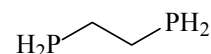
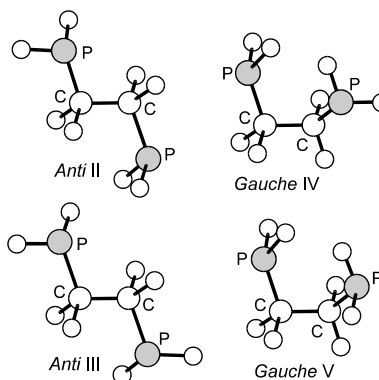


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MW $\text{C}_2\text{H}_8\text{P}_2$ **1,2-Diphosphinoethane**
1,2-Ethanediylobisphosphine C_1 (*Anti* II)
 C_2 (*Gauche* V)
 C_2 (*Anti* III)
 C_1 (*Gauche* IV)

Four conformers, two P–C–C–P *anti* and two P–C–C–P *gauche* with different orientations of the phosphino groups, were assigned. *Anti* II was found to be the most stable conformer that possesses a dipole moment different from zero. *Anti* II is 3.4(5) kJ mol^{−1} more stable than *Gauche* V, 3.5(5) kJ mol^{−1} more stable than *Anti* III and 4.7(6) kJ mol^{−1} more stable than *Gauche* IV. *Anti* II displays tunneling splitting in the ground vibrational state. The tunneling frequency is 8.387(48) MHz in *Anti* II. Tunneling is absent in the first excited state of the C–C torsion. The agreements between results of MP2/6-31G** calculations and experimental data are good in all cases where the latter are available. The tendency to prefer P–C–C–P *anti* conformation is in accord with the general *gauche* effect. Intramolecular repulsion may be important in at least some of the *gauche* conformations, leading to a stabilization of *anti* conformers by repulsive forces as well.



Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand. **50** (1996) 875.