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Short Note

2-(2-Imino-1-methylimidazolidin-4-ylidene)hydrazinecarbothioamide

Ahmed A. Al-Amiery [1,2,]*, Abdul Amir H. Kadhum [1] and Abu Bakar Mohamad [1]

[1] Department of Chemical & Process Engineering, Universiti Kebangsaan Malaysia, 43600 Bangi Selangor, Malaysia

[2] Applied Chemistry division, Applied Science Department, University of Technology (UOT), Baghdad, Iraq

* Author to whom correspondence should be addressed; E-Mail: dr.ahmed1975@gmail.com; Tel.: +6-0-192-903-670.

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Abstract: A new thiosemicarbazone, 1-methyl-2-imino-N-(methanethialdiamine)-yl-4-iminoimidazolidin was synthesized and its UV-VIS, IR, and NMR spectroscopic data and CHN analysis are presented.

Keywords: 2-(2-imino-1-methylimidazolidin-4-ylidene)hydrazinecarbothioamide; thiosemicarbazide; thiosemicarbazones

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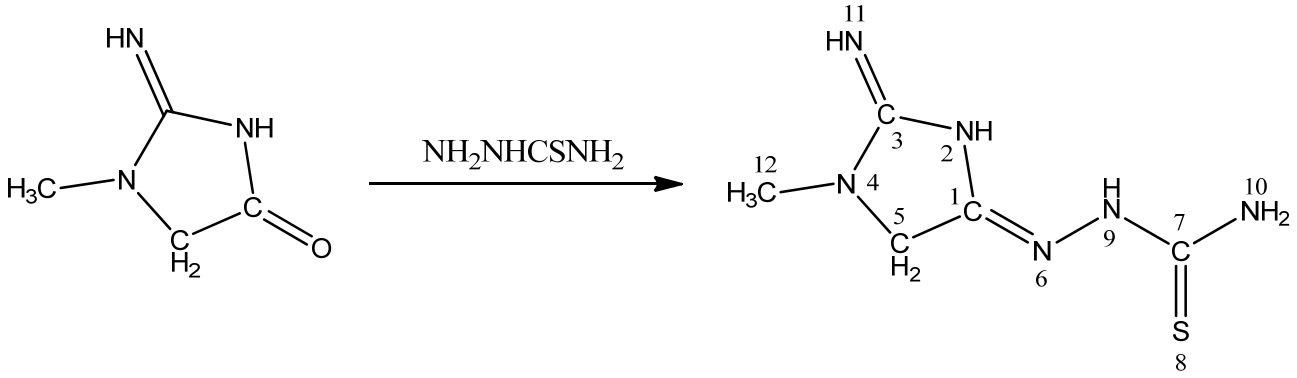
The chemistry of thiosemicarbazones has received considerable attention because of their variable bonding modes, promising biological implications, structural diversity, and ion-sensing ability [1,2]. They have been used as drugs and are reported to possess a wide variety of biological activities against bacteria, fungi, and certain type of tumors, and they are also a useful model for bioinorganic processes [3]. In continuation of previous studies [4–14], we have focused on synthesis of new heterocyclic compounds, and herein we are reporting the synthesis of 1-methyl-2-imino-N-(methanethialdiamine)-yl-4-iminoimidazolidin as new molecule (Scheme **1**).

Scheme 1. Synthesis of 1-methyl-2-imino-N-(methanethialdiamine)-yl-4-iminoimidazolidin.



Experimental

Synthesis of 2-(2-Imino-1-methylimidazolidin-4-ylidene)hydrazinecarbothioamide

A mixture of 1-methyl-4-oxo-2-iminoimidazolidin (2.26 g, 0.02 mol) and thiosemicarbazide (1.82 g, 0.02 mol) in 100 mL of ethanol was refluxed for 3 h. The solvent was evaporated on a rotary evaporator. The title compound was washed with cold ethanol, and dried under vacuum over P_4O_{10}. Yield 70%, (light brown) [7].

Melting point: 153 °C.

UV-VIS in DMF 255 and 322 nm.

FT-IR spectroscopy; 3421 cm^{-1} (N-H stretching vibrations, NH_2); 1631 cm^{-1} (C=N) and 1618 cm^{-1} (C=N).

^{1}H-NMR (300 MHz, DMSO-d_6): 1.80 (s, 1H, NH), 2.20 (s, 3H, CH_3), 2.70 (s, 2H, CH_2), 8.00 (s, 1H, NH), 9.10 (s, 1H, NH) and 10.90 (s, 1H, NH).

Elemental analysis: C, 32.25 (31.91); H, 5.41 (5.11); N, 45.13 (44.74).

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