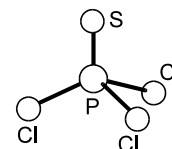


154  
MW

 $\text{Cl}_3\text{PS}$ 
**Thiophosphoryl trichloride**  
Phosphorothioic trichloride

 $\text{C}_{3v}$   
 $\text{PSCl}_3$ 

$r_0$	$\text{\AA}$	$\theta_0$	deg
P=S	1.8863(14)	S=P-Cl	116.273(34)
P-Cl	2.0072(6)		
$r_s$	$\text{\AA}^{\text{a}}$	$\theta_s$	deg <sup>a</sup>
P=S	1.8867(10)	S=P-Cl	116.220(30)
P-Cl	2.0059(5)		
$r_z$	$\text{\AA}^{\text{b}}$	$\theta_z$	deg <sup>b</sup>
P=S	1.8835(7)	S=P-Cl	116.35(2)
P-Cl	2.0093(3)		
$r_e$	$\text{\AA}^{\text{a) c}}$	$\theta_e$	deg <sup>a) c</sup>
P=S	1.8805(20)	S=P-Cl	116.348(60)
P-Cl	2.0042(10)		


<sup>a</sup>) Uncertainties were not estimated in the original paper.

<sup>b</sup>) Including Morse anharmonicity constant  $a(\text{S}=\text{P}) = a(\text{P}-\text{Cl})$  as a parameter in a fit, resulting in a value of  $2.17(9) \text{ \AA}^{-1}$ .

<sup>c</sup>) Estimated from the  $r_z$  structure.

 Firth, S., Davis, R.W.: J. Mol. Spectrosc. **179** (1996) 32.

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