

reported in this paper, the dihedral angle is 51.6° and the geometry of the CuBr₄²⁻ ion, although intermediate between square planar and tetrahedral, is nearer to square planar than the high-temperature form of the CuCl₄²⁻ salt. The N—Br distance is 3.480 Å (ave.) and the H—Br distance is 2.66 Å (ave.). In other compounds studied in this laboratory, where both the CuCl₄²⁻ salt and the CuBr₄²⁻ salt of the same cation have been prepared, the tetrabromocuprate(II) ion has usually shown a larger dihedral angle than the tetrachlorocuprate(II) ion (Table 6). This is as expected for the larger Br atom since distortion towards a tetrahedral geometry will lessen ligand–ligand repulsions. This argument would hold for the bis(NMPH) salts if the tetrabromocuprate(II) is compared directly with the low-temperature form of the tetrachlorocuprate(II). The high-temperature form contains disordered organic cations which exhibit decreased hydrogen bonding; it is therefore able to adopt a more tetrahedral configuration. The role of hydrogen bonding in CuCl₄²⁻ ions has been discussed previously (Geiser & Willett, 1984), and in CuBr₄²⁻ versus CuCl₄²⁻ ions (Place & Willett, 1987a).

In the NMPH salt, the distances and angles within the cations are normal. The lattice is held together with hydrogen bonding between the ammonium nitrogen N(9) and the Br ions. The N(9)—Br(1) distance is 3.485, H(9A)—Br(1) is 2.726 Å. N(9)—Br(2) is 3.476, H(9B)—Br(2) is 2.593 Å. The packing shows distinct layers of anions and cations. The 2-phenylethyl groups form a contiguous layer with the charged methyl-ammonium group alternating either side of, and protruding from, this layer.

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Three Forms of (Triphenylarsine)diiodine: Two Polymorphs of C₁₈H₁₅AsI₂ and a 1:3/2 Toluene Solvate C₁₈H₁₅AsI₂.3/2C₇H₈

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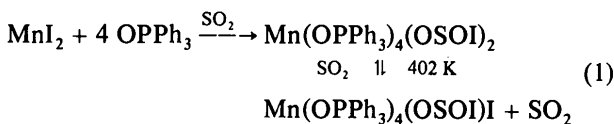
Abstract. (I): C₁₈H₁₅AsI₂, *M_r* = 560.05, orthorhombic, *P*2₁2₁2₁, *a* = 10.990 (4), *b* = 12.056 (4), *c* = 13.963 (3) Å, *V* = 1850.0 Å³, *Z* = 4, *F*(000) = 1048, *D_x* = 2.01 Mg m⁻³, Mo *K*α radiation, λ = 0.71069 Å, μ = 5.04 mm⁻¹, *T* = 293 K, *R* = 0.037 for

2880 reflexions with *F* > 3σ(*F*). (II): C₁₈H₁₅AsI₂, *M_r* = 560.05, monoclinic, *P*2₁/*c*, *a* = 9.228 (3), *b* = 10.079 (2), *c* = 20.348 (3) Å, β = 93.78 (2)°, *V* = 1888.4 Å³, *Z* = 4, *F*(000) = 1048, *D_x* = 1.97 Mg m⁻³, Mo *K*α radiation, λ = 0.71069 Å, μ = 4.94 mm⁻¹, *T* = 293 K, *R* = 0.059 for 1585 reflexions with *F* > 3σ(*F*). (III): C₁₈H₁₅AsI₂.1.5C₇H₈, *M_r* = 698.16, rhombohedral indexed on hexagonal axes, *R*3̄*c*, *a*

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= 13.302 (2), $c = 53.929$ (7) Å, $V = 8263.9$ Å³, $Z = 12$, $F(000) = 4044$, $D_x = 1.68$ Mg m⁻³, Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 3.39$ mm⁻¹, $T = 293$ K, $R = 0.065$ for 951 reflexions with $F > 3\sigma(F)$. The title molecule is composed of an As—I—I shaft with three phenyl fins projecting from the As atom. The As—I bond lengths of 2.641 (1), 2.653 (2) and 2.638 (2) Å for (I), (II) and (III) respectively are similar and I—I distances are identical within their e.s.d.'s [3.005 (1) (I), 3.005 (2) (II), 3.002 (2) Å (III)]. Unlike (III), where molecular conformation is dictated by crystallographic C_3 symmetry, the diiodine is displaced from its central location above the arsenic lone pair in (I) and (II) [I(1)—I(2)—As(1) 174.8 (1) (I), 174.3 (1)^o (II)].

Introduction. Diiodine is capable of forming charge-transfer complexes with various Lewis bases by accepting an electron pair into its σ_u^* orbital. Several structures of this type have been reported covering a range of donor groups, *e.g.* $>N$ (von Pritzkow, 1975), $>Se$ (Maddox & McCullough, 1966), NCS^{*-} (Hartl & Steidl, 1977), NC^{*-} (Fröhlich & Tebbe, 1982), Br^- (Emge *et al.*, 1985), I^- (Runsink, Swen-Walstra & Migchelsen, 1972), where * signifies the donor atoms; however, the title molecule is the first example involving arsenic. The present work forms part of a general investigation into the reaction of small molecules with complexed manganese (McAuliffe, Barratt, Benson, Gott & Tanner, 1985). It focuses in particular on the interaction of SO_2 with a suspension of $MnI_2/OAsPh_3$ in various solvents and follows directly from similar investigations of the analogous phosphine oxide system, which is outlined in (1) (Gott, Fawcett, McAuliffe & Russell, 1984). By contrast, a solid with ligand-to-manganese ratio of 3:1 was produced on adding SO_2 to the corresponding arsenic system. Also, the crystalline solid most readily isolated from this system by thermal decomposition contained the title molecule, a product of ligand reduction, with (III) appearing after the initial SO_2 addition and (I) and (II) as sublimates instead of the semi-reversible SO_2 desorption seen in the phosphine oxide reaction.



Experimental. Purple/red crystals of (I) and (II) were sublimed at 373 K *in vacuo* from a solid, which analysed as $Mn(OAsPh_3)_3I_2(SO_2)_2$ and was itself prepared by adding sulfur dioxide to a suspension of $MnI_2/OAsPh_3$ in propyl acetate. Dark orange (III) crystallized from the toluene solution remaining after filtering off an $MnI_2/OAsPh_3$ suspension, which had been kept under a sulfur dioxide atmosphere for two days.

Table 1. *Details of data collection, structure solution and refinement*

	(I)	(II)	(III)
Crystal dimensions	All crystals selected for data collection had an oval profile, max. dimension 0.2 mm		
Crystal mounting	Lindemann tube		
Diffractometer	Enraf-Nonius CAD-4		
Radiation	Graphite-monochromatized Mo $K\alpha$		
Lattice parameters	Least-squares refinement on setting angles of 25 reflexions		
Lattice reflexions range (°)	4.7 to 7.7	7.1 to 10.1	3.5 to 7.1
Scan width (°)	0.7+0.35 tan θ	0.7+0.35 tan θ	0.8+0.35 tan θ
Scan speed (° min ⁻¹)	0.8 to 5	2 to 5	1.2 to 5
Scan type	$\omega/2\theta$		
Intensity standards	$\bar{2}24, 303, 04\bar{2}$	$20\bar{6}, 206, 23\bar{2}$	$\bar{1}30, \bar{2}0\bar{4}, \bar{3}1\bar{2}$
Fluctuation in standards (%)	± 1.5	± 1	± 1.5
h, k, l range	$-13 \leq h \leq 2$ $0 \leq k \leq 14$ $-16 \leq l \leq 16$ 1 to 25	$0 \leq h \leq 10$ $0 \leq k \leq 11$ $-24 \leq l \leq 24$ 1 to 25	$0 \leq h \leq 15$ $-15 \leq k \leq 0$ $-63 \leq l \leq 63$ 1 to 25
θ range (°)	1 to 25		
No. of reflexions	4065	2538	3328
$I > 0$	2880	1585	951
$F > 3\sigma(F)$ after merging	(Friedel pairs unmerged)		
Corrections	Lp only, absorption and decomposition ignored		
R_{int}	0.018	0.001	0.038
Structure solution	Normal heavy-atom techniques		
Refinement	Full-matrix least squares using <i>SHELX76</i> (Sheldrick, 1976) with non-hydrogen atoms treated anisotropically*		
Hydrogen atoms	Constrained to chemically reasonable positions		
H vibrational parameters	Individual isotropic	Overall isotropic [0.06 (1) Å]	Overall isotropic [0.16 (2) Å]
Final R	0.037	0.059	0.065
wR	0.046	0.050	0.063
$w = k/[\sigma^2(F) + gF^2]$	$k = 0.2687$ $g = 0.0016$	1.6321 0.00039	5.2360 0.00010
Max. Δ/σ	0.004	0.023	0.037
Fluctuations in final ΔF synthesis (e Å ⁻³)	+1.2, -1.5	+1.1, -0.9	+1.0, -1.2
Atomic scattering factors	<i>International Tables for X-ray Crystallography</i> (1974)		

* The absolute configuration of crystal (I) was determined by η refinement (Rogers, 1981) using a specially modified version of *SHELX76*. η quickly converged to 0.92 (5) indicating that the correct enantiomorph had been chosen. \mathcal{R} was also evaluated (Hamilton, 1965) and at 1.109 supported the above assignment. The toluene in (III) was intersected asymmetrically by a crystallographic diad. This resulted in each molecular site being occupied by a disordered superposition of two molecules and necessitated constraining the benzene ring to be a regular hexagon. The ring hydrogens were placed in chemically reasonable positions but those attached to the methyl carbon were ignored.

All details of data collection, structure solution and refinement are presented in Table 1.

Discussion. A molecule of (I) is illustrated in Fig. 1. Atomic coordinates are presented in Table 2* and

* Lists of structure factors, anisotropic vibrational parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44355 (45 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

selected bond lengths and angles in Table 3. The crystal packing of (III) is indicated in Fig. 2.

(Triphenylarsine)diiodine is composed of a heavy-atom shaft with phenyl fins projecting from the As atom. In (III) the molecule has assumed C_3 symmetry so that the benzene rings are equivalent [I(2)—As(1)—C(1)—C(2) -45.5 (7°)]; however, asymmetric environments in forms (I) and (II) have twisted the rings relative to the I(2)—As(1) bond [I(2)—As(1)—C(1)—C(2) -48.1 (7) (I), -42 (1) (II); I(2)—As(1)—C(7)—C(8) -7.9 (6) (I), -62 (1) (II); I(2)—As(1)—C(13)—C(14) -49.8 (7) (I), -53 (1) ($^\circ$) (II)]. In addition to the above deformation, examination of the I—I—As and I—As—C angles and I(1)—I(2)—As(1)—C(13) torsion angles [176.8 (2) (I), 165.8 (5) ($^\circ$) (II)] indicates that the diiodine has been displaced away from C(13) and the central location occupied in (III). All three As—I bonds are strong, [As—I 2.641 (1) (I), 2.653 (2) (II), 2.638 (2) \AA (III)], resembling those in iodoarsines, e.g. *meso-o*-phenylenebis(iodomethylarsine) where the two As—I bonds are 2.693 (3) and 2.581 (3) \AA (Henrick, Raston, White & Wild, 1977). Lone-pair donation has led to considerable changes in the triphenylarsine moiety, whose C—As—C angles range from 99.2 (3) to 100.8 (3) ($^\circ$) (mean 100.1 ($^\circ$)) and As—C bond lengths are distributed between 1.935 (7) and 1.966 (7) \AA (mean 1.957 \AA) prior to complex formation (Sobolev, Belsky, Chernikova & Akhmadulina, 1983). By comparison all C—As—C angles in the diiodine adducts are significantly increased and, although the As—C bond lengths show some overlap, their mean values are reduced [1.921 (I), 1.919 (II), 1.926 \AA (III)], implying enhanced *s* character in the As—C bonds. These changes are mirrored in the diiodine, where, by comparison with the gaseous uncomplexed molecule [I—I = 2.662 \AA (Karle, 1955)] the extended I—I bonds [3.005 (1) (I), 3.005 (2) (II), 3.002 (2) \AA (III)] show a marked decrease in bond number, *n* [I—I = 3.000 \AA corresponds to *n* = 0.4 (Bürgi, 1975)].

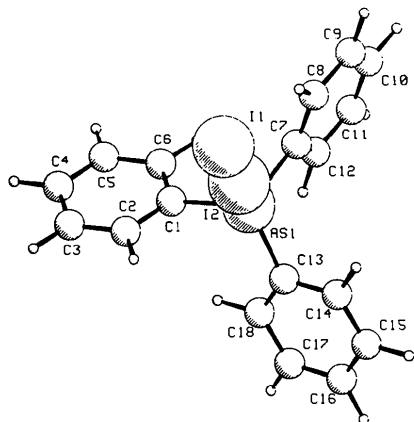


Fig. 1. Orthorhombic (triphenylarsine)diiodine (I) drawn using PLUTO (Motherwell & Clegg, 1978), indicating the common labelling scheme used for all three structures.

Table 2. Fractional atomic coordinates [$\times 10^4$ except for I and As in (I) and (III) $\times 10^5$] and vibrational parameters ($\text{\AA}^2 \times 10^4$) for non-hydrogen atoms

	x	y	z	U_{eq}
(I)				
I(1)	32965 (7)	13638 (5)	59217 (4)	637
I(2)	27220 (5)	33082 (4)	46537 (3)	449
As(1)	23931 (7)	51066 (6)	36053 (5)	419
C(1)	2186 (8)	6360 (7)	4448 (5)	493
C(2)	1384 (10)	6262 (9)	5197 (7)	698
C(3)	1296 (11)	7117 (10)	5844 (8)	850
C(4)	2033 (13)	8075 (9)	5751 (8)	856
C(5)	2823 (12)	8142 (9)	5012 (10)	912
C(6)	2906 (11)	7292 (8)	4351 (8)	737
C(7)	3824 (7)	5380 (7)	2848 (5)	397
C(8)	4868 (8)	4758 (7)	2995 (6)	513
C(9)	5885 (7)	4944 (9)	2412 (7)	575
C(10)	5824 (9)	5726 (8)	1719 (6)	577
C(11)	4806 (8)	6358 (8)	1569 (6)	590
C(12)	3779 (7)	6167 (7)	2135 (6)	484
C(13)	1094 (7)	5140 (7)	2698 (6)	467
C(14)	988 (9)	4262 (10)	2078 (8)	698
C(15)	131 (11)	4294 (11)	1360 (9)	833
C(16)	-633 (10)	5192 (11)	1283 (9)	848
C(17)	-519 (12)	6054 (11)	1888 (11)	1015
C(18)	354 (10)	6034 (9)	2616 (9)	737
(II)				
I(1)	869 (1)	-865 (1)	2500 (1)	601
I(2)	2582 (1)	873 (1)	1635 (1)	520
As(1)	3906 (2)	2596 (2)	892 (1)	475
C(1)	4033 (19)	4253 (18)	1339 (7)	530
C(2)	2877 (19)	4683 (19)	1650 (8)	617
C(3)	2898 (21)	5950 (22)	1967 (9)	719
C(4)	4104 (23)	6727 (20)	1960 (9)	638
C(5)	5286 (19)	6239 (18)	1649 (9)	588
C(6)	5283 (21)	5053 (17)	1354 (8)	555
C(7)	2734 (15)	2890 (16)	91 (7)	374
C(8)	2459 (16)	1810 (16)	-324 (8)	443
C(9)	1573 (19)	1973 (18)	-896 (9)	580
C(10)	955 (19)	3199 (21)	-1042 (9)	617
C(11)	1258 (16)	4256 (20)	-631 (8)	564
C(12)	2147 (15)	4145 (20)	-56 (8)	527
C(13)	5849 (16)	2165 (15)	652 (8)	455
C(14)	6843 (18)	1859 (15)	1142 (8)	483
C(15)	8280 (19)	1614 (17)	1001 (10)	597
C(16)	8652 (18)	1743 (19)	362 (11)	715
C(17)	7658 (19)	2025 (15)	-126 (9)	529
C(18)	6229 (18)	2293 (18)	6 (9)	615
(III)				
I(1)	0	0	83434 (2)	1639
I(2)	0	0	89000 (2)	963
As(1)	0	0	93892 (3)	795
C(1)	1427 (7)	210 (7)	9527 (2)	812
C(2)	1893 (8)	-430 (8)	9427 (2)	1324
C(3)	2934 (9)	-286 (10)	9522 (2)	1426
C(4)	3511 (10)	501 (9)	9713 (2)	1292
C(5)	2980 (8)	1090 (8)	9814 (2)	1081
C(6)	1944 (7)	957 (9)	9719 (1)	1053
C(7)	2814 (11)	2572 (11)	2325 (2)	747 (56)
C(8)	3595 (11)	3590 (11)	2448 (2)	833 (54)
C(9)	3411 (11)	3745 (11)	2697 (2)	932 (70)
C(10)	2446 (11)	2883 (11)	2822 (2)	1268 (126)
C(11)	1665 (11)	1865 (11)	2699 (2)	1012 (74)
C(12)	1849 (11)	1710 (11)	2450 (2)	1012 (66)
C(13)	2924 (24)	2356 (24)	2073 (7)	1521 (122)

$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

Table 3. Selected bond lengths (\AA) and angles ($^\circ$)

	(I)	(II)	(III)
I(1)—I(2)	3.005 (1)	3.005 (2)	3.002 (2)
I(2)—As(1)	2.641 (1)	2.653 (2)	2.638 (2)
As(1)—C(1)	1.929 (8)	1.90 (2)	1.926 (8)
As(1)—C(7)	1.924 (7)	1.92 (1)	
As(1)—C(13)	1.909 (8)	1.94 (2)	
I(1)—I(2)—As(1)	174.8 (1)	174.3 (1)	180
I(2)—As(1)—C(1)	108.7 (2)	108.5 (5)	112.8 (2)
I(2)—As(1)—C(7)	109.5 (2)	109.3 (5)	
I(2)—As(1)—C(13)	119.2 (2)	117.7 (5)	
Average phenyl C—C	1.38	1.38	1.39
Phenyl C—C e.s.d.	0.01–0.02	0.02	0.01

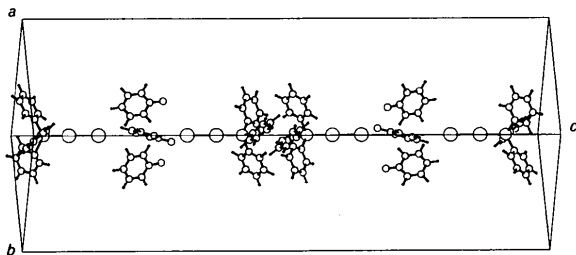


Fig. 2. Packing in $1:\frac{1}{2}$ (triphenylarsine)diiodine toluene solvate (III). Two other identical columns generated by centring operations, $\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{3}$ and $\frac{1}{3}$, $\frac{2}{3}$, $\frac{2}{3}$ complete the cell contents. Half the disordered toluene molecules have been omitted for clarity.

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Structure of Pentaqua(L-threonine)holmium(III) Trichloride

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Abstract. $[\text{Ho}(\text{H}_2\text{O})_5(\text{C}_4\text{H}_9\text{NO}_3)]\text{Cl}_3$, $M_r = 480.5$, orthorhombic, $P2_12_12_1$, $a = 10.508$ (3), $b = 7.395$ (2), $c = 18.708$ (4) Å, $V = 1453.7$ Å³, $Z = 4$, $D_m = 2.19$, $D_x = 2.20$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 6.22$ mm⁻¹, $F(000) = 928$, $T = 298$ (2) K. Final $R = 0.040$ for 2700 observed reflections. The structure is that of a linear polymer. The threonine molecule coordinates to Ho *via* chelation through the hydroxy O and one of the carboxyl O atoms. The second carboxyl O atom is coordinated to Ho of a symmetry-related molecule to form polymeric chains along *a*. Ho is eight-coordinate with a coordination polyhedron in the form of a distorted square antiprism.

Introduction. The complexes of hydroxycarboxylic acids with lanthanide ions were investigated by Grenthe

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(1972, and references therein). The results of these investigations show that hydroxycarboxylate ions coordinate to metal ions as chelate ligands *via* the hydroxy O and one of the carboxyl O atoms. In this paper we have determined the structure of the title compound, in order to elucidate how the coordination mode might change if the hydroxycarboxylic acid contained an additional amine group.

Experimental. Crystals of the title compound were obtained from an aqueous solution of HoCl_3 and L-threonine; density by flotation in bromoform/ethylene bromide. Intensity data with $2\theta_{\text{max}} = 65.0^\circ$ (Mo $K\alpha$ radiation) collected from crystal of size $0.20 \times 0.25 \times 0.40$ mm, Syntex $P2_1$ diffractometer, $\theta:2\theta$ scan with scan rate $3.0\text{--}29.3^\circ \text{min}^{-1}$, systematic absences $h00$