



range of 32 to 43 mg. Three rats were observed for seven days following withdrawal of the hormone. The glycosuria immediately disappeared from the two animals which had excreted glucose during the injection period.

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STRAIN ENERGIES OF CYCLIC HYDROCARBONS¹

THE strain energies of cyclic hydrocarbons have long been of interest to chemists. Since the discovery of appreciable energy barriers to rotation about single bonds, it has been apparent that this phenomenon may contribute a strain energy² in addition to the long-recognized deviation from tetrahedral bond angles. Conn, Kistiakowsky and Smith² discussed the relative energy contents of five- and six-membered cyclic hydrocarbons with zero, one and two double bonds without being able to obtain agreement between calorimetric values and theory. It is the purpose of this communication to point out that by recognizing the non-planarity of the cyclopentane ring³ it is possible to obtain substantial agreement.

The calculations leading to the values in Table 1 are based on the well-established (though not very

¹ The material in this communication was presented as a part of the American Chemical Society Award in Pure Chemistry address, Pittsburgh, 1943. Publication and further work have been delayed by war activities.

² J. B. Conn, G. B. Kistiakowsky and E. A. Smith, *Jour. Am. Chem. Soc.*, 61: 1868, 1939. These authors state that Dr. V. Schomaker first suggested this possibility to them.

³ J. G. Aston, H. L. Fink and S. C. Schumann, *Jour. Am. Chem. Soc.*, 65: 341, 1943.

TABLE 1
STRAIN ENERGIES (KCAL. PER MOLE)

	Bond angles	Single bond twist	Total calc.	Exper.
Cyclopentane	2.6	6.6	9.2	7
Cyclopentane (planar)* ..	(0.1)	(14.0)	(14.1)*	(7)*
Cyclopentene	2.6	5.6	8.2	6
Cyclopentadiene—1, 3	7	0	7	6
Cyclohexane (chair form) ..	0	0	0	(0)
Cyclohexane (boat form)* ..	(0)	(5.6)	(5.6)*	(0)*
Cyclohexene	0	1.5	1.5	1
Cyclohexadiene—1, 3	0	4	4	4

* Hypothetical, unstable forms.

precise) values of 2,800 cal. per mole for the potential barrier⁴ about an ethane-like single bond (staggered position having minimum energy) and 6×10^{-12} erg per radian² for the force-resisting⁵ distortion of the bond angles about a carbon atom. Several amounts and types of puckering of cyclopentane were considered in order to estimate the energy of the stable position. In the column headed "Bond Angles" are given the energies needed to bend the bond angles below their equilibrium values. To compute the twist energy, each single bond in the ring is considered separately. The energy needed to twist an ethane molecule into a similar configuration is taken as the contribution for that bond. In considering orientations adjacent to the double bond in the olefins, it is assumed that the equilibrium position is still the staggered one (if two single bonds were bent into a two-membered ring). This is confirmed by results for the simpler olefins. While the agreement in Table 1 is not perfect, it is within the various uncertainties present.

The experimental values in Table 1 are based on hydrogenation data² for the olefins and on combustion data⁶ for the two naphthenes. The basic, no-strain heat of olefin hydrogenation is taken as that of trans 2-butene. For the diene hydrogenation, the value for 1,3-butadiene is adjusted for the effect of substitution on each end with the trans 2-butene-ethylene difference.

It is planned, when circumstances permit, to refine these calculations by detailed consideration of the force constants and spectra of the molecules involved. At that time additional details of these calculations can be given.

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⁴ K. S. Pitzer, *Chem. Rev.*, 27: 39, 1940.

⁵ Rough average of values given by T. Y. Wu, "Vibration Spectra and Structure of Polyatomic Molecules," National University of Peking, Kun-ming (1939).

⁶ H. M. Huffman, private communication.