unsaturated ketones or their enols formed are preferentially hydrogenated to saturated ketones, as illustrated in Scheme 1 in the case of *o*-cresol, it may be calculated that the hydrogenation of cresols will give 67% yield of methylcyclohexanone as the intermediate. It will be noted that this value does not differ so much from those estimated from the present stereochemical results.

TABLE 2

ESTIMATED YIELDS OF METHYLCYCLOHEXANONE INTERMEDIATES

Compound	Yield of *cis* isomer of methylcyclohexanol (%): At initial stage of hydrogenation	Yield of *cis* isomer of methylcyclohexanol (%): Formed in hydrogenation of methylcyclohexanone[a]	Estimated yield of methylcyclohexanone intermediate (%)
o-Cresol	100	64	61
m-Cresol	87	49	61
p-Cresol	80	70	70

[a] Mean values of the results obtained in phenol and cyclohexanol solutions.

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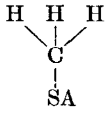
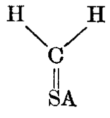
Hybridization of the Carbon Atom in Chemisorbed Hydrocarbon Species

Hybridization of the carbon atom of some small symmetric chemisorbed hydrocarbon species can readily be described by application of the group theory. This theory was applied by us to the adsorbed methyl radical (I) and the αα-diadsorbed methylene radical (II),



(I)



(II)

where SA represents a surface atom.

By representing each hybrid orbital by a vector pointing in the appropriate direction and using the rule that the character of the corresponding reducible representation equals the number of vectors which have not shifted by the symmetry operation, we found that for (I) (symmetry group C_{3v}) $\Gamma_\sigma = 2A_1 + E$. The four atomic orbitals necessary for constructing the set of four hybrid orbitals, must consist of two orbitals of A_1 symmetry and one of E symmetry. Using the character table, we found for the carbon atom the A_1 orbitals s, p_z, and d_{z^2} and the E orbitals (p_x, p_y), $(d_{x^2-y^2}, d_{xy})$, and

(d_{xz}, d_{yz}). If it is assumed that d orbitals (or a higher s orbital) are not used for energetic reasons, it can be concluded that the carbon atom of (I) uses sp^3 (or more correct: spp^2) hybrids.

For (II) (symmetry group C_{2v}) we found that $\Gamma_\sigma = 2A_1 + B_1$. In this case, the A_1 orbitals s, p_z, $d_{x^2-y^2}$ and d_{z^2} and the B_1 orbitals p_x and d_{xz} are found. It follows therefore that the σ bonds consist of sp_xp_z hybrids. However, we should also consider the six possible π bonds which will transform by the symmetry operation in the same way as a set of six vectors attached to the three atoms surrounding the carbon atom. The two vectors on each atom must lie in a plane perpendicular to the bond with the carbon atom and also be at right angles in respect of each other. By application of the various symmetry operations we derived that $\Gamma_\pi(\perp) = A_2 + 2B_2$ and $\Gamma_\pi(\|) = A_1 + 2B_1$.

Considering $\Gamma_\pi(\perp)$ it may be found that the appropriate orbital for A_2 is d_{xy} and those for B_2 are p_y and d_{yz}. Again, the d orbitals are neglected for energetic reasons, so that only p_y is left. In the case of $\Gamma_\pi(\|)$, the energetically allowed orbitals belonging to the irreducible representations A_1 and B_1, have been used already for the formation of the σ bonds. For the bonding of the methylene radical to the metal surface, one σ hybrid and one p_y orbital—the latter being perpendicular to the plane of the adsorbed species—are available.

This conclusion is in agreement with the suggestion of Rooney (*1*) that bonding of $\alpha\alpha$-diadsorbed intermediates takes place by means of one σ bond and one π bond.

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Announcement

The Fourth International Congress on Catalysis will be held from 23 to 29 June 1968 in Moscow. The theme of the Congress will be "Principles of the Prediction of Catalytic Action."

For copies of the circulars, submission of papers (abstracts are due not later than July 15, 1967, and papers not later than September 15, 1967), and other information, please apply to Dr. B. D. Polkovnikov, Secretary, Fourth International Congress on Catalysis, Leninskii Prosp. 47, Institute of Organic Chemistry, Academy of Sciences of the USSR, Moscow B-334, USSR.