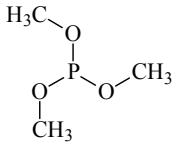
455 **$C_3H_9O_3P$** **Trimethyl phosphite** **C_1 ($\pm ag^+g^+$)**
ED, DFT Trimethoxyphosphine **C_1 ($\pm aa^+g^+$)**
calculations **C_s (ag^-g^+)**

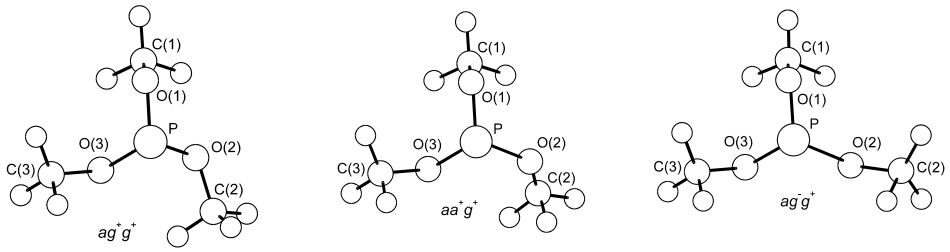


r_a	Å [a])
P–O(1)	1.609(4)
P–O(2)	1.632(4)
P–O(3)	1.651(4)
O(1)–C(1)	1.451(10)
O(2)–C(2)	1.441(10)
O(3)–C(3)	1.442(10)
C–H [b])	1.090(4)

θ_α	deg [a])
O(1)–P–O(2)	98.2(9)
O(2)–P–O(3)	96.1(9)
O(1)–P–O(3)	103.8(9)
P–O(1)–C(1)	121.6(12)
P–O(2)–C(2)	116.9(12)
P–O(3)–C(3)	116.2(12)
O–C–H [b])	113(3)
C(1)–O(1)–P–lp [c])	174(2)
C(2)–O(2)–P–lp [c])	37(5)
C(3)–O(3)–P–lp [c])	35(5)
C(1)–O(1)–P–O(2)	45(3)
C(1)–O(1)–P–O(3)	–54(3)
C(2)–O(2)–P–O(3)	–84(6)
C(2)–O(2)–P–O(1)	171(6)
C(3)–O(3)–P–O(1)	–93(7)
C(3)–O(3)–P–O(2)	167(7)

The molecule was found to exist as a mixture of $\pm ag^+g^+$ (78(13)%), $\pm aa^+g^+$ (14(21)%) and ag^-g^+ (9(11)%). The differences in the chemically equivalent but symmetry inequivalent bond distances and angles in the same conformer and in the corresponding bond lengths and angles of different conformers were assumed at the values from B3PW91/6-311+G* calculations. The dihedral angles were refined for the main conformer, while the dihedral angles in the other conformers were assumed at the values from DFT calculations. Staggered conformation was assumed for each methyl group. The structural parameters are listed for the ag^+g^+ conformer.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors including a systematic error.
[b]) Mean value.
[c]) lp is the lone pair on the P atom, assumed to lie in a plane containing the P–O bond and bisecting the opposite O–P–O angle.



Belyakov, A.V., Dalhus, B., Haaland, A., Shorokhov, D.J., Volden, H.V.: J. Chem. Soc., Dalton Trans. (2002) 3756.

Replaces II/25C (**3**, 1410)