

# A common conformation of stabilized triphenyl phosphonium ylidic diesters with bulky alkoxy groups

Castañeda, Fernando

Silva, Paul

Garland, M. Teresa

Shirazi, Ata

Bunton, Clifford A.

The phosphonium ylidic diesters, methyl and ethyl isopropyl and, methyl and ethyl t-butyl triphenylphosphoranylidene malonates, 1a,b and 2a,b, respectively, have the syn-anti conformation in solution, as in the crystal, and the bulkier alkoxy group is oriented towards phosphorus. The  $^1\text{H}$  NMR spectra show that in 1a,b, the isopropyl group is oriented towards the face of a phenyl group, consistent with shielding in the  $^1\text{H}$  signals, and examination of the  $^1\text{H}$  coupled  $^{13}\text{C}$  NMR spectra allows assignment of the acyl carbon signals. Computed bond lengths and angles for isolated molecules are similar to those in the crystal, and the geometry and the NMR spectra indicate extensive ylidic resonance. Estimated partial atomic charges on the ester oxygens are more negative when they are oriented towards, rather than away from, phosphorus.