

enhanced in case of *Draschlera australiensis* at both dilutions.

The compounds thus inhibit fungal growth to a considerable extent. Some of them compare well with the fungicidal activity of sodium pentachloro phenate as is evident from Table I.

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Fe(II), Co(II), Ni(II) AND Cu(II) PERCHLORATE COMPLEXES WITH AMINOPYRINE

S. V. TATWAWADI, A. P. SINGH AND K. K. NARANG*

Department of Pharmaceutics, Institute of Technology, Banaras Hindu University, Varanasi 221 005, India

* Department of Chemistry

ABSTRACT

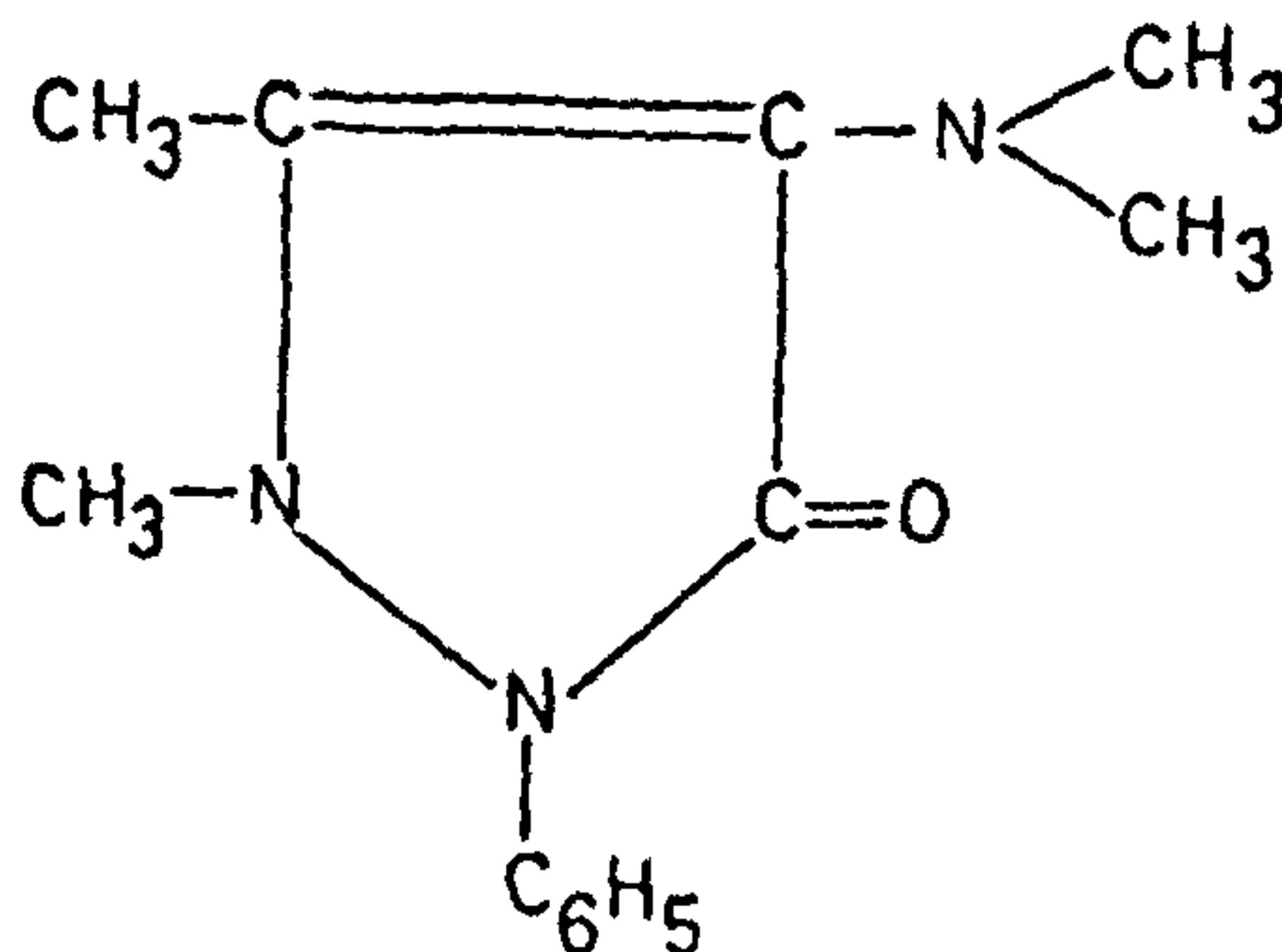
Aminopyrine complexes with metal(II) perchlorate of the types $[M(AMP)_2 \cdot 2H_2O](ClO_4)_2$, $[M(AMP)_2](ClO_4)_2$ and $[M(AMP)_2 \cdot H_2O](ClO_4)_2$, where M = Fe(II), Co(II), Ni(II) and Cu(II), AMP = aminopyrine, were prepared and characterised by analysis, molar conductance, magnetic measurements, electronic and infrared spectral studies.

INTRODUCTION

AMINOPYRINE (2,3-dimethyl, 4-dimethylamino-1-phenyl-3-pyrazolin-5-one) acts as a bidentate ligand and belongs to the pyrazole group. It has antipyretic and analgesic properties¹. Metal complexes with aminopyrine² (Structure I) and antipyrine³ have been reported. In view of our interest in the metal complexes of drugs, we report here the metal(II) perchlorate complexes of aminopyrine.

EXPERIMENTAL

Freshly prepared metal(II) perchlorate solutions in dilute ethanol and aminopyrine (E. Merck grade) were reacted in 1:2 (M:Drug) molar ratios. The complexes, which were precipitated or crystallised, were washed with dilute ethanol and dried in a desiccator. Metal part, drug and anion in the complexes were



Aminopyrine
(Structure I)

* To whom the correspondence should be addressed.

estimated using standard procedures^{4,5}. Physico-chemical data were recorded on ECIL conductivity bridge, Cahn magnetic balance, Perkin Elmer IR (621, 720) and Cary-14 spectrophotometers.

RESULTS AND DISCUSSION

The complexes of Fe(II) and Co(II) are yellow and brown respectively while the complexes of Ni(II) and Cu(II) are green in colour. They are soluble in water as well as in methanol. The molar conductance values in water fall within the range reported for 1:2 electrolyte⁶. This shows that perchlorate anion in complexes is readily ionisable in the solution.

The magnetic moments indicate that Fe(II) and Ni(II) complexes are spin-free octahedral. The magnetic moments of Co(II) and Cu(II) complexes show high spin tetrahedral and square pyramidal structures respectively⁷. The electronic spectral data (Table I) support the magnetic moments. The electron paramagnetic resonance study of Cu(II) perchlorate aminopyrine complex ($g_{\parallel} \approx 2.2573$) $>$ $g_{\perp} = 2.0490$) suggests its square pyramidal structure⁸⁻¹⁰.

INFRARED SPECTRA

The negative shifts in $\nu(\text{C}=\text{O})$ by $\sim 50 \text{ cm}^{-1}$ ¹¹ and $\nu(\text{C}-\text{N})$ by $\sim 30 \text{ cm}^{-1}$ ¹² in copper(II) complex suggest that aminopyrine has two sites of coordination with metal. In other complexes, however, a strong band at 1090 cm^{-1} due to ionic perchlorate¹³ overlaps the $\nu\text{C}-\text{N}$ vibration. The perchlorate vibrations between $1085-1090 \text{ cm}^{-1}$ and $620-625 \text{ cm}^{-1}$ are due to ν_3 and ν_4 modes respectively. A weak band ν_1 is observed at 940 cm^{-1} in the complexes and it is due to crystal field effect¹⁴. The absence of splitting of these bands indicates tetrahedral symmetry of the perchlorate and hence its ionic nature¹⁵. The coordinated water absorbs between $3400-3500 \text{ cm}^{-1}$ $\nu(\text{O}-\text{H})$ in Fe(II), Ni(II) and Cu(II) complexes. Bending vibration of H_2O overlaps with the carbonyl frequency. The H_2O rocking frequencies occur between $835-845 \text{ cm}^{-1}$ indicating that water is coordinated to the metal ion¹⁶. The non-ligand M-O and M-N vibrations are observed at $450-400 \text{ cm}^{-1}$ and $330-300 \text{ cm}^{-1}$ respectively (Table II)^{16,17}.

TABLE I

Electronic spectral data of the complexes of Fe(II), Co(II), Ni(II) and Cu(II) perchlorate complexes

Complexes	Intraligand transitions (cm^{-1})	Band positions (cm^{-1}), assignments and the values of $10 Dq$, β' , β and LFSE (K. Cal/mole)			
[Fe(AMP) ₂ · 2H ₂ O] (ClO ₄) ₂	37735 (46083, 41666, 37037)*	10400 ⁵ T _{2g} → ⁵ E _g 10 Dq (cm^{-1}) 10400			
[Co(AMP) ₂] (ClO ₄) ₂	40816, 37037	8264 ⁴ A ₂ (F) → ⁴ T ₂ (F) 10 Dq (cm^{-1}) 8264	14282 ⁴ A ₂ (F) → ⁴ T ₁ (F) β' (cm^{-1}) B 1031	25974 ⁴ A ₂ (F) → ⁴ T ₁ (P) ν_2/ν_1 LFSE 1.7 30.99	
[Ni(AMP) ₂ · 2H ₂ O] ClO ₄) ₂	46511, 37735	8368 ³ A _{2g} (F) → ³ T _{2g} (F) 10 Dq (cm^{-1}) 8368	15151 ³ A _{2g} (F) → ³ T _{1g} (F) β' (cm^{-1}) B 1045	25641 ³ A _{2g} (F) → ³ T _{1g} (P) ν_2/ν_1 LFSE 1.81 31.38	
[Cu(AMP) ₂ · H ₂ O] (ClO ₄) ₂	40000, 36363	14599 $d_{xy} \rightarrow d_{x^2-y^2}$ 10 Dq (cm^{-1}) 14599	$d_{x^2-y^2} \rightarrow d_{xy}$	$d_{yz} \rightarrow d_{z^2}$	

* UV spectrum of aminopyrine.

TABLE II
Analytical data and some important IR frequencies (cm^{-1}) of Fe(II), Co(II), Ni(II) and Cu(II) perchlorate complexes with aminopyrine

Compounds	Temperature of decomposition ($^{\circ}\text{C}$)	Elemental analysis, %		Drug estimated	Δ Conductance $\text{ohm}^{-1}\text{cm}^2\text{mole}^{-1}$	Magnetic moment (B.M.)	$\nu(\text{C}=\text{O})$ cm^{-1}	$\nu(\text{M}-\text{O})$	$\nu(\text{M}-\text{N})$
		Metal	Perchlorate						
[Fe(AMP) $_2$ 2H $_2$ O](ClO $_4$) $_2$	195	7.49 (7.44)	26.50 (61.35)	61.31 (61.35)	241	5.12	1610 s 1670 s*	415 w	320 w
[Co(AMP) $_2$ (ClO $_4$) $_2$	181	8.11 (8.19)	27.59 (27.64)	64.14 (64.17)	252	4.52	1620 s	400 w	325 w
[Ni(AMP) $_2$ 2H $_2$ O](ClO $_4$) $_2$	210	7.72 (7.80)	26.64 (26.39)	61.16 (61.11)	230	3.10	1620 s	435 w	330 w
[Cu(AMP) $_2$ H $_2$ O](ClO $_4$) $_2$	178	8.56 (8.49)	26.79 (26.82)	62.30 (62.26)	268	1.85	1605 s	450 m	300 w

* Carbonyl frequency of free aminopyrine. The values in parenthesis are calculated values.

On the basis of foregoing discussion, the structure of Fe(II) and Ni(II) complexes may be octahedral, Co(II) complex tetrahedral while that of Cu(II) complex square pyramidal.

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TOPOLOGY AND PHYSICAL PROPERTIES OF ALICYCLIC COMPOUNDS

R. S. LALL

Chemistry Department, St. Andrew's College, Gorakhpur 273 001, India

ABSTRACT

A correlation between the topological indices and the physical properties of the saturated alicyclic hydrocarbons is reported. Boiling points, refractive indices, specific gravities and the bond energies vary linearly with the mean and root mean square values of the Wiener number while the heat of formation varies linearly with the reciprocal of W_{rms} .

INTRODUCTION

RECENTLY the molecular graph theory^{1,2} has been applied to various systems of conjugated hydrocarbons³⁻⁶ in the framework of Hückel molecular orbital theory. The topological characterization of cyclic systems was developed by Trinajstić and others^{7,8}. The Wiener number⁹ was found to be most useful in characterizing the monocycles. In monocyclic structures the topological index was found to be sensitive to the change in ring size and also to their physical and chemical properties¹⁰. Various other topological indices were also introduced, e.g., Rouvray's index¹¹, Randić index¹², Platt index¹³ and Hosoya index¹⁴. Trinajstić interrelated these indices and developed a relationship for monocyclic systems⁷.

In our previous work¹⁵ we have defined the root mean square value of the Wiener number (W_{rms}) and derived a relationship between some physical properties of *n*-alkanes and the mean value of the Wiener number (\bar{W}). In the present work we have developed a relationship between the mean and the root mean square values of the Wiener number and some physical properties of the saturated alicyclic hydrocarbons.

THEORY

The molecular graph *G* of a hydrocarbon system is a set of edges representing the C-C bonds and vertices representing the carbon atoms. The distance matrix¹⁶ *D*(*G*), associated with *G*, is defined as a *N* × *N* matrix where *N* is the number of vertices in the graph *G*.