Synthesis, IR/Raman, and Quantum-Chemical Structural Analysis of New Octathiotetraphosphetane Ammonium Salts

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ABSTRACT: New octathiotetraphosphetane ammonium salts are obtained based on the reaction of white phosphorus (P_4) and elemental sulfur with aliphatic mercaptans in the presence of amines (morpholine, methylmorpholine, pyrrolidine, and N,N-dimethylbenzylamine). Both the salts and novel Cu(I) chloride complex with the pyperidinium salt of octathiotetraphosphetane are characterized by IR/Raman spectroscopy in combination with DFT methods. The comparative spectral analysis reveals clear spectral features, characteristic for a $P_4S_8^{4-}$ anion, which are present in IR and Raman spectra of all the compounds obtained. © 2010 Wiley Periodicals, Inc. Heteroatom Chem 22:24–30, 2011; View this article online at wileyonlinelibrary.com. DOI 10.1002/hc.20651

INTRODUCTION

Ammonium salts of octathiotetraphosphetanes as heterocyclic compounds bearing various functional groups in molecules would be expected to possess a wide set of useful properties. Earlier, these salts were obtained by the interaction of white phosphorus with polysulfides and amines along with other cyclic thiophosphates; their structures were determined by the vibrational spectra and X-ray diffraction analysis [1–4].

Using another approach, recently we have reported a new reaction of white phosphorus (P₄) and elemental sulfur with aliphatic mercaptans in the presence of amines **1a–c**, which resulted in formation of ammonium salts of 1,2,3,4tetramercapto-1,2,3,4-tetrathioxotetraphosphetane **2a–c** [5,6]. Their structures determined by the X-ray diffraction were identified as supramolecular structures formed by realization of intermolecular interactions, including N–H…S and C–H…S ones. Centrosymmetric thiotetraphosphetane molecules are connected with four amine molecules by strong hydrogen bonds. From the point of view of charge distribution in crystal, the sphere-like associates are formed [5,6].

In this work, we report about new octathiotetraphosphetane ammonium salts and some of their derivatives as well as their spectral (IR/Raman) characteristics to compare their structure with those previously described [1–6].

RESULTS AND DISCUSSION

Continuing the research of this reaction, we have used a range of secondary and tertiary amines, in particular, morpholine **1d**, methylmorpholine **1f**,

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pyrrolidine **1e**, and *N*,*N*-dimethylbenzylamine **1g** to synthesize new ammonium salts by the interaction of white phosphorus, sulfur, and butanethiol or 3-methylbutane-1-thiol. The reaction proceeds easily at 5–30°C, according to the previously described method for compounds **2a–c** [5,6]. Corresponding products **2d–g** were light yellow powders formed with yield 8–15%, being rather stable in solid as well as in an aqueous solution. Their composition is confirmed by the elemental analysis data.



 $\begin{aligned} & R' = R'' = Et (a); \ R' = H, \ R'' = Et (b); \ R' = H, \ R'' = (CH_{2})_5 (c), \\ & R' = H, \ R'' = (CH_2CH_{2})_2O (d); \ R' = H, \ R'' = (CH_{2})_4 (e) \\ & R' = Me, \ R'' = (CH_2CH_{2})_2O (f), \ R' = CH_2C_6H_5, \ R'' = Me (g) \\ & R = Bu \ ; \ i\text{-Am} \end{aligned}$

In NMR ³¹P spectra of compounds **2d–g**, a singlet at 121–123 ppm is assigned to this type of salts. Besides, in the reaction mixture after separation of corresponding salts, the residue remains (δ_p 98 ppm), which is not crystallized and decomposed at vacuum distillation. Because of poor quality of crystals of compounds **2d–g**, we were unable to determine their structure by the X-ray diffraction. Thus, vibrational spectroscopy was applied to their structural analysis.

The experimental Raman and IR spectra of salts 2a-g, registered at 25°C, are given in Figs. 1-4, respectively. Characteristic bands of the cationic fragments of the compounds, found in the 3600-700 cm⁻¹ spectral range (Figs. 3 and 4), will be described later on the discussion of the spectra of the compounds **2c** and **5c**. Several bands of strong and medium intensities, observed in 700–375 cm⁻¹ (IR) and in 700-50 cm⁻¹ (Raman) spectral ranges (Figs. 1 and 2), are assigned to the $P_4S_8^{4-}$ anion [2]. Pronounced differences in frequencies of IR and Raman bands in this spectral range suggest that the rule of mutual exclusions takes place in our case, similar to the case of $[K_4][P_4S_8] \cdot 2H_2O[2]$. Hence, a center of symmetry would be expected in the structure of the anion in the salts **2a–g**.

Nevertheless, the quantum-chemically optimized $[P_4S_8]^{4-}$ structure of the D_{4h} symmetry did not correspond to minimum on potential energy surface, as its computed spectrum comprised one imaginary frequency. Optimization of a starting geometry of the isolated $[P_4S_8]^{4-}$ anion of the C_1 symmetry, taken



FIGURE 1 IR spectra of 2a (A), 2b (B), 2c (C), 2d (D), 2e (E), 2f (F), and 2g (G) salt in the selected spectral range 700– 350 cm^{-1} .

directly from the X-ray data for **2c** [6], resulted in a structure with potential energy ~1 kcal/mol lower than the above-mentioned D_{4h} -form. Computed geometrical parameters of this C_1 structure are in a reasonably good agreement with the corresponding X-ray values [6] (Table 1).

The Raman and IR bands of the $[P_4S_8]^{4-}$ anion calculated for the C_1 structure, corresponding to minimum on potential energy surface, agree very well with the experimental spectra of 2a (Figs. 5 and 6). The strongest Raman bands at 323, 363, and 177 cm⁻¹ are assigned to symmetric and antisymmetric stretching of P-P bonds and "breathing" vibration of the anion, respectively, whereas the strongest IR bands 660 and 565 cm⁻¹ are assigned to symmetric and antisymmetric stretching of P-S bonds, respectively. These IR and Raman bands can be used as reliable spectroscopic markers for the $[P_4S_8]^{4-}$ anion in the structures of new compounds 2a-g. It should be noted that our computationally assisted assignments differ from the earlier empirical interpretation of IR/Raman spectra of related compound $[K_4][P_4S_8] \cdot 2H_2O$ [2]. For example, the authors [2] assigned strong Raman bands at 363 and 177 cm⁻¹ to vPS and to lattice vibrations, respectively, whereas

	Bond (Å)			Angles (Å)		
	Bond (Å)	X-ray	Calculated	Angles (Å)	X-ray	Calculated
	P1–P2	2.288	2.360	P1-P2-P8	90.03	89.077
	P1–P7	2.297	2.360	P2–P8–P7	89.97	89.071
	P8–P7	2.288	2.361	P1–P7–P8	90.03	89.106
	P2-P8	2.297	2.362	P7–P1–P2	89.97	89.107
	P1–S4	1.962	2.013	S4–P1–S6	118.47	116.448
P7 01 000	P1–S6	1.992	2.022	S3–P2–S5	118.75	116.429
	P2–S3	1.978	2.012	S10-P8-S12	118.47	116.448
	P2–S5	1.989	2.022	S9-P7-S11	118.75	116.429
	P7–S9	1.978	2.013			
	P7–S11	1.992	2.022			
30	P8–S10	1.962	2.012			
	P8–S12	1.989	2.022			

TABLE 1 Some Experimental and Computed Bond Lengths (Å) and Angles (°) of the [P₄S₈]⁴⁻ Anion

IR bands at 662 cm⁻¹ and 394 cm⁻¹ were interpreted as in-plane deformations of PPP and ν PS, respectively.

In continuation of the study of P,S-containing ligands ability to the complexation with transition dmetals, we investigated the behavior of one of salts of octathiotetraphosphetane, namely pyperidinium salt, **2c** in the reaction with copper(I)chloride. Owing to the presence of four donor sulfur atoms and cyclic structure of its molecule, such ligand would be expected to form a copper(I) complex with copper coordination via the sulfur atoms of the ligand, as we have earlier established by means of the X-ray data for the copper(I)complex with triisopropyltetrathiophosphate [8]. Thus, the reaction of salt **2c**



FIGURE 2 Raman spectra of **2a** (A), **2b** (B), **2c** (C), **2d** (D), **2e** (E), **2f** (F), and **2g** (G) salts in the selected spectral range 700–50 cm⁻¹.



FIGURE 3 Raman spectra of 2c (A) and 5c (B).



FIGURE 4 IR spectra of 2c (A) and 5c (B).

with Cu(I)Cl in the ratio 1:4 ligand:metal in acetonitrile or in methanol at 50–60°C was conducted. As a result, the yellow powder was obtained, which decomposed at temperature higher than 300°C.

Note that earlier authors of the work on the synthesis of ammonium salt of thiophosphate [1] have mentioned the formation of the cyclothiophosphates of some metals, in particular, of the yellow-brown cyclothiophosphate with Cu(II). However, the properties of these compounds were not described.

In the NMR 31 P spectrum of new compound **5c**, a signal of phosphorus at 122 ppm, unchanged relative to **2c** spectrum, is observed. According to the EPR data, copper in this compound remains its monovalent state, i.e., Cu(I). The elemental analysis data agree with the composition of the supposed complex **5c**.





FIGURE 5 Selected region of the experimental Raman spectra of **2c (2)** and **5c (3)** in comparison with the calculated Raman spectra of the $[P_4S_8]^{4-}$ anion (1) and $[P_4S_8]^{4-}$ -(CuCl)₄ (4).

To further obtain support for the supposed structure, IR and Raman spectra of 5c were registered at 25°C and compared with the spectra of starting salt **2c** (Figs. 3 and 4). In the 3600–700 cm⁻¹ spectral range, characteristic Raman bands of the pyperidinium cations are observed. For example, νCH_2 peaks at 2980–2880 cm⁻¹ of 5c are red-shifted by $\sim 20 \text{ cm}^{-1}$ relative to the spectrum of **2c**. Several new bands, appearing in the 1650–700 cm⁻¹ range of the spectra of **5c** but are absent from the spectra of 2c, can be assigned to vibrations of the pyperidinium cations coordinated to CuCl. It is remarkable that several common bands are observed in 700-50 cm⁻¹ range of Raman spectra of salt 2c and complex 5c (Fig. 3), which are unequivocally assigned above to vibrations of $[P_4S_8]^{4-}$ anion in the compounds **2a–g**. So, we can be sure that $[P_4S_8]^{4-}$ anion is present in the structure of both the ligand 2c and complex 5c.

In the IR spectrum of the complex **5c** (Fig. 4, **B**), ν CH₂ bands at 2980–2880 cm⁻¹ and ν NH₂⁺ bands at 2463–2367 cm⁻¹ are registered at approximately the same frequencies as in the spectrum of **2c**, though



FIGURE 6 Selected region of the experimental IR spectra of **2c (2)** and **5c (3)** in comparison with the calculated Raman spectra of the $[P_4S_8]^{4-}$ anion (1) and $[P_4S_8]^{4-}$ -(CuCl)₄ (4).

 νNH_2^+ bands decreased in intensities. In the IR spectrum of the complex **5c**, δNH_2^+ bands at 1600 and 1553 cm⁻¹ are more separated than in the spectrum of the salt 2c (1600 and 1583 cm⁻¹). The IR bands of scissoring (δCH_2) and wagging (wCH_2) vibrations of the pyperidinium cation (1450-1388 cm⁻¹) and 1128–1056 cm⁻¹ of rocking (ρ CH₂) vibrations in the spectrum of 5c shift or transform their contours relative to the spectrum of **2c**. The IR ρ CH₂ band, which is registered at 777 cm⁻¹ in the spectrum of **2c**, disappears in the spectrum of **5c**, but a new band 430 cm⁻¹ of the pyperidinium cycle skeletal deformation is observed instead. As in the case of the Raman spectra (Fig. 3), common bands of vibrations of the $[P_4S_8]^{4-}$ anion are observed in the 700–350 cm⁻¹ range of IR spectra of the salt **2c** and complex 5c (Fig. 4). Bands at 657 and 567 cm^{-1} of ν P–S (A, Fig. 4) are split in the spectrum of complex **5c** that can point to distortion of the $[P_4S_8]^{4-}$ anion in the complex, though the ν P–P band at 390 cm⁻¹ remains unchanged. All the above-mentioned spectroscopic features demonstrate that both pyperidinium and $[P_4S_8]^{4-}$ fragments of the ligand are influenced by complexation with CuCl.



FIGURE 7 Optimized possible structure of the anionic part of the complex 5c.

To further clarify the suggested structure of the complex 5c, quantum-chemical modeling was carried out. A selected model was the $[P_4S_8]^{4-}$ anion surrounded by four neutral molecules of CuCl. An optimized structure, shown in Fig. 7, demonstrates that the anion retains its structure when each of the sulfur atoms is coordinated by CuCl. The calculated Raman and IR spectra of this model agree reasonably well with the experimental spectra of **5c** (Figs. 5 and 6). Quantum-chemical simulations reproduce the experimentally observed splitting of $v_{as}PS$ and v_{s} PS bands, which suggest that CuCl molecules coordinate the ligand **2c** via sulfur atoms. According to the calculations, ν Cu–Cl band should appear at 250 cm⁻¹ and Cu...S vibrations are predicted to produce bands in the 200-50 cm⁻¹ spectral region. So, several IR/Raman bands in low-frequency region of the spectra of complex 5c additional in comparison with the spectrum of "free" ligand 2c may be assigned either to vCu–Cl or to the metal-ligand vibrations.

It should be noted that the computed spectra of another model of $(CuCl)_4[P_4S_8]^{4-}$, where four CuCl molecules are situated roughly in the plane of a P_4 ring, were in a much worse agreement with the experimental spectra.

Thus, a series of new ammonium salts of octathiotetraphosphetane **2a–g**, and a Cu(I)Cl complex **5c** with pyperidinium salt **2c** are obtained. In the complex **5c**, all sulfur atoms of the octathiotetraphosphetane ligand **2c** are coordinated by the copper(I) atoms. The IR/Raman analysis reveals common spectral characteristics corresponding to the $P_4S_8^{4-}$ anion for all the compounds obtained in this work, which demonstrates that, regardless of the character of the compounds formed, their structure comprises a $P_4S_8^{4-}$ moiety.

EXPERIMENTAL

NMR spectra were measured on a Bruker MSL-400 (162.0 MHz, ¹H) and on a Bruker CXP-100 (36.48 MHz, ³¹P) spectrometers. IR spectra of all compounds were recorded on a FTIR spectrometer "Tensor 27" (Bruker) in the 4000–400 cm⁻¹ middle IR range at an optical resolution of 4 cm⁻¹. Solid samples were prepared as KBr pellets. Far-IR spectra of 2a were recorded on a FTIR spectrometer "IFS-66v/s'' (Bruker) in the 600–100 cm⁻¹ range at an optical resolution of 4 cm⁻¹. Solid sample, mixed with Nujol, was placed between polyethylene plates. FT Raman spectra were recorded on a Bruker RAM II module (using a Ge detector) attached to a Bruker Vertex 70 FTIR spectrometer in the 4000-10 cm⁻¹ range at an optical resolution of 4 cm⁻¹. The Nd:YAG laser with a wavelength of 1064 nm (power of 500 mW) was used as a source of excitation. The samples were placed in a standard cylindrical aluminum sample pan.

Solvents and amines were purified by standard methods. Butanethiol and 3-methylbutane-1thiol were obtained from Sigma-Aldrich Rus LLC (Moscow, Russia). All preparations were carried out in argon atmosphere.

*Tetraammonium Salts of 1,2,3,4-tetramercapto-1,2,3,4-tetrathioxotetraphosphetane (***2a–g***)*

General Procedure. Amine (32.7 mmol) was added dropwise to a stirred mixture of 1 g P₄ (32.3 mmol), 2.1 g (64.6 mmol) sulfur, thiol (32.6 mmol) in CH₃CN (8 mL) at 15–30°C. The mixture was stirred until the reaction was complete (complete conversion of P₄) \approx 1–2.5 h. The reaction mixture was allowed to stand for 15 h at room temperature. Then the precipitated crystals of **2a**-g were separated from the solution by decantation, washed with acetonitrile (3 × 5 mL) and diethyl ether (2 × 5 mL) and dried. The filtrate was evaporated and corresponding dialkyldisulfide was distilled from the residue by means of thin layer distillation Physical, analytical and spectral data for **2a–c** were published in [5,6].

Tetra(*morpholinium*) *Salt of 1,2,3,4-tetramercapto-1,2,3,4-tetrathioxotetraphosphetane* (**2d**). Yield 10%. mp 178–183°C. ¹H NMR (D₂O), δ : 3.29–3.32 (m, 16H, NCH₂), 3.93–3.95 (m, OCH₂, 16H); ³¹P NMR (D₂O), δ : 122.6. Anal. Calcd for C₁₆H₄₀N₄O₄P₄S₈ (732): C 26.23; H 5.46; N 7.65; P 16.9; S 34.9. Found: C 26.75; H 5.41; N 7.34; P 17.31; S 34.46.

Tetra(*pyrrolidinium*) *Salt of 1,2,3,4-tetramercapto-1,2,3,4-tetrathioxotetraphosphetane* (**2e**). Yield 8%. mp 175–179°C. ³¹P NMR (D₂O), δ : 125. Anal. Calcd for C₁₆H₄₀N₄P₄S₈ (668): C 28.74; H 5.99; N 8.38; P 18.56; S 38.3. Found: C 28.43; H 6.23; N 8.41; P 18.72; S 37.82.

Tetra(*N*-*methylmorpholinium*) Salt of 1,2,3,4tetramercapto - 1, 2, 3, 4 - tetrathioxotetraphosphetane (**2f**). Yield 11%. mp 138–145°C. ¹H NMR (CD₃OD), δ: 2.88 (s, 12H, CH₃), 3.2 (m, 16H, NCH₂), 3.94 (m, 16H, OCH₂); ³¹P NMR (D₂O), δ: 121. Anal. Calcd for $C_{20}H_{48}N_4O_4P_4S_8$ (788): C 30.46; H 6.09; N 7.1; P 15.7; S 32.48. Found: C 30.36; H 6.23; N 6.97; P 15.98; S 32.09.

Tetra(*N*,*N*-dimethylbenzylammonium) Salt of 1,2, 3, 4-tetramercapto-1, 2, 3, 4-tetrathioxotetraphosphetane (**2g**). Yield 15%. mp 111–115°C. ¹H NMR (CD₃OD), δ: 2.83 (s, 24H, CH₃), 4.32 (s, 8H, N-CH₂), 7.48–7.54 (m, 20H, H_{Ar}); ³¹P NMR (D₂O), δ: 123. Anal. Calcd for C₃₆H₅₆N₄P₄S₈ (924): C 46.75; H 6.06; N 6.06; P 13.4; S 27.7. Found: C 47.16; H 6.30; N 5.96; P 13.03; S 27.3.

Tetra(dithiopyperidinium)tetraphosphetane Copper(I)chloride (**5c**)

CuCl 0.14 g (1.4 mmol) was added gradually to a stirred mixture of 0.25 g (0.3 mmol) tetraphosphetane **2c** in 15–20 mL acetonitrile or methanol at 28°C, and then the reaction mixture was stirred for 2 h at 50–60°C or 35–40°C, respectively. During this time, a white compound was converted to light-yellow one. After cooling of the reaction mixture to the room temperature, the yellow precipitate was filtered from the solution and dried to give complex **5c** (0.24 g, 61.5%); mp >300°C (decompos.). Anal. Calcd. for C₂₀H₄₈N₄P₄S₈Cu₄Cl₄ (1117): C 21.40; H 3.97; N 4.99; S 22.87; P 11.0. Found: C 21.12; H 3.25; N 4.77; S 22.93; P 10.2.

Computations

All quantum-chemical calculations were carried out using the Gaussian-03 suite of programs [7]. The hybrid metageneralized gradient DFT approximation M05-2X [9,10] was used in combination with

I _{IR} (km·mol ^{−1})/ I _{Raman} (Å ⁴ ·amu)	Assignment ^b
449/0	v _{as} P–S
0/2	
4/6	
0/29	vs P–S
238/1	-
6/5	
80/0	vas P–P
0/56	
0/120	ν _s Ρ–Ρ
2/3	δPS_2
0/0	δSPP
38/ 0	δPS_2
0/ 6	Deformation of anion
1/ 31	
0/ 69	"Breathing" of anion, δ_s PPP
0/ 20	δ_{as} PPP
1/ 1	ωPS_2
0/ 32	
4/ 1	r PS ₂
0/ 0	τPS_2
0/ 1	
0/3	
0/0	Deformation of anion
	$I_{IR} (km \cdot mol^{-1})/I_{Raman} (Å^4 \cdot amu)$ $449/0$ $0/2$ $4/6$ $0/29$ $238/1$ $6/5$ $80/0$ $0/56$ $0/120$ $2/3$ $0/0$ $38/0$ $0/6$ $1/31$ $0/69$ $0/20$ $1/1$ $0/32$ $4/1$ $0/0$ $0/1$ $0/3$ $0/0$

TABLE 2 Calculated Vibrational Spectra of the $\left[\mathsf{P}_4\mathsf{S}_8\right]^{4-}$ Anion

 $a \times 2$, degeneracy.

^{*b*} ν , stretching; δ , bending; ω , wagging; r, rocking; τ , twisting; s, symmetrical; as, antisymmetrical.

a standard 6-31G* basis set. All stationary points were characterized as minima by the analysis of the Hessian matrices. The simulated spectra are obtained by convolution of computed band intensities with a Lorentzian lineshape function (f.w.h.m. = 20 cm⁻¹ for the $[P_4S_8]^{4-}$ model and 10 cm⁻¹ for the $[P_4S_8]^{4-}$ (CuCl)₄ model). Calculated IR and Raman spectra of $[P_4S_8]^{4-}$ model are summarized in Table 2.

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