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Correction to "Reactions Between Azolium Salts and Nucleophilic Reagents VII"*

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The exchange rate data in the last three columns of Table 1 on p. 3504 should be corrected as follows: For 9.86 2.4 5.5 read 7.96 21.9 48. For 32.5 30, read 17.5 60.

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Mean Amplitudes of Vibration for Small Molecules Containing Sulphur

Part IV. SO_2FCl and SO_2FBr

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The mixed sulphuryl halides SO_2FCl and SO_2FBr were investigated in continuation of the previous vibrational analyses of small molecules containing sulphur.[1–3] Structural parameters were transferred from the related molecules SO_2F_2, SO_2Cl_2, and $SOBr_2$.

An initial approximate harmonic force field for SO_2FCl was set up with the aid of the previously developed force fields for SO_2F_2[2] and SO_2Cl_2.[1] The final force field for SO_2FCl was produced so as to make it fit exactly the set of observed frequencies:[4] (A') 1228, 823, 627, 480, 430, 195 cm^{-1} and (A'') 1455, 505, 308 cm^{-1}. This force field is given in Table 1 in terms of the F matrix on the basis of symmetry coordinates specified elsewhere[5] (atom number 1 is chosen to be F).

The final force constants for SO_2FCl were tentatively transferred to SO_2FBr along with a value of 2.5 mdyn/Å assumed for the S–Br stretching. Table 1 includes the refined force field after adjusting of the force constants in order to make them fit exactly the observed frequencies:[6] (A') 1225.8, 812.2, 601.3, 458, 305, 244 cm^{-1} and (A'') 1455.2, 489, 262 cm^{-1}.

The final force fields were used to calculate the mean amplitudes of vibration, which are shown in Table 2. The table includes the calculated interatomic distances for all the types of bonded and nonbonded atom pairs. These values contain the precise information on the applied structural parameters.

The present analysis was performed independently of a similar investigation by Ramaswamy and Jayaraman,[7] which has appeared recently. Their mean amplitudes are in generally good agreement with the present results (*cf.* Tables 3 and 4). The mentioned investigators[7] have based their analysis on vibrational assignments similar to those adopted here with one noticeable exception. They propose that 294 cm^{-1} from Pfeiffer[8] should be assigned as the

Table 1. Symmetry force constants (mdyn/Å).

Species A' for SO_2FCl					
10.472					
−0.560	4.544				
−0.060	−0.024	3.425			
−0.030	−0.015	−0.188	1.137		
0.003	0.005	−0.254	0.569	1.359	
0.016	−0.001	0.035	0.517	0.571	1.259
Species A' for SO_2FBr					
10.421					
−0.587	4.500				
−0.126	0.012	2.424			
0.006	−0.123	−0.304	1.835		
0.068	−0.139	−0.559	1.391	2.263	
0.093	−0.080	−0.257	1.210	1.343	1.862
A'' SO_2FCl			A'' SO_2FBr		
10.835			10.769		
0.007	0.760		−0.026	0.711	
0.000	0.001	0.349	−0.038	0.011	0.270

Table 2. Mean amplitudes of vibration (u) at $T = 0$ and 298 K with calculated interatomic distances (R); Å units.

Distance	SO_2FCl			SO_2FBr		
	(R)	$u(0)$	$u(298)$	(R)	$u(0)$	$u(298)$
S=O	(1.406)	0.0346	0.0347	(1.405)	0.0346	0.0348
S−F	(1.530)	0.0415	0.0426	(1.530)	0.0416	0.0428
S−Cl	(2.010)	0.0409	0.0440			
S−Br				(2.270)	0.0407	0.0483
O···O	(2.477)	0.0524	0.0556	(2.481)	0.0524	0.0554
F···Cl	(2.694)	0.0730	0.1061			
F···Br				(2.885)	0.0621	0.0836
O···F	(2.381)	0.0574	0.0624	(2.380)	0.0580	0.0632
O···Cl	(2.783)	0.0584	0.0690			
O···Br				(3.016)	0.0588	0.0749

lowest SO_2FCl frequency rather than 195 cm^{-1}. [4,9] In our initial set of calculated frequencies for SO_2FBr we obtained 173 cm^{-1} for the lowest frequency, which is below the corresponding value in SO_2FCl. This feature gives support to the mentioned re-assignment. Nevertheless we were able to adjust the force field of SO_2FBr to the observed frequencies within reasonable magnitudes of the force constants. Hence we believe that the question of the assignment of the lowest frequency in SO_2FCl is not yet definitively settled.

In Tables 3 and 4 the mean amplitudes for corresponding distances in nine molecules containing sulphur are compared. In most of the cases the mean amplitudes for related distances are found to have characteristic values.

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Table 3. Comparison between mean amplitudes (in Å at 298 K) for bonded atom pairs in some small molecules containing sulphur.

Distance	SF_4[a]	SOF_4[b]	SOF_2[c]	$SOCl_2$[d]	$SOBr_2$[c]	SO_2F_2[e]	SO_2Cl_2[f]	SO_2FCl	SO_2FBr
S=O		0.034	0.035[g]	0.036[g]	0.036[g]	0.034[g]	0.035[g]	0.034[g,h] 0.035[g,i]	0.035[g,h] 0.035[g,i]
S−F	0.043[j] 0.046[k]	0.040[j] 0.042[k]	0.044[g]			0.041[g]		0.042[g,h] 0.043[g,i]	0.043[g,h] 0.043[g,i]
S−Cl				0.052[g]			0.048[g]	0.049[g,h] 0.044[g,i]	
S−Br					0.051[g]				0.049[g,h] 0.048[g,i]

[a] From Cyvin.[3] [b] From Cyvin.[10] [c] From Müller *et al.*[11] Cited by Cyvin.[12] [d] From Hargittai and Cyvin.[1] Cited by Cyvin.[12] [e] From Cyvin and Hargittai.[2] [f] From Hargittai and Cyvin.[1] [g] Rounded off to three decimals. [h] From Ramaswamy and Jayaraman.[7] [i] Present calculations. [j] Equatorial F atom. [k] Axial F atom.

Table 4. Comparison between mean amplitudes (in Å at 298 K) for nonbonded atom pairs in some small molecules containing sulphur.

Distance	SF_4[a]	SOF_4[b]	SOF_2[c]	$SOCl_2$[d]	$SOBr_2$[c]	SO_2F_2[e]	SO_2Cl_2[f]	SO_2FCl	SO_2FBr
O···O						0.060[g]	0.067[g]	0.058[g,h] 0.056[g,i]	0.056[g,h] 0.055[g,i]
F···F	0.113[l] 0.060[m] 0.071[n]	0.069[l] 0.050[m] 0.085[n]	0.061			0.060[g]			
F···Cl								0.104[g,h] 0.106[g,i]	
F···Br									0.081[g,h] 0.084[g,i]
Cl···Cl				0.096[g]			0.099[g]		
Br···Br					0.103				
O···F		0.067[j] 0.058[k]	0.069			0.060[g]		0.060[g,h] 0.062[g,i]	0.059[g,h] 0.063[g,i]
O···Cl				0.077[g]			0.069[g]	0.065[g,h] 0.069[g,i]	
O··Br					0.087				0.073[g,h] 0.075[g,i]

[a–k] See footnotes to Table 3. [l] Equatorial-equatorial F atoms. [m] Axial-axial F atoms. [n] Equatorial-axial F atoms.

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