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Molecular Structure of Bis(trimethylsilyl) Hypophosphite $HP(OSiMe_3)_2$ by Gas-Phase Electron Diffraction and Quantum Chemistry

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Abstract—Geometric parameters and conformation of the bis(trimethylsilyl)hypophosphite molecule were determined by gas-phase electron diffraction and quantum-chemical calculations. The molecule has an asymmetric structure, including an asymmetric $P(OSiMe_3)_2$ group. The principal geometric parameters are as follows: (r_a; in parentheses are standard deviations): bond lengths: P–O 1.616 and 1.633(1), Si–O 1.670(1), Si–C 1.892(1), C–H 1.097(3) Å; bond angles: OPO 100.8(8), POSi 133.3, and 138.4(3)°; torsion angles about P–O bonds 120(2) and 41.(3)°; and torsion angles about Si–O bonds are 145 and –178(4)°.

Three-coordinate phosphorus compounds with active trimethylsilyl group on phosphorus and P–H bond are highly reactive and undergo diverse transformations. Various organophosphorous compounds are formed, for example, by reactions with unsaturated and carbonyl compounds [1–3]. For this reason it is important to determine the structure of such compounds. The structure of the bis(trimethylsilyl) hypophosphite molecule was previously studied by gas-phase electron diffraction [4], but neglecting rotation of methyl groups about Si–C bonds in a molecule containing four rotation axes prevented assessment of the molecular conformation. This problem can only be solved by a combined gas-phase electron diffraction and quantum-chemical study. This was the aim of the present work.

Quantum-chemical calculations and normal-coordinate analysis. Geometry and conformations of the bis(trimethylsilyl) hypophosphite molecule were calculated at the HF/6-31G* and HF/6- 31G** levels of theory [5]. It was demonstrated that the C_s conformation is 1.75 kcal mol^{-1} more stable then the asymmetric C_1 conformation. The calculations were performed both with full geometry optimization and with partial constraints. Namely, it was assumed that respective P–O, Si–O, as well as all C–H bond lengths are equal. Therewith, for the C_s conformation one imaginary vibration correspons to a frequency was revealed. This fact indicates that the transition state on the potential energy surface more symmetrical conformer. The theoretical geometric parameters for the C_1 model are given in Table 1. As seen, the results calculated at different levels of theory are very similar, and the energy difference is only about 0.15 kcal mol^{-1}. The main contribution to this difference is due to variation in the P–O bond length.

The location of the phosphorus lone electron pair (l_p) is determined by the $\angle l_p$PO angle of 118.47°. In this case, $\angle l_p$PH is equal 118.6°, that is l_p is located on the symmetry pseudo-axis of the HPO_2 fragment (Fig. 1). In any case, lone pair should reside in the plane that passes through the P–H bond and the bisector of the OPO bond angle or a bisector close to it due to the asymmetry of the HPO_2 fragment.

Table 2 shows the principal vibration amplitudes some of which were refined in the structural analysis. The calculated amplitudes for the Si–P and P–O bonds in $HP(OSiMe_3)_2$ nicely fit those calculated for $Me_2Si(OSiMe_3)_2$ and $P(OMe_3)_3$ at the BPW91/6-311G* level of theory [6]. The reported electron-diffraction vibration amplitudes of Si–C bond in organosilicon compounds [7–12] span the range 0.050–0.061 Å.

Noteworthy are large amplitudes for C···C distances in $HP(OSiMe_3)_2$. For example, for the $C^8 \cdots C^{11}$ distance (Fig. 1) the amplitude is up to 0.9 Å, implying considerable torsion vibrations about Si–O, Si–C, and P–O bonds. The results of normal-coordinate analysis indicate that the calculated (gas phase) and

Table 1. Geometric parameters of $HP(XSiMe_3)_2$ molecules (X = O, S)

Parameter	$HP(OSiMe_3)_2$					$HP(SSiMe_3)_2$	
	HF/6-31*[a]	HF/6-31*[b]	HF/6-31**	B3LYP/6-31**	experiment, r_a, $\angle_\alpha$	HF/6-31**	B3LYP/6-31**
Interatomic distations, Å							
P^1–X^2	1.615	1.623	1.615	1.645	1.616 (1)	2.120	2.154
P^1–X^3	1.632	1.623	1.632	1.662	1.633	2.130	2.166
X–Si	1.670	1.669	1.670	1.695	1.670	2.186	2.199
d(P–X)	0.017	0.0	0.017	0.017	–	0.010	0.012
d(X–Si)	0.055	0.046	0.055	0.030	–	0.060	0.045
Si–C	1.881	1.882	1.882	1.883	1.892 (1)	1.883	1.886
C–H	1.087	1.087	1.087	1.095	1.097 (3)	1.086	1.095
P–H	1.411	1.408	1.408	1.438	1.408[c]	1.397	1.421
Independent bond and torsion, deg							
XPX	102.6	102.6	102.5	103.4	100.8 (8)	108.4	109.9
$XSiC^{6,9}$	105.9	106.1	105.9	105.2	105.4 (3)	103.6	103.5
$X^2SiC^{7,8}$	109.4	109.4	109.4	109.5	109.0	110.6	110.6
$X^3SiC^{10,11}$	109.3	109.4	109.3	109.5	109.0	110.1	110.0
d(XSiC)	3.5	3.3	3.5	4.3	–	7.1	7.1
PX^3Si^5	133.5	134.9	133.5	128.4	133.3 (3)	103.7	101.9
PX^2Si^4	138.7	138.8	138.7	135.2	138.4	111.5	110.4
SiCH	111.3	111.2	111.2	111.3	111.2 (9)	111.0	111.1
HPX_{av}	98.6	97.4	97.4	96.6	98.6[c]	97.3	95.8
$X^2PX^3Si^5$	121.4	122.4	121.4	113.8	120.2 (22)	104.9	100.5
$X^3PX^3Si^4$	45.6	45.3	45.4	50.4	41.0 (34)	52.9	56.0
$PX^2Si^4C^6$	151.9	152.0	151.8	153.2	144.6 (37)	155.6	161.8
$PX^3Si^5C^9$	–176.4	–177.1	–176.3	–169.8	–178.1	–178.1	–179.8
Dependent bond and torsion, deg							
$PX^2Si^4C^7$	31.8	32.4	31.7	33.1	26.8 (39)	36.6	43.0
$PX^2Si^4C^8$	–89.5	–88.5	–89.5	–88.1	–97.7 (36)	–86.5	–79.7
$PX^3Si^5C^{10}$	64.3	63.4	64.3	72.1	64.1 (39)	63.0	60.8
$PX^3Si^5C^{11}$	–58.5	–57.5	–56.4	–49.9	–60.4 (34)	–59.0	–61.2
l_pPH	118.6	–	–	–	118.1	–	–
HPX^2Si^4	–52.6	–54.1	–52.6	–46.5	–59.3 (33)	–45.8	–40.5
HPX^3Si^5	–138.3	–138.3	–138.2	–146.2	–139.2 (23)	–153.1	–159.1
$l_pPX^2Si^4$	177.9	–	–	–	172.0	–	–
$l_pPX^3Si^5$	–11.1	–	–	–	–10.7	–	–
R factor, %				7.16/7.30			

[a] Unconstrained calculations; [b] Constrained calculations (see text); [c] Fixed values. Parenthesized values are standard deviations.

experimental frequencies of the crystalline sample fairly fit each other [13].

The number of fundamental frequencies in a molecule is given by 3*N* – 6 (where *N* is the number of atoms in the molecule). Consequently, the number of fundamental frequencies in $HP(OSiMe_3)_2$ is 84. We omitted from Table 3 all frequencies with intensities below or equal 1 and gave only ν_{CH}, α_{HCH}, and α_{SiCH} frequencies whose experimental values are available. Like with C–H stretching vibrations, the number of in-plane α_{HCH} and α_{SiCH} vibrations is 18 in each group. Therewith, the frequencies are nearly the same or differ by 1–2 cm^{-1}. For the region below 670 cm^{-1} we give all calculated frequencies. The lowest frequencies are due to torsion vibrations about P–O and O–Si bonds. According to the normal-coordinate analysis, the frequencies of torsion vibrations about Si–C bonds are in the region 100–150 cm^{-1}. Unscaled torsion force constants (mdyn) are as follows: P–O 0.042 and 0.069, O–Si 0.030 and 0.055, and Si–C 0.043–0.053. These values reflect a high asymmetry of the molecule as a whole and large vibration amplitudes for nonbonded atoms.

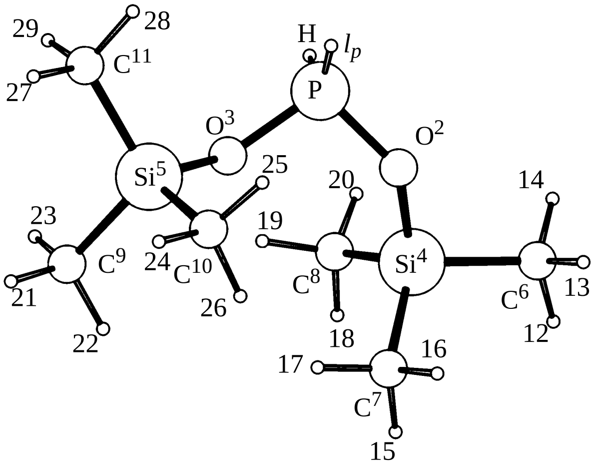

Fig. 1. Molecular conformation of bis(trimethylsilyl) hypophosphite and atom numbering scheme.

Structural analysis. The molecular geometry of bis(trimethylsilyl) hypophosphite was refined by molecular intensity $sM(s)$ and radial distribution $f(r)$ curves (Figs. 2 and 3). To this end, the KCED program developed by Norwegian researches and modified by one of us was used. In this program, the geometry of the bis(trimethylsilyl)hypophosphite molecule is specified by the Z matrix with the following independent structural parameters: P–O, Si–O, Si–C, and C–H bond lengths OPO, POSi, OSiC, and SiCH bond angles. Taking into account the closeness of the first two parameters, we imposed constraints and refined P–O and Si–O bond lengths in group with the following corrections (HF/6-31G* data, Table 1): d(P–O) 0.017, $d(\text{Si–O}) = r(\text{Si–O}) - r(\text{P–O}) = 0.054$ Å. Six Si–C bond lengths and all C–H bond lengths in the methyl groups are set to be equal on the basis of theoretical calculations. The $O–Si–C_3$ fragments, according to the calculation results, possess C_s symmetry: The $OSiC^{6,9}$ bond angles are smaller that $OSiC^{7,8}$ and $OSiC^{10,11}$ by 3.6°. We used this value in the final calculations. The POSi bond angles differ by 5°, that leads to their strong correlation. Therefore, we used the constraint $d(\text{POSi}) = \angle \text{POSi}_4 - \angle \text{POSi}_5$ (5.1°). Unstable results arose upon independent refinement of the $\tau(PO^2Si^4C^6)$ and $\tau(PO^3Si^5C^9)$ torsion angles that define the conformation of the molecule as a whole. For this reason, we imposed constraints on these parameters. The symmetry of the methyl groups is assumed to be C_3. The final geometric parameters and vibration amplitudes of the bis(trimethylsilyl) hypophosphite molecule are given in Tables 1 and 2. As seen from the correlation matrix given below ($\times 10^2$), strong correlations between refined parameters are absent [in matrix $^{a–c}$ at l denote refinement in group with fixed differences, Table 2; $l(\text{Si}\cdots\text{H})$ values relate to the $Si(CH_3)_3$ groups].

Table 2. Principal mean vibration amplitudes in $HP(OSiMe_3)_2$, Å

Parameter	r_{ij}	Calculation	Experiment
P–O	1.62	0.046	0.046 (1)
O–Si	1.67	0.047	0.048
C–Si	1.89	0.054	0.055(1)
C–H	1.10	0.079	0.093(3)
$P\cdots Si^4$	3.07	0.080	0.078 (3)^a
$P\cdots Si^5$	3.03	0.093	0.091
$O^2\cdots C^6$	2.83	0.098	0.096
$O^2\cdots C^7$	2.90	0.094	0.092
$O^2\cdots C^8$	2.90	0.099	0.097
$O^3\cdots C^9$	2.83	0.097	0.095
$O^3\cdots C^{10}$	2.90	0.097	0.095
$O^3\cdots C^{11}$	2.90	0.096	0.094
$C^6\cdots C^7$	3.10	0.108	0.106
$C^6\cdots C^8$	3.10	0.108	0.106
$C^9\cdots C^{10}$	3.10	0.108	0.106
$C^9\cdots C^{11}$	3.10	0.108	0.106
$C^7\cdots C^8$	3.17	0.109	0.107
$P\cdots C^6$	4.37	0.127	0.130 (17)^b
$P\cdots C^7$	4.12	0.203	0.206
$P\cdots C^9$	4.46	0.117	0.120
$Si^5\cdots C^7$	4.65	0.556	0.560
Si···Si	4.69	0.265	0.268
$O^2\cdots C^{10}$	4.20	0.258	0.261
$C^7\cdots C^{10}$	4.45	0.475	0.606
$P\cdots C^8$	3.62	0.200	0.094 (9)^c
$P\cdots C^{10}$	3.74	0.272	0.166
$P\cdots C^{11}$	3.80	0.278	0.172
$Si^5\cdots O^2$	3.93	0.194	0.088
$O^3\cdots C^7$	3.83	0.454	0.347
$O^3\cdots C^8$	3.49	0.409	0.303
$Si^4\cdots C^9$	5.22	0.454	–
$Si^4\cdots C^{10}$	5.03	0.237	–
$O^3\cdots C^6$	5.04	0.173	–
$C^6\cdots C^{10}$	6.61	0.274	–
$C^6\cdots C^{11}$	7.90	0.730	–
$C^7\cdots C^9$	4.87	0.810	–
$C^7\cdots C^{11}$	6.44	0.622	–
$C^8\cdots C^9$	5.02	0.722	–
$C^8\cdots C^{10}$	5.83	0.475	–
$C^8\cdots C^{11}$	6.25	0.902	–
$C^6\cdots C^9$	7.13	0.455	–
Si···H	2.50	0.126	0.140 (5)

[a–c] Criteria for group refinement. Parenthesized values are standard deviations.

r(P–O, Si–O)	100																	
r(Si–C)	–1	100																
r(C–H)	–21	14	100															
∠OPO	–8	12	11	100														
∠POSi	–28	–29	0	–21	100													
∠CSiO	9	–32	–15	–36	42	100												
∠SiCH	13	–29	–27	–78	31	61	100											
$\tau(PO^2Si^4C^6)$	2	11	2	22	–45	–51	–28	100										
$\tau(O^3PO^2Si^4)$	0	0	6	–17	25	31	12	–66	100									
$\tau(Si^5O^3PO^2)$	0	–9	–10	–78	2	5	62	13	–42	100								
l(P–O, Si–O)	19	9	–9	8	–3	–10	–7	9	0	–8	100							
l(Si–C)	–13	–12	4	4	14	–3	–1	4	0	–2	38	100						
l(CH)	3	–6	–1	8	–1	–11	–10	4	1	–8	28	32	100					
l^a	10	–18	–6	–1	19	54	8	–30	19	–12	24	18	13	100				
l^b	0	6	2	–23	10	9	20	–8	–14	27	2	6	0	8	100			
l^c	2	0	0	5	–2	–5	–6	30	5	–21	11	9	6	5	–9	100		
l(Si···H)	8	7	4	40	13	15	–22	–2	24	–41	24	7	17	15	12	6	7	100

Table 3. Normal-coordinate analysis of $HP(OSiMe_3)_2$ [a]

Calculation, HF/6-31G**				Experiment [13]	
cm^{-1}	I_{IR}	Raman	PED, %	IR	Raman
2958	23	112	$80\nu_{CH}$	2960 s	2962 s
2909	1	10	$80\nu_{CH}$	2904 w	2903 w
2178	226	125	$99\nu_{PH}$	2173 m	2172 m
1457	6	–	$69\alpha_{HCH}$	1464 v.w	–
1410	17	1	$87\alpha_{HCH}$	1415 w	1415 w
1283	41	10	$88\alpha_{HCH}$	1269 v.w	1265 w
1063	162	9	$29\nu_{SiO}$ $+11\nu_{PO}$ $+$ $45\alpha_{OPH}$	1070 s	–
1030	63	15	$24\nu_{SiO}$ $+$ $32\nu_{PO}$ $+$ $39\alpha_{OPH}$	1036 m	1040 v.w
988	366	3	$75\alpha_{OPH}$	977 m	977 v.w
920	7	3	$41\nu_{PO}$ $+$ $32\alpha_{OPH}$	895 sh	897 v.w
878	253	1	$67\alpha_{SiCH}$	–	–
862	306	2	$52\alpha_{SiCH}$	–	–
858	–	–	$60\alpha_{SiCH}$	850 v.s	846 v.w
765	38	3	$55\alpha_{SiCH}$ $+$ $15\nu_{SiC}$	759 m	759 v.w
692	–	–	$43\nu_{SiC}$	–	695 v.w
690	–	–	$49\nu_{SiC}$ $+$ $11\alpha_{SiCH}$	696 w	–
678	15	4	$83\nu_{SiC}$	–	–
668	12	7	$23\nu_{SiO}$ $+$ $27\nu_{SiC}$ $+$ $19\nu_{PO}$	–	–
654	3	1	$17\nu_{SiO}$ $+$ $42\nu_{SiC}$ $+$ $13\nu_{PO}$	–	655 v.w
573	13	11	$15\nu_{SiO}$ $+$ $37\nu_{SiC}$ $+$ $13\nu_{PO}$	–	575 m
553	6	25	$30\nu_{SiO}$ $+$ $36\nu_{SiC}$ $+$ $16\nu_{PO}$	–	561 s
385	24	–	$50\alpha_{OPO}$	–	–
279	21	1	$36\alpha_{OSiC}$	–	298 w
266	14	–	$52\alpha_{OSiC}$	–	–
212	5	–	$35\alpha_{CSiC}$ $+$ $32\alpha_{OSiC}$	–	208 w
204	5	–	$46\alpha_{CSiC}$ $+$ $10\alpha_{OSiC}$	–	–
183	1	1	$43\alpha_{CSiC}$	–	–
178	–	–	$40\alpha_{CSiC}$ $+$ $18\alpha_{OSiC}$	–	172 w
156	–	–	$79\tau_{CSi}$	–	–

Table 3. (Contd.)

Calculation, HF/6-31G**				Experiment [13]	
cm^{-1}	I_{IR}	Raman	PED, %	IR	Raman
152	–	–	$69\tau_{CSi}$	–	–
150	–	–	$48\tau_{CSi} + 14\alpha_{OSiC}$	–	–
147	–	–	$82\tau_{CSi}$	–	–
131	–	–	$97\tau_{CSi}$	–	–
130	–	–	$97\tau_{CSi}$	–	–
119	–	–	$29\nu_{PO} + 36\nu_{PO}Si$	–	–
84	–	–	$80\nu_{PO}Si$	–	–
54	–	–	$42\nu_{PO} + 48\tau_{OSi}$	–	–
34	–	–	$52\nu_{PO} + 28\tau_{OSi}$	–	–
20	–	–	$34\nu_{PO} + 40\tau_{OSi}$	–	–
17	–	–	$41\nu_{PO} + 44\tau_{OSi}$	–	–

[a] (I_{IR}, I_{Raman}) Calculated IR and Raman intensities. (ν, α, and τ) Stretching, bending and torsion vibrations, respectively.
[b] The intensities of the vibration bands below 178 cm^{-1} are less than 1.

Nevertheless, it was impossible to avoid correlations at all. Thus, ∠OPO correlates with ∠SiCH [the O···O and Si···H distances in the trimethylsilyl groups are 2.50 Å, see also the radial distribution curve $f(r)$, Fig. 3].

The POSi bond angles (133° and 138°) are enlarged as compared with the angle at the oxygen atom in ethers like MeOMe (112°) and are typical for silyl ethers, such as $(MeH_2Si)_2O$, $(Me_2HSi)_2O$, $(H_3Si)_2O$, and some other compounds (Tables 1.2 and 1.6 in [4]; see also [6]). The enlargement of the bond angle at the oxygen atom in such compounds is probably explained by interaction of the oxygen lone electron pair with *d* orbitals of silicon. Indirect evidence for this assumption comes from *ab initio* calculations of the geometry of the $HP(SSiMe_3)_2$ molecule (Table 1). The POSi bond angles in $HP(OSiMe_3)_2$ differ by 5°. This may be associated with different mutual orientations of the phosphorous and oxygen lone electron pairs.

Thus, the molecule in the gas phase possesses an asymmetric structure, with the $P(OSiMe_3)$ fragment being also asymmetric. We made an attempt to perform structural analysis for the asymmetric conformation of the whole molecule and the $P(OSiMe_3)$ fragment of C_2 symmetry. In this case, the fit of the theoretical molecular intensity and radial

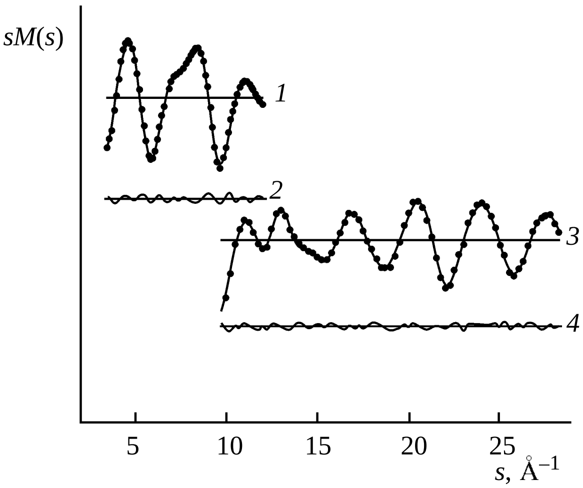

Fig. 2. (*1, 2*) Molecular intensity curves. (Points) Experiment and (solid lines) calculation. (*3, 4*) $\Delta = sM(s)_{exp} - ksM(s)_{calc}$.

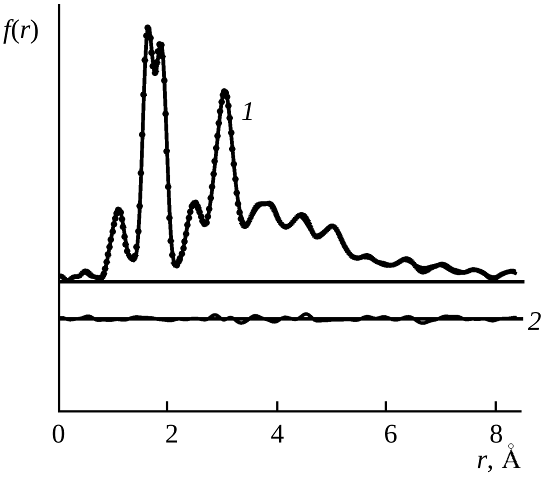

Fig. 3. Radial distribution curves. (Points) Experiment and (solid line) calculation. $\Delta = f(r)_{exp} - kf(r)_{calc}$.

distribution curves to experimental proved to be unsatisfactory. Moreover, a short contact between $OSiCH_3$ hydrogens was observed.

For the sake of comparison, we performed quantum-chemical calculation of the thio analog of bis(trimethylsilyl) hypophosphite, $HP(SSiMe_3)_2$, at the HF/6-31G* level of theory with certain constratints, as well as at the HF/6-31G* and B3LYP/6-31G** levels of theory (Table 1). The calculations resulted in an asymmetric molecular conformation with an asymmetric $P(SSiMe_3)_2$ fragment, which is in principle close to what is observed with $HP(OSiMe_3)_2$. Bond angles around the sulfur atom are different. One of them in the PS^2SiC^6 chain is close to that found in sulfides [15] and that in the other chain, PS^3SiC^9, is enlarged as compared with the first one by 9°. The SPS bond angle in the hypothiophosphite is markedly enlarged as compared with the OPO bond angle in the hypophosphite. Nevertheless, the sums of phosphorus bond angles in the two molecules are the same and close to 100°. Furthermore, the O···O (2.5 Å) and S···S (3.5 Å) distances are equal to double the van der Waals radii of oxygen (1.29 Å) and sulfur (1.82 Å).

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