Supporting Information

Deoxygenation of Dithiirane 1-Oxides with Lawesson's Reagent Leading to the Corresponding Dithiiranes

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Contents

(1) ORTEP drawing (Figure S1) and CIF file of **1,1,3,3-tetramethylindane-2-spiro-3'-dithiirane 1'-oxide (1e)**

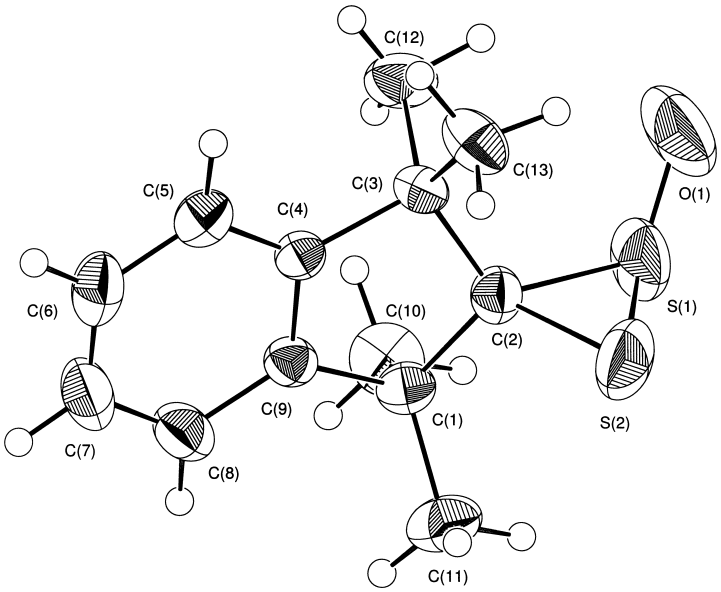

Figure S1

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1,1,3,3-tetramethylindane-2-spiro-3’-dithiirane 1’-oxide

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The study of the titled structure was undertaken to establish its three dimensional structure. Geometries are tabulated below. All diagrams and calculations were performed using maXus (Bruker Nonius, Delft & MacScience, Japan).
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Submission details

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Johnson, C. K. (1976). ORTEP-II. A Fortran Thermal-Ellipsoid Plot Program. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). J. Appl. Cryst. 27, 435.

Sheldrick, G. M. (1997). SHELXL97. Program for the Refinement of Crystal Structures. University of G¥"ottingen, Germany.

Blessing, R.H. (1995), Acta. Cryst. A51, 33-38.

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(2) ORTEP drawing (Figure S2) and CIF file of **3,3-di(1-adamantyl)dithiirane (3c)**

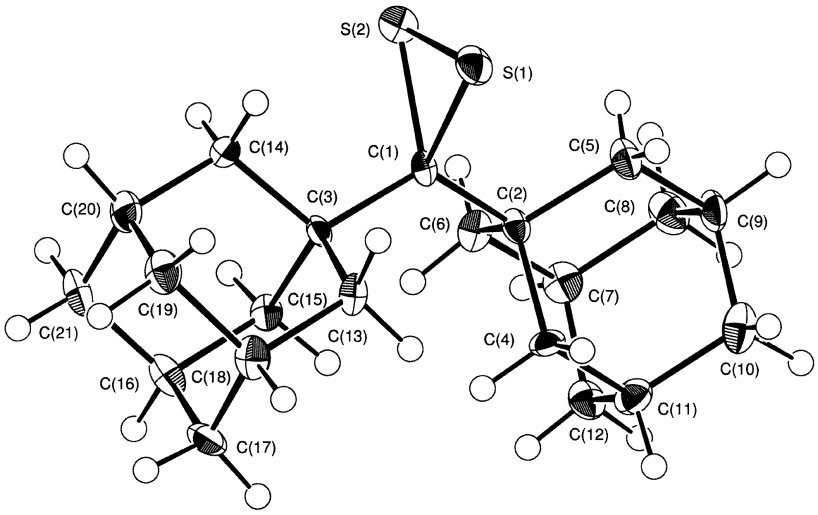

Figure S2

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The study of the titled structure was undertaken to establish its three
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Mackay, S., Gilmore, C. J.,Edwards, C., Stewart, N. & Shankland, K. (1999). maXus Computer Program for the Solution and Refinement of Crystal Structures. Bruker Nonius, The Netherlands, MacScience, Japan & The University of Glasgow.

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Blessing, R.H. (1995), Acta. Cryst. A51, 33-38.

#===END

(3) An ^{1}H NMR spectrum of **3-*t*-butyl-3-phenyldithiirane (3d)** (Figure S3)
(on the way to obtaining the analytical sample)

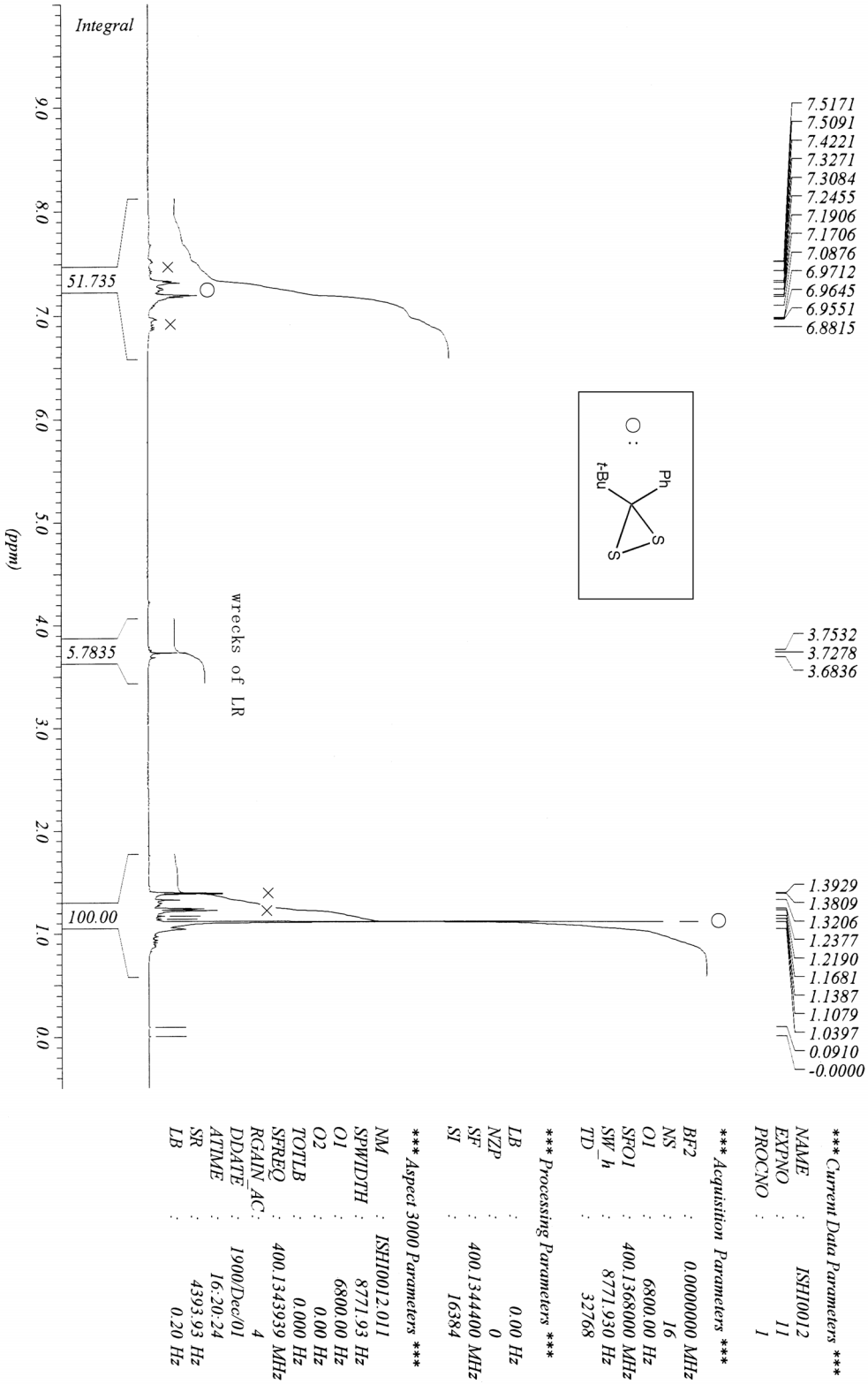


Figure S3

(4) An ^{1}H NMR spectrum of **1,1,3,3-tetramethylindane-2-spiro-3'-dithiirane (3e)** (the 10:1 mixture of **3e** and the thioketone) (Figure S4)

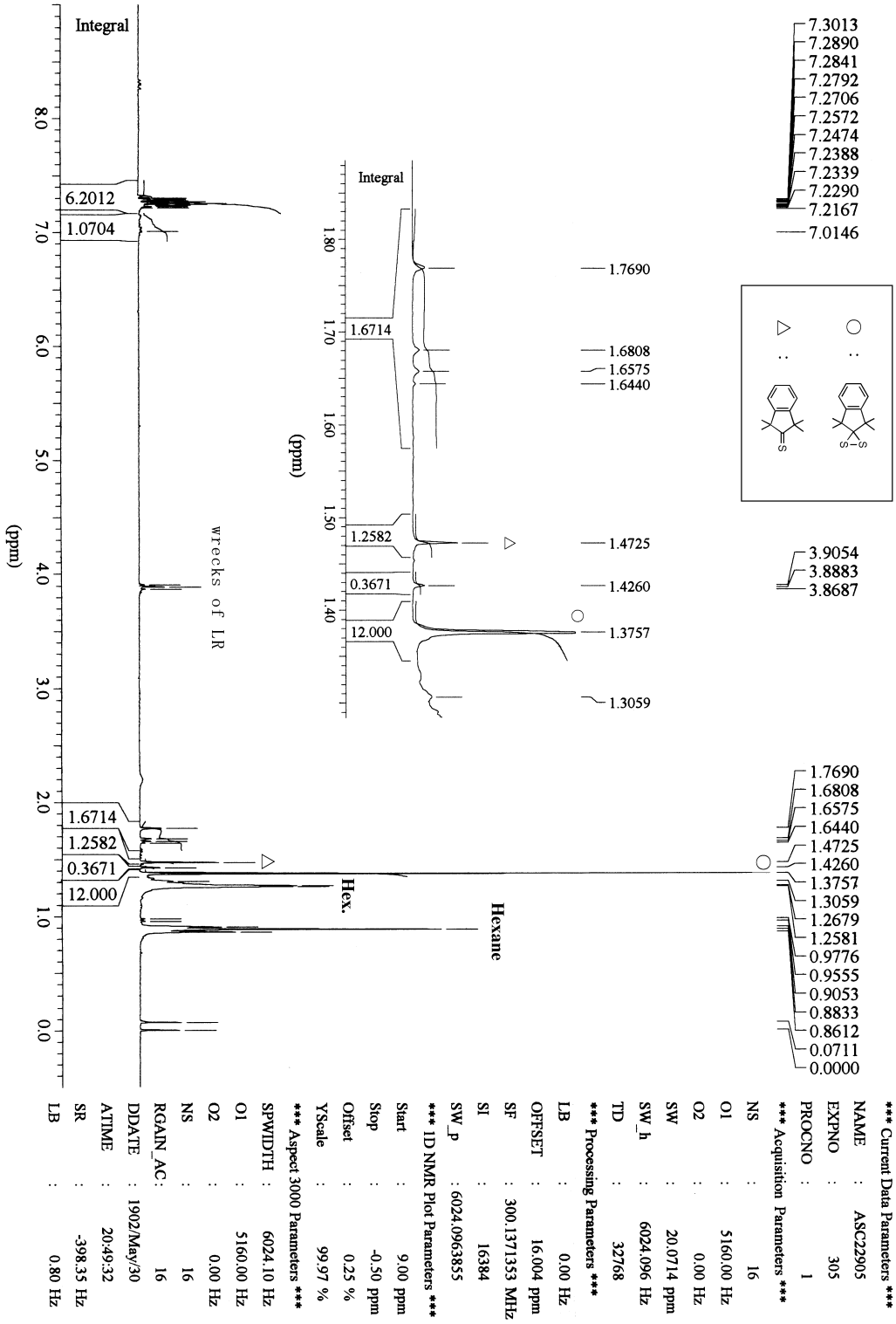
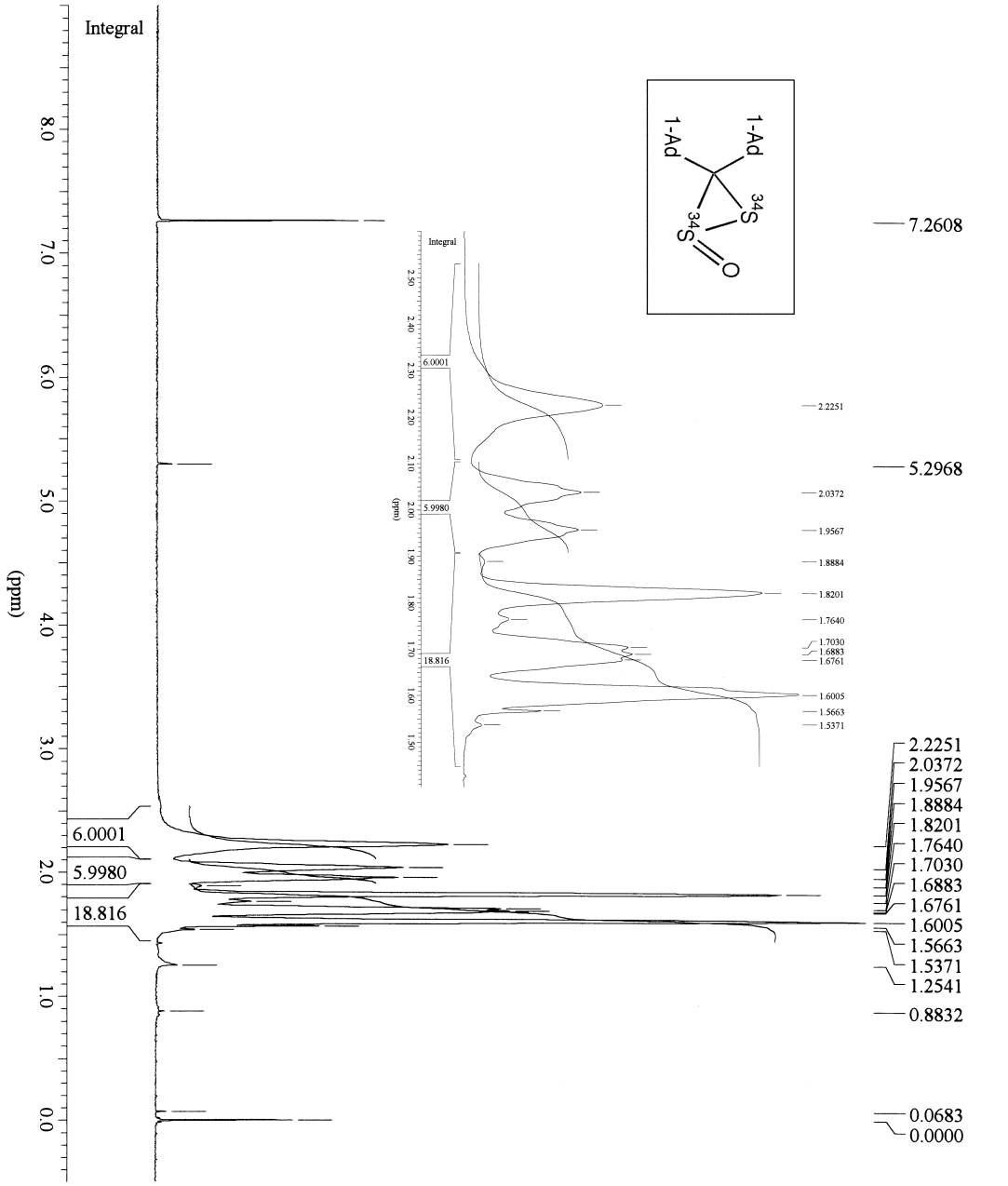


Figure S4

(5) An ^{1}H NMR spectrum of **3,3-di(1-adamantyl)-$^{34}S_2$-dithiirane 1-oxide (10)** (Figure S5)

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EXPNO     :  213
PROCNO    :  1

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O2        :  0.00 Hz
SW        :  19.9868 ppm
SW_h      :  4000.000 Hz
TD        :  16384

*** Processing Parameters ***
LB        :  0.00 Hz
OFFSET    :  15.041 ppm
SF        :  200.1323407 MHz
SI        :  8192
SW_p      :  4000.0000000

*** 1D NMR Plot Parameters ***
Start     :  9.00 ppm
Stop      :  -0.50 ppm
Offset    :  1.42 %
YScale    :  100.00 %

*** Aspect 3000 Parameters ***
SPWIDTH   :  4000.00 Hz
O1        :  3351.00 Hz
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NS        :  40
RGAIN_AC  :  16
DDATE     :  1901/Nov/21
ATIME     :  17:18:47
SR        :  2341.72 Hz
LB        :  0.20 Hz
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Figure S5

(6) An ^{1}H NMR spectrum of **3,3-di(1-adamantyl)-$^{34}S_2$-dithiirane (12)** (Figure S6)

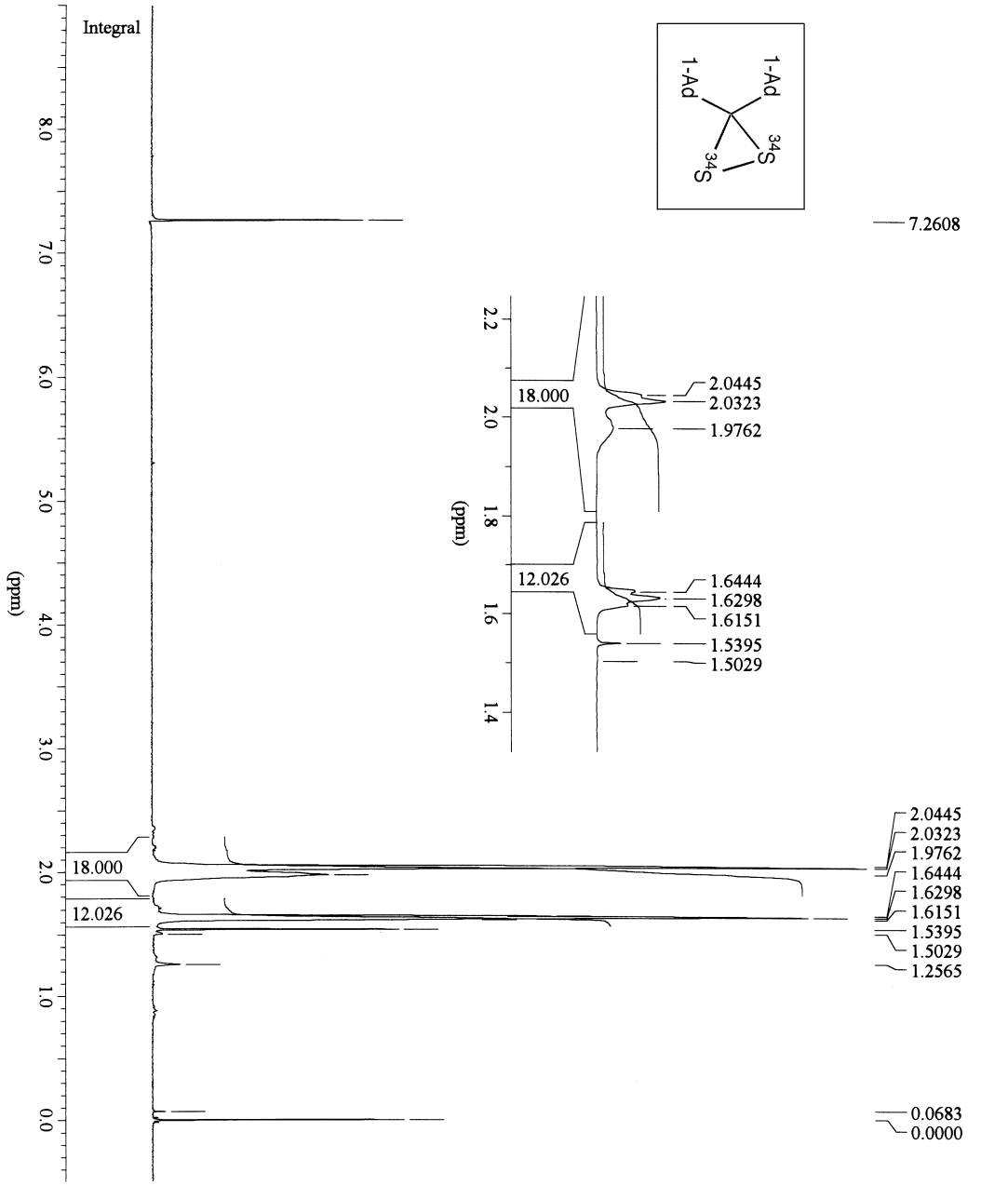

Figure S6

(7) A mass spectrum of **3,3-di(1-adamantyl)-$^{34}S_2$-dithiirane (12)** (Figure S7)

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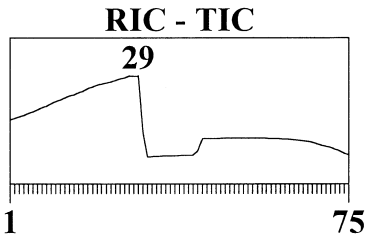
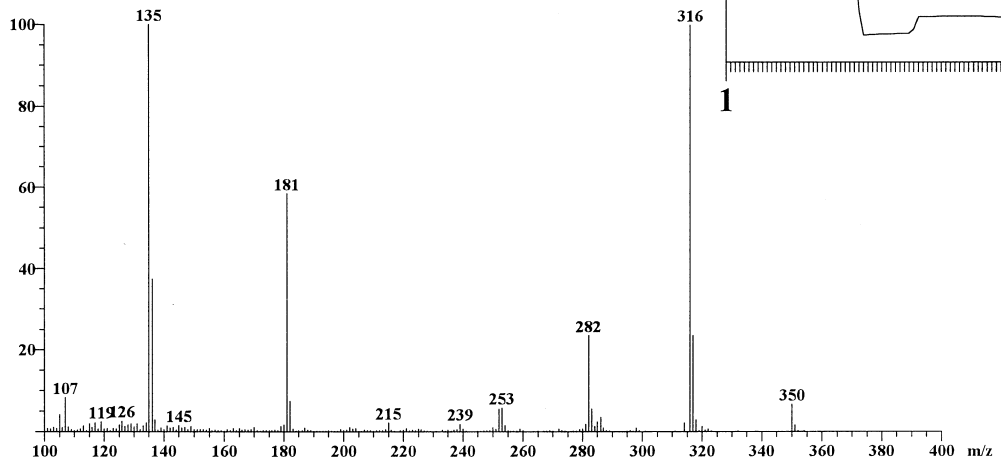
File: REMI08 **Date Run: 11-29-2001** **Time Run: 19:35:33**
Sample:
Instrument: JEOL JMS600 **Run By: jeol**
Inlet: Probe **Ionization mode: EI+** **Printed by: jeol**

Scan: 24 (Max Inten : 1048575) R.T.: 0:53.4 (Max Inten : 1048575)
Base: m/z 135; 100%FS (Max Inten : 1048575) TIC: 7034025
(Max Inten : 1048575)





Mass Table Threshold: 5% of Base **Displayed TIC: 4002337**

Mass	%Base	Mass	%Base	Mass	%Base	Mass	%Base
107.1	8.3	181.1	58.5	253.0	5.7	316.2	99.7
135.0	100.0	182.1	7.4	282.2	23.5	317.2	23.4
136.1	37.5	252.1	5.6	283.2	5.5	350.1	6.7

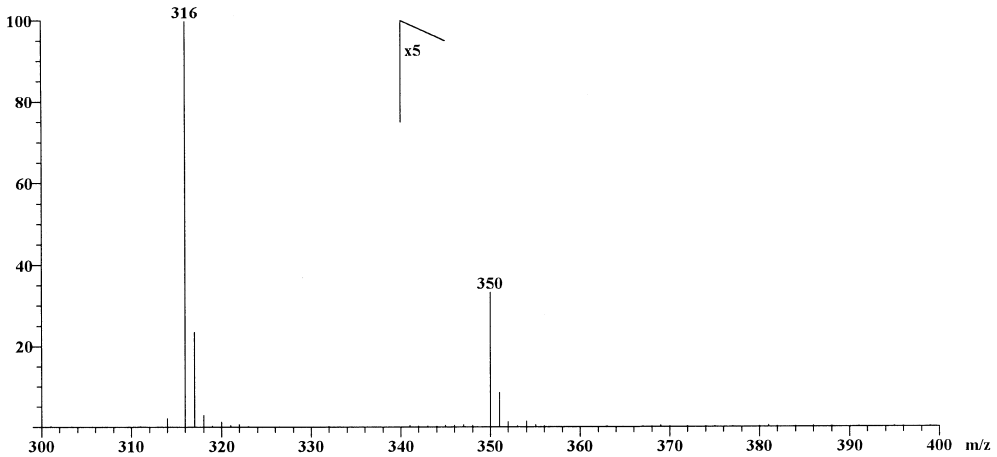


Figure S7