PERHYDROFULLERENES AS AKKUMULATORS OF HYDROGEN

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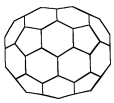
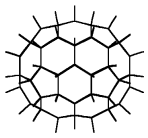
The carbon dodecahedron claster C_{20} may be considered as a parent fullerene. Then its hydrogenated form $C_{20}H_{20}$ - dodecahedrane presents the only known up to the present fully hydrogenated fullerene - perhydrofullerene (PHF). It is known that all attempts to prepare other PHF remained so far unsuccessful, though partly hydrogenated forms up to $C_{60}H_{36}$ are known. There is a reason to believe that failure in synthesis of $C_{60}H_{60}$ is due to strong unbonded interactions arising between hydrogen atoms in the outer shell of C_nH_n molecules embracing the carbon skeleton of PHF.



C_{70}



$C_{70}H_{70}$

In the author's opinion another important reason of the strong strain arising in molecules of PHF, may consist in straightening bent *cys*-decalin (6+6) and *cys*-indan (6+5) fragments on the spherical surface of fullerene. The curvature reduction of a spherical surface in the greater fullerenes (C_{70}, C_{80}, C_{180} etc) should lead to highly strained PHF. Nevertheless quantum mechanical (PM3) calculation of such structures showed that energy for one methine group CH - the unit of PHF structure (E_{CH}) is close to energy for the same group in well known macrocyclic hydrocarbons annulenes C_nH_n (see the table). For comparison the calculated data of the unstable tetrahedrane and the quite stable cubane are also presented.

Formula	Bond energy, *kcal/mol*		Formula	Bond energy, *kcal/mol*	
	E	E_{CH}		E	E_{CH}
Annulenes			Polyhedranes		
C_6H_6	-1315	-219,1	C_4H_4	-751,8	-187,9
$C_{18}H_{18}$	-3911	-217,3	C_8H_8	-1670	-208,8
$C_{30}H_{30}$	-6523	-217,4	$C_{20}H_{20}$	-4499	-224,9
$C_{42}H_{42}$	-9133	-217,5	$C_{60}H_{60}$	-13050	-217,5
$C_{54}H_{54}$	-11745	-217,5	$C_{70}H_{70}$	-15139	-216,3
$C_{66}H_{66}$	-14355	-217,5	$C_{80}H_{80}$	-17213	-215,2

Thus, we believe that PHF must be quite real compounds. In the context of their tending to stabilize by transformation in the more stable fullerenes on the account of easy splitting off hydrogen, PHF can be accumulators of hydrogen. It is quite possible that a partial dehydrogenization can happen by weak heating of PHF or in milder conditions - by action of usual catalysts of hydrogenation-dehydrogenation (Pt, Pd, Ni). One more application of PHF may be based on their markedly better than for fullerenes solubility in non-polar solvents typical for saturated cage hydrocarbons. The last property can be of decisive importance in analysis and separation of complex mixtures of sparingly soluble fullerenes by transforming them into PHF.