

N. Sheppard	In Honour of Professor Dušan Hadži's 60th Birthday	A foreword to the festschrift dedicated to professor Hadži	1—5
R. Blinc	The Soft Mode in H-Bonded Ferroelectrics Revisited	The soft pseudo spin mode description of the dynamics of order-disorder transition and the nature of the soft tunneling modes in KH_2PO_4 type ferroelectrics is discussed	7—13
S. Bratos	Infrared Band Shapes of van der Waals and Hydrogen Bonded Liquids. Comparison of Band Shaping Mechanisms	Band shaping mechanisms are presented, different relaxation mechanisms are compared and structure of the OH stretching band is discussed	15—22
C. A. Chatzidimitriou-Dreismann and E. Lippert	A Statistical Description of Molecular Dynamical Processes in Liquids. Application to FIR Absorption Spectroscopy	Derivation and validity of the generalized fluctuation-dissipation theorem (FDT) in quantum statistics is discussed. Generalized FDT delivers a microscopic interpretation of the theorem of minimum entropy production (TMEP).	23—40
Lj. Golič and I. Leban	The Crystal Structure of Ammonium Hydrogen Maleate	Crystal structure of ammonium hydrogen maleate ($\text{NH}_4^+\text{C}_4\text{H}_3\text{O}_4^-$) has been determined by X-ray diffraction method. It is isostructural with the potassium salt. Two types of H-bonds are present in the struc-	

	ture: intermolecular bond $\text{NH}\dots\text{O}$ connecting NH_4^+ with maleate ions and intramolecular bond in the maleate ion ($\text{O}\dots\text{O} = 0.2432(2)$ nm).	41—45
E. Grech, Z. Malarski, and L. Sobczyk	[NH...N]⁺ Hydrogen Bonds in Crystalline Salts of Monoaza- and Diaza-bicyclo[2.2.2]octane Infrared spectra of homoconjugated cations of 1,4-diazabicyclo[2.2.2]octane (DABCO) and azabicyclo[2,2,2]octane (ABCO) with acids are studied. Hydrogen bond bands are broad and show strong temperature effect. Evans transmission windows are found and hydrogen bond vibration is determined at ca 100 cm^{-1} .	47—53
P. L. Huyskens and G. G. Siegel	Dipole Moments of H-Bonded Complexes Equations used in determination of the dipole moments in liquid phase are discussed. Experimental dipole data for alcohols, carboxylic acids, amides, amines, anilines and pyridines is presented. Experimental method is discussed.	55—73
R. Janoschek	The Electrostatic Model in the Theory of H-Bonds Proton donor and acceptor electrostatic interaction is treated by perturbation theory. Electrostatic potential of proton acceptor is indicator for H-bond properties.	75—83
M. Kertesz, J. Koller, and A. Ažman	Application of the Intermediate Exciton Formalism to H₂ Molecular Chains Intermediate exciton theory at ab-initio level applied to a model insulator of H ₂ molecular chains shows that the correlation corrections to the forbidden energy gap are large.	85—89
A. Kivinen, H. Auvinen, J. Huuskonen, and K. Väkiparta	Hydrogen Bonding Properties of Pharmaceuticals. Part 1. 2,3,4,5-Tetraiodo, Tetrabromo and Tetra-chloropyrroles as Medium-Strong Proton Donors Heteroassociation of 2,3,4,5-tetraiodopyrrole and its bromo and chloro analogues	

- with acetone, tetrahydrofuran, pyridine, dimethylsulphoxide, and hexamethyl phosphoric triamide in carbon tetrachloride have been studied by IR spectroscopy. Acid base pair formation constants and $\Delta\nu$ NH frequency shifts are determined and irregular NH-stretching absorption is discussed. 91—97
- J. Kroon and J. A. Kanters**
The Two Fundamental H-Bond Types in Acid Salts Displayed in the Dimorphs of Potassium Hydrogen Tartrate
 Two modifications of the acid potassium salt of tartaric acid have been determined by X-ray analysis. One modification contains A-type H-bonds, whereas in the other one B-type H-bonds occur. 99—104
- J.-M. Leclercq, P. Dupuis, and C. Sándorfy**
Possibility of a Double Well Potential in the Proton Bridge of Visual Pigments and Bacteriorhodopsin
 It is shown that if a vibration is governed by a double well potential, the resonance Raman spectrum might reflect only one of the two wells which may be the less populated one. It is suggested that such a situation could exist for the chromophore of visual pigments. 105—119
- D. Lucas, L. J. Allamandola and G. C. Pimentel**
Matrix Isolation Infrared Spectra of Hydrogen Halide and Halogen Complexes with Nitrosyl Halides
 Infrared spectra of nitrosyl halide complexes ($XNO \cdot HX$ and $XNO \cdot X_2$, $X = Cl, Br$) in matrices have been measured. Relative frequency shifts ($\Delta\nu/\nu$) of νXH , $\nu XN-O$ and $\nu X-NO$ modes are presented. Structure and charge distribution of the complexes are discussed. 121—128
- Y. Maréchal**
Quantitative IR Spectroscopy of H-Bonds: Intensities of ν_s Bands
 The measurements of the intensities of ν_s bands ($X-H \dots Y$) of H-bonds show an anomalous behaviour upon deuteration, which can be an indication of the peculiar electronic structure of H-bonds. 129—132

D. J. Millen	<p>Microwave Spectroscopic Investigations of Hydrogen-Bonded Dimers and the Directional Character of Hydrogen Bonds</p> <p>Geometry and bending force constants obtained from microwave spectra are used to explore the directional character of hydrogen bonds. Lone-pair directions correlate with observed geometries of gas-phase dimers, but not for hydrogen bonded structures in the solid state. These contrasting results can be understood in terms of bending potential functions. . . .</p>	133—145
A. Novak	<p>Intermolecular Hydrogen Bond Vibrations</p> <p>Hydrogen bond stretching frequencies and force constants are given as well as correlations with AH stretching frequencies. The role of AH . . . B vibrations on breadth and structure of AH-stretching band is discussed and behaviour of the νOH . . . O Raman bands during phase transition of squaric acid and cesium dihydrogen phosphate is studied. . . .</p>	147—169
I. Olovsson	<p>The Electron Density of the Hydrogen Bond</p> <p>Electron distribution in hydrogen bonds of weak and intermediate strengths and the electron densities of the monomer are discussed. A modification of the monomer densities is noticeable in very strong hydrogen bonds. . . .</p>	171—190
W. J. Orville-Thomas and H. Ratajczak	<p>Matrix Isolation and Molecular Orbital Studies of Water</p> <p>A review of the infrared evidence and theoretical predictions on association of water; dimers and trimers with open chain structures and higher multimers in cyclic forms are expected to be present. . . .</p>	191—205

C. N. R. Rao,
S. Ganguly,
and H. R. Swamy

Vibrational Spectroscopic Studies of Phase Transitions in Organic Molecular Crystals and Dicarboxylic Acids

Order disorder transitions in 2,3-benzothio-
thiophene and cyclopentyl-1-thiaethane
and vibronic effects in the phase transi-
tions of the alkali metal salts of TCNQ
have been investigated. Crystalline forms
of methylcyclohexane have been establish-
ed by infrared spectroscopy. Transitions in
malonic, succinic and glutaric acids lead
to changes in frequencies and intensities
of IR and Raman bands.

207—221

N. D. Sokolov

Mode Coupling in Molecular Complexes

A—Z and A...B mode interactions (A—Z
...B system) is described by a coupling
parameter. Some empirical findings and
regularities are interpreted quantitatively
by this parameter.

223—231

J. C. Speakman
and K. W. Muir

Basic Salts with »Very Short« Hydrogen Bonds; the Crystal Structure of α -Picoline-N-oxide Hemyhydrochloride Sesquihydrate (Dunlop's Salt)

The structure of $\text{BHB}^+ \text{Cl}^- \cdot 3\text{H}_2\text{O}$, Dun-
lop's Salt, has been determined by X-ray
diffraction (1040 reflexions, $R = 3.7\%$).
The cation contains a strong hydrogen
bond ($\text{O} \dots \text{O} = 241.4(3) \text{ pm}$) across a cry-
stallographic centre of symmetry; whilst
the Cl^- is strongly bonded to a water mole-
cule ($\text{Cl}^- \dots \text{O} = 297(1) \text{ pm}$), symmetri-
sed by disorder, between $\text{Cl}^- \dots \text{H}-\text{OH}/$
 $\text{HO}-\text{H} \dots \text{Cl}^-$, across a twofold axis. The
IR spectrum is almost identical with that
of the hemihydrobromide $\text{BHB}^+ \text{Br}^-$

233—248

E. Spinner

Vibrational Spectroscopy of Compounds with Very Short Hydrogen Bonds. The Aqueous Bisformate Ion. Comparison with Two Solid Salts and Some Comments on Broad OH Absorption Continua

The infrared and Raman spectra of aque-
ous bisformate ions $(\text{HCO}_2)_2\text{H}^-$, $(\text{HCO}_2)_2\text{D}^-$,
 $(\text{DCO}_2)_2\text{H}^-$, $(\text{DCO}_2)_2\text{D}^-$, the isotopic mixture

(HCO₂)(DCO₂)H⁻ and corresponding Na⁺ and K⁺ salts in solid state have been investigated and compared with the results of ab-initio molecular orbital calculations. The continuum character of the OH band, reflecting high variability of the potential energy curves that make up the potential energy hyper surface, is discussed.

CROATICA
CHEMICA ACTA

Croat. Chem. Acta Vol. 55 No. 1—2

1—270 (1982)

Zagreb, 1. srpnja 1982

SADRŽAJ

V počastitev šestdesetletnice profesorja Dušana Hadžija . . . N. Sheppard	1—5
Mehki načini nihanja v feroelektrikih z vodikovimi vezmi . . . R. Blinc	7—13
Oblika nihajnih trakov van der Waalsovih tekočin in tekočin z vodikovimi vezmi. Primerjava mehanizmov, ki vplivajo na njihovo obliko . . . S. Bratos	15—22
Statistični opis dinamičnih procesov molekul v tekočinah. Uporaba ab- sorpcijske spektroskopije v daljnem infrardečem območju . . . C. A. Chatzidimitriou-Dreismann in E. Lippert	23—40
Kristalna struktura amonijevega hidrogen maleata . . . Lj. Golič in I. Leban	41—45
Vodikove vezi (NH \cdots N) ⁺ v kristalih soli mono-aza in diaza-biciklo[2,2,2]- oktana E. Grech, Z. Malarski in L. Sobczyk	47—53
Dipolni momenti vodikovo vezanih kompleksov . . . P. L. Huyskens in G. G. Siegel	55—73
Elektrostatski model v teoriji vodikove vezi. R. Janoschek	75—83
Uporaba formalizma vmesnih ekscitonov na molekulski verigi H ₂ . . . M. Kertesz, J. Koller in A. Ažman	85—89
Vodikove vezi v farmacevtskih substancah. Prvi del. 2,3,4,5-tetrajodo-, tetrabromo- in tetrakloropirrol kot srednje močni protonski donorji . . . A. Kivinen, H. Auvinen, J. Huuskonen in K. Väkiparta	91—97
Kalijev hidrogen tartronat: dva osnovna tipa H-vezi . . . J. Kroon in J. A. Kanters	99—104
Možnost dvojnega potencialnega minimuma v protonskem mostu v vidnih pigmentih in bakteriorodopsinu . . . J.-M. Leclercq, P. Dupuis in C. Sandorfy	105—119
Infrardeči spektri simetrično izoliranih aduktov med nitrozilovimi halo- genidi in vodikovimi halogenidi ali halogeni . . . D. Lucas, L. J. Allamandola in G. C. Pimentel	121—128
Kvantitativna infrardeča spektroskopija H-vezi: intenzitete ν_8 trakov . . . Y. Maréchal	129—132
Mikrovalovne spektroskopske raziskave vodikovo vezanih dimerov in usmerjeni značaj vodikovih vezi D. J. Millen	133—145
Medmolekulska nihanja vodikove vezi A. Novak	147—169
Elektronska gostota vodikove vezi I. Olovsson	171—190
Matrična izolacija in študij vode z metodo molekulskih orbital . . . W. J. Orville-Thomas in H. Ratajczak	191—205

Študij faznih prehodov v organskih molekulskih kristalih in dikarbonskih kislinah z vibracijsko spektroskopijo	
. . . C. N. R. Rao, S. Ganguly in H. R. Swamy	207—221
Nihajne sklopitve v molekulskih kompleksih	N. D. Sokolov
Bazične soli z zelo kratkimi vodikovimi vezmi; kristalna struktura adukta α -pikolin- <i>N</i> -oksid-hemivodikovklorid trihidrat (Dunlopova sol)	223—231
. . . J. C. Speakman in K. W. Muir	233—248
Vibracijska spektroskopija spojin z zelo kratkimi vodikovimi vezmi. Vodni bisformatni ion. Primerjava z dvema solmi v kristaliničnem stanju in nekaj opomb na široke, zvezne vibracijske trakove OH	
. . . E. Spinner	249—269

CROATICA
CHEMICA ACTA

Croat. Chem. Acta Vol. 55 No. 1—2

1—270 (1982)

Zagreb, July 1, 1982

**The contents of CCA may be reproduced, citing the original form
in any medium without prior permission**

CONTENTS

In Honour of Professor Dušan Hadži's 60th Birthday . . . Norman Sheppard	1—5
The Soft Mode in H-Bonded Ferroelectrics Revisited . . . Robert Blinc	7—13
Infrared Band Shapes of van der Waals and Hydrogen Bonded Liquids. Comparison of Band Shaping Mechanisms Savo Bratos	15—22
A Statistical Description of Molecular Dynamical Processes in Liquids. Application to FIR Absorption Spectroscopy . . . C. A. Chatzidimitriou-Dreismann and Ernst Lippert	23—40
The Crystal Structure of Ammonium Hydrogen Maleate . . . Ljubo Golič and Ivan Leban	41—45
[NH \cdots N] ⁺ Hydrogen Bonds in Crystalline Salts of Monoaza- and Diaza- -bicyclo[2.2.2]octane . . . Eugeniusz Grech, Zbigniew Malarski, and Lucjan Sobczyk	47—53
Dipole Moments of H-Bonded Complexes . . . Pierre L. Huyskens and Georges G. Siegel	55—73
The Electrostatic Model in the Theory of H-Bonds . . . Rudolf Janoschek	75—83
Application of the Intermediate Exciton Formalism to H ₂ Molecular Chains . . . Miklós Kertesz, Jože Koller, and Andrej Ažman	85—89
Hydrogen Bonding Properties of Pharmaceuticals. Part 1. 2,3,4,5-Tetraiodo, Tetrabromo and Tetrachloropyrroles as Medium-Strong Proton Donors . . . Antti Kivinen, Helena Auvinen, Jarmo Huuskonen, and Keijo Väkiparta	91—97
The Two Fundamental H-Bond Types in Acid Salts Displayed in the Dimorphs of Potassium Hydrogen Tartronate . . . Jan Kroon and Jan A. Kanters	99—104
Possibility of a Double Well Potential in the Proton Bridge of Visual Pigments and Bacteriorhodopsin . . . Jean-Marie Leclercq, Paul Dupuis and Camille Sándorfy	105—119
Matrix Isolation Infrared Spectra of Hydrogen Halide and Halogen Com- plexes with Nitrosyl Halides . . . Donald Lucas, Louis J. Allaman- dola, and George C. Pimentel	121—128
Quantitative IR Spectroscopy of H-Bonds: Intensities of ν_s Bands . . . Yves Maréchal	129—132
Microwave Spectroscopic Investigations of Hydrogen-Bonded Dimers and the Directional Character of Hydrogen Bonds . . . Douglas James Millen	133—145

Continued on inside back cover

Continued from outside back cover

Intermolecular Hydrogen Bond Vibrations	Aleksander Novak	147—169
The Electron Density of the Hydrogen Bond	Ivar Olovsson	171—190
Matrix Isolation and Molecular Orbital Studies of Water . . .	William James Orville-Thomas and Henryk Ratajczak	191—205
Vibrational Spectroscopic Studies of Phase Transitions in Organic Molecular Crystals and Dicarboxylic Acids . . .	Chintamani Nagesha Ramachandra Rao, Somnath Ganguly, and Humachadakatte Ramachandra Swamy	207—221
Mode Coupling in Molecular Complexes	Nikolai D. Sokolov	223—231
Basic Salts with Very Short Hydrogen Bonds; the Crystal Structure of α -Picoline- <i>N</i> -oxide Hemihydrochloride Sesquihydrate (Dunlop's Salt) . . .	J. Clare Speakman and Kenneth W. Muir	233—248
Vibrational Spectroscopy of Compounds with Very Short Hydrogen Bonds. The Aqueous Bisformate Ion. Comparison with Two Solid Salts, and Some Comments on Broad OH Absorption Continua . . .	Ernest Spinner	249—269