BIBLIOGRAPHY OF FIVE MEMBERED RINGS

Mathematical Papers.

(1) Marzec, C. J., and Day, L. A., *An ecact description of five-membered ring configurations. I Parameterization via an amplitude S, and angle* Γ*, the pseudorotation amplitude q and phase angle P, and the bond lengths*, Journal of Biomolecular Structure & Dynamics, **10**, no. 6, (1993), 1091–1123. This is the paper we will discuss the most, since most of the equations are written down and discussed there.

(2) Abillon, E., *Geometry of the five-membered ring. Mathematical demonstration of the pseudorotation formulae*, Biophysics of Structure and Mechanism, **8**, (1982), 257–270. This paper derives many concrete relationships between the internal coordinates, and derives certain symmetric conformations purely geometrically.

(3) Kapovich, M., Millson, J. J., *The symplectic geometry of polygons in Euclidean space*, Journal of Differential Geometry, **44**, (1996), 479–513. This paper studies the mathematical structure of the space of all polygon conformations, and the flows on that space induced by rotating "flaps".

(4) Hausmann, J-C., Knutson, A., *Polygon spaces and Grassmannians*, L' Enseignement Mathèmatique, **43**, (1997), 173–198. This paper follows up on the previous one and develops the connection between the space of all polygon conformations and mathematical spaces called Grassmannians. In particular, on the pentagon space two complex coordinates are said to exist; these may be related to the coordinates proposed by Marzec and Day.

(5) Banchoff, T. F., *Frenet frames and theorems of Jacobi and Milnor for space polygons (Global geometry of polygons III)*, Rad Jugoslavenske Akademije Zanosti i Umjetnosti, **396**, (1982), 101–108. This contains some interesting results on the total absolute torsion of of polygonal curves. It is of only mild interest.

Chemistry papers.

(1) Marzec, C. J., and Day, L. A., *An exact description of five-membered ring configurations. II Applications to furanose rings in DNA and RNA, analysis of errors, and bond angle bending energy*, Journal of Biomolecular Structure & Dynamics, **10**, no. 6, (1993), 1125–1155. This paper shows what values of their four coordinates occur in practise in furanose rings.

(2) Cremer, D., Pople, J. A., *A general definition of ring puckering coordinates*, Journal of the Americal Chemical Society, **97**, no. 6, March 19, (1975), 1354–1358. This paper defines some general coordinates of puckered polygons in space. It is the foundation of Marzec and Day's theory for pentagons, but it also applies to hexagons. But the authors do not give a complete coordinate decription of these rings.

(3) Cai, M., Huang, Y., Liu, J., Krishnamoorthi, R., *Solution conformations of proline rings in proteins studied by NMR spectroscopy*, Journal of Biomolecular NMR, **6**, (1995), 123–128. A good source of information on proline conformations.

(4) De Leeuw, H. P. M., Haasnoot, C. A. G., Altona, C., *Empirical Correlations between conformational parameters in β-furanoside fragments derived from a staistical survey of crystal structures of nucleic acid constituents*, Israel Journal of Chemistry, **20**, (1980), 108–126. This work contains some useful approximate formulae. They are mathematically unsatisfactory because they are based on endocyclic torsion angles, which cannot exactly satisfy analogues of the Cremer-Pople identities except in very special cases. However, it is ironic that these formulae gave smaller statistical errors than did the Cremer-Pople formulae, and this lead to a period of controversy.

(5) Levitt, M., Warshel, A., *Extreme conformational flexibility of the furanose ring in DNA and RNA*, Journal of the American Chemical Society, **100**, no. 9, April 26, (1978), 2607–2613. This paper still gives a reasonable overview of the energetic characteristics of furanose rings and how pseudorotation fits into the picture. The title is in retrospect a bit of an exaggeration.