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Infrared absorption spectra of benzyl phenyl sulphide dibenzyl disulphide and dibenzyl sulphoxide*

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The ever increasing realisation of the biochemical, medical and industrial importance of organic sulphur compounds has evoked a great interest in the spectroscopic studies of these molecules. The infrared absorption spectra of several aromatic sulphur compounds have been studied by various workers (Barnard *et al* 1949, Shrieber 1949, Amstutz *et al* 1951, Cymerman and Willis 1951, Green 1962, Green 1968, Allum *et al* 1968, Mallick *et al* 1973). No information is, however, available on the vibrational analysis of benzyl phenyl sulphide, dibenzyl disulphide and dibenzyl sulphoxide (hereafter referred to as BPS, DBDS and DBSO respectively). The present investigation has therefore been undertaken with a view to presenting detailed vibrational assignments of the infrared bands of these molecules.

The chemicals DBDS and DBSO of AR quality were obtained from M/S Riedel de Haeng, Germany while BPS of same quality was obtained from M/S Tokyo Chemical Co., Japan. The infrared absorption spectra were recorded on Perkin-Elmer (model 577) IR grating spectrophotometer in the region 200–4000 cm^{-1} in solid phase using KBr pellet technique.

The vibrational assignments have been made assuming C_s point group symmetry for each of the three molecules. The assignments are based essentially on the magnitudes and relative intensities of the observed bands. In addition, assignments in related molecules have been utilized to serve as guidelines in the present analysis. A correlation of the observed fundamental phenyl vibrations in the infrared spectra of BPS, DBDS and DBSO molecules alongwith their relative intensities, symmetry species and proposed assignments have been presented in Table 1. The numbering of phenyl modes follows Wilson (1934). The wave-

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Table 1. Assignment of fundamental phenyl ring vibrations in BPS, DBDS and DBSO molecules

	BPS	DBDS	DBSO		Assignment	VIBR. No.
	Band (cm^{-1})	Band (cm^{-1})	Band (cm^{-1})	Sym. species		
1	n.i	3080(w)	3082(w)	a′	ν(C-H)	20a
2	n.i	n.i.	3064(w)	a′	ν(C−H)	20b
3	3045(s)	n.i.	3042(ms)	a′	ν(C-H)	2
4	n.i.	3025(m)	n.i.	a′	ν(C-H)	13
5	3015(s)	3010(m)	3010(s)	a′	ν(C-H)	7b
6	1590(s)	1585(s)	1588(m)	a′	ν(C-C)	8a
7	1570(s)	1569(s)	1571(m)	a′	ν(C-C)	8b
8	1481(s)	1478(s)	1476(vs)	a′	ν(C-C)	19a
9	1440(s)	1436(s)	1437(vs)	a′	ν(C-C)	19b
10	1309(w)	1318(vw)	1628(w)	a′	ν(C-C)	14
11	1292(s)	1280(m)	1382(m)	a′	β(C-H)	3
12	1175(w)	1173(w)	1169(w)	a′	β(C-H)	9a
13	1150(m)	1132(m)	1145(m)	a′	β(C-H)	9b
14	1062(s)	1061(s)	1062(vs)	a′	β(C-H)	15
15	1020(s)	1021(s)	1018(vs)	a′	β(C-H)	18a
16	999(s)	999(s)	991(s)	a′	Ring	1
17	619(m)	619(m)	617(m)	a′	α(C-C-C)	6b
18	1081(s)	1100(s)	1098(s)	a′	X-sens.	7a
19	815/802(m)	800(m)	804(m)	a′	X-sens.	12
20	481/471(s)	465(s)	465(vs)	a′	X-sens.	6a
21	232(s′)	229(m)	n.i.	a′	X-sens.	18b
22	960(m)	969(n)	962(m)	a″	γ(C-H)	5
23	913(m)	909(m)	910(s)	a″	γ(C-H)	17a
24	891(w)	n.i.	881(m)	a″	γ(C-H)	10a
25	860(m)	860(m)	860(m)	a″	γ(C-H)	11
26	764(s)	765(s)	768(vs)	a″	γ(C-H)	17b
28	686(s)	691(s)	692(vs)	a″	ϕ(C-C)	4
26	403(w)	n.i.	n.i.	a″	ϕ(C-C)	16a
29	564(w)	564(w)	559(w)	a″	X-sens	16b
30	214(s)	210(s)	n i.	a″	X-sens.	10b

n.i.-not investigated ; w-weak ; m-medium ; s-strong ; v-very ; ν-stretching ; β-in-plane bending , γ-out-of-plane bending ; α-angle deformation ; ϕ-torsional deformation ; X-substitutent The letter in parantheses against the wave number indicates the relative intensity of the band.

numbers, intensities and proposed assignments for the internal vibrations of the intermediate groups have been reported in Table 2.

Table 2. Vibrational modes of the intermediate group (in cm^{-1})

Nature*	BPS	DBDS	DBSO
CH_2 strasy	2908(s)	2944(s)	2943(s)
CH_2 strasy	2880(s)	2890(s)	2895(s)
CH_2d	1428(s)	1398(s)	1398(s)
CH_2w	1230(s)	1220(s)	1240(s)
CR_2r	735(s)	755(s)	752(s)
C-S str	670(s)	660(s)	672(s)
S-S str	n.a.	505(m)	n.a.
CSOd	n.a.	n.a.	360/320(m)

*asy-asymmetric ; sy-symmetric ; str-stretch ; d-deformation ; w-wag ; r-rock ; s-strong ; m-medium ; n.a.-not applicable.

The frequencies of vibrations of a number of modes that are not substituent-sensitive have been observed in the usually accepted regions (Whiffen 1956, Green 1961, Green 1962, Stephenson *et al* 1961, Jacobsen and Bentley 1964, Garrigou-Lagrange *et al* 1958, Green 1968) and have been properly identified in Table 1. The substituent-sensitive vibrations, on the other hand, have been located by comparison with assignments in related molecules (Mallick *et al* 1973, Allum *et al* 1968). The vibrations arising due to the respective intermediate groups in the molecules under consideration have been identified in Table 2 These assignments are in agreement with Trotter and Thompson 1946, Cymerman and Willis 1951, Wiberley *et al* 1960, Allum *et al* 1968, Green 1968.

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