Crystal structure of tetraphenylphosphonium thiocyanate, $(C_6H_5)_4P(SCN)$

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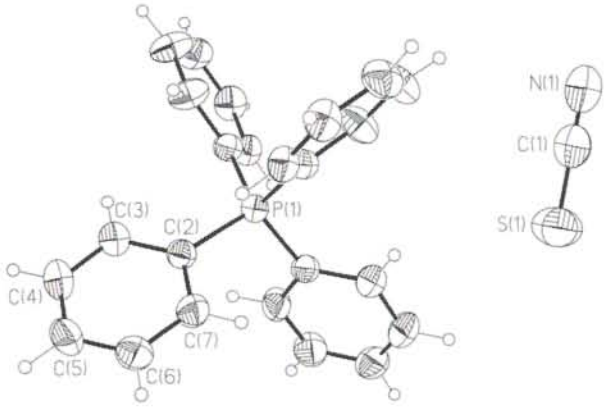

Abstract

$C_{25}H_{20}NPS$, tetragonal, $I\bar{4}$ (No. 82), $a = 11.829(3)$ Å, $c = 7.330(2)$ Å, $V = 1025.7$ Å^3, $Z = 2$, $R_{gt}(F) = 0.036$, $wR(F^2) = 0.099$, $T = 293$ K.

Source of material

Stoichiometric amounts of tetraphenylphosphonium chloride and potassium thiocyanate were dissolved in acetonitrile. The precipitate of KCl was removed by filtration. Single crystals were grown by slow evaporation of the solvent.

Discussion

In the structure the SCN anions are disorded. A similar anion disorder is found in the structure of KSCN [1, 2].

Table 1. Data collection and handling.

Crystal:	white block, size 0.40 × 0.42 × 0.45 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.46 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	60°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1171, 1076
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1001
$N(param)_{refined}$:	75
Programs:	SHELXL-97 [3], CT26_97 [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(3)	8g	0.00021	–0.24433	0.05418	0.069(3)
H(4)	8g	–0.08880	–0.36290	0.26600	0.069
H(5)	8g	–0.21413	–0.28917	0.47914	0.069
H(6)	8g	–0.25924	–0.09559	0.47740	0.069
H(7)	8g	–0.16455	0.02591	0.27494	0.069

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	4f	0.5	0	1/2	0.5980(6)	0.110(3)	0.134(4)	0.060(3)	–0.030(2)	0	0
C(1)	4f	0.5	0	1/2	0.817(2)	0.057(4)	0.068(5)	0.075(8)	–0.006(4)	0	0
N(1)	4f	0.5	0	1/2	0.971(2)	0.050(4)	0.18(1)	0.09(1)	–0.001(5)	0	0
P(1)	2a		0	0	0	0.0307(2)	U_{11}	0.0318(4)	0	0	0
C(2)	8g		–0.0730(1)	–0.0973(1)	0.1459(2)	0.0356(7)	0.0343(7)	0.0327(8)	–0.0038(6)	–0.0007(6)	0.0006(6)
C(3)	8g		–0.0511(1)	–0.2134(2)	0.1426(3)	0.0352(8)	0.0380(8)	0.046(1)	0.0010(6)	0.0002(8)	0.0026(8)
C(4)	8g		–0.1044(2)	–0.2833(2)	0.2675(3)	0.047(1)	0.0383(8)	0.060(1)	–0.0061(7)	–0.000(1)	0.0096(9)
C(5)	8g		–0.1794(2)	–0.2397(2)	0.3917(3)	0.061(1)	0.051(1)	0.049(1)	–0.0147(9)	0.007(1)	0.010(1)
C(6)	8g		–0.2043(2)	–0.1249(2)	0.3933(4)	0.069(1)	0.055(1)	0.049(1)	–0.009(1)	0.023(1)	–0.004(1)
C(7)	8g		–0.1496(2)	–0.0538(2)	0.2722(3)	0.063(1)	0.0387(9)	0.047(1)	–0.0034(8)	0.017(1)	–0.0044(8)

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