

Short Note

## Synthesis and Characterization of N,N'-(propane-1,2-diyl)dicarbamothioyl)dibenzamide

Gülşah Kurt \* and Bedrettin Mercimek

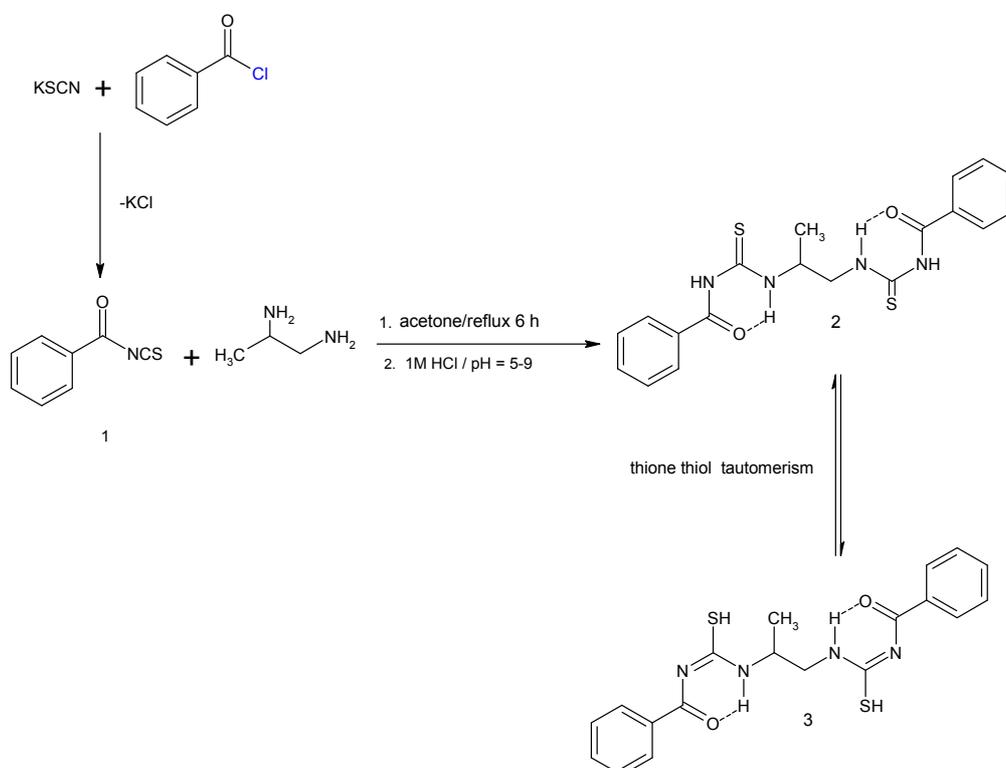
Department of Chemistry, Faculty of Education, Selcuk University, Meram 42099 Konya, Turkey

\* Author to whom correspondence should be addressed; E-Mail: g\_kurt\_81@hotmail.com

Tel. +90 332 8220; Fax: +90 332 323 82 25

Received: 9 September 2008 / Accepted: 3 November 2008 / Published: 7 November 2008

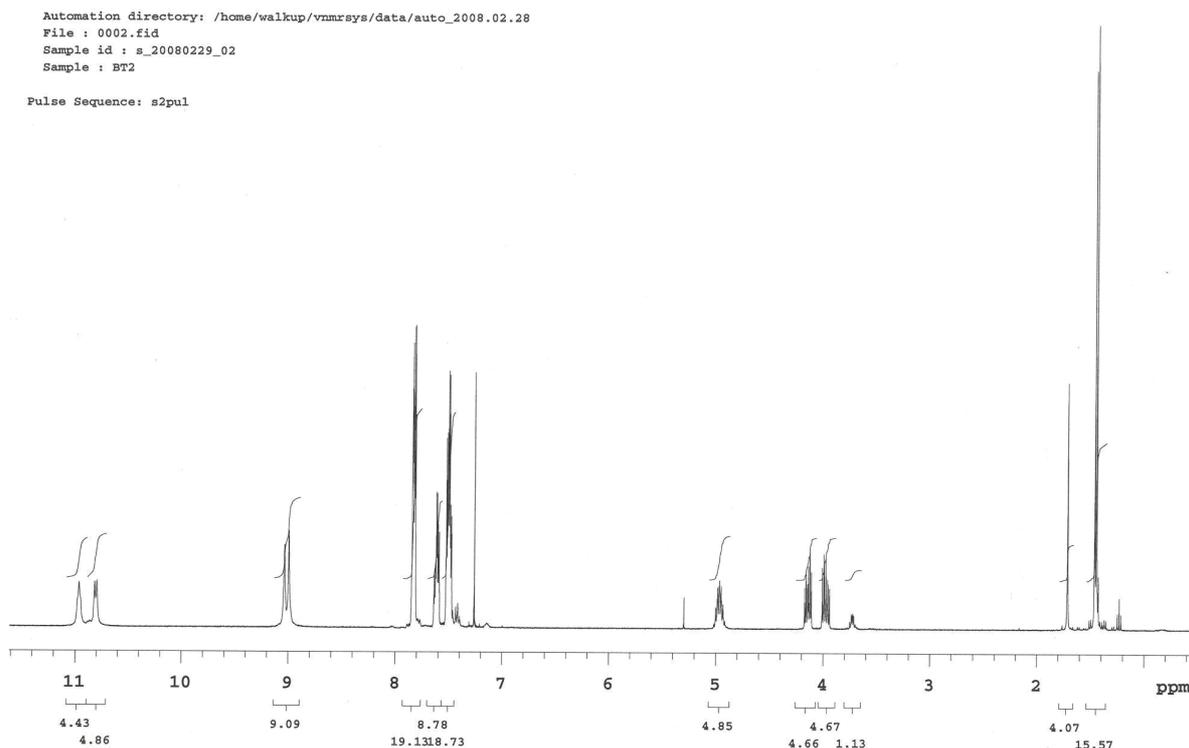
**Keywords:** Benzoylthiourea, benzoyl isothiocyanate, amine.



Benzoylthioureas have found some interest due to their biological activity [1], spectroscopic and structural properties [2,3], or as synthetic building blocks [4]. Here, we report the convenient

preparation of a new representative of this type of compounds. Benzoyl isothiocyanate (**1**) was prepared by known methods reported in the literature [5]. Benzoyl isothiocyanate (21 ml) was added to a solution of 1,2-diaminopropane (17 ml) in anhydrous acetone. The resulting mixture was refluxed for 6 h. Finally, the mixture was cooled in an ice bath and 1M HCl (250 ml) was added. The yellow precipitate was collected by filtration and it was washed with diethyl ether. The title compound **2** thus obtained was recrystallized from EtOH/CH<sub>2</sub>Cl<sub>2</sub>.

**Scheme 1.** <sup>1</sup>H NMR spectrum of **2**.



Color: yellow.

Mp 162-163°C.

Elemental analysis: Found: C, 57.5; H, 5.1; N, 13.9; S, 16.0. Calc. for C<sub>19</sub>H<sub>20</sub>N<sub>4</sub>S<sub>2</sub>O<sub>2</sub>: C, 57.0; H, 5.0; N, 14.0; S, 16.0.

<sup>1</sup>H NMR: δ (CDCl<sub>3</sub>, 400.1 MHz): 11.00 (s, 1H, NH-CO); 10.96 (d, 1H, NH-CO); 9.04 (s, 1H, NH); 8.99 (s, 1H, NH); 7.84–7.52 (m, 10H, PhH); 5.03–4.98 (m, 1H, CH); 4.19–3.99 (m, 2H, CH<sub>2</sub>); 1.46–1.44 (d, 3H, CH<sub>3</sub>).

<sup>13</sup>C NMR: δ (CDCl<sub>3</sub>, 100.0 MHz): 185.2 (C=S); 164.0 (C=O); 135.6–127.2 (C=C<sub>arom</sub>); 47.5 (CH); 46.9 (CH<sub>2</sub>); 18.7 (CH<sub>3</sub>).

IR (KBr) ν<sub>max</sub>/cm<sup>-1</sup>: 3350–3300 (N-H), 3161 (C-H<sub>aromatic</sub>), 3038 (CH<sub>3</sub>), 2935–2859 (C-H<sub>aliphatic</sub>), 1980–1835 (C=C), 1677 (C=O), 1540–1258 (C-N), 1189, 1162 (C=S).

UV-vis (CH<sub>2</sub>Cl<sub>2</sub>, abs): 240; 400.

**Table 1.** Thermal analysis of **2**.

Sample	Stage	TG results temperature range (°C)	DTA results temperature peak (°C)	Weight loss (%) Found/Calculated	Evolved moiety
<b>2</b>	I	180–240	226.71	43.684/44.75	C <sub>6</sub> H <sub>5</sub> CONHCSNH
	II	240–340	282.56	44.884/44.75	C <sub>6</sub> H <sub>5</sub> CONHCSNH

## References

1. Xu, X.Y.; Qian, X.H.; Li, Z.; Huang, Q.C.; Chen, G. *J. Fluorine Chem.* **2003**, *121*, 51-54.
2. Zhou, W.Q.; Yang, W.; Qiu, L.H.; Zhang, Y.; Yu, Z.F. *J. Mol. Struct.* **2005**, *749*, 89-95.
3. Arslan, H.; Külçü, N.; Flörke, U. *Spectrochim. Acta Pt. A* **2006**, *64*, 1065–1071
4. Kodomari, M.; Suzuki, M.; Tanigawa, K.; Aoyama, T. *Tetrahedron Lett.* **2005**, *46*, 5841-5843.
5. Binzet, G.; Arslan, H.; Flörke, U.; Külçü, N.; Duran, N. *J. Coordination Chem.* **2006**, *59*, 1395–1406.

© 2008 by the authors; licensee Molecular Diversity Preservation International, Basel, Switzerland.  
This article is an open-access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/3.0/>).