

Is Dodecahedral P₂₀ Special?

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The laboratory study of phosphorus clusters by laser-based mass spectrometric methods indicates, tentatively, that P⁺²¹ may be special. A plausible interpretation might place a P⁺ ion interior to a dodecahedral P₂₀ molecule. *Ab initio* quantum mechanical methods have been applied to the P₂₀ molecule using contracted gaussian basis sets as large as (9s 6p 4d 3f) on each phosphorus atom. At the highest level of theory, dodecahedral P₂₀ is predicted to lie 23 kcal/mol above five separated P₄ molecules.

Key words : Phosphorus clusters - P₂₀ - Dodecahedra