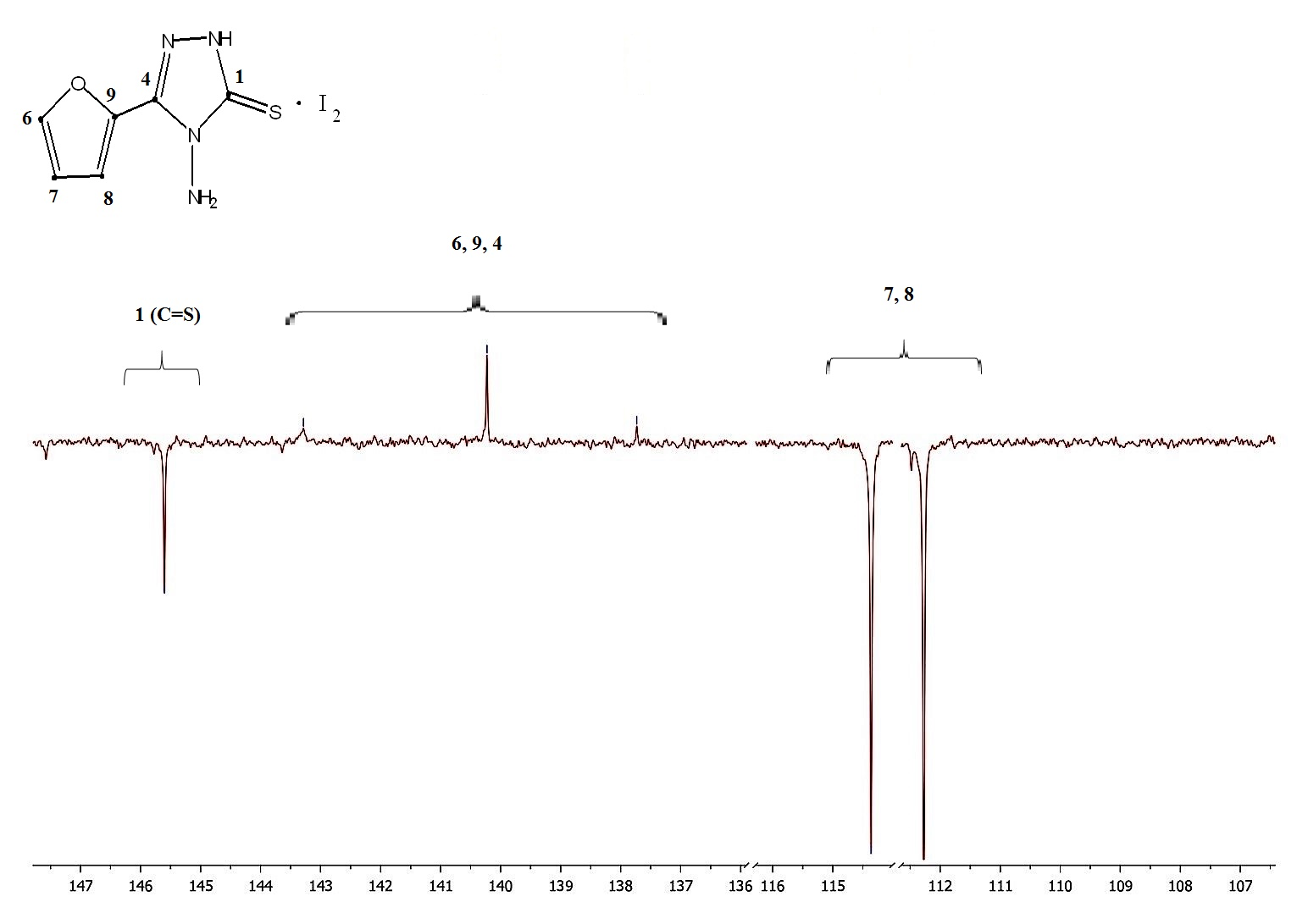
**Figure S 2:** Raman spectrum of C6H6N4OS∙I2

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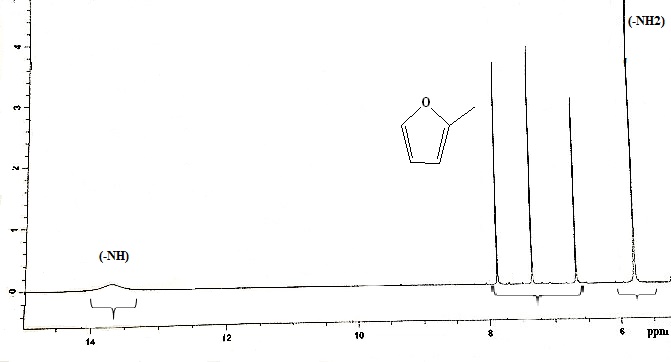
**Figure S 3**: FT-IR spectrum of C6H6N4OS∙I2

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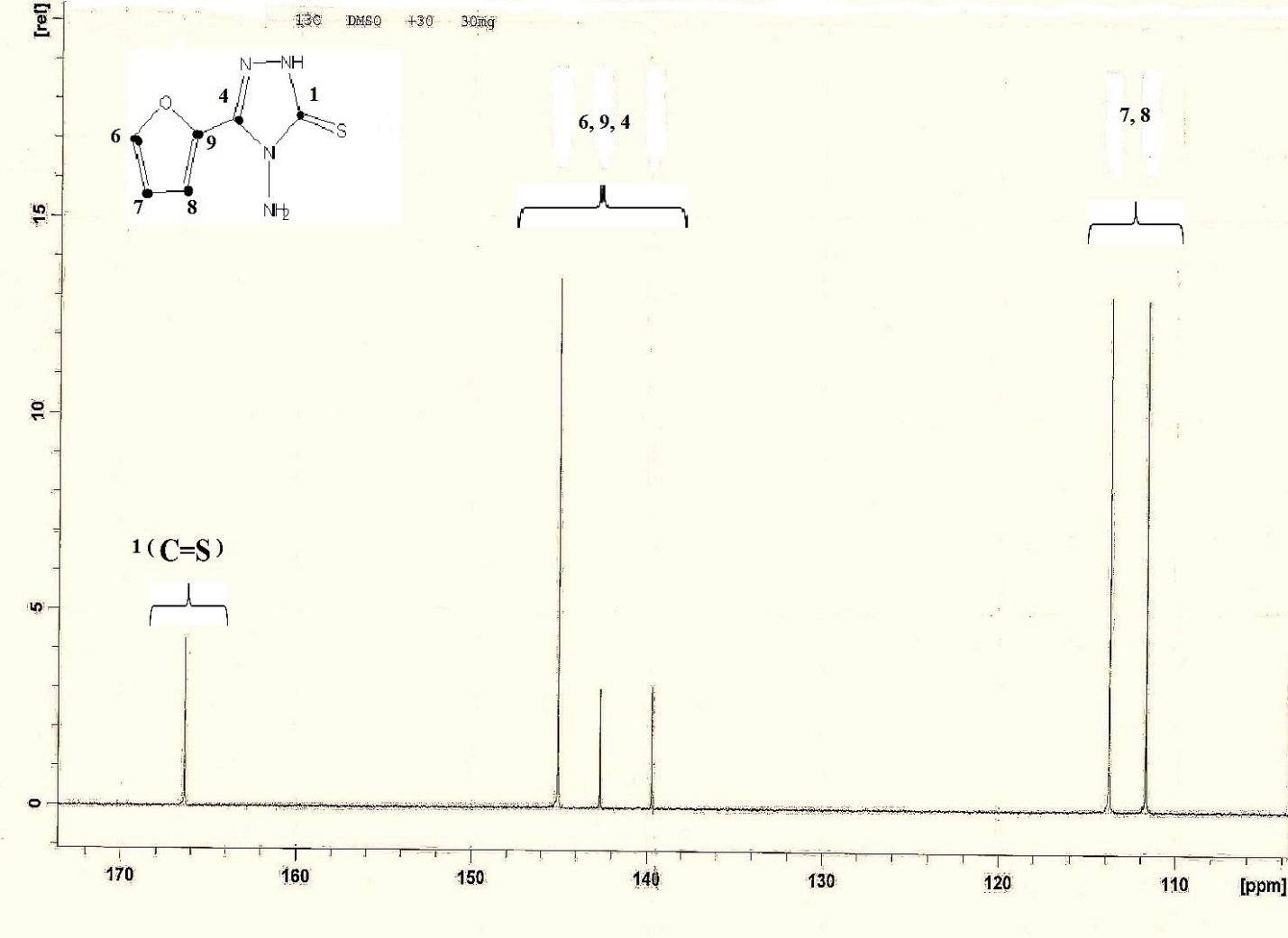
**Figure S 4**: 1H NMR (250 MHz, DMSO) of C6H6N4OS∙I2

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**Figure S 5**: 13C NMR (62.9 MHz, DMSO) of C6H6N4OS∙I2

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**Figure S 6**: 1H NMR (600 MHz, DMSO) of *4-amino-5-(furan-2-yl)-4H-1,2,4-triazole-3-thione*

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**Figure S 7**: 13C (151 MHz, DMSO) of *4-amino-5-(furan-2-yl)-4H-1,2,4-triazole-3-thione*