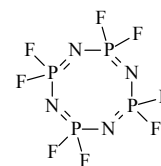


**206** **F<sub>8</sub>N<sub>4</sub>P<sub>4</sub>**ED, *ab initio* and DFT calculations**2,2,4,4,6,6,8,8-Octafluoro-2λ<sup>5</sup>,4λ<sup>5</sup>,6λ<sup>5</sup>,8λ<sup>5</sup>-cyclotetraphosphaza-1,3,5,7-tetraene**  
2,2,4,4,6,6,8,8-Octafluoro-1,3,5,7,2,4,6,8-tetraazatetraphosphocine**S<sub>4</sub>** (see comment)

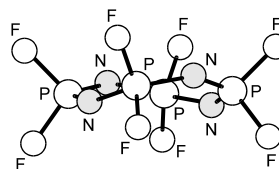
| $r_a$ | $\text{\AA}^a$ | $\theta_a$      | deg <sup>a)</sup> |
|-------|----------------|-----------------|-------------------|
| P–N   | 1.520(5)       | P–N–P           | 141.2(9)          |
| P–F   | 1.554(5)       | N–P–N           | 122.9(10)         |
|       |                | F–P–F           | 98.0(6)           |
|       |                | P–N–P–N         | 30.4(22)          |
|       |                | N–P–N–P         | 26.6(48)          |
|       |                | $h(\text{N})^b$ | $\pm 0.299(22)$   |
|       |                | $h(\text{P})^b$ | $\pm 0.031(63)$   |



The N–PF<sub>2</sub>–N moieties were assumed to have C<sub>2v</sub> symmetry. An equally good fit was obtained in the ED analysis for molecular models of S<sub>4</sub> and D<sub>2d</sub> symmetry.

The nozzle was at room temperature.

HF/6-31G\* and B3LYP/6-31G\* calculations indicated that only the S<sub>4</sub> conformer corresponds to a minimum on the energy hypersurface.



<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Out-of-plane coordinate of N or P.

Elias, A.J., Twamley, B., Haist, R., Oberhammer, H., Henkel, G., Krebs, B., Lork, E., Mews, R., Shreeve, J.M.: J. Am. Chem. Soc. **123** (2001) 10299.