

## Spectroscopic Studies on Ethylene Molecules

## III. Coriolis Coupling Coefficients \*

S. J. CYVIN and B. N. CYVIN

*Institutt for teoretisk kjemi, Norges tekniske høgskole, Trondheim, Norway*

The various types of Coriolis coupling in ethylene type molecules are specified in the standard work of Herzberg.<sup>1</sup> Further theoretical considerations of this problem have been reported elsewhere.<sup>2</sup> Here we wish to present a complete set of values of  $\zeta$  for ethylene, ethylene-d<sub>4</sub> and ethylene-t<sub>4</sub> as obtained from a recently developed harmonic force field for these molecules.<sup>3</sup>

Table I. Coriolis coupling coefficients  $\zeta^a[i,j]$ .

Type	$a[i,j]$	C <sub>2</sub> H <sub>4</sub>	C <sub>2</sub> D <sub>4</sub>	C <sub>2</sub> T <sub>4</sub>
$B_{1g} \times B_{2g}$	$x[5,8]$	0.833	0.858	0.883
	$x[6,8]$	-0.554	-0.514	-0.469
	$x[9,7]$	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

\* This project has been supported by *Norges tekniske høgskoles fond* (1964).

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

$$\zeta^a = L^{-1} C^a \tilde{L}^{-1}$$

$$\zeta^a = \tilde{L} G^{-1} C^a \tilde{L}^{-1}$$

$$\zeta^a = \tilde{L} \bar{C}^a L$$

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

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Received May 28, 1964.

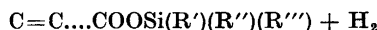
## Über Reaktionen von Triäthylsilan mit einigen ungesättigten Carbonsäuren

GERT PETTERSSON

*Organisch-chemisches Institut der Universität, Lund, Schweden*

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:<sup>1</sup>



II. Das Hydrosilan wird an die Kohlenstoff-Kohlenstoff-Doppelbindung unter Bildung einer Silacarbonsäure addiert:<sup>2,3</sup>

