Theoret. Chim. Acta (Berl.) 40, 352 (1975)

Erratum

Electronic Structure of Saturated Hydrocarbons in the Semi-Empirical Equivalent Orbital Method

2. "Through Space Interactions" from the Data for Diamond and Neopentane

Pavel N. Dyachkov and Alexandr A. Levin

Theoret. Chim. Acta (Berl.) **36**, 181 (1975)

Received May 30, 1975

The symmetry assignment obtained on the pages 192–193 holds for the zone center only. For $q \neq 0$ the valence band structure may be obtained using the matrix elements:

$$H_{aa} = c + 2\beta_t \cos q$$
$$H_{cc} = a + 2p \cos q$$
$$H_{ab} = \beta_A + \beta_w \exp(iq) + \beta_A \exp(-iq) + \beta_w \exp(-i2q)$$
$$H_{ac} = d + s \exp(iq) + \delta_m \exp(-iq)$$
$$H_{bc} = s + d \exp(iq) + \delta_m \exp(i2q)$$
$$H_{ae} = d + s \exp(-iq) + \delta_m \exp(iq)$$
$$H_{cd} = b + 2k \cos q$$
$$H_{ce} = g + g \exp(-iq)$$
$$H_{cf} = f + f \exp(-iq)$$

The corresponding dispersion curves are shown in Fig. 1.

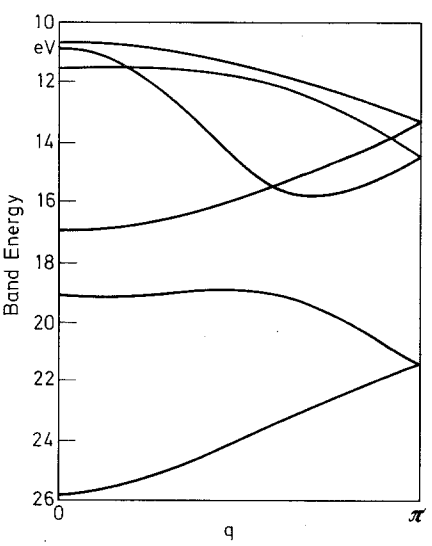

Fig. 1. Band structure of polyethylene valence band

Dr. A. Levin
Academy of Science of the USSR
Institute for General and Inorganic Chemistry
Leninskii prospect 31
Moscow V-71, USSR