Spectroscopic Studies on Ethylene Molecules

III. Coriolis Coupling Coefficients *

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The various types of Coriolis coupling in ethylene type molecules are specified in the standard work of Herzberg.[1] Further theoretical considerations of this problem have been reported elsewhere.[2] Here we wish to present a complete set of values of ζ for ethylene, ethylene-d_4 and ethylene-t_4 as obtained from a recently developed harmonic force field for these molecules.[3]

Table 1. Coriolis coupling coefficients $\zeta^{\alpha}[i,j]$.

Type	$\alpha[i,j]$	C_2H_4	C_2D_4	C_2T_4
$B_{1g}\times B_{2g}$	$x[5,8]$	0.833	0.858	0.883
	$x[6,8]$	−0.554	−0.514	−0.469
$B_{2u}\times B_{1u}$	$x[9,7]$	0.870	0.886	0.898
	$x[10,7]$	−0.492	−0.464	−0.440
$B_{3u}\times A_u$	$x[11,4]$	0.840	0.813	0.786
	$x[12,4]$	−0.542	−0.583	−0.619
$A_g\times B_{2g}$	$y[1,8]$	0.497	0.549	0.640
	$y[2,8]$	−0.041	−0.426	−0.445
	$y[3,8]$	0.867	0.719	0.626
$B_{2u}\times A_u$	$y[9,4]$	0.492	0.464	0.440
	$y[10,4]$	0.870	0.886	0.898
$B_{3u}\times B_{1u}$	$y[11,7]$	0.542	0.583	0.619
	$y[12,7]$	0.840	0.813	0.786
$A_g\times B_{1g}$	$z[1,5]$	−0.016	−0.125	−0.261
	$z[1,6]$	0.873	0.860	0.875
	$z[2,5]$	−0.266	0.220	0.337
	$z[2,6]$	−0.473	−0.462	−0.314
	$z[3,5]$	−0.964	−0.967	−0.905
	$z[3,6]$	0.116	−0.216	−0.369
$B_{2u}\times B_{3u}$	$z[9,11]$	0.058	0.139	0.210
	$z[9,12]$	0.998	0.990	0.978
	$z[10,11]$	−0.998	−0.990	−0.978
	$z[10,12]$	0.058	0.139	0.210
$A_u\times B_{1u}$	$z[4,7]$	0	0	0

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The desired quantities are obtainable by means of any one of the matrix relations

$$\zeta^{\alpha} = L^{-1}\, C^{\alpha}\, \tilde{L}^{-1}$$
$$\zeta^{\alpha} = \tilde{L}\, G^{-1}\, C^{\alpha}\, \tilde{L}^{-1}$$
$$\zeta^{\alpha} = \tilde{L}\, \bar{C}^{\alpha}\, L$$

For the theoretical basis and explanation of symbols, see *e.g.*[2,4] The numerical results are presented in Table 1, where the indices $[i,j]$ are consistent with the conventional numbering of ethylene frequencies.[4]

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2. Meal, J. H. and Polo, S. R. *J. Chem. Phys.* **24** (1956) 1119; Cyvin, B. N., Cyvin, S. J. and Kristiansen, L. A. *J. Chem. Phys.* **39** (1963) 1967.
3. Cyvin, B. N. and Cyvin, S. J. *Acta Chem. Scand.* **17** (1963) 1831.
4. Meal, J. H. and Polo, S. R. *J. Chem. Phys.* **24** (1956) 1126.

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Über Reaktionen von Triäthylsilan mit einigen ungesättigten Carbonsäuren

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Nach unseren jetzigen Kenntnissen kann ein Hydrosilan – $HSi(R')(R'')(R''')$, wo R', R'' und R''' Halogenatome oder Kohlenwasserstoffreste sind – mit ungesättigten Carbonsäuren nach einer der folgenden Möglichkeiten reagieren:

I. Das Hydrosilan ergibt mit der Carboxylgruppe einen Silylester:[1]

$$C{=}C....COOH + HSi(R')(R'')(R''') \rightarrow$$
$$C{=}C....COOSi(R')(R'')(R''') + H_2$$

II. Das Hydrosilan wird an die Kohlenstoff-Kohlenstoff-Doppelbindung unter Bildung einer Silacarbonsäure addiert:[2,3]

$$C{=}C....COOH + HSi(R')(R'')(R''') \rightarrow$$
$$C{-}CH....COOH$$
$$|$$
$$Si(R')(R'')(R''')$$