ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

2019. Том 60, № 2 *Февраль* *DOI: 10.26902/JSC_id39212*

SUPPLEMENTARY MATERIALS TO:

SPECTROSCOPIC PROPERTIES AND THEORETICAL STUDIES OF 5-ETHYLSULPHONYL-2-PHENYL-BENZOXAZOL: RELATION BETWEEN THE FRONTIER MOLECULAR ORBITALS AND OPTICAL PROPERTIES

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Table S1

Calculated wavenumbers, observed FT-IR bands, and assignments of 5-ethylsulphonyl-2-phenyl-benzoxazole

Assignments (% PED)[a]	Experiment[b] (cm^{-1})	B3LYP/ 6–311++G(*d*,*p*) (unscaled) (cm^{-1})	B3LYP/ 6–311++G(*d*,*p*) (scaled)[c] (cm^{-1})	Mode
1	2	3	4	5
$\upsilon_s(CH)_{PhII}(99)$	–	3214	3076	93
$\upsilon_{as}(CH)_{PhII}(98)$		3209	3072	92
$\upsilon_s(CH)_{PhI}$ (99)	3067(w)	3205	3068	91
$\upsilon_{as}(CH)_{PhI}(100)$		3203	3066	90

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1	2	3	4	5
$\upsilon_{as}(CH)_{PhII}(100)$		3196	3059	89
$\upsilon_{as}(CH)_{PhI}(100)$		3190	3053	88
$\upsilon_{as}(CH)_{PhI}(100)$		3180	3044	87
$\upsilon_{as}(CH)_{PhI}(100)$		3169	3033	86
$\upsilon_{as}(CH_2)(36)+ \upsilon_{as}(CH_3)(63)$		3128	2994	85
$\upsilon_{as}(CH_2)(57)+ \upsilon_{as}(CH_3)(52)$	2980(w)	3109	2976	84
$\upsilon_{as}(CH_2)(8)+ \upsilon_{as}(CH_3)(91)$		3101	2968	83
$\upsilon_{s}(CH_2)(98)$	2939(w)	3061	2930	82
$\upsilon_{s}(CH_3)(100)$		3040	2909	81
$\upsilon(PhII)_{ring}(35)+\upsilon(N=C)(17)+ \upsilon(PhI)_{ring}(12)$	1619(m)	1652	1595	80
$\upsilon(PhII)_{ring}(40)+ \upsilon(PhI)_{ring}(10)$		1643	1584	79
$\upsilon(PhII)_{ring}(15)+ \upsilon(PhI)_{ring}(45)$		1635	1575	78
$\upsilon(PhII)_{ring}(13)+ \upsilon(PhI)_{ring}(50)$		1617	1556	77
$\upsilon(N=C)(30)+\upsilon(N–C)(12)$	1556(s)	1586	1531	76
$\upsilon(N=C)(6)+ \upsilon(PhI)ring(26)+\rho(CH)_{PhI}(52)$	1481(m)	1519	1453	75
$\delta_{as}(CH_3)(62)$	1449(s)	1506	1444	74
$\delta_{as}(CH_3)(63)$		1495	1433	73
$\upsilon(PhII)_{ring}(37)+\rho(CH)_{PhI}(28)$	1423(s)	1483	1425	72
$\upsilon(PhI)_{ring}(24)+ \rho(CH)_{PhI}(44)$		1477	1416	71
$sci(CH_2)(33)$	1402(sh)	1456	1405	70
$\upsilon(N=C)(10)+ \upsilon(PhII)_{ring}(48)+\rho(CH)_{PhII}(27)$		1453	1400	69
$\delta_{s}(CH_3)(96)$	1345(m)	1417	1347	68
$\upsilon(PhII)_{ring}(66)$		1380	1327	67
$\upsilon(PhI)_{ring}(24)+\rho(CH)_{PhI}(62)$	1312(vs)	1356	1293	66
$\upsilon(PhI)_{ring}(39)$	1274(m)	1341	1291	65
$\upsilon_{as}(SO_2)(6)+\gamma(CH_2–S)(21)+\gamma(CH_2–CH_3)(21)$	1262(m)	1313	1264	64
$\upsilon(N=C)(10)+\upsilon(C–N–C)(10)+\upsilon(PhI)_{ring}(21)+\rho(CH)_{PhII}(10)+\upsilon(PhII)_{ring}(4)$		1306	1255	63
$\upsilon(C–O)(6)+\upsilon_{as}(SO_2)(9)+ \upsilon(C–N)(6)+\upsilon(PhII)_{ring}(6)+\rho(CH)_{PhII}(49)$	1238(s)	1282	1229	62
$\upsilon_{as}(S–O)(35)+\gamma(CH_2–S)(11)+\gamma(CH_2– CH_3)(30)$		1271	1218	61
$\upsilon(C–N)(35)+\upsilon(PhII)ring(4)+\rho(CH)_{PhII}(24)$		1258	1212	60
$\upsilon_{as}(S–O)(41)+\gamma(CH_2– CH_3)(24)$	1200(w)	1255	1205	59

1	2	3	4	5
υ(C–O)(28)+ υ(N=C)(6)+υ(PhII)$_{ring}$(12)+ρ(CH)$_{PhII}$(25)	1172(w)	1218	1174	58
υ(PhI)$_{ring}$(15)+ρ(CH)$_{PhI}$(65)		1255	1144	57
υ(PhI)$_{ring}$(16)+ρ(CH)$_{PhI}$(76)	1129(vs)	1185	1127	56
υ(PhII)$_{ring}$(24)+ρ(CH)$_{PhII}$(64)		1144	1094	55
υ_s(S–O)(15)+υ_{as}(S–C$_{phII}$)(3)+υ(PhI)$_{ring}$(4)+ρ(CH)$_{PhI}$(18)	1065(m)	1108	1066	54
υ_s(S–O)(28)+υ_{as}(S–C$_{phII}$)(3)+υ(PhI)$_{ring}$(12)+ρ(CH)$_{PhI}$(11)		1101	1058	53
υ(CH$_2$– CH$_3$)(38)+γ(CH$_2$–CH$_3$)(6)+γ(CH$_3$)(25)	1042(s)	1078	1037	52
υ_s(S–O)(8)+ υ(C9–O)(16)+υ(PhI)$_{ring}$(11)+ρ(CH)$_{PhI}$(21)+ ρ(N1–C9–O1)(11)		1066	1032	51
υ_s(S–O)(11)+υ(PhII)$_{ring}$(4)+t(CH$_2$)(20)+τ(CH$_2$ –CH$_3$)(24)		1056	1015	50
υ_s(S–O)(20)+υ(S–C3)(3)+ υ(PhI)$_{ring}$(11)+υ(PhII)$_{ring}$(12)+ρ(CH)$_{PhI}$(10)		1053	1011	49
υ(PhI)$_{ring}$(14)+ρ(CH)$_{PhI}$(22)+ ρ(C–C–C)$_{phI}$(19)	1020(w)	1039	1009	48
υ(PhI)$_{ring}$(72)+ρ(C–C–C)$_{phI}$(4)		1016	985	47
τ(PhI)(87)	977(w)	1005	981	46
τ(PhI)(83)		992	969	45
υ(CH$_2$–CH$_3$)(47)+ υ(CH$_2$–S)(5)+γ(CH$_3$)(25)		986	944	44
τ(PhII)(88)	942(w)	938	962	43
τ(PhI)(88)		925	948	42
υ(C3–S)(4)+υ(PhI)$_{ring}$(4)+ υ(PhI)$_{ring}$(3)+υ(C9–O1)(12)+ ρ(C6–O1–C9)(13)+ρ(O1–C9–N1)(5)	919(m)	935	918	41
υ(C–N)(10)+υ(C9–O1)(30)+ υ(PhII)$_{ring}$(16)+ υ(C6–O1)(3)+ρ(O1–C9–N1)(4)+ρ(O1–C9–N1)(7)		934	912	40
τ(H4–C4–C3–S1)(23)+τ(C6–C5–C4–H4)(18)+τ(N–C5–C4–H4)(29)+τ(H4–C4–C3–C2)(17)	885(m)	918	895	39
τ(PhI)$_{ring}$(100)		861	840	38
υ(C6–O1)(14)+υ(C5–N)(3)+ υ(PhII)$_{ring}$(41)+ ρ(CH)$_{PhII}$(4)+τ(H4+C4+C5+N1)(3)	815(s)	838	812	37
τ(H7–C7–C6–N)(21)+τ(H7–C7–C6–C5)(8)+τ(H8–C8–C3–S)(11)+τ(H8–C8–C7–H7)(14)+ +τ(C3–C8–C7–H7)(15)		826	806	36
τ(N–C9–O1–C6)(4)+τ(O1–C9–N–C5)(4)+τ(H14–C14–C13–H12)(6)+ +τ(H12–C12–C13–C14)(5)+τ(H11–C11–C10–C9)(4)+τ(N1–C9–C10–C11)(10)+ +τ(C10–C11–C12–H12)(8)+τ(H15–C15–C10–C9)(5)+τ(O1–C9–C10–C15)(8)+ +τ(C10–C15–C14–H14)(9)+τ(C11–C12–C13–H13)(6)+τ(C15–C14–C13–H13)(6)	781(vs)	791	772	35
γ(CH$_2$–CH$_3$)(35)+τ(H2a–C12–S–O2)(12)+τ(H2b–C2–S–O2)(10)		785	759	34

1	2	3	4	5
τ(N–C5–C6–O1)(10)+τ(O1–C9–C10–C15)(8)+τ(C6–C5–C4–H4)(7)+ +τ(C5–C6–O1–C9)(4)+τ(C6–C5–N–C9)(8)+τ(H7–C7–C6–C5)(8)+ +(C4–C5–C6–C7)(11)+(H4–C4–C3–C8)(4)+(C8–C7–C6–C5)(8)	733(vs)	764	746	33
υ(C3–S1)(11)+ υ(CH_2–S)(10)+υ(PhII)$_{ring}$(4)+γ(C5–C6–O1)(7)+ +γ(C6–C5–N)(4)+γ(PhII)$_{ring}$(12)		729	713	32
τ(N–C9–O1–C6)(12)+τ(H7–C7–C6–C5)(4)+τ(O1–C9–N–C5)(10)+τ(PhI)$_{ring}$(16)+ +τ(O1–C9–C10–C11)(4)+τ(N–C9–C10–C11)(6)+τ(O1–C9–C10–C15)(4)+τ(N–C9–C10–C11)(5)		719	702	31
υ(C9–C10)(9)+ υ(PhI)$_{ring}$(10)+ ρ(PhI)$_{ring}$+(30)+ρ(O1–C9–N)(3)		704	692	30
τ(PhI)$_{ring}$(99)	688(s)	698	681	29
υ(S–CH_2)(27)+γ(C6–C5–N)(4)+γ(C5–C6–O1)(4)+γ(C6–C5–N)(4)+τ(C8–C3–S–O3)(7)		678	664	28
δ(PhI)$_{ring}$(78)	614(m)	631	621	27
υ(S–CH_2)(13)+γ(C3–S1–CH_2)(3)+τ(N–C5–C4–C3)(3)+τ(PhII)$_{ring}$(38)		618	603	26
υ(C6–O1)(4)+ υ(C3–S)(6)+υ(PhII)$_{ring}$(8)+δ(PhII)$_{ring}$(36)	592(m)	599	590	25
δ(PhII)$_{ring}$(19)+δ(PhII)$_{ring}$(13)+δ(O1–C9–C10)(11)+δ(N–C9–C10)(11)+ +δ(C7–C6–O1)(5)C10)(11)+δ(C9–C10–C15)(6)		557	554	24
δ(SO_2)(18)+τ(C4–C3–S1–O2)(4)+τ(CH_2–S1–O2)(19)+τ(C8–C3–S1–O2)(4)+τ(CH_3–CH_2–O2)(11)		513	504	23
τ(RingIII)(15)+τ(PhI)$_{ring}$(46)+τ(N–C9–C10–C11)(3)		499	487	22
υ(S–CH_2)(8)+γ(C3–S1–CH_2)(7)+τ(O2–S–CH_2)(10)+τ(C4–C3–S1–O2)(5)+τ(C8–C3–S1–O2)(6)		488	479	21
τ(PhII)$_{ring}$(35)+τ(C5–C5–N–C9)(4)+τ(C7–C6–O1–C9)(3)		434	425	20
υ(S–CH_2)(10)+γ (O2–S–C3)(6)+ γ(C4–C3–S1)(5)+τ(C4–C3–S1–O3)(7)+τ(PhII)$_{ring}$(3)		425	418	19
τ(PhI)$_{ring}$(98)		410	400	18
υ(S–CH_2)(9)+δ(SO_2)(7)+γ(C3–S1–CH_2)(6)+δ(O3–S–CH_2)(13)+ γ(CH_3–CH_2–S)(5)+ +τ(C4–C3–S1–O3)(7)		365	360	17
γ(O2–S–CH_2)(7)+γ(C3–S–CH_2)(11)+γ(C9–C10–C15)(3)		361	355	16
υ(S–C3)(16)+υ(C9–C10)(19)+ γ(C9–C10–C11)(4)+γ(C11–C10–C15)(7)		337	329	15
γ(O2–S–C3)(9)+ γ(N–C5–C4)(4)+γ(C7–C6–O1)(4)+ γ(C3–S–CH_2)(5)+ +γ(C9–C10–C11)(8)+ γ(C9–C10–C15)(6)+τ(H2a–C2–CS–C3–C9)(3)		302	298	14
γ(CH_2–S–C3)(3)+ γ(C3–S–O)(11)+γ(O2–S–CH_2)(5)		298	294	13
γ(SO_2)(8)+γ(O2–S–CH_2)(5)+γ(CH_3–CH_2–S)(4)+τ(PhII)$_{ring}$(5)+τ(N–C5–C6–C7)(4)+ +τ(C7–C6–O1–C9)(3)+τ(C8–C3–S1–O2)(5)+τ(CH_3–CH_2)(17)+τ(CH_3–CH_2–S)(16)			248	12
γ(O2–S–CH_2)(10)+γ(CH_3–CH_2–S)(5)+τ(CH_3–CH_2)(19)+τ(CH_3–CH_2–S)(38)		164	216	11

1	2	3	4	5
υ(S–C3)(16)+υ(C9–C10)(7)+γ(O2–S–CH_2)(5)+γ(CH_3–CH_2–S)(14)+ +τ(C4–C3–S–O2)(3)+τ(C8–C3–S–O2)(4)			210	10
υ(S–C3)(7)+γ(O3–S–CH_2)(3)+ γ(CH_3–CH_2–S)(3)+τ(N–C5–C6–C7)(3)+ +τ(C7–C6–O1–C9)(6)+τ(C7–C8–C3–S1)(3)+τ(C12–C11–C10–C9)(4)+ +τ(C14–C15–C10–C9)(4)		203	199	9
γ(O3–S–C3)(3)+γ(C3–S–CH_2)(17)+ γ(O3–S–C8)(4)+γ(CH_3–CH_2–S)(3)+ +τ(N–C5–C4–C3)(4)+τ(C4–C5–N1–C9)(4)+τ(C11–C10–C9–O1)(6)+ +τ(C14–C15–C10–C9)(7)		164	162	8
δ(C4–C3–S)(20)+δ(O1–C9–C10)(5)+δ(O1–C9–C10)(5)+δ(N1–C9–C10)(4)+ +δ(C8–C3–S1)(14)+δ(C9–C10–C11)(6)+δ(C9–C10–C15)(8)+τ(H2a–C2–S–O2)(19)		156	155	7
τ(C5–C4–C3–S)(5)+τ(CH_2–S–C3)(13)+τ(H2a–C2–S–O2)(3)+ +τ(C8–C3–S–O2)(6)+τ(C7–C8–C3–S)(6)+τ(N1–C9–C10–C15)(4)+ +τ(CH_3–CH_2–S–O)(14)+τ(CH_3–CH_2–S–C3)(12)		104	102	6
γ(C4–C3–S1)(6)+ γ(O1–C9–C10)(16)+ γ(N1–C9–C10)(16)+ γ(C8–C3–S1)(8)+ +γ(O3–S–C3)(3)+ γ(C9–C10–C11)(9)+ γ(C9–C10–C15)(9)		78	78	5
γ(C3–S–C2)(7)+τ(C4–C3–S–O3)(4)+τ(C8–C3–S–O2)(6)+τ(C19–C9–O1–C7)(4)+ +τ(C19–C9–N1–C5)(5)+τ(CH_2–S–C3)(12)+τ(C4–C3–S–C2)(5)+ +τ(C1–C2–S–C3)(13)+τ(C1–C2–S–O3)(7)		69	67	4
τ(C4–C3–SO_2)(6)+τ(C8–C3–SO_2)(10)+τ(C6–O1–C9–C10)(22)+ +τ(N1–C9–C10–C11)(9)+τ(O1–C9–C10–C15)(15)+ +τ(N1–C9–C10–C15)(4)+τ(C1–C2–S–C3)(3)		55	54	3
τ(C5–C4–C3–S1)(3)+τ(C4–C5–N1–C9)(3)+τ(C8–C3–S–O2)(6)+ +τ(C7–C8–C3–S1)(4)+τ(C8–C3–S–C2)(4)+τ(O1–C9–C10–C11)(5)+ +τ(N1–C9–C10–C11)(13)+τ(O1–C9–C10–C15)(11)+τ(N1–C9– C10–C15)(21)			34	2
τ(C4–C3–S–C2)(7)+τ(C4–C3–S–O2)(13)+τ(C5–C4–C3–S)(5)+ +τ(N1–C5–C4–C3)(4)+τ(C10–C9–O1–C6)(5)+τ(C10–C9–N1–C5)(5)+ +τ(C4–C3–S–C2)(16)+τ(C8–C3–S–O3)(6)+τ(C8–C7–C6–O1)(3)+ +τ(C8–C3–S–C2)(8)+τ(O1–C9–C10–C11)(3)		32	31	1

[a]*Abbreviations*: ν is bond stretching; δ is in-plane deformation; γ is out-of-plane deformation; sci is scissoring; t is twisting; τ is torsion; w is wagging; ρ is rocking; PhI is *para*-substitued phenyl ring; PhII is trisubstitued phenyl ring; RingIII is benzoxazole ring; as is antisymmetric; and s is symmetric; % of PED is given in brackets for B3LYP.

[b]vs is very strong; s is strong; m is medium; w is weak; sh is shoulder.

[c]Scaled with quantum mechanics force field (SQMFF) methodology [19]