SAINS MALAYSIANA

www.ukm.my/jsm

UNIVERSITI KEBANGSAAN MALAYSIA
The National University of Malaysia

SAINS MALAYSIANA is published by Penerbit UKM and as of 2011 it will be published monthly (twelve issues a year). It contains articles on Earth Sciences, Health Sciences, Life Sciences, Mathematical Sciences and Physical Sciences. Articles are published in Malay or English.

The primary purpose of this journal is to act as a channel for the publication of research work undertaken at Universiti Kebangsaan Malaysia as well as other institutions.

All correspondence pertaining to articles and related matters should be addressed to:

Editor-in-Chief
SAINS MALAYSIANA
Faculty of Science and Technology
Universiti Kebangsaan Malaysia
43600 UKM Bangi, Selangor D.E. MALAYSIA
Tel: 603-89215423, Fax: 603-89256086
E-mail: jsm@ukm.my

- Subscription
- Poster

ISSN 0126-6039

SAINS MALAYSIANA is indexed and abstracted in ISI Thomson Reuters (Science Citation Index Expanded/SciSearch®, Journal Citation Reports/Science Edition), SCOPUS, Chemical Abstracts, Google-Scholar, MyAis and Zentralblatt MATH.

Google™ Custom Search Search

SJR SCImago Journal & Country Rank

EST MODUS IN REBUS

Home
Journal Rankings
Journal Search
Country Rankings
Country Search
Compare
Map Generator
Help
About Us

Show this information in your own website

Indicator 2002-2009 Value
SJR 0.03
Cites per doc 0.14
Total cites 25

Display journal title

Just copy the code below and paste within your html page:
<a href="http://www.scimagoj

How to cite this website?

SJR is developed by:
SCIMAGO LAB

Powered by SCOPUS

Journal Search

Search query

in Journal Title Search

Exact phrase

Sains Malaysiana

Country: Malaysia

Subject Area: Multidisciplinary

Subject Category: Multidisciplinary Q4

Publisher: Universiti Kebangsaan Malaysia. **Publication type:** Journals. **ISSN:** 01266039

Coverage: 2006-2010

H Index: 3

Charts Data

SJR indicator vs. Cites per Doc (2y)

The SJR indicator measures the scientific influence of the average article in a journal, it expresses how central to the global scientific discussion an average article of the journal is. Cites per Doc. (2y) measures the scientific impact of an average article published in the journal, it is computed using the same formula that journal impact factor ™ (Thomson Reuters).

Citation vs. Self-Citation

Evolution of the total number of citations and journal's self-citations received by a journal's

SAINS MALAYSIANA
www.ukm.my/jsm
UNIVERSITI KEBANGSAAN MALAYSIA

EDITORIAL BOARD

sains malaysiana

Editor-In-Chief

R. Abd-Shukor

Editors

Bioscience and Biotechnology
Halimah Abdullah Sani

Chemistry
Musa Ahmad

Engineering Geology
Abdul Ghani Rafek

Environmental Science and Natural Resources
Choong Chee Yen/Mohd Talib Latif

Food Science and Nutrition
Wan Aida Wan Mustapha

Geology
Hamzah Mohamed

Health Sciences
Suzana Shahar

Materials Science
Abdul Razak Daud

Mathematics
Mohd Salmi Md Noorani

Physics
Supian Samat

Statistics
Zaidi Isa

International Advisory Board

Biodiversity
Abdul Latiff Mohamad
Universiti Kebangsaan Malaysia, Malaysia

Environmental Chemistry and Chemical Education
J.O. Hill
La Trobe University, Australia

Environmental Science
P. Brimblecombe
University of East Anglia, UK

T. Kunz
Boston University, USA

Food Science
S. Hill
The University of Nottingham, UK

Materials Chemistry
M. Oyama
Kyoto University , Japan

Mathematics
I. Pop
University of Cluj, Romania

Molecular Biology
Farid Khan
The University of Manchester, UK

SCOPE

Sains Malaysiana is a refereed journal committed to the advancement of scholarly knowledge and research findings of the several branches of science and technology. The journal publishes articles, reviews, and research notes whose content and approach are of interest to a wide range of scholars.

Sains Malaysiana is published by an autonomous Editorial Board drawn from the Faculty of Science and Technology, Universiti Kebangsaan Malaysia . In addition, distinguished scholars from local and foreign universities are appointed to serve as advisory board members and referees.

SUBMISSION PROCEDURE

The Journal publishes manuscripts written in the Malay and English language. Manuscript submitted to the journal for publication should be original contribution and must not have been previously published or is under consideration simultaneously by any other publication.

Two copies of the manuscript, typed with double spacing on A4 paper not exceeding 15 pages, should be submitted to the *Editor-in-Chief, Sains Malaysiana, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor Darul Ehsan, Malaysia.*

An author(s) whose manuscript has been accepted for publication will be required to send a hard copy as well as the electronic file of the final edited version of the manuscript. While a manuscript is under consideration, be sure to inform the editor of any change in address.

FORMAT AND STYLE

The title of a manuscript should be concise, descriptive and preferably not exceeding 15 words. The manuscript must include an abstract, describing its main points within 150 - 250 words in the Malay and English language. For authors who are unable to provide the Malay version of the abstract, the editor will provide assistance.

In general, the contents should comprise of Introduction, Materials and Methods, Results and Discussion, Conclusion, Acknowledgement and References. The manuscript should be supplied with 3-5 keywords.

All illustrations including figures, charts and graphs, must be labelled and supplied on pages separate from the text. The desired placement in the text should be clearly indicated. These illustrations should be referred to and numbered serial, as figures. All illustrations should be clearly drawn in permanent ink or photographed in sharp black and white and reproduced in the form of high - contrast glossy prints or digital images and provided in camera ready form.

References in the text should be denoted by giving the name(s) of the author(s). All alphabetically ordered references list should be included at the end of the manuscript. All references cited in the text must appear in the reference list. Authors are responsible for the accuracy and completeness of all information in the reference. Manuscripts must conform to the references in Penerbit UKM style or the Chicago Manual of Style (University of Chicago Press). The references style adopted should be consistent throughout the manuscript.

COPYRIGHT

It is the author's responsibility to ensure that his or her submitted work does not infringe any existing copyright. Authors should obtain permission to reproduce or adapt copyrighted material and provide evidence of approval upon submitting the final version of a manuscript.

REVIEW PROCESS

Manuscripts will be reviewed by the Editorial Board and at least one independent referee. Decisions regarding the publication of a manuscript will be based on the Board's recommendations. The manuscript will be evaluated based on its appropriateness for *Sains Malaysiana,* contribution to the discipline, cogency of analysis, conceptual breadth, clarity of presentation and technical adequacy. Manuscripts submitted by members of the journal's Editorial Board are subjected to the same review procedure.

PROOFS, OFF-PRINTS AND ADDRESS

One set of proofs will be sent to the author(s) to be checked for printer's errors and it is the responsibility of the author(s) to submit corrections to the Editorial Board. Each author will be provided with 20 free off-prints of the article after publication and one complimentary copy of the journal in which the manuscript appears. Please indicate the address of the author(s) (including phone numbers, fax numbers and/or e-mail addresses) to who correspondence may be sent.

» Volume 36 • Number 1 • July 2007

Gadolinium(III) Complexes with Dialkyldithiocarbamates and 1,10-Phenantroline Kompleks (Gadolinium(III) dengan Dialkilditiokarbamat dan 1, 10 Fenantrolina)

Indah Raya, and Ibrahim Baba, and Bohari Mohd Yamin, and Djulia Onggo, (2007) *Gadolinium(III) Complexes with Dialkyldithiocarbamates and 1,10-Phenantroline Kompleks (Gadolinium(III) dengan Dialkilditiokarbamat dan 1, 10 Fenantrolina).* Sains Malaysiana , 36 (1). pp. 15-20. ISSN 01266039

Official URL: http://pkukmweb.ukm.my/~jsm/english_journals/vol36num1_2007/vol36num1_07page15-20.html

Affiliations

Universiti Kebangsaan Malaysia. Faculty of Science and Technology. School of Chemical Sciences and Food Technology
Universiti Kebangsaan Malaysia. Faculty of Science and Technology. School of Chemical Sciences and Food Technology
Universiti Kebangsaan Malaysia. Faculty of Science and Technology. School of Chemical Sciences and Food Technology

Abstract

A new series of gadolinium complexes with mixed ligands, dialkyl dithiocarbamate and 1,10-Phenantroline were successfully synthesized using "in situ" methods. Microelemental analysis data of complexes are in agreement with the general formula Gd[S2CNR'R"]3Phen (R' = ethyl, methyl; R" = butyl, heptyl, isopropyl, isobutyl, benzyl and cyclohexyl; Phen = 1,10-phenantroline). These complexes have been characterized using elemental analysis, infrared, thermogravimetric analysis, conductivity and magnetic measurements. Infrared spectra of complexes showed the thioureide n(C-N) bands were in the region of 1450 - 1490 cm-1. The single n(C-S) bands appeared in the region of 959 – 1003 cm-1 and n(C-H) bands in the region of 2853-2931 cm-1. The crystal structure of tris(N,N-methylbenzyldithiocarbamate)(1,10-phenantroline) gadolinium(III) adopts a triclinic system (space group P1) with a distorted dodecahedron geometry with a = 11.04(6) Å , b = 12.65(7) Å, c = 17.13(10) Å, a =73.86o(8) b =74.54o(8) g = 72.34o(8) and Z = 2. Three dithiocarbamates and one phenanthroline ligands were coordinated to the central Gd atom in bidentate manner.

[Satu siri kompleks logam gadolinium baru dengan dialkilditiokarbamat dan 1,10-fenantrolin telah berjaya disintesis secara "in-situ". Hasil analisis bersetuju dengan formula umum Gd[S2CNR'R"]3Phen (R' = metil, etil; R" = butil, heptil, isopropil, isobutil, benzil dan sikloheksil; Phen = fenantrolina). Kompleks telah diciri dengan analisis unsur, spektroskopi inframerah, analisis termogravimetri, pengukuran kemagnetan dan pengukuran konduktiviti. Spektrum inframerah kompleks menunjukkan jalur tioureida n(C-N) berada di sekitar 1450-1490 cm-1, Manakala jalur tunggal n(C-S) pula berada di kawasan 959-1003 cm-1 dan jalur n(C-H) berada di kawasan 2853-2931 cm-1. Struktur hablur tris(N,N-metilbenzilditiokarbamat)(1,10-fenantrolin)gadolinium(III) menunjukkan sistem hablur triklinik (kumpulan ruang P1) dengan geometri *dodekahedron terherot* dengan a = 11.04(6) Å, b = 12.65(7) Å, c = 17.13(10) Å, a =73.86o(8) b =74.54o(8) g = 72.34o(8) and Z = 2. Tiga molekul ditiokarbamat dan satu molekul fenantrolina memebentuk ikatan kelat kepada atom Gd secara bidentat].

Item Type: Journal
Keywords: Gadolinium; dithiocarbamate; crystal structure
Subjects: Q Science, Computer Science
ID Code: 2814

Brown, D. A., Glass, W. K. & Burke, M. A. 1976. The general use of IR spectral criteria in disscussions of the bonding and structure of metal dithiocarbamate. Spectrochem. Acta 32A:137-143. SEEK

Coucouvanis, D. & Fackler, J. P. Jr. 1976. Square-planar sulphur complexes. Inorganic Chem. 6: 2047-2053. SEEK

Criado, J. J., Fernandez, I. & Macias, B. 1990. Novel chelates of Pd(II) dithiocarbamates, spectroscopic studies and thermal behaviour. Inorg. Chem. Acta 174:67-75 SEEK

Haas, W. & Schwarz, T. 1963. NH4 diethanol dithiocarbamate a reagent for the spectrophotometric determination of Mo and U. Microchem. Ichonal. Acta 58: 253-259. SEEK

Hursthouse, M. B., Malik, M. A., Motervalli, M. & O'Brien, P. 1992. The crystal and molecular structure of N,N-dimethyldiselenocarbamatocadmium(II): cadmium and zinc dimethyldiselenocarbamates as precursors for selenides. SEEK

Polyhedron 11: 45-48. SEEK

Nomura, R., Takabe, A., & Matsuda, H. 1987. Facile synthesis of antimony dithiocarbamate complexes. Polyhedron 6: 411-416. [SEEK]

Sharma, H., Watanabe, H., Tamura, H., Yasui, H., Matsushita, R. & Takada, J. 1998. Insulin-mimetic vanadyl-dithiocarbamate complexes. Inorg. Chim. Acta 283: 175-183. [SEEK]

Sheldrick, G. M. 1996. SAINT V4, Software reference manual, Siemens Analytical X-ray System, Madison, WI, USA. [SEEK]

Sheldrick, G. M. 1996. SADABS, Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen, Germany. [SEEK]

Sheldrick, G. M. 1997. SHELXTL V 5.1, Software reference manual, Bruker AXS, Inc., Madison, WI, USA. [SEEK]

Siddal, T. H. & Steward, W. E. 1970. Preparation and studies of magnetic and spectroscopic properties of alkyl ammonium lanthanide tetrakis (N,N-dialkyldithiocarbamates). J. Inorg Nuclear Chem. 32: 1147-1158. [SEEK]

Siemens, 1996, SMART and SAINT. Area Detector Control and Integration Software. Siemens Analytical X-Ray Systems, Inc., Madison, Wisconsin, USA. [SEEK]

Su, C., Tan, M., Tang, N., Gan, X. & Liu, W. 1997. Synthesis, structure and spectroscopic properties of dimmethylammonium lanthanide tetrakis(N, N-dimmethyldithiocarbamate). Polyhedron 16: 1643-1650. [SEEK]

Tang, N., Zhu, H., Tan, M., Gan, X. & Wang, A. 1991. Synthesis and characterisation of dimethylammonium lanthanide (monomethyldithiocarbamate). Polyhedron 16:1643-1650 . [SEEK]

Thorn, G.D., & Ludwig, R.A., 1962. The dithiocarbamates abd related compounds. New York: Elsevier Pub.Co. [SEEK]

Venkatachalam, V., Ramalingam, K., Casellato, U. & Graziani, R. 1997. Structural and electronic effect of alkyl substituents on the main group dithiocarbamato complexes: crystals and molecular structures of tris(N,N'-iminodiethanoldithiocarbamato)metal(III) complexes (M = As, Sb and Bi) and cyclic voltammetric studies on substituted dithiocarbamates. Polyhedron 16(7): 1211-1221. [SEEK]

Zhu, H., Tang, N., Gan, X., Wang, A. & Tan, M. 1993. Synthesis and characterization of light lanthanide piperidinocarbodithioate complexes. Polyhedron 12: 945-991. [SEEK]

Sains Malaysiana 36(1): 15-20 (2007)

Gadolinium(III) Complexes with Dialkyldithiocarbamates and 1,10-Phenantroline

(Kompleks Gadolinium(III) dengan Dialkilditiokarbamat dan 1, 10 Fenantrolina)

Indah Raya, Ibrahim Baba, Bohari Mohd Yamin & Djulia Onggo
School of Chemical Sciences & Food Technology
Faculty of Science and Technology, Universiti Kebangsaan Malaysia
43600 Bangi, Selangor, D.E. Malaysia

ABSTRACT

A new series of gadolinium complexes with mixed ligands, dialkyl dithiocarbamate and 1,10-Phenantroline were successfully synthesized using "in situ" methods. Microelemental analysis data of complexes are in agreement with the general formula $Gd[S_2CNR'R"]_3Phen$ (R' = ethyl, methyl; R" = butyl, heptyl, isopropyl, isobutyl, benzyl and cyclohexyl; Phen = 1,10-phenantroline). These complexes have been characterized using elemental analysis, infrared, thermogravimetric analysis, conductivity and magnetic measurements. Infrared spectra of complexes showed the thioureide n(C-N) bands were in the region of 1450 - 1490 cm^{-1}. The single n(C-S) bands appeared in the region of 959 – 1003 cm^{-1} and n(C-H) bands in the region of 2853-2931 cm^{-1}. The crystal structure of tris(N,N-methylbenzyldithiocarbamate)(1,10-phenantroline) gadolinium(III) adopts a triclinic system (space group P$\bar{1}$) with a distorted dodecahedron geometry with a = 11.04(6) Å , b = 12.65(7) Å, c = 17.13(10) Å, a =73.86°(8) b =74.54°(8) g = 72.34°(8) and Z = 2. Three dithiocarbamates and one phenanthroline ligands were coordinated to the central Gd atom in bidentate manner.

Keywords: Gadolinium; dithiocarbamate; crystal structure

ABSTRAK

Satu siri kompleks logam gadolinium baru dengan dialkilditiokarbamat dan 1,10-fenantrolin telah berjaya disintesis secara "in-situ". Hasil analisis bersetuju dengan formula umum $Gd[S_2CNR'R"]_3Phen$ (R' = metil, etil; R" = butil, heptil, isopropil, isobutil, benzil dan sikloheksil; Phen = fenantrolina). Kompleks telah diciri dengan analisis unsur, spektroskopi inframerah, analisis termogravimetri, pengukuran kemagnetan dan pengukuran konduktiviti. Spektrum inframerah kompleks menunjukkan jalur tioureida n(C-N) berada di sekitar 1450-1490 cm^{-1}, Manakala jalur tunggal n(C-S) pula berada di kawasan 959-1003 cm^{-1} dan jalur n(C-H) berada di kawasan 2853-2931 cm^{-1}. Struktur hablur tris(N,N-metilbenzilditiokarbamat)(1,10-fenantrolin)gadolinium(III) menunjukkan sistem hablur triklinik (kumpulan ruang P$\bar{1}$) dengan geometri dodekahedron terherot dengan a = 11.04(6) Å, b = 12.65(7) Å, c = 17.13(10) Å, a =73.86°(8) b =74.54°(8) g = 72.34°(8) and Z = 2. Tiga molekul ditiokarbamat dan satu molekul fenantrolina memebentuk ikatan kelat kepada atom Gd secara bidentat.

Kata kunci: Gadolinium; ditiokarbamat; struktur hablur

RUJUKAN/REFERENCES

Brown, D. A., Glass, W. K. & Burke, M. A. 1976. The general use of IR spectral criteria in disscussions of the bonding and structure of metal dithiocarbamate. *Spectrochem. Acta* 32A:137-143.

Coucouvanis, D. & Fackler, J. P. Jr. 1976. Square-planar sulphur complexes. *Inorganic Chem.* 6: 2047-2053.

Criado, J. J., Fernandez, I. & Macías, B. 1990. Novel chelates of Pd(II) dithiocarbamates, spectroscopic studies and thermal behaviour. *Inorg. Chem. Acta* 174:67-75

Haas, W. & Schwarz, T. 1963. NH_4 diethanol dithiocarbamate a reagent for the spectrophotometric determination of Mo and U. *Microchem. Ichonal. Acta* 58: 253-259.

Hursthouse, M. B., Malik, M. A., Motervalli, M. & O'Brien, P. 1992. The crystal and molecular structure of N,N-dimethyldiselenocarbamatocadmium(II): cadmium and zinc dimethyldiselenocarbamates as precursors for selenides. *Polyhedron* 11: 45-48.

Nomura, R., Takabe, A., & Matsuda, H. 1987. Facile synthesis of antimony dithiocarbamate complexes. *Polyhedron* 6: 411-416.

Sharma, H., Watanabe, H., Tamura, H., Yasui, H., Matsushita, R. & Takada, J. 1998. Insulin-mimetic vanadyl-dithiocarbamate complexes. *Inorg. Chim. Acta* 283: 175-183.

Sheldrick, G. M. 1996. SAINT V4, Software reference manual, Siemens Analytical X-ray System, Madison, WI, USA.

Sheldrick, G. M. 1996. SADABS, Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen, Germany.

Sheldrick, G. M. 1997. SHELXTL V 5.1, Software reference manual, Bruker AXS, Inc., Madison, WI, USA.

Siddal, T. H. & Steward, W. E. 1970. Preparation and studies of magnetic and spectroscopic properties of alkyl ammonium lanthanide tetrakis (N,N-dialkyldithiocarbamates). *J. Inorg.Nuclear Chem.* 32: 1147-1158.

Siemens, 1996, *SMART* and *SAINT*. Area Detector Control and Integration Software. Siemens Analytical X-Ray Systems, Inc., Madison, Wisconsin, USA.

Su, C., Tan, M., Tang, N., Gan, X. & Liu, W. 1997. Synthesis, structure and spectroscopic properties of dimmethylammonium lanthanide tetrakis(*N*, *N*-dimmethyldithiocarbamate). *Polyhedron* 16: 1643-1650.

Tang, N., Zhu, H., Tan, M., Gan, X. & Wang, A. 1991. Synthesis and characterisation of dimethylammonium lanthanide (monomethyldithiocarbamate). *Polyhedron* 16:1643-1650 .

Thorn, G.D., & Ludwig, R.A., 1962. The dithiocarbamates abd related compounds. New York: Elsevier Pub.Co.

Venkatachalam, V., Ramalingam, K., Casellato, U. & Graziani, R. 1997. Structural and electronic effect of alkyl substituents on the main group dithiocarbamato complexes: crystals and molecular structures of tris(*N,N'*-iminodiethanoldithiocarbamato)metal(III) complexes (M = As, Sb and Bi) and cyclic voltammetric studies on substituted dithiocarbamates. *Polyhedron* 16(7): 1211-1221.

Zhu, H., Tang, N., Gan, X., Wang, A. & Tan, M. 1993. Synthesis and characterization of light lanthanide piperidinocarbodithioate complexes. *Polyhedron* 12: 945-991.

« previous content next »

Home Editorial Board Guide for Authors Contents, Abstract and References Malay

Sains Malaysiana 36(1)(2007): 15-20

Gadolinium(III) Complexes with Dialkyldithiocarbamates and 1,10-Phenantroline

(Kompleks Gadolinium(III) dengan Dialkilditiokarbamat dan 1,10 Fenantrolina)

INDAH RAYA, IBRAHIM BABA, BOHARI MOHD YAMIN & DJULIA ONGGO

ABSTRACT

A new series of gadolinium complexes with mixed ligands, dialkyl dithiocarbamate and 1,10-Phenantroline were successfully synthesized using "in situ" methods. Microelemental analysis data of complexes are in agreement with the general formula Gd[S_2CNR'R"]$_3$Phen (R' = ethyl, methyl; R" = butyl, heptyl, isopropyl, isobutyl, benzyl and cyclohexyl; Phen = 1,10-phenantroline). These complexes have been characterized using elemental analysis, infrared, thermogravimetric analysis, conductivity and magnetic measurements. Infrared spectra of complexes showed the thioureide ν(C-N) bands were in the region of 1450 - 1490 cm^{-1}. The single ν(C-S) bands appeared in the region of 959 – 1003 cm^{-1} and ν(C-H) bands in the region of 2853-2931 cm^{-1}. The crystal structure of tris(N,N-methylbenzyldithiocarbamate) (1,10-phenantroline) gadolinium(III) adopts a triclinic system (space group P?) with a distorted dodecahedron geometry with a = 11.04(6) Å , b = 12.65(7) Å, c = 17.13(10) Å, α =73.86°(8) β =74.54°(8) γ = 72.34°(8) and Z = 2. Three dithiocarbamates and one phenanthroline ligands were coordinated to the central Gd atom in bidentate manner.

Keywords: Gadolinium; dithiocarbamate; crystal structure

ABSTRAK

Satu siri kompleks logam gadolinium baru dengan dialkilditiokarbamat dan 1,10-fenantrolin telah berjaya disintesis secara "in-situ". Hasil analisis bersetuju dengan formula umum Gd[S_2CNR'R"]$_3$Phen (R' = metil, etil; R" = butil, heptil, isopropil, isobutil, benzil dan sikloheksil; Phen = fenantrolina). Kompleks telah diciri dengan analisis unsur, spektroskopi inframerah, analisis termogravimetri, pengukuran kemagnetan dan pengukuran konduktiviti. Spektrum inframerah kompleks menunjukkan jalur tioureida ν(C-N) berada di sekitar 1450-1490 cm^{-1}, Manakala jalur tunggal ν(C-S) pula berada di kawasan 959-1003 cm^{-1} dan jalur ν(C-H) berada di kawasan 2853-2931 cm^{-1}. Struktur hablur tris(N,N-metilbenzilditiokarbamat)(1,10-fenantrolin)gadolinium(III) menunjukkan sistem hablur triklinik (kumpulan ruang P?) dengan geometri dodekahedron terherot dengan a = 11.04(6) Å , b = 12.65(7) Å, c = 17.13(10) Å, α =73.86°(8) β =74.54°(8) γ = 72.34°(8) and Z = 2. Tiga molekul ditiokarbamat dan satu molekul fenantrolina memebentuk ikatan kelat kepada atom Gd secara bidentat.

Kata kunci: Gadolinium; ditiokarbamat; struktur hablur

INTRODUCTION

A number of dithiocarbamate complexes with striking structural features and wide range of applications has been reported. These complexes were widely used in industries of agriculture, pharmaceutical and medicine (Coucovanis & Fackler 1976; Hursthouse et al. 1992). Almost all of the dithiocarbamate complexes with lanthanide were prepared in inert atmosphere using anhydrous lanthanides salts (Siddal & Steward 1970; Tang et al. 1991; Zhu et al. 1993). Su et al. (1997) synthesized complexes of lanthanide dithiocarbamate together with 1,10-phenantroline by using small amount of dialkyldithiocarbamate ligands (dialkyl = monomethyl, dimethyl and diethyl). However, another method to synthesize [Ln(S_2CNR'R")$_3$Phen] was by reacting of [Ln(S_2CNR'R")$_3$] with 1,10-phenantroline (Tang et al. 1991). The main difficulty with this method was to prepare [Ln(S_2CNR'R")$_3$] but once the complexes formed it was easily hydrolyzed. To avoid this problem the preparation was carried out in dry solvents.

This paper reports the synthesis and characterization of a series of gadolinium(III) complexes with various dithiocarbamate ligands and the crystal structure of tris(*N,N*-methylbenzyldithiocarbamate)(1,10-phenantroline) gadolinium(III), [Gd(MBzdtc)$_3$Phen]. This particular technique has successfully been used to synthesize seven types of dialkyldithiocarbamate complexes with gadolinium i.e. *ethylbutyldithiocarbamate* (EBudtc$^-$), *heptylmethyldithiocarbamate* (HMdtc$^-$), *ethylisopropyldithiocarbamate* (EiPrdtc$^-$), *methylisobutyldithiocarbamate* (MiBudtc$^-$), *methylbenzyldithiocarbamate* (MBzdtc$^-$), *ethylbenzyldithiocarbamate* (EBzdtc$^-$) and *ethylcyclohexyldithiocarbamate* (EChdtc$^-$).

EXPERIMENTAL

INSTRUMENTATION

The melting point of the compounds was determined by Electrothermal IA 9100. Elemental analysis were recorded

on Fison EA 1108, IR spectra were recorded as KBr discs in the range 4000 – 500 cm^{-1} and 500 - 200 cm^{-1} using Perkin Elmer FTIR Model GX. The magnetic property was measured with Sherwood Scientific Magnetic susceptibility balance. Thermal analysis was carried out on Mettler Toledo Model STGA/SDTA 851. The electrical conductivity was measured by Philips conductivity bridge Model PR 9645. X-ray structure determination was carried out by Bruker SMART APEX and the accompanying SHELXTL programming suite.

CHEMICALS

Acetonitrile (Hmbg Chemical), dialkylamine and ethanol (Fluka Chemical), carbon disulphide and methanol (Ajax Chemical Ltd), dichloromethane (R & M Chemical), gadolinium(III) chloride and 1,10-phenantroline (Merck) were used as supplied without further purification.

X-RAY CRYSTALLOGRAPHY

Room-temperature diffraction data were collected on a Bruker SMART APEX area-detector diffractometer (MoK_α radiation, λ=0.71073 Å) on a crystal size 0.50×0.19×0.05 mm^3 over the $1.76< \theta <27.0$ range (Siemens, 1996). The structure was solved and refined by using the SHELXS (Sheldrick 1997). The final *R* (I>2/s(I)) and *Rw* values were 0.07 and 0.1820, respectively. All non-hydrogen atoms were refined anisotropically. The perspective view of the molecule was obtained using SHELXTL (Sheldrick 1996).

SYNTHESIS OF DITHIOCARBAMATE COMPLEXES

A solution of potassium dithiocarbamate was synthesized using a technique published by Thorn and Ludwig (1962). An ethanolic solution of potassium hydroxide (30 mL) was added drop wise to dialkylamine (30 mmol) and CS_2 (30 mmol) by and stirred vigorously at temperature below 15°C for 30 minutes. A gadolinium trichloride solutions (10 mmol) was added to 1,10-phenantroline (10 mmol) in boiling water. The dithiocarbamate complexes were synthesized by the reaction between potassium dithiocarbamate and 1,10-phenantroline gadolinium trichloride solutions. The mixture was heated for 10 minutes and then allowed to stand for five minutes until a precipitate was formed. Recrystallization was performed by using a mixture of dichloromethane and methanol (2:1 v/v) with crystal started to appear in about four days.

RESULT AND DISCUSSION

Microelemental analysis and melting points data are shown in Table 1, while magnetic and conductivity data are shown in Table 2. The elemental analysis data of complexes are in agreement with the general formula $M[S_2CNR'R'']_3Phen$ [R' = ethyl, methyl; R'' = butyl, heptyl, isopropyl, isobutyl, benzyl and cyclohexyl; M = Gd(III); Phen = 1,10-phenantroline; n = 3]. The magnetic measurement data has proven that all gadolinium dithiocarbamate complexes in Table 2 are paramagnetic and electrical conductivity data showed that all complexes are non-electrolytes.

Important IR peaks of the complexes have been reported in Table 3. The ν(C=N) modes appeared in the region of thioureide band which is in 1450 – 1490 cm^{-1}, while ν(C=S) modes appeared in the region 959 – 1003 cm^{-1} (Brown 1976; Haas & Schwarz 1963). The absence of splitted of ν(C=S) bands in the range of 959 – 1003 cm^{-1} indicated a bidentate nature of the chelation of the dithiocarbamate ligands (Criado et al. 1990; Nomura et al. 1987). The molar conductance data, in range 46-55 $m.ohm^{-1}$, showed that all complexes were non-electrolytes indicating that the ligand was coordinated to the metal ions as uninegatively charged bidentate species (Su et al. 1997). The highest energy of ν(C=N) and ν(C=S) bands observed for $Gd(EBudtc)_3Phen$ may be due to the electron donating

TABLE 1. Analytical and physical data of $Gd(S_2CNR'R'')_3Phen$ complexes

Complexes	Colour	Yield (%)	Melting point (°C)	Found (Calculated) (%)				
				C	H	N	S	M
$Gd(EBudtc)_3Phen$	White	66	138-140	46.414 (45.89)	5.731 (5.91)	8.728 (8.02)	21.476 (22.15)	17.30 (18.11)
$Gd(HMdtc)_3Phen$	White	45	118-119	48.599 (49.25)	7.220 (6.72)	8.249 (7.19)	18.65 (20.04)	16.56 (17.05)
$Gd(EiPrdtc)_3Phen$	White	62	126-128	43.48 (43.68)	6.02 (5.58)	7.767 (8.34)	22.83 (23.19)	17.97 (18.12)
$Gd(MiBudtc)_3Phen$	White	71	118-121	42.83 (43.48)	5.54 (6.27)	8.249 (8.25)	21.333 (22.92)	17.81 (17.94)
$Gd(MBzdtc)_3Phen$	Cream	86	143-145	50.517 (50.404)	4.009 (4.45)	7.272 (7.53)	20.393 (20.7)	15.64 (16.32)
$Gd(EBzdtc)_3Phen$	White	83	145-148	51.01 (50.69)	4.67 (4.64)	6.809 (7.03)	19.881 (19.73)	16.70 (15.45)
$Gd(EChdtc)_3Phen$	Yellow White	88	122-124	48.291 (49.59)	6.016 (6.02)	6.006 (7.17)	19.165 (20.19)	15.30 (15.82)

effect of the ethyl and butyl group compare to the other groups (Venchatalam et al. 1997).

The thermograms of thermal gravimetric (TGA) analysis of complexes in static nitrogen were shown in Figure 1. The thermogram of $Gd(MBzdtc)_3Phen$ and $Gd(EBzdtc)_3Phen$ showed a decomposition temperature above 360°C that indicate both complexes possess good thermal stability. While $Gd(HMdtc)_3Phen$ and $Gd(MiBudtc)_3Phen$ complexes started to decompose at 280°C. However, $Gd(EiPrdtc)_3Phen$ and $Gd(EChdtc)_3Phen$ complexes were less stable than other; because they decomposed at below 110°C as illustrated in Figure 1.

TABLE 2. Magnetic moment and electrical conductivity of $Gd(S_2CNR'R'')_3Phen$ complexes

Complexes	Magnetic Moment μ_{eff} (B.M.)	Electrical Conductivity σ, $(ohm\text{-}m)^{-1}$
$Gd(EBudtc)_3Phen$	7.92	46
$Gd(HMdtc)_3Phen$	7.95	53
$Gd(EiPrtc)_3Phen$	7.20	51
$Gd(MiBudtc)_3Phen$	7.78	50
$Gd(MBzdtc)_3Phen$	7.27	55
$Gd(EBzdtc)_3Phen$	7.79	55
$Gd(EChdtc)_3Phen$	7.68	48

X-RAY CRYSTALLOGRAPHY

A suitable crystal was obtained for $Gd[MBzdtc]_3Phen$. The compound crystallized in triclinic system with space group $P\bar{1}$. The crystal data and refinement parameter are given Table 4. Table 5 showed selected bond distances and angles. The molecular structure of the compound shown in (Figure 2) supports the elemental and spectroscopic data given in Table 1, 2 and 3.

One phenantroline and three methylbenzyldithiocarbamate ligands were chelated to

TABLE 3. Infrared data for $Gd(S_2CNR'R'')_3Phen$ complexes

Complexes	Frequency (cm^{-1})				
	ν(C-H)	ν(C-N)	ν(C=S)	ν(Gd-N)	ν(Gd-S)
$Gd(EBudtc)_3Phen$	2929.3	1489.1	1001.4	363.8	273.8
$Gd(HMdtc)_3Phen$	2925.5 2853.6	1485.3	987.7	363.5	276.1
$Gd(EiPrdtc)_3Phen$	2973.2	1467.3	999.8	359.1	277.8
$Gd(MiBudtc)_3Phen$	2915.1	1476.5	989.8	363.6	278.4
$Gd(MBzdtc)_3Phen$	2928.3	1471.3 1451.7	959.7	363.8	276.8
$Gd(EBzdtc)_3Phen$	2927.9	1471.0 1451.0	959.4	361.5	277.2
$Gd(EChdtc)_3Phen$	2930.3	1450.7	1002.8	358.2	277.4

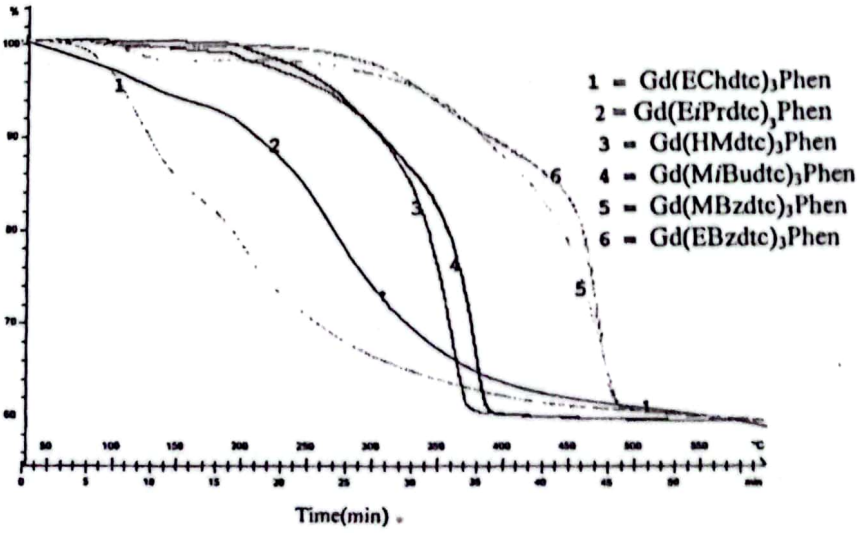

FIGURE 1. Thermogram of TGA analysis in nitrogen for $Gd(S_2CNR'R'')_3Phen$ complexes

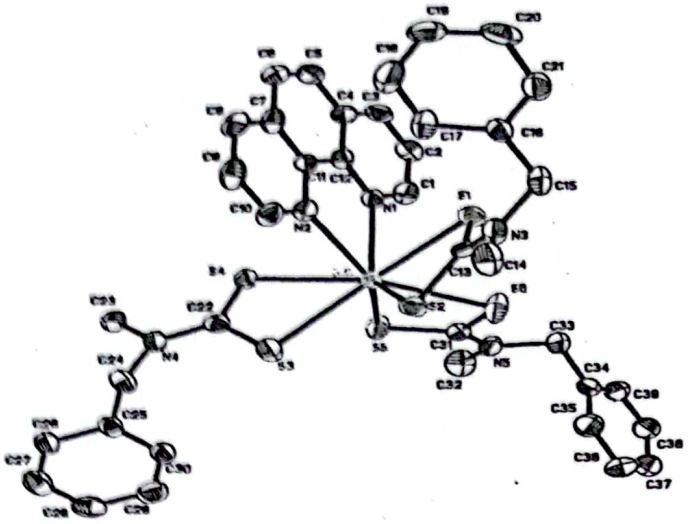

FIGURE 2. ORTEP Plot of gadolinium tris(*N,N*-methylbenzyldithiocarbamate)1,10-phenantroline with displacement 50 % probability ellipsoid

TABLE 4. Crystallographic data for $Gd[S_2CN(CH_3)(C_7H_7)]_3Phen$

Compound	$Gd[S_2CN(CH_3)(C_7H_7)]_3Phen$
Empirical Formula	$C_{39}H_{38}N_5S_6Gd$
Formula weight	926.35
Temperature	273 K
Wavelength A	0.71073
Crystal system	Triclinic
Space group	$P\tau$
a Å	11.04 (6)
b Å	12.65 (7)
c Å	17.13 (10)
α /°	73.86 (8)
β /°	74.54 (10)
γ /°	72.34 (9)
V (Å^3)	2147 (21)
Z	2, 1.433 Mg/m^3
D/Mgm^{-3}	1.860
F (000)	934
Crystal size	0.45 × 0.25 x 0.16 mm^3
Refinement method	Full matrix least-square
θ range (°)	2.21 - 25.00°
Final R indices $I > 2\sigma(I)$	$R_1 = 0.0625$, $wR_2 = 0.1788$
R indices (all data)	$R_1 = 0.1710$, $wR_2 = 0.2697$

Gd(III) atom in bidentate manner via nitrogen and sulphur atoms respectively, in a distorted dodecahedron geometry. The bond angles of S(1)-Gd-S(2), S(3)-Gd-S(4), S(5)-Gd-S(6) are 60.9(7)°, 61.50(8)° and 61.9(7)° respectively. The C-S bonds have an average distance of 1.77° and the mean S–C–S angle is of 117.5°. The thioureide C–N bond distances of N(3)-C(13), N(4)-C(22) and N(5)-C(31) [1.391(15)Å; 1.37(2)Å and 1.339(19)] are shorter than the other CN bond, which are indicative of a partial double bond character (C=N) as suggested by infrared spectra data (1450 – 1490 cm^{-1}).

CONCLUSION

The elemental, spectroscopic and crystallographic data showed that new compounds of gadolinium dithiocarbamate phenantroline have been successfully synthesized. The dithiocarbamate anions and bidentate nitrogen from 1,10-phenantroline were chelated to the gadolinium atom to form the eight coordinated mixed-ligand compounds. The crystallographic studies of $Gd[S_2CN(CH_3)(C_7H_7)]_3Phen$ compounds showed that the dithiocarbamate and nitrogen ligands coordinated in bidentate manner.

TABLE 5. Selected bond distances (Å) and angles (°) for $Gd[S_2CN(CH_3)(C_7H_7)]_3Phen$

Gd(1)-N(1)	2.588(16)	S(4)-C(22)	1.737(15)
Gd(1)-N(2)	2.650(14)	S(5)-C(31)	1.762(16)
Gd(1)-S(1)	2.992(11)	S(6)-C(31)	1.831(18)
Gd(1)-S(2)	2.967(14)	N(3)-C(14)	1.517(19)
Gd(1)-S(3)	2.936(13)	N(3)-C(15)	1.53(2)
Gd(1)-S(4)	3.010(15)	N(4)-C(22)	1.391(17)
Gd(1)-S(5)	2.965(15)	N(4)-C(24)	1.522(17)
Gd(1)-S(6)	2.937(14)	N(3)-C(13)	1.37(2)
S(1)-C(13)	1.750(14)	N(4)-C(23)	1.529(19)
S(2)-C(13)	1.777(16)	N(5)-C(31)	1.339(19)
S(3)-C(22)	1.788(15)	N(5)-C(32)	1.47(2)
N(5)-C(33)	1.527(19)		
N(1)-Gd(1)-N(2)	64.4(5)	N(1)-Gd(1)-S(2)	128.0(3)
N(1)-Gd(1)-S(3)	136.0(4)	N(1)-Gd(1)-S(1)	71.5(5)
N(1)-Gd(1)-S(6)	95.4(3)	N(1)-Gd(1)-S(4)	78.4(3)
N(2)-Gd(1)-S(1)	72.9(5)	N(1)-Gd(1)-S(5)	92.1(4)
N(2)-Gd(1)-S(2)	81.8(4)	N(2)-Gd(1)-S(4)	76.2(4)
N(2)-Gd(1)-S(3)	87.8(4)	N(2)-Gd(1)-S(5)	141.7(3)
S(1)-Gd(1)-S(4)	60.9(3)	N(2)-Gd(1)-S(6)	144.4(3)
S(2)-Gd(1)-S(1)	143.77(17)	S(2)-Gd(1)-S(4)	132.06(14)
S(3)-Gd(1)-S(1)	134.3(3)	S(3)-Gd(1)-S(4)	61.5(2)
S(5)-Gd(1)-S(1)	130.22(18)	S(3)-Gd(1)-S(2)	75.8(3)
S(5)-Gd(1)-S(2)	134.4(3)	S(3)-Gd(1)-S(5)	90.2(3)
S(5)-Gd(1)-S(4)	69.4(2)	S(3)-Gd(1)-S(6)	123.8(3)
S(6)-Gd(1)-S(1)	73.0(3)	S(6)-Gd(1)-S(5)	61.9(2)
S(6)-Gd(1)-S(2)	90.2(4)	S(6)-Gd(1)-S(4)	130.7(4)

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the research grant provided by The Malaysian Government IRPA 09-02-02-0048-EA144 and scholarship for Indah Raya from TPSDP Hasanuddin University Indonesia, X-ray Crystallography laboratory for structure determination and technical support from School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia. Many thanks to Chemistry Department of Institut Teknologi Bandung, Indonesia for measuring the magnetic properties of the compounds.

REFERENCES

Brown, D. A., Glass, W. K. & Burke, M. A. 1976. The general use of IR spectral criteria in disscussions of the bonding and structure of metal dithiocarbamate. *Spectrochem. Acta* 32A: 137-143.

Coucouvanis, D. & Fackler, J. P. Jr. 1976. Square-planar sulphur complexes. *Inorganic Chem* 6: 2047-2053.

Criado, J. J., Fernandez, I. & Macias, B. 1990. Novel chelates of Pd(II) dithiocarbamates, spectroscopic studies and thermal behaviour. *Inorg. Chem. Acta* 174: 67-75

Haas, W. & Schwarz, T. 1963. NH_4 diethanol dithiocarbamate a reagent for the spectrophotometric determination of Mo and U. *Microchem. Ichonal. Acta* 58: 253-259.

Hursthouse, M. B., Malik, M. A., Motervalli, M. & O'Brien, P. 1992. The crystal and molecular structure of N,N-dimethyldiselenocarbamatocadmium(II): cadmium and zinc dimethyldiselenocarbamates as precursors for selenides. *Polyhedron* 11: 45-48.

Nomura, R., Takabe, A. & Matsuda, H. 1987. Facile synthesis of antimony dithiocarbamate complexes. *Polyhedron* 6: 411-416.

Sharma, H., Watanabe, H., Tamura, H., Yasui, H., Matsushita, R. & Takada, J. 1998. Insulin-mimetic vanadyl-dithiocarbamate complexes. *Inorg. Chim. Acta* 283: 175-183.

Sheldrick, G. M. 1996. SAINT V4, Software reference manual, Siemens Analytical X-ray System, Madison, WI, USA.

Sheldrick, G. M. 1996. SADABS, Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen, Germany.

Sheldrick, G. M. 1997. SHELXTL V 5.1, Software reference manual, Bruker AXS, Inc., Madison, WI, USA.

Siddal, T. H. & Steward, W. E. 1970. Preparation and studies of magnetic and spectroscopic properties of alkyl ammonium lanthanide tetrakis (N,N-dialkyldithiocarbamates). *J. Inorg. Nuclear Chem.* 32: 1147-1158.

Siemens. 1996. *SMART* and *SAINT*. Area Detector Control and Integration Software. Siemens Analytical X-Ray Systems, Inc. Madison, Wisconsin, USA.

Su, C., Tan, M., Tang, N., Gan, X. & Liu, W. 1997. Synthesis, structure and spectroscopic properties of dimmethylammonium lanthanide tetrakis(*N*, *N*-dimmethyldithiocarbamate). *Polyhedron* 16: 1643-1650.

Tang, N., Zhu, H., Tan, M., Gan, X. & Wang, A. 1991. Synthesis and characterisation of dimethylammonium lanthanide (monomethyldithiocarbamate). *Polyhedron* 16: 1643-1650.

Thorn, G.D. & Luding R.A. 1962. The dithiocarbonates and related compounds. New York: Elsevier Pub. Co.

Venkatachalam, V., Ramalingam, K., Casellato, U. & Graziani, R. 1997. Structural and electronic effect of alkyl substituents on the main group dithiocarbamato complexes: crystals and molecular structures of tris(*N*,*N*'iminodiethanoldithiocarbamato)metal(III) complexes (M = As, Sb and Bi) and cyclic voltammetric studies on substituted dithiocarbamates. *Polyhedron* 16(7): 1211 – 1221.

Zhu, H., Tang, N., Gan, X., Wang, A. & Tan, M. 1993. Synthesis and characterization of light lanthanide piperidinocarbodithioate complexes. *Polyhedron* 12: 945-991.

School of Chemical Sciences & Food Technology
Faculty of Science and Technology
Universiti Kebangsaan Malaysia
43600 Bangi, Selangor, D.E.
Malaysia

Received: 4 October 2006
Accepted: 5 January 2007

Journal Search

SCIENCE CITATION INDEX EXPANDED - JOURNAL LIST

Total journals: 8091

|A|B|C|D|E|F|G|H|I|J|K|L|M|N|O|P|Q|R|S|T|U|V|W|X|Y|Z|

"S" Journals 1-10 (of 386)

SABRAO JOURNAL OF BREEDING AND GENETICS
Semiannual
ISSN: 1029-7073
EMILUZ PRINTING INDUSTRIES INC, #1 LA UNION ST, SAN FRANCISCO DEL MONTE, QUEZON CITY, PHILIPPINES, 00000
Coverage
Science Citation Index Expanded
BIOSIS Previews

SADHANA-ACADEMY PROCEEDINGS IN ENGINEERING SCIENCES
Bimonthly
ISSN: 0256-2499
INDIAN ACAD SCIENCES, C V RAMAN AVENUE, SADASHIVANAGAR, P B #8005, BANGALORE, INDIA, 560 080
Coverage
Science Citation Index Expanded
Current Contents - Engineering, Computing & Technology

SAFETY SCIENCE
Monthly
ISSN: 0925-7535
ELSEVIER SCIENCE BV, PO BOX 211, AMSTERDAM, NETHERLANDS, 1000 AE
Coverage
Science Citation Index Expanded
Current Contents - Engineering, Computing & Technology

SAINS MALAYSIANA
Quarterly
ISSN: 0126-6039
UNIV KEBANGSAAN MALAYSIA, FAC ALLIED HEALTH SCI, JALAN RAJA MUDA ABDUL AZIZ, KUALA LUMPUR, MALAYSIA,50300
Coverage
Science Citation Index Expanded
Zoological Record

SAJOG-SOUTH AFRICAN JOURNAL OF OBSTETRICS AND GYNAECOLOGY
Tri-annual
ISSN: 0038-2329
SA MEDICAL ASSOC HEALTH & MEDICAL PUBL GROUP, 21 DREYER ST, 4TH FLOOR, SANCLARE BLDG, CLAREMONT, SOUTH AFRICA, 7700
Coverage
Science Citation Index Expanded

SALUD I CIENCIA
Bimonthly
ISSN: 1667-8982
SOC IBEROAMERICANA INFORMACION CIENTIFICA-S I I C, AVE BELGRANO 430-C1092AAR, BUENOS AIRES, ARGENTINA, 00000
Coverage
Science Citation Index Expanded

SAMJ SOUTH AFRICAN MEDICAL JOURNAL
Monthly
ISSN: 0256-9574
SA MEDICAL ASSOC, BLOCK F CASTLE WALK CORPORATE PARK, NOSSOB STREET, ERASMUSKLOOF EXT3, PRETORIA, SOUTH AFRICA, 0002
Coverage
Science Citation Index
Science Citation Index Expanded
Current Contents - Clinical Medicine
BIOSIS Previews

SAMPE JOURNAL
Bimonthly

ISSN: 0091-1062
SAMPE PUBLISHERS, 1161 PARKVIEW DRIVE, COVINA, USA, CA, 91722
Coverage
Science Citation Index Expanded
Current Contents - Engineering, Computing & Technology

SANG THROMBOSE VAISSEAUX

Monthly
ISSN: 0999-7385
JOHN LIBBEY EUROTEXT LTD, 127 AVE DE LA REPUBLIQUE, MONTROUGE, FRANCE, 92120
Coverage
Science Citation Index Expanded

SANTE PUBLIQUE

Bimonthly
ISSN: 0995-3914
SOC FRANCAISE SANTE PUBLIQUE, 2 RUE DU DOYEN JACQUES PARISOT, BP 7, VANDOEUVRE-LES-NANCY CEDEX, FRANCE, 54501
Coverage
Science Citation Index Expanded

"S" Journals 1-10 (of 386)

FORMAT FOR PRINT
