

SEMIEMPIRICAL AND *ab initio* STUDY OF THE NATURE OF THE C—S BOND IN SULFONIUM YLIDES

Vladimír KRÁL, Zdeněk ARNOLD and Zdeněk HAVLAS

*Institute of Organic Chemistry and Biochemistry,
Czechoslovak Academy of Sciences, 166 10 Prague 6*

Received June 30th, 1980

The importance of *d*-orbitals for the interpretation of properties of sulfonium ylides is demonstrated on the basis of semiempirical and *ab initio* calculations. The calculated C—S bond length values are sensitive to inclusion of *d*-orbitals into the AO basis set. Even a high quality basis (4-31 G) without *d*-orbitals leads to C—S bond lengths which are significantly larger than the experimental ones whereas bases including *d*-orbitals afford satisfactory agreement. Inclusion of *d*-orbitals results in charge reduction on the atoms C and S and in a substantially increased order of the bond between these atoms. The decrease of total energy which results from inclusion of *d*-orbitals is related to $(d-p)_n$ bonding overlap between the atoms S and C.

Participation of outer shell *d*-orbitals in the chemical bond and reactivity represents one of the central problems related to chemistry of the second row elements. For sulfur-containing compounds, *d*-orbitals were frequently considered in order to explain some experimental facts, such as interatomic distances¹, geometric arrangement^{2,3} and barriers to rotation⁴. Wolfe and coworkers² investigated the geometric arrangement of α -sulfinyl and α -sulfonyl carbanions with inclusion of *d*-orbitals. Koch and Moffat³ discussed the stability of conformers of aryl sulfones on the basis of $2p-3d$ conjugation with various arrangements of the $2p_z$ electron pair relative to the sulfonyl group. Hoffmann and coworkers⁵ investigated theoretical aspects connected with the role of $3d$ orbitals in the bonds in sulfur-containing three-membered rings and showed their significance for the overlap population. The observed barrier to internal rotation in α -sulfonyl carbanions has been also explained by the participation of *d*-orbitals⁶.

The successful interpretations of experimental facts conditioned by the use of *d*-orbitals have led to an overestimation of their importance even in cases, where the calculated *d*-orbital population was not large enough, *e.g.* the shape of molecules of PF_5 , ClF_3 and SF_4 was explained on the basis of participation of $3d$ -orbitals, although the same conclusions were obtained using the *sp* basis⁷. It was shown by *ab initio* calculations of some systems that the assumption of significant participation of *d*-orbitals which should explain the properties of the studied compounds,

is incorrect^{8,9}. The *d*-orbital participation in carbanions, adjacent to a sulfur atom, has been a subject of a non-empirical MO study¹⁰. The authors ascribed a small significance to $(p-d)_\pi$ conjugation in the ground state. Minyayev and coworkers¹¹ assume a small importance of *d*-orbitals for the barrier to rotation or inversion of sulfur-, selenium- or tellurium-containing ylides. Coulson¹² infers that inclusion of the outer shell *d*-orbitals into the basis set would undoubtedly improve the wave function, but no definite conclusion in the chemical sense may be derived from the small *d*-orbital population. The outlined situation made it necessary to find a more general criterion for classification of the *3d*-orbitals participation in the system under study. Ratner and Sabin¹³ deduced the significance of *d*-orbitals on the basis of symmetry. The symmetry criterion is fundamental but ineffective for molecules lacking a higher degree of symmetry. A method for determination of *d*-orbital participation in chemical reactions on the basis of spin and spatial symmetry conservation has been elaborated by Fueno and coworkers¹⁴⁻¹⁶. This method, which is up to this time

the most general one, was applied to the simplest idealized sulfonium ylide $\text{H}_2\text{S}^{(+)}\text{—CH}_2^{(-)}$ (*I*) which serves as a model for the existing ylides¹⁷. It was found for several chosen molecular geometries that the coefficient λ , which is negative when the *sp* basis is used, turns positive after inclusion of *d*-orbitals. This resulted in postulating a significant *d*-orbital participation in this molecule. The role of *d*-orbitals in the model compound *I* is demonstrated by analysis of expansion coefficients of the HOMO wave function and also by change of charge distribution when *d*-orbitals are included¹⁷.

The significant *d*-orbital participation for sulfonium ylides does not follow from quantum chemical calculations only. The existence of this phenomenon is supported also by experimental data. The partial double bond created by $\text{C}_{2p}\text{—S}_{3d}$ overlap should hinder a rotation around the C—S bond. In this way, it is possible to explain the observation of magnetically non-equivalent methyl groups¹⁸. Substitution of hydrogen atom in the methyl group makes the two remaining hydrogen atoms non-equivalent^{18,19}. As an experimental proof of *d*-orbital participation we may consider the results of a measurement of basicities of ammonium and sulfonium ylides derived from dimethyl malonate²⁰. It was found that basicity of sulfonium betaines is by four orders of magnitude lower than the basicity of the corresponding nitrogen-containing betaines²⁰. It may be assumed that the lower basicity of sulfonium ylides is the result of lower electron density in the anionic system, caused by transfer of the negative charge towards the sulfur atom with participation of vacant *d*-orbitals. In the present report the nature of the C—S bond in stabilized and non-stabilized ylides as well as the role of *d*-orbitals in this bond is investigated on a semi-empirical and non-empirical level.

CALCULATIONS

CNDO/2 Method was used with original parameters²¹ in *sp* and *spd* bases. In PCILO (ref.²²) calculations the bond polarities were optimized for each conformation. *Ab initio* calculations were executed with the bases STO-3G, 4-31G (ref.²³) (GAUSSIAN 70 computer program²⁴) and also with the bases described by Rauk²⁵ [S(5s2*spd*), C(3s1*p*), H(1s)] and Roos²⁶ [S(10s6*pd*/6s4*pd*), C(7s3*p*/4s2*p*), H(4s/2s)²⁷] either without or with inclusion of *d*-orbitals (HONDO computer program²⁸). Geometric arrangements of the ylide *I* were taken from ref.²⁹. Geometric arrangement on the ylide carbon atom (Fig. 1) was optimized in STO-3G and 4-31G bases (STO-3G: $\alpha = 30^\circ$, 4-21G: $\alpha = 15^\circ$); geometries of the ylides *II*—*VI* were taken from ref.³⁰. The C—S bond lengths were optimized *ab initio* (GAUSSIAN 70, HONDO) using the STO-3G, 4-21G bases as well as the basis given by Roos (without or with inclusion of *d*-orbitals). Charge distribution was investigated semiempirically (CNDO/2; *sp, spd*) and *ab initio* in the bases STO-3G, 4-31G. The GAUSSIAN 70 computer program does not involve *d*-type functions and, consequently, no information on significance of the *d*-type functions in sulfonium ylides can be obtained from calculations performed using this program.

RESULTS AND DISCUSSION

⁽⁻⁾ ⁽⁺⁾
Length of the C—S Bond in Sulfonium Ylides

Table I presents comparison of the experimentally determined C—S bond lengths in sulfonium ylides with values calculated either by CNDO/2 method (*sp* and *spd*) or *ab initio* (bases STO-3G, 4-31G and that given by Roos). Comparison of the ⁽⁻⁾ ⁽⁺⁾ ylide C—S bond length with that of a single C—S bond (1.79—1.84, ref.³⁶) or

TABLE I
Experimental and Calculated S—C Bond Lengths (*r*. 10, nm) in Sulfonium Ylides

Compound	X-Ray	CNDO/2 <i>sp</i>	CNDO/2 <i>spd</i>	STO-3G	4-31G	HONDO	
						without <i>d</i>	with <i>d</i>
<i>I</i>	—	1.81	1.66	1.778	1.801 ^a	1.825	1.695
<i>II</i>	—	1.81	1.66	1.80	—	—	—
<i>III</i>	1.73 ^b	1.81	1.72	1.80	—	—	—
<i>IV</i> ^c	1.71 ^d	1.81	1.71	1.795	—	—	—
<i>V</i>	—	1.80	1.71	—	—	—	—
<i>VI</i>	—	1.81	1.70	—	—	—	—
<i>VII</i>	1.707 ^e	—	—	—	—	—	—
<i>VIII</i>	1.721 ^f	—	—	—	—	—	—
<i>IX</i>	1.745 ^g	—	—	—	—	—	—

^a Ref.²⁹; ^b ref.³¹; ^c PCILO calculation 0.182 nm; ^d ref.³²; ^e ref.³³; ^f ref.³⁴; ^g ref.³⁵.

TABLE II
Charge Densities (Q_A) and Bond Orders (W_{AB}) in the Studied Ylides

Compound	Atom A	Q_A (CNDO/2)		Bond	W_{AB} (CNDO/2)		Q_A^a (GAUSSIAN)	
		<i>sp</i>	<i>spd</i>		<i>sp</i>	<i>spd</i>	STO-3G	4-21G
I	⁺ (S)	0.300	0.202	C—S	0.705	1.732	0.318	0.173
	⁻ (C)	-0.314	-0.274				-0.448	-0.711
II	⁺ (S)	0.349	0.134	C—S	0.792	1.725	0.464	—
	⁻ (C)	-0.379	-0.286				-0.424	
III	⁺ (S)	0.316	0.161	C—S	0.741	1.494	0.540	—
	⁻ (C)	-0.231	-0.140				-0.269	
	C(N)	0.105	0.126	(C)—C	1.225	1.120	0.041	
	N	-0.249	-0.214	C=N	2.730	2.788	-0.266	
IV	⁺ (S)	0.283	0.206	C—S	0.733	1.358	0.509	
	⁻ (C)	-0.184	-0.176	(C)—C	1.312	1.179	-0.246	
	C(O)	0.242	0.267	C—O	1.681	1.749	0.088	
	O	-0.401	-0.347				-0.346	
V	⁺ (S)	0.293	0.195	C—S	0.745	1.404	—	—
	⁻ (C)	-0.225	-0.210	(C)—C	1.251	1.123		
	C(O)	0.255	0.269	C—O	1.602	1.679		
	O	-0.428	-0.372					
VI	⁺ (S)	0.330	0.234	C—S	0.797	1.433	—	—
	⁻ (C)	-0.266	-0.248	(C)—S	1.241	1.127		
	C(O)	0.399	0.416	C—O	1.564	1.628		
	O	-0.480	-0.432					

^a Gross atomic charges.

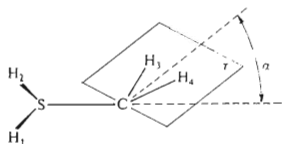


FIG. 1
Spatial Arrangement of Ylide I

a $C_{sp^2} = S$ double bond (1.635–1.66) (ref.³⁷) shows that the ylide bond has a considerable double bond character. Similar C—S bond lengths were found in thiourea (1.71) (ref.³⁸) and thioacetamide (1.713) (ref.^{39,40}). The marked shortening of the

C—S bond as compared with a single C—S bond cannot be ascribed solely to the opposite charges acting along this bond. As follows from studies on ammonium ylides³⁸, there is no marked shortening of the $\overset{(+)}{N}-\overset{(-)}{C}$ bond, and thus the $\overset{(-)}{C}-\overset{(+)}{S}$ bond length is influenced by another factor: participation of *d*-orbitals in the $(p-d)_n$ bonding interaction.

The effect of inclusion of *d*-orbitals within semiempirical (CNDO/2) and *ab initio* procedures on the calculated C—S bond length is demonstrated on the model ylide I. When comparing the results achieved by both methods we are aware of the fact, that the starting *sp* basis of semiempirical calculations is not good enough to prevent large changes of calculated total energy caused necessarily by inclusion of *d*-orbitals (*spd* basis). The reverse is true for *ab initio* calculations where the starting basis of Roos²⁶ is already of sufficient quality. Comparison of results achieved with and without inclusion of *d*-orbitals demonstrates their specific importance for sulfonium ylides. Inclusion of *d*-orbitals results in a decrease of total energy, HOMO orbital energies and in a marked shortening of the optimized C—S bond length as well.

Charge Distribution

Calculated characteristics of charge distribution exhibit a marked change when 3*d*-orbitals on the sulfur atom are included (Table II). For non-stabilized sulfonium ylides the inclusion of *d*-orbitals results in a charge decrease on both the atoms S and

C. Charge distribution in these compounds reflects the effect of *d*-orbital participation. When *d*-orbitals are included the charge separation is markedly reduced, the effect being caused by interaction of the $d(S)-p(C)$ orbitals. This conclusion may be deduced from the C—S bond order calculated in the basis including *d*-orbitals (Table II), as well as from the values of overlap integrals (0.25–0.28) between $3d_{yz}(C)$ atomic orbitals.

Two mechanisms of stabilization are probably operating in molecules of stabilized ylides. The first and certainly more significant one is delocalisation of the negative charge over the electronegative atoms of the stabilizing groups as described in ref.³⁰. The second mechanism of stabilization consists in *d*-orbital participation. As shown by analysis of charge distribution in stabilized ylides, for sulfonium betaines the negative charge can be transferred in a reversed direction towards the sulfur atom with participation of vacant *d*-orbitals. Consequently, electron density in the anionic system decreases, with simultaneous increase of the C—S bond order. The inclusion

TABLE III
Wave Functions and HOMO Orbital Energies for the Studied Ylides

Compound	Method (basis)	i^a MO index	Θ_i^b	$\epsilon_i, \text{kJ mol}^{-1}$
I^c	CNDO/2 (<i>sp</i>)	7	$0.394s(\text{C}) - 0.799p_z(\text{C}) -$ $- 0.211p_y(\text{S}) + 0.212s(\text{H}_1)$	-1 049.15
	CNDO/2 (<i>spd</i>)	7	$-0.297s(\text{C}) - 0.317p_y(\text{C}) +$ $+ 0.661p_z(\text{C}) + 0.288p_y(\text{S}) +$ $+ 0.401d_{yz}(\text{S}) - 0.219s(\text{H}_1) +$ $+ 0.205s(\text{H}_2)$	-1 219.55
	<i>ab initio</i> STO-3G	13	$-0.500 2s(\text{C}) + 0.830 2p_z(\text{C}) +$ $+ 0.222 3p_y(\text{S}) - 0.215 1s(\text{H}_1)$	- 381.75
	4-31G	13	$0.464 2p_{zi}(\text{C}) + 0.583 2p_{z0}(\text{C}) +$ $- 0.211 1s_0(\text{H}_1) - 0.244 1s_0(\text{H}_1)$	- 651.65
	<i>ab initio</i> ^d (HONDO) (<i>sp</i>)	13	$0.383p_z(\text{C}) + 0.656p_z(\text{C}) +$ $+ 0.225s(\text{H}_1) - 0.245s(\text{H}_2)$	- 610.49
	<i>ab initio</i> ^d (HONDO) (<i>spd</i>)	13	$-0.386p_z(\text{C}) - 0.612p_z(\text{C}) -$ $- 0.233s(\text{H}_1) + 0.245s(\text{H}_2) -$ $- 0.136d_{yz}(\text{S})$	- 653.65
II	CNDO/2 (<i>sp</i>)	13	$-0.362s(\text{C}) - 0.784p_z(\text{C}) +$ $+ 0.230p_y(\text{S})$	- 917.87
	CNDO/2 (<i>spd</i>)	13	$-0.247s(\text{C}) - 0.294p_y(\text{C}) -$ $- 0.669p_z(\text{C}) + 0.280p_y(\text{S}) -$ $- 0.380d_{yz}(\text{S})$	-1 086.69
	<i>ab initio</i>	21	$-0.489 2s(\text{C}) - 0.822 2p_z(\text{C}) +$ $+ 0.249 3p_y(\text{S})$	- 337.64
III	CNDO/2 (<i>sp</i>)	21	$-0.724p_z(\text{C}) + 0.466p_z(\text{N}_{\text{CN}}) +$ $+ 0.451p_z(\text{N}_{\text{CN}})$	- 858.80
	CNDO/2 (<i>spd</i>)	21	$-0.357s_{yz}(\text{S}) - 0.627p_z(\text{C}) +$ $+ 0.426p_z(\text{N}_{\text{CN}}) + 0.422p_z(\text{N}_{\text{CN}})$	- 985.35
	STO-3G	33	$-0.757 2p_z(\text{C}) + 0.451 2p_z(\text{N}_{\text{CN}})$ $+ 0.439 2p_z(\text{N}_{\text{CN}})$	- 528.25
IV	CNDO/2 (<i>sp</i>)	23	$-0.618p_z(\text{C}) + 0.537 p_z(\text{O}) +$ $+ 0.547p_z(\text{O})$	- 958.83
	CNDO/2 (<i>spd</i>)	23	$0.293d_{yz}(\text{S}) + 0.556p_z(\text{C}) -$ $- 0.498p_z(\text{O}) - 0.538p_z(\text{O})$	-1 047.84
	STO-3G	35	$-0.692 2p_z(\text{C}) + 0.516 2p_z(\text{O}) +$ $+ 0.498 2p_z(\text{O})$	- 457.89

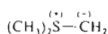
TABLE III
(Continued)

Compound	Method (basis)	i^a MO index	Θ_i^b	$\epsilon_i, \text{kJ mol}^{-1}$
V	CNDO/2 (<i>sp</i>)	28	$-0.630p_z(\text{C}) + 0.526p_z(\text{O}) + 0.539p_z(\text{O})$	- 931.00
	CNDO/2 (<i>spd</i>)	28	$0.294d_{yz}(\text{S}) + 0.564p_z(\text{C}) - 0.489p_z(\text{O}) - 0.531p_z(\text{O})$	-1 024.99
VI	CNDO/2 (<i>sp</i>)	35	$0.639p_z(\text{C}) - 0.512p_z(\text{O}) - 0.539p_z(\text{O})$	- 959.62
	CNDO/2 (<i>spd</i>)	35	$0.294d_{yz}(\text{S}) + 0.554p_z(\text{C}) - 0.482p_z(\text{O}) - 0.551p_z(\text{O})$	-1 046.52

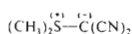
i^a Serial number of MO; b chosen terms with C_i 0.20; c total energy calculated *ab initio* (basis of Roos and Siegbahn) without *d*-orbitals amounts to $-1.1076992 \cdot 10^6 \text{ kJ mol}^{-1}$, with *d*-orbitals $-1.1079181 \cdot 10^6 \text{ kJ mol}^{-1}$; d symbols *p* and *s* denote Gaussian functions with largest exponents.



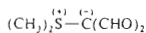
I



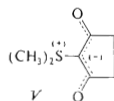
II



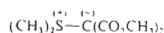
III



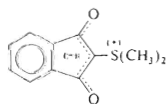
IV



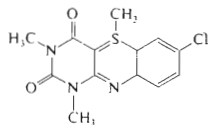
V



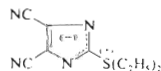
VI



VII



VIII



IX

of d -orbitals results in a decrease of charge separation on the S and C atoms and of charges on electronegative atoms of stabilizing groups. There is a decrease in the

$\text{C}=\text{C}$ bond index and increase in the $\text{C}-\text{X}$ ($\text{X} = \text{O}, \text{N}$) bond order (decreasing enolate character of the bond).

The role of d -orbitals may be demonstrated on the basis of analysis of the HOMO wave function. With neglect of d -orbitals, HOMO of non-stabilized ylides is represented mainly by the lone electron pair orbital. Inclusion of d -orbitals leads to a substantial change of the wave function (Table III). It follows from the expansion coefficients values that the resulting decrease in orbital energies is caused by a π -overlap between the relevant $3d$ -orbital of the sulfur atom and $2p$ -orbital of the carbon atom (a decrease in total energy as a consequence of overlap stabilization between $3d_{yz}(S)$ and $2p_z(C)$). It further follows from *ab initio* calculations that bases without d -orbitals lead for non-stabilized ylides to HOMO with a nodal plane on the C—S bond which disappears on inclusion of d -orbitals. For stabilized ylides the HOMO wave function is localized on the ylide carbon atom and on the stabilizing groups. Inclusion of d -orbitals results in delocalization into the region of the C—S bond. In stabilized sulfonium ylides, the $2p_z$ -orbitals of electronegative atoms (O, N) are significantly populated. It follows from comparison of the C—S bond orders (CNDO/2, *spd*, Table II) in carbonyl-stabilized ylides that participation of d -orbitals operates most significantly in the ylide VI. For non-stabilized ylides this stabilization mechanism is the only one possible and it is therefore substantially more significant than for the stabilized ylides.

The importance of d -orbitals for a reliable quantum chemical description of sulfonium ylides may be inferred also from a comparison of calculated and experimental dipole moments³⁰. Calculated dipole moments strongly depend on the used AO basis³⁰. Inclusion of d -orbitals leads to a charge reduction on S and C atoms (Table II) and, consequently, to a marked decrease in the calculated dipole moments. Dipole moments, calculated without inclusion of d -orbitals either semiempirically or by the *ab initio* method, are significantly higher than the experimental values. On the other hand, the values calculated with inclusion of d -orbitals (CNDO/2, *spd*) are close to the experimental data³⁰.

On the basis of our results we can thus conclude that a reasonable quantum chemical description of sulfonium ylides requires inclusion of d -orbitals into the AO basis set.

REFERENCES

1. Pauling L.: J. Phys. Chem. 56, 361 (1952).
2. Wolfe S., Rauk A., Csizmadia I. G.: J. Amer. Chem. Soc. 91, 1567 (1969).
3. Koch H. P., Moffat W. E.: Trans. Faraday Soc. 47, 7 (1951).
4. Jordan T., Smith H. W., Lohr L. L. jr, Lipscomb W. N.: J. Amer. Chem. Soc. 85, 846 (1963).
5. Hoffmann R., Fujimoto H., Sivenson J. R., Wan C. C.: J. Amer. Chem. Soc. 95, 7644 (1973).
6. Jordan T., Smith H. W., Lohr L. L. jr, Lipscomb W. N.: J. Amer. Chem. Soc. 85, 846 (1963).
7. Manne R.: Theor. Chim. Acta 6, 312 (1966).
8. Nakatsuji H., Mussher J. Y.: Chem. Phys. Lett. 34, 77 (1974).
9. Van Der Woon C. P., Drago R. S.: J. Amer. Chem. Soc. 94, 3035 (1972).

10. Bernardi F., Csizmadia I. G., Mangini A., Schlegel H. B., Whangbo M., Wolfe S.: *J. Amer. Chem. Soc.* **97**, 2209 (1975).
11. Minyayev R. M., Minkin V. I., Sadekov I. D., Nabaka V. I.: *Zh. Obshch. Khim.* **47**, 1294 (1977).
12. Coulson C. A.: *Nature (London)* **221**, 1106 (1969).
13. Ratner M. A., Sabin J. R.: *J. Amer. Chem. Soc.* **93**, 3542 (1971).
14. Yamaguchi K., Fueno T., Fukutome H.: *Chem. Phys. Lett.* **22**, 461 (1973).
15. Yamaguchi K., Fueno T., Fukutome H.: *Chem. Phys. Lett.* **22**, 466 (1973).
16. Yamaguchi K., Fueno T.: *Chem. Phys. Lett.* **22**, 471 (1973).
17. Tatsumi K., Yoshioka Y., Yamaguchi K., Fueno T.: *Tetrahedron* **32**, 1705 (1976).
18. Ratts K. W.: *Tetrahedron Lett.* **1966**, 4707.
19. Cook A. F., Moffat J. C.: *J. Amer. Chem. Soc.* **90**, 740 (1968).
20. Nejland O. Ja., Kalnin C. V.: *Zh. Org. Khim.* **4**, 140 (1968).
21. Pople J. A., Beveridge D. L.: *Approximate Molecular Orbital Theory*. McGraw-Hill, NY 1970.
22. Claverie P., Daudey J. P., Diner S., Giessner-Prettre G., Gilbert M., Langlet I., Malrieu J. P., Pincelli U., Pullman B.: *QCPE* **12**, 220 (1980).
23. Ditchfield R., Hehre W. J., Pople J. A.: *J. Chem. Phys.* **54**, 724 (1971).
24. Hehre W. J., Lathan W. A., Ditchfield R., Newton M. D., Pople J. A.: *QCPE* **12**, 236
25. Rauk A., Csizmadia I. G.: *Can. J. Chem.* **46**, 1205 (1968).
26. Roos B., Siegbahn P.: *Theor. Chim. Acta* **17**, 199 (1970).
27. Huzinaga S.: *J. Chem. Phys.* **42**, 1293 (1965).
28. King H. F., Dupuis M., Rys J.: *QCPE* **12**, 338 (1980).
29. Bernardi F., Schlegel M. B., Whangbo M., Wolfe S.: *J. Amer. Chem. Soc.* **99**, 5633 (1977).
30. Král V., Arnold Z., Jehlička V., Exner O.: *This Journal* **45**, 1236 (1980).
31. Christensen A. T., Witmore W. G.: *Acta Crystallogr. Sect. B* **25**, 73 (1969).
32. Kulpe S.: Private communication.
33. Christensen A. T., Thom E.: *Acta Crystallogr. Sect. B* **27**, 581 (1971).
34. Schaefer J. P., Reed L. L.: *J. Amer. Chem. Soc.* **94**, 908 (1972).
35. Atwood J. L., Mayfield H. T.: *Cryst. Struct. Commun.* **1978**, 739.
36. Sutton L. E. (Ed): *Tables of Interatomic Distances*. The Chemical Society, London 1958.
37. Karle I. L., Estlin S. A., Britts K.: *Acta Crystallogr.* **22**, 273 (1967).
38. Kunchur N. R., Truter M. R.: *J. Chem. Soc.* **1958**, 2551.
39. Truter M. R.: *J. Chem. Soc.* **1960**, 997.
40. Král V., Arnold Z.: *This Journal* **45**, 92 (1980).

Translated by M. Tichý.