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Molecular Structure of Diphenyl Sulfide in the Gas Phase

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Abstract—Gas-phase electron diffraction and quantum-chemical calculations were used to study the molecular structure of diphenyl sulfide. It is shown that the diphenyl sulfide molecule (PhS_2) possesses C_2 symmetry. The main geometrical parameters are as follows: r_a(C–S) 1.774(2) Å, $r_a(C–C)_{av}$ 1.401 Å, ∠CSC 103.4(11)°, ∠SCC 122.5 and 117.9(6)°, and $\angle CCC_{av}$ 120.0°. The torsion angles about C–S bonds τ(CSCC) are –49.6(1.4)°.

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Among diphenyl derivatives of trivalent nitrogen and phosphorus, gas-phase molecular structures were studied for $HNPh_2$ [1] and $HPPh_2$ [2]. Of diphenyl derivatives of the oxygen group compounds, data are available for diphenyl ether OPh_2 [3]. The question on the molecular structure of diphenyl sulfide in the gas phase is still open, since Hargittai and co-workers [4, 5] failed to determine its conformation unambiguously. It was reasonable, using the intensities recorded in [4], to reinvestigate the molecular structure of diphenyl sulfide with the aim to compare the structural parameters of $HNPh_2$ and OPh_2, on the one hand, and those of $HPPh_2$ and SPh_2 on the other. The central atoms in these molecules posses a lone electron pair (LEP).

Diphenyl ether has an unsymmetrical conformation with different torsion angles about C–O bonds. Structural data for diphenyl sulfide are scarce. There were determined only two main geometric parameters: C–S bond length and CSC bond angle [4]. Later Hargittai [5] suggested that the Ph_2S molecule possesses a symmetric C_2 conformation. To determine the conformation of diphenyl sulfide, it was necessary first of all to conduct a theoretical study by various quantum-chemical methods. These methods permit to predict the molecular symmetry, calculate theoretical vibration frequencies, perform normal coordinate analysis, and estimate mean vibration amplitudes for nonbonded distances between carbon atoms in different phenyl groups.

Theoretical calculations. Table 1 shows selected results of conformational calculations of PhS_2 at different levels of theory [6]. The atom numbering is shown in Fig. 1. As follows from HF/6-31G**, B3LYP/6-31G**, HF/6-31G*, and B3LYP/6-31G* calculations, the C_2 structure is preferred by energy over C_s. Geometry optimization starting from the unsymmetrical conformation, too, led to a C_2 conformation. Moreover, the C_s conformation proved to possess one imaginary vibration frequency. This finding indicates that the C_s conformation corresponds to the transition state of the diphenyl sulfide molecule in the gaseous state. Nevertheless, we performed normal coordinate analysis for both the C_2 and C_s conformations. However, it proved difficult to decide between these two conformations on the basis of the normal-coordinate analysis (Table 2). Normal-coordinate analysis is used in gas-phase electron diffraction to estimate mean vibration amplitudes. In principle, they can be estimated experimentally by gas-phase electron diffraction method alone, but for such a complex molecule it is very difficult, particularly for C···C, C···H, H···H distances between different cycles, because of strong correlations of amplitudes

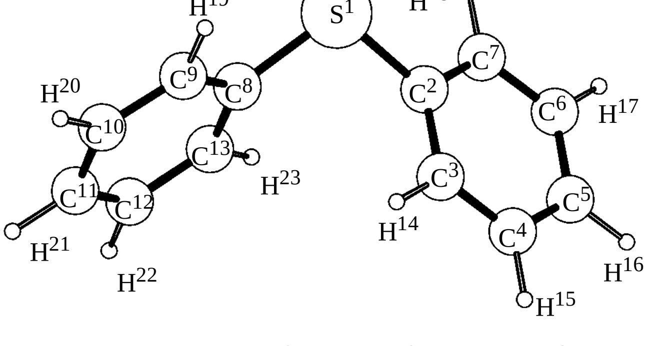

Fig. 1. Molecular conformation of diphenyl sulfide.

Table 1. Results of ab initio calculations and gas-phase electron diffraction analysis of diphenyl sulfide

Parameter	C_2 symmetry				C_s symmetry		Experiment, r_a	
	B3LYP/6-31G**	B3LYP/6-31G*	HF/6-31G**	HF/6-31G*	B3LYP/6-31G**	HF/6-31G*		
Bond lengths, Å								
S–C	1.795	1.795	1.788	1.788	1.796	1.786	1.774	(2)
C^2–C^3	1.402	1.402	1.391	1.391	1.401	1.390	1.405	
C^3–C^4	1.394	1.394	1.383	1.382	1.395	1.385	1.397	
C^4–C^5	1.397	1.398	1.388	1.388	1.396	1.386	1.401	(1)
C^5–C^6	1.395	1.395	1.383	1.383	1.396	1.386	1.398	
C^6–C^7	1.396	1.396	1.388	1.388	1.395	1.385	1.399	
C^7–C^2	1.400	1.400	1.387	1.387	1.401	1.390	1.405[a]	
C^3–H^{14}	1.085	1.086	1.074	1.075	1.085	1.075		
C^4–H^{15}	1.086	1.087	1.075	1.076	1.086	1.076		
C^5–H^{16}	1.086	1.087	1.075	1.076	1.086	1.076		
C^6–H^{17}	1.086	1.087	1.075	1.076	1.086	1.076		
C^7–H^{18}	1.085	1.086	1.074	1.075	1.085	1.075		
Bond and torsion angles, deg								
CSC	103.7	103.7	102.8	102.8	104.1	104.7	103.4	(11)
SC^2C^3	122.2	122.2	121.4	121.9	120.1	120.2	122.5	
SC^2C^7	118.0	118.0	119.0	118.0	120.1	120.2	117.9	(6)
$C^3C^2C^7$	119.7	119.7	119.6	119.6	119.8	119.6	119.6[a]	
$C^2C^3C^4$	119.9	119.9	120.1	120.1	120.0	120.1	120.0	
$C^3C^4C^5$	120.5	120.5	120.3	120.3	120.1	120.1	120.4	(1)
$C^4C^5C^6$	119.6	119.6	119.8	119.8	120.0	120.0	119.6	
$C^5C^6C^7$	120.3	120.3	120.1	120.1	120.1	120.1	120.4	
$C^6C^7C^2$	120.1	120.1	120.2	120.1	120.0	120.1	120.0[a]	
$\tau(C^8C^1C^2C^3)$	–46.0	–46.5	–58.9	–58.6	91.6	91.5	–49.6	(1.4)
$\tau(C^2C^1C^8C^{13})$	–46.0	–46.5	–58.9	–58.6	180.0	180.0	–49.6	(1.4)
E, au	–861.8613	–861.302448	–857.558954	–857.577490	–861.318183	–857.576574		
R factor, %							4.5	

[a] Dependent parameters. [b] Parenthesized values are δ_{LS}.

and geometric parameters, which increases estimation uncertainties.

Table 3 lists the calculated mean vibration amplitudes. The amplitudes for the SPh fragments are identical irrespective of the level of theory. Reliability of the calculation methods can be judge about by the C–C, C–H, C···C, and C···H amplitudes of phenyl fragments (Table 3). The calculated values fit well the experimental data for benzene. It is to be noted that we used the same approach for studying phenyl derivatives of nitrogen and phosphorous.

Structural analysis. The molecular geometry of diphenyl sulfide is determined by the following independent parameters: S–C, C–C, and C–H bond lengths and CSC, SCC, CCC, and CCH bond angles. It is assumed that the phenyl rings are planar. The molecular conformation is determined by torsion angles about the C–S bond. For the symmetric C_2 conformation they are equal. In view of the results of quantum-chemical calculations, structural analysis of the C_s conformation was not performed.

The refinement of structural parameters was performed by the least-squares method, using the computer program developed by M.B. Zuev, on the basis of the experimental intensities *I*(*s*) measured in [4]. Before analysis these *I*(*s*) values were transformed

Table 2. Normal coordinate analysis of diphenyl sulfide

C_2 symmetry B3LYP/6-31G**			C_s symmetry B3LYP/6-31G**			Exp. IR
ν, cm^{-1}	Int.	*PED*, %^{a,b}	ν, cm^{-1}	Int.	*PED*, %^{a,b}	
3114	6.4	νCH(86)	3120	5.3	νCH(96)	
3114	11.0	νCH(84)	3117	10.0	νCH(96)	
3109	1.9	νCH(96)	3114	12.9	νCH(82)	
3109	43.8	νCH(96)	3109	25.4	νCH(73)	
3102	20.0	νCH(88)	3105	20.8	νCH(80)	
3102	18.9	νCH(92)	3096	22.6	νCH(96)	
3091	10.7	νCH(92)	3095	8.8	νCH(82)	3060 s
3091	10.4	νCH(92)	3087	2.3	νCH(81)	
3083	0.4	νCH(88)	3086	0.1	νCH(92)	
3083	1.8	νCH(90)	3080	3.2	νCH(96)	
1593	3.1	νCC(60)	1595	34.8	νCC(48)	
1589	4.6	νCC(56)	1589	16.2	νCC(58)	1577 vs
1583	0.2	νCC(64)	1582	1.4	νCC(52) + αCCH(10)	
1579	4.8	νCC(64) + αCCH(10)	1581	0.8	νCC(68)	
1474	9.4	νCC(26) + αCCH(60)	1476	35.6	νCC(19) + αCCH(51)	
1473	41.4	νCC(28) + αCCH(62)	1473	20.0	νCC(19) + αCCH(56)	1476 s
1439	6.6	νCC(30) + αCCH(44)	1438	7.1	νCC(31) + αCCH(55)	
1433	6.2	νCC(28) + αCCH(68)	1435	7.7	νCC(32) + αCCH(52)	1442 s
1315	2.3	νCC(46) + αCCH(46)	1320	0.8	νCC(41) + αCCH(42)	
1314	1.0	νCC(36) + αCCH(44)	1310	2.3	νCC(52) + αCCH(42)	
1293	0.9	νCC(56) + αCCH(24)	1289	2.9	νCC(75)	
1280	0.3	νCC(62)	1284	0	νCC(41) + αCCH(26)	
1171	0.5	νCC(12) + αCCH(74)	1175	1.1	νCC(13) + αCCH(59)	
1170	1.2	νCC(12) + αCCH(70)	1168	2.3	νCC(12) + αCCH(74)	1157 w
1151	0.03	νCC(10) + αCCH(72)	1152	0	νCC(12) + αCCH(74)	
1150	0.1	νCC(12) + αCCH(72)	1151	0.3	νCC(10) + αCCH(74)	
1079	2.9	νCS(26) + αCC(34)	1080	3.5	νCC(24) + νCS(26)	
1072	0.8	νCC(42) + αCCH(30)	1076	1.6	νCC(43) + αCCH(17)	
1070	3.2	νCC(44) + αCCH(28)	1068	2.8	νCC(44) + αCCH(32)	
1066	16.1	νCS(24) + αCC(39)	1065	19.6	νCC(52)	1082 s
1018	2.0	νCC(56)	1019	12.0	νCC(61)	
1017	17.7	νCC(62)	1016	9.8	νCC(60)	1025 s
983	0.2	νCC(24) + αCCH(48)	984	5.4	νCC(22) + αCCC(53)	
983	7.6	νCC(28) + CC(48)	980	3.8	νCC(22) + αCCC(52)	999 w
982	0.0	γCC(16) + αCCC(48)	974	0	γCH(63) + τCC(16)	
968	0.4	γCH(66) + τCC(12)	963	0.1	γCH(51) + τCC(29)	
967	0.1	γCH(69) + τCC(14)	949	0	γCH(74) + τCC(16)	
945	0.2	γCH(74) + τCC(14)	938	0.1	γCH(74) + τCC(15)	
944	0.3	γCH(72) + τCC(14)	909	1.1	γCH(76)	
894	2.1	γCH(72)	877	1.0	γCH(75)	
892	0.1	γCH(74)	833	0	γCH(78) + τCC(18)	
829	0.1	γCH(76) + τCC(16)	821	0.2	γCH(79) + τCC(10)	
827	14.8	γCH(76) + τCC(12)	745	28.1	γCH(69) + γCS(13)	
740	52.5	γCH(82)	727	43.2	γCH(79) + γCS(11)	736 vs
731	20.5	γCH(86)	694	14.4	γCS(35) + αCCC(14)	
689	7.3	νCS(18) + αCCC(14)	685	12.6	γCH(42) + γCS(11) + αCCC(10)	
688	17.1	γCH(34)	682	8.6	νCS(17) + γCH(44)+τCC(33)	688 s
683	6.2	γCS(16) + αCCC(14) + αCH(40)	678	11.6	νCS(13) + αCCC(23)	

Table 2. (Contd.)

C_2 symmetry B3LYP/6-31G**			C_s symmetry B3LYP/6-31G**			Exp. IR
ν, cm^{-1}	Int.	*PED*, %[a,b]	ν, cm^{-1}	Int.	*PED*, %[a,b]	
679	0.2	νCS(20) + αCH(12)	611	0.3	αCCC(64) + αCCH(16)	
610	0.0	νCS(20) + αCCH(16)	610	0	αCCC(64) + αCCH(16)	
610	9.8	αSCC(27) + αCH(28)	509	9.6	αCSC(30) + γCS(26) + τCC(14)	617 w
460	9.7	γCS(58) + αCH(12)	464	3.5	γCS(60) + γCH(12)	515 s
429	0.1	νCS(46) + αCCC(12)	432	1.5	νCS(29)	
406	0.4	νCS(16) + αCC(34)	405	0	τCC(62) + γCH(30)	
400	0.0	νCS(12) + αCC(36) + αCH(12)	399	1.9	νCS(33) + αCSC(10)	
399	1.5	τCC(56) + αCH(26)	399	0	τCC(58) + γCH(32)	402 s
268	2.3	αSCC(64)	275	0.2	αSCC(84)	
265	0.5	νCS(30) + αSCC(34)	257	1.1	αSCC(32) + τCS(40)	
197	0.8	αCSC(16) + αCC(32)	200	0.4	αSCC(31) + τCC(28)	
170	1.2	γCS(26) + αCC(44)	171	0.1	γCS(26) + τCC(49)	
62	0.0	αCSC(44) + αCS(22)	68	0.2	αCSC(47) + γCS(28)	
31	0.2	τCS(54) + αCSC(23)	34	0	τCS(83)	
18	1.5	τCS(90)				

[a] (*PED*) Potential energy distribution, contributions below 10% are omitted. [b] (ν, α, γ, τ) Stretching, bending, wagging, and torsion vibrations, respectively.

Table 3. Mean atomic vibration amplitudes in diphenyl sulfide

Parameter	Experiment			Calculation	Parameter	Experiment			Calculation
	r_{ij}, Å	u_{ij}, Å		u_{ij}, Å		r_{ij}, Å	u_{ij}, Å		u_{ij}, Å
C–S	1.77	0.054	(2)	0.050	$C^5\cdots C^8$	5.3	0.362	(46)[e]	0.138
C–C	1.40	0.044	(1)	0.046	$C^6\cdots C^8$	5.0	0.400		0.176
C–H	1.12	0.077	(3)	0.075	$C^6\cdots C^9$	5.0	0.407		0.183
$S\cdots C^3$	2.80	0.068	(2)[a]	0.066	$C^4\cdots C^{10}$	5.5	0.702		0.478
$S\cdots C^7$	2.73	0.071		0.069	$C^5\cdots C^{11}$	5.2	0.508		0.284
$C\cdots C$	2.80	0.063		0.069	$C^5\cdots C^9$	5.2	0.532		0.308
$C^2\cdots C^8$	2.8	0.087		0.085	$C^3\cdots C^8$	3.2[f]			0.215
					$C^3\cdots C^{13}$	3.5[f]			0.285
$S\cdots C^4$	4.08	0.067	(3)[b]	0.064	$C^3\cdots C^9$	3.5[f]			0.434
$S\cdots C^6$	4.04	0.070		0.067	$C^3\cdots C^{11}$	3.5[f]			0.368
$C^7\cdots C^8$	3.9	0.192		0.189	$C^4\cdots C^9$	4.6[f]			0.436
$C\cdots C$	2.43	0.055	(1)[c]	0.055	$C^4\cdots C^{12}$	5.5[f]			0.308
$S\cdots C^5$	4.6	0.074	(4)[d]	0.065	$C^5\cdots C^{10}$	6.3[f]			0.328
$C^4\cdots C^8$	4.5	0.191		0.182	$C^6\cdots C^{10}$	6.3[f]			0.216
$C^3\cdots C^{12}$	4.6	0.308		0.299					
$C^7\cdots C^9$	4.1	0.144		0.135					
$C^3\cdots C^{10}$	4.6	0.471		0.462					
$C^4\cdots C^{11}$	4.6	0.374		0.365					
$C^3\cdots C^{12}$	4.6	0.308		0.299					

[a–e] Groups of refined amplitudes. [f] Fixed amplitudes.

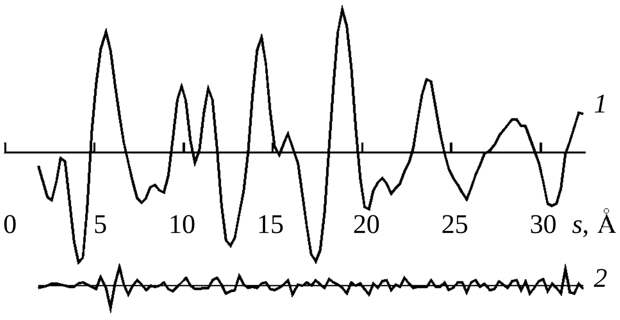

Fig. 2. (*1*) Experimental molecular intensity curve of diphenyl sulfide *sM*(*s*) and (*2*) $\Delta sM(s) = sM(s)_{\mathrm{exp}} - ksM(s)_{\mathrm{calc}}$.

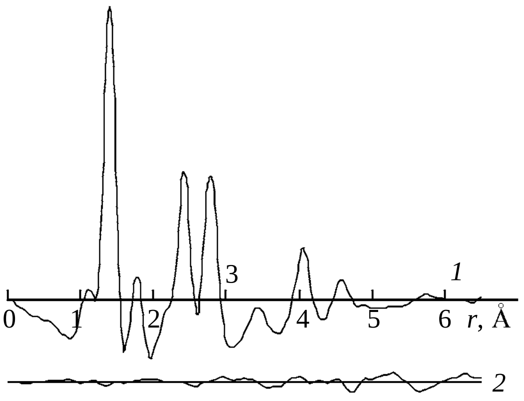

Fig. 3. (*1*) Experimental radial distribution curve of diphenyl sulfide *rf*(*r*) and (*2*) $\Delta rf(r) = rf(r)_{\mathrm{exp}} - krf(r)_{\mathrm{calc}}$.

into reduced molecular intensity functions *sM*(*s*) which were used in the refinement. The atomic coordinates were calculated using a *Z* matrix analogous to that used in quantum-chemical calculations. The independent parameters of the phenyl ring are 5 C–C distances and four endocyclic CCC angles at the C^3, C^4, C^5, and C^6 atoms. In this case, the C^2–C^7 distance and two endocyclic angles at C^7 and C$_2$ (Fig. 1) are dependent. The *G* functions are calculated from the tabulated values in [7]. The use of observed intensity *I*(*s*) and background *B*(*s*) functions allows prompt identification of *B*(*s*) regions which need to be corrected. The final results are obtained in the form of reduced *sM*(*s*) functions.

The independent parameters C–C and CCC of the phenyl ring were refined in groups. The base parameters were the C$_2$–C$_3$ bond length and C^{2}C^{3}C^4 bond angle. The corrections for the C^3–C^4, C^4–C^5, C^5–C^6, and C^6–^{3}C^7 distances and CCC angles at C^4, C^5 and C^6 were taken from the theoretical calculations. The refinement results are listed in Table 1. Together with geometric parameters we also refined torsion angles about C–S bonds and mean vibration amplitudes u_{ij} (Table 3). As accepted in most electron diffraction studies, the amplitudes of nonbonded distances were refined in groups. Below is shown the correlation matrix of diphenyl sulfide [correlation coefficients ($\times 10^2$); the groups of refined parameters (a)–(e) correspond to the those in Table 2]. The strongest correlations are between C–C bond distances and CCC bond angles, as well as the SCC bond angle and group of amplitudes for the C···C and C···S (2.80) distances.

Figures 2 and 3 compare the observed and calculated *sM*(*s*) and *f*(*r*) curves. The observed *f*(*r*) curve shows the distribution of internuclear distances, Å: 1.1 (C–H), 1.4 (C–C), 1.8 (C–S), 2.4 (C···C distances of type 1–3), 2.8 (diagonal distances of C···C type in the phenyl rings), and 3.6 [S···C^3 (S···C^7)]. Short C···C distances for different cycles (4.1 Å) were assigned to the S···C^4 (S···C^5) and C···C distances, and the peak at 4.6 Å corresponds to the C···C and S···C^6 distances. All peaks are well resolved. The two last peaks at *r* 5.8 and 6.7 Å correspond to long C···C distances between different phenyl rings.

It is to be noted that the C–C$_{ipso}$ distances are longer than the other distances. This follows from the theoretical and, naturally, observed data, because the refinement was made in groups. The average C–C bond distance is 1.401 Å, and the CC$_{ipso}$C bond angle is reduced by 0.2–0.4° according to the theoretical data (Table 1). The CSC bond angle, according to our present data, is 103.4°. This result agrees with the respective values for diphenyl sulfide {103.7(1.3)° [4]}, bis(2-pyridyl) sulfide {104.4(1.7)° [8]}, and bis(4-sulfenylphenyl) sulfide {103.5(1.3)° [9]}. In sulfides with saturated substituents, except for (t-Bu)$_2$S and (*iso*-Bu)$_2$S, the CSC bond angle is no larger than 100°. The increase of the bond angle in aromatic sulfides is attributed to steric factors [10, 11].

Thus, the present study showed that gaseous diphenyl sulfide possesses C_2 symmetry with torsional angles about the C–S bonds of 49.6°. It is to be noted that the theoretical values of this parameter, obtained at the HF and DFT levels of theory, differ by 12° and are determined by the shortest C^2···C^{13} and C^3···C^8 distances of 3.22 Å (HF) and 3.27 Å (DFT). In any case, both distances are about 0.3 Å smaller than the sum of the van der Waals radii of carbon atoms (3.50–3.60 Å). From observed data, these distances are

	Parameter	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	r(C–S)	100														
2	r(C–C)	43	100													
3	r(C–H)	–3	8	100												
4	SC^2C^3	–17	–47	5	100											
5	$C^2C^3C^4$	–46	–98	–5	47	100										
6	CSC	–5	57	–3	–53	–61	100									
7	τ	4	–37	–1	–7	40	45	100								
8	u(C–S)	1	–2	8	2	0	–2	1	100							
9	u(C–C)	16	23	0	–4	–24	5	–5	26	100						
10	u(C–H)	–6	–1	6	1	2	–1	0	0	–3	100					
11	u^a	–4	–9	10	–73	9	17	33	3	7	0	100				
12	u^b	–3	5	1	–57	–4	19	19	4	10	0	60	100			
13	u^c	6	6	–1	1	–5	0	0	14	38	0	8	7	100		
14	u^d	–1	3	6	3	–3	0	–1	3	9	0	–3	–8	6	100	
15	u^e	–1	10	3	–6	–11	22	2	1	2	0	0	0	1	12	100

3.21 Å. The phenyl ring possesses C_s symmetry, and the $C^3C^2C^7$ bond angle is smaller than 120° by 0.4°. Note that the latter parameter is dependent.

The oxygen analog of diphenyl sulfide, diphenyl ether, possesses C_1 symmetry in the gas phase [1]. According to ab initio calculations, the C_2 conformation is more stable than C_s by as little as 0.05 kcal mol^{-1} [1]. These results agree with data in [12], according to which $\Delta E(C_s–C_2)$ varies within 0.30–0.49 kcal mol^{-1}. The situation is analogous to that following from ab initio calculations for diphenyl sulfide. However, as mentioned above, the C_s conformation in diphenyl sulfide has one imaginary frequency. According to the B3LYP/6-31G* results [13], the conformation of diphenyl ether has C_1 symmetry. This fact prompted us [3] to reinvestigate the geometry of diphenyl ether in the gas phase.

Domenicano [14] performed a detailed analysis of the effect of a heteroatom connected to the phenyl group on the deformation of the D_{6h} symmetry of the benzene ring. Suitable objects for such research are phenol, diphenyl ether, and diphenyl sulfide, for which experimental and theoretical data are available. As follows from microwave spectral data, the hydroxy group in phenol shortens the C_{ipso}–C bonds by 0.001–0.004 Å compared with the other bonds and increases the $CC_{ipso}C$ bond angle to 120.8(4)° [15]. In diphenyl ether, as follows from theoretical data, the $C_{ipso}C$ bond length is practically the same for C_2 and C_1 symmetries, and the $CC_{ipso}C$ bond angle is increased to 120.6° [1]. In diphenyl sulfide, the C_{ipso}–C bond length (1.401 Å) is increased by 0.004 Å as compared with the average value 1.395 Å. The $CC_{ipso}C$ bond angle is decreased to 119.6° (Table 1). These changes can be explained by charge redistribution on carbon atoms (Fig. 4). Since the independent refinement of phenyl CCC bond angles results in unrealistic values due to strong correlations, the deformation of the benzene ring is expedient to determine from the theoretical results.

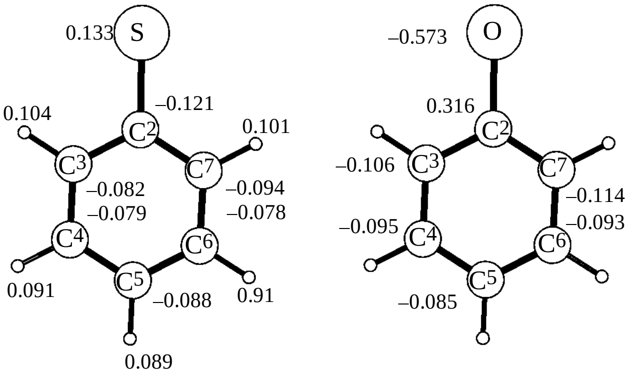

Fig. 4. Atomic charges in diphenyl sulfide as given by HF/6-31G** calculations.

Thus, diphenyl ether and diphenyl sulfide have different conformations. This is not surprising, since, as follows from the charge distributions in the sulfide and ether (Fig. 4), the LEP in oxygen is more active than in sulfur.

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