Mean Amplitudes of Vibration, Force Constants and Coriolis Coupling Constants of $ZXY_2(C_{2v})$ and $ZXY_3(C_{3v})$ Type Molecules and Ions

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For a large number of $ZXY_3(C_{3v})$ and $ZXY_2(C_{2v})$ molecules and ions symmetry force constants, mean amplitudes of vibration for bonded and nonbonded distances and Coriolis coupling constants have been calculated.

In the last years several papers have appeared dealing with the calculation of mean amplitudes of vibration. They were almost exclusively obtained by solving the secular equation

$$|\Sigma G^{-1} - \Delta E| = 0 \quad (1)$$

given by CYVIN¹ with drastic approximations of neglecting off-diagonal elements. This procedure has inappropriately frequently been referred to as CYVIN's method. Already MÜLLER² has pointed out that the calculation of the Σ matrix is better when using the equation

$$\Sigma = L \Delta L' \quad (2)$$

given by CYVIN. The physical basis for this has been discussed². In this paper mean amplitudes of vibration for several molecules and ions shall be calculated according to (2), i.e. after initial calculation of force constants. In the cases of the molecules the values obtained can be useful for electron diffraction studies.

I. Frequencies of the Normal Vibrations, Molecular Data and Symmetry Coordinates

References for the data on which the calculations for the $ZXY_3(C_{3v})$ compounds are based are given in Table I. The frequencies are taken from the most recent papers. In some cases the assignment of $\delta_{as}(XY_3) = \nu_5(E)$ and $\delta(ZXY) = \rho(XY_3) = \nu_6(E)$ is not completely clear^{8,10} but this has almost no effect on the results except on the values for the

mean amplitudes for the nonbonded distances and the ζ_{55} and ζ_{66} values as shown for $BrSiCl_3$ and $ISiBr_3$, where the calculations have been done with the assignments of ν_5 and ν_6 interchanged. References for the corresponding data of the $ZXY_2(C_{2v})$ type compounds are summarized in Table 2.

For the four-atomic molecular models (C_{2v} symmetry) the applied symmetry coordinates are specified elsewhere³. Those for the XY_3Z model of symmetry C_{3v} are also to be published⁴. But since this latter paper probably will not appear before the present article we reproduce the appropriate coordinates in the following for the sake of convenience. R and D are used to designate the $X-Y$ and $X-Z$ distances, respectively, and the equilibrium YXY angle is $2A$. The three angle bendings α_i are opposite to the corresponding $X-Y$ stretchings r_i (for $i = 1, 2, 3$). The three bendings γ_i have atoms in common with the corresponding r_i 's.

$$S_1(A_1) = 3^{-1/2}(r_1 + r_2 + r_3),$$

$$S_2(A_1) = d,$$

$$S_3(A_1) = \left\{ \frac{R}{3[R(4 - \sec^2 A) + D]} \right\}^{1/2} \cdot [(4 - \sec^2 A)^{1/2} R(\alpha_1 + \alpha_2 + \alpha_3) - D(\gamma_1 + \gamma_2 + \gamma_3)].$$

$$S_{1a}(E) = 6^{-1/2}(2r_1 - r_2 - r_3),$$

$$S_{2a}(E) = 6^{-1/2} R(2\alpha_1 - \alpha_2 - \alpha_3),$$

$$S_{3a}(E) = 6^{-1/2} (RD)^{1/2} (2\gamma_1 - \gamma_2 - \gamma_3).$$

$$S_{1b}(E) = 2^{-1/2}(r_2 - r_3),$$

$$S_{2b}(E) = 2^{-1/2} R(\alpha_2 - \alpha_3),$$

$$S_{3b}(E) = 2^{-1/2} (RD)^{1/2} (\gamma_2 - \gamma_3).$$

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ZXY ₃	$F_{11}(A_1)$	$F_{12}(A_1)$	$F_{13}(A_1)$	$F_{22}(A_1)$	$F_{23}(A_1)$	$F_{33}(A_1)$	fre- quencies	References structural data
OPF ₃	7.4210	0.2709	0.0875	11.8329	-0.1335	0.6240	7	11, 12
OPCl ₃	3.5053	0.0522	0.1073	10.0661	-0.0658	0.3153	8	11, 13
OPBr ₃	3.3046	0.0173	0.1510	9.7296	-0.0482	0.2229	8	11
OVF ₃	5.4011	0.0767	0.0098	7.8041	-0.0185	0.2381	7	1,56 Å; 1,86 Å; 109° ^a
OVCl ₃	3.0422	0.0106	0.0152	7.6040	-0.0133	0.1572	8	11
OVBr ₃	2.6214	0.0012	0.0392	7.4828	-0.0147	0.1350	8	1,56 Å; 2,36 Å; 112° ^a
ClReO ₃	9.1352	0.0025	-0.0012	1.5902	-0.0104	0.5992	9	11
BrReO ₃	9.0941	0.0033	-0.0010	1.3635	-0.0104	0.3838	9	2,42 Å; 1,70 Å; 109° ^a
SPO ₃ ²⁻	6.9025	0.1072	0.0156	2.8149	-0.3043	0.7129	8	14 ^b
HPO ₃ ²⁻	7.6252	-0.0075	0.0727	3.0970	-0.0045	0.7529	8	14
FPO ₃ ²⁻	7.4087	0.3157	0.1452	4.7818	-0.2158	0.7743	8	14
HOP ₃ ²⁻	7.2691	0.9808	0.1891	5.5507	-0.1915	0.7657	8	14
SSO ₃ ²⁻	7.5571	0.1370	0.0463	2.9498	-0.2705	0.8578	8	14
HSO ₃ ⁻	8.5723	0.0496	0.0960	3.9345	-0.0223	0.9526	8	14
FSO ₃ ⁻	8.7284	0.0914	0.1332	4.6595	-0.2983	0.8977	8	14
ClSO ₃ ⁻	8.5101	0.0398	-0.0286	2.7528	-0.3561	0.5418	8	14
HOSO ₃ ⁻	8.2066	0.5346	0.2077	5.5977	-0.2495	0.9742	8	14
HOS ₃ ⁻	6.4072	0.0850	0.0171	4.6411	-0.0184	0.5118	8	14
SReO ₃ ⁻	8.0423	-0.0031	0.0016	4.0378	-0.0110	0.4014	8	14
FCrO ₃ ⁻	6.9060	0.0329	0.0194	3.3730	-0.0354	0.3579	8	1,53 Å; 1,53 Å; 109.5° ^a
ClCrO ₃ ⁻	6.9102	-0.0311	0.0097	2.3727	-0.0903	0.2509	8	14
NOSO ₃ ⁻	7.4245	0.0403	0.0007	7.9661	-0.0068	0.3935	8	1,58 Å; 1,75 Å; 109.5° ^a
FCIO ₃	8.6437	-0.0376	0.0875	3.9221	-0.3038	0.8491	8	14
HOCIO ₃	8.1621	-0.0020	0.1109	3.9372	-0.2953	0.9162	8	14
FSiH ₃	2.8525	0.0021	-0.0019	5.5564	-0.0903	0.2444	10	10
ClSiH ₃	2.8411	0.0033	-0.0004	3.0233	-0.0112	0.2003	10	10
BrSiH ₃	2.8387	0.0032	-0.0003	2.4723	-0.0081	0.1854	10	10
ISiH ₃	2.8183	0.0027	-0.0002	1.9480	-0.0059	0.1652	10	10
HSiF ₃	6.5981	-0.0050	0.0566	3.0666	-0.0036	0.4434	10	10
HSiCl ₃	3.4043	-0.0015	0.0835	2.9205	-0.0028	0.2397	10	10
HSiBr ₃	3.1643	-0.0055	0.1445	2.8644	-0.0025	0.1691	10	10
FSiCl ₃	3.6585	0.1275	0.0536	5.3458	-0.0583	0.2072	10	10
BrSiCl ₃	4.0313	0.4028	0.0883	2.3638	-0.1835	0.2211	10	10
ClSiBr ₃	2.9537	0.2461	0.1190	2.9452	-0.1070	0.1895	10	10
ISiCl ₃	3.6506	0.3485	0.0649	2.2625	-0.1964	0.1864	10	10
ClSiI ₃	2.3158	0.1663	0.1147	2.7594	-0.0679	0.1307	10	10
ISiBr ₃	4.5306	0.3209	0.1011	1.3487	-0.1666	0.1574	10	10
FG ₃ H ₃	2.6591	0.0003	-0.0001	4.2990	-0.0043	0.1953	10	10
ClG ₃ H ₃	2.6567	-0.0016	-0.0004	2.5420	-0.0011	0.1701	10	10
BrG ₃ H ₃	2.6435	-0.0164	-0.0080	2.3600	-0.1941	0.1613	10	10
IG ₃ H ₃	2.6317	-0.0012	-0.0011	1.7208	-0.0018	0.1394	10	10
HGeCl ₃	2.9613	0.0206	0.0108	2.7304	-0.0009	0.1935	10	10
HGeBr ₃	2.4848	-0.0014	0.0395	2.6225	-0.0006	0.1547	10	10
ClGeBr ₃	2.5719	0.0793	0.0340	2.4380	-0.0321	0.1445	10	10
BrSnCl ₃	2.5697	0.0396	0.0064	2.1475	-0.0159	0.1007	10	10
ClSnBr ₃	2.2475	0.0275	0.0142	2.2453	-0.0132	0.1251	10	10
BrTiCl ₃	2.9991	0.2891	0.0279	2.2677	-0.0479	0.1035	10	10
ClTiBr ₃	2.5824	0.1455	0.0362	2.5194	-0.0359	0.1020	10	10

Table 1a. Symmetry force constants for species A_1 (in $\text{myn}/\text{\AA}$).^a Estimated values, in the order d_{X-Z} , d_{X-Y} , angle $Y-X-Y$. ^b Angles assumed to be tetrahedral for all the following ions and molecules (the frequencies of Ref.¹⁰ have not been corrected for anharmonicities. This has been done by NAGARAJAN in a physically unreasonable way (see^{10,14})).

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ZXY ₃	F_{44} (E)	F_{45} (E)	F_{46} (E)	F_{55} (E)	F_{56} (E)	F_{66} (E)
OPF ₃	5.8924	— 0.0492	0.1181	0.4113	0.0017	0.7121
OPCl ₃	2.7457	— 0.0630	0.1498	0.2518	0.0063	0.3643
OPBr ₃	2.4832	— 0.0915	0.1472	0.1759	0.0106	0.2650
OVF ₃	4.7718	— 0.0070	0.0153	0.1510	0.0002	0.2903
OVC1 ₃	2.6042	— 0.0164	0.0322	0.1029	0.0017	0.2111
OVBr ₃	2.2656	— 0.0327	0.0519	0.0821	0.0033	0.1643
ClReO ₃	7.8090	— 0.0002	0.0014	0.4154	— 0.0019	0.1879
BrReO ₃	7.8325	0.0001	0.0011	0.3813	— 0.0014	0.1553
SPO ₃ ²⁻	5.6993	— 0.1038	0.0537	0.7944	0.0035	0.4984
HPO ₃ ²⁻	6.2890	— 0.0711	0.1498	0.6232	0.0073	0.3801
FPO ₃ ²⁻	6.8917	— 0.0918	— 0.0490	0.7896	0.0033	0.4536
HOPO ₃ ²⁻	6.2168	— 0.1033	0.0507	0.8182	0.0030	0.4577
SSO ₃ ²⁻	6.6138	— 0.1009	0.0397	0.8552	0.0023	0.4237
HSO ₃ ⁻	7.7792	— 0.0831	0.1694	0.7624	0.0081	0.4552
FSO ₃ ⁻	8.9817	— 0.1141	0.0513	1.0294	0.0026	0.5347
ClSO ₃ ⁻	7.7783	— 0.1164	0.0143	1.0119	0.0008	0.1778
HOSO ₃ ⁻	7.7501	— 0.1272	0.0578	1.0416	0.0030	0.5621
HOSSeO ₃ ⁻	6.1997	— 0.0077	0.0056	0.5026	— 0.0001	0.3516
SReO ₃ ⁻	6.7006	— 0.0001	0.0028	0.3262	— 0.0053	0.2843
FCrO ₃ ⁻	5.9542	— 0.0155	0.0075	0.4236	0.0002	0.2203
ClCrO ₃ ⁻	5.9932	— 0.0145	0.0052	0.4119	0.0001	0.1729
NOSO ₃ ⁻	6.4109	0.0000	0.0019	0.4752	— 0.0032	0.3071
FCIO ₃	9.8175	— 0.0936	0.0403	1.0380	0.0016	0.5321
HOCIO ₃	8.5458	— 0.0950	0.0456	0.9918	0.0017	0.5769
FSiH ₃	2.7306	0.0013	0.0032	0.1940	— 0.0138	0.2834
ClSiH ₃	2.7286	0.0001	0.0016	0.1998	— 0.0083	0.1956
BrSiH ₃	2.7312	0.0001	0.0013	0.1988	— 0.0067	0.1681
ISiH ₃	2.7563	0.0001	0.0010	0.1959	— 0.0050	0.1343
HSiF ₃	5.5612	— 0.0454	0.0544	0.3074	0.0021	0.2573
HSiCl ₃	2.8061	— 0.0498	0.0100	0.1835	0.0013	0.1667
HSiBr ₃	2.3122	— 0.0896	0.0036	0.1561	0.0011	0.1475
FSiCl ₃	4.4170	— 0.0493	0.0799	0.1686	0.0060	0.2811
BrSiCl ₃	2.8078	— 0.0368	0.1058	0.1107	0.0010	0.3038
	2.7982	— 0.0717	0.0456	0.2383	0.0071	0.1413
ClSiBr ₃	2.4154	— 0.0700	0.1246	0.1260	0.0097	0.2360
ISiCl ₃	2.7226	— 0.0300	0.1042	0.0908	— 0.0000	0.3032
ClSiI ₃	1.8249	— 0.0688	0.0940	0.1002	0.0096	0.1531
ISiBr ₃	2.3543	— 0.0485	0.1286	0.0808	0.0033	0.2176
	2.3410	— 0.1060	0.0532	0.1874	0.0070	0.0941
FGeH ₃	2.6502	— 0.0001	0.0009	0.1696	— 0.0134	0.2274
ClGeH ₃	2.6427	— 0.0000	0.0007	0.1703	— 0.0095	0.1679
BrGeH ₃	2.6378	0.0000	0.0006	0.1697	— 0.0079	0.1465
IGeH ₃	2.6230	0.0000	0.0005	0.1633	— 0.0068	0.1238
HGeCl ₃	2.4235	— 0.0105	— 0.0000	0.1433	0.0001	0.1320
HGeBr ₃	2.0101	— 0.0292	— 0.0005	0.1179	0.0002	0.1156
ClGeBr ₃	1.9836	— 0.0283	0.0368	0.1084	0.0035	0.1579
BrSnCl ₃	2.3135	— 0.0016	0.0055	0.0566	— 0.0001	0.1470
ClSnBr ₃	1.9199	— 0.0093	0.0149	0.0706	0.0008	0.1264
BrTiCl ₃	2.5578	— 0.0113	0.0233	0.0701	0.0005	0.1439
ClTiBr ₃	2.1902	— 0.0316	0.0379	0.0864	0.0046	0.1227

Table 1 b. Symmetry force constants for species *E* (in mdyne/Å).

II. Force Constants

The symmetry force constants calculated according to the "Kopplungsstufenverfahren" of FADIN^{15,6,8} are given in Tables 1 and 2. The force constants with respect to internal coordinates are not listed, because they are not necessary for the calculation of the amplitudes of vibration. The values obtained from the "Kopplungsstufenverfahren" are the better, the more characteristic the vibrations

are. But, in any case, the accuracy of the *F* values is good enough for the calculation of reliable amplitudes of vibration.

III. Mean Amplitudes of Vibration

The mean amplitudes of vibration have been calculated from the force constants as usual¹, employing a suitable computer program. The values for

ZXY ₂ (C _{2v})	F ₁₁ (A ₁)	F ₁₂ (A ₁)	F ₁₃ (A ₁)	F ₂₂ (A ₁)	F ₂₃ (A ₁)	F ₃₃ (A ₁)	F ₄₄ (B ₁)	F ₄₅ (B ₁)	F ₅₅ (B ₁)	References fre- quencies	structural data
OCH ₂	4.3205	—	0.0417	12.0516	0.4241	1.1712	4.2122	0.0038	0.5925	8	15
OC ₂ D ₂	4.4022	0.3015	—	12.2027	0.1716	1.1976	4.3025	0.0200	0.6188	8	15
HCO ₂ ⁻	11.2122	—	0.0501	4.3265	0.0425	3.0090	7.3388	0.3362	0.4814	8	15
DCO ₂ ⁻	11.3447	0.0272	—	4.4160	0.1127	3.0376	7.0965	0.1849	0.4782	8	15
OCO ₂ ⁻ (unident.)	10.4421	1.8784	—	6.4575	0.9791	3.4030	6.7457	0.5469	0.9522	14	15
OCO ₂ ⁻ (bident.)	8.4774	1.3315	—	9.8812	1.1004	3.5395	5.1096	0.5663	0.8928	14	15
OCF ₂	7.7108	1.1301	—	14.1936	0.6749	2.7086	5.5169	0.5602	0.7753	8	15
OCCL ₂	3.7659	0.4611	—	13.1326	0.2746	1.3427	3.2149	0.4191	0.4062	8	15
OCBr ₂	3.0868	0.4141	—	13.3390	0.2112	1.2558	2.9865	0.3394	0.2677	8	15
SCF ₂	5.9638	1.6175	—	9.5236	0.8296	1.7696	4.9530	0.2892	0.4523	8	15
SCCl ₂	3.8469	0.9837	—	6.5812	0.2035	0.4880	2.7859	0.2698	0.2954	8	1,63 Å; 1,32 Å; 112° ^a
FCIF ₂	2.4001	0.3222	—	3.8007	0.1029	1.0568	3.4472	0.1266	0.4322	8	15
FBrF ₂	2.6928	0.1455	—	3.7600	0.0245	0.9561	3.2074	0.0284	0.4005	14	15
HONO ₂	10.7291	0.5967	—	4.7530	0.5920	1.8923	8.7011	0.4305	1.0717	8	1,40 Å; 1,22 Å; 135° ¹⁶
DONO ₂	10.7138	0.5074	—	4.9876	0.8741	2.3315	8.4546	0.3101	0.8066	14	1,40 Å; 1,22 Å; 135° ¹⁶
(CH ₃)NO ₂	11.1841	0.5762	—	4.6008	0.6051	2.1205	7.9930	0.1820	0.4915	8	15
PN ₂ O ₂	10.5872	0.5158	—	4.0241	0.2834	1.1037	10.3615	0.2966	0.7612	8	15
ClNO ₂	10.2986	0.0703	—	4.9349	0.3181	0.7662	9.2358	0.1307	0.3638	8	15

Table 2. Symmetry force constants (in mdyn/Å). ^a Estimated, in the order d_{X-Z}, d_{X-Y}, angle Y-X-Y.

0° and 298,2°K are given in Tables 3 and 4. For the reason given above they are believed to be more reliable than previously published ones, for instance the calculations of NAGARAJAN et. al.^{14, 15a} (see also¹ where other incorrect values for Ge and Si compounds are cited).

IV. Coriolis Coupling Constants

The band contours in the infrared spectra of gaseous compounds are essentially dependent on the Coriolis coupling constants. In the case of symmetrical top molecules and especially for spherical top compounds the ζ values can be obtained from the contours.

We have calculated type E × E ζ values for the molecules ZXY₃ according to the method of MEAL and POLO¹⁷:

$$\zeta^\alpha = L^{-1} \cdot C^\alpha \cdot (L^{-1})'. \quad (3)$$

However, only the physically interpretative diagonal elements of the ζ matrices are given (Table 4). They effect the band contours of the corresponding vibrations. In the present case the sum rule is

$$\zeta_4 + \zeta_5 + \zeta_6 = I_A/2 I_B.$$

It should be realized that reliable ζ values can only be calculated from force constants or eigenvectors L if the latter are accurate enough, because Coriolis coupling constants are strongly dependent on the force constants, contrary to the mean amplitudes of vibration.

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ZXY ₃	ζ_{44}	ζ_{55}	ζ_{66}	$T = 0$				$T = 298.2^\circ\text{K}$			
				u_{X-Y}	u_{X-Z}	$u_{Y...Y}$	$u_{Y...Z}$	u_{X-Y}	u_{X-Z}	$u_{Y...Y}$	$u_{Y...Z}$
OPF ₃	0.57	— 0.61	0.55	0.0385	0.0339	0.060	0.054	0.0390	0.0340	0.069	0.058
OPCl ₃	0.75	— 0.71	0.64	0.0428	0.0353	0.060	0.058	0.0464	0.0354	0.085	0.068
OPBr ₃	0.86	— 0.80	0.78	0.0407	0.0357	0.051	0.059	0.0464	0.0359	0.090	0.077
OVF ₃	0.39	— 0.48	0.68	0.0394	0.0364	0.072	0.065	0.0404	0.0366	0.098	0.079
OVCl ₃	0.58	— 0.57	0.74	0.0411	0.0366	0.068	0.067	0.0459	0.0369	0.112	0.090
OVBr ₃	0.76	— 0.71	0.82	0.0384	0.0368	0.058	0.067	0.0465	0.0371	0.119	0.097
ClReO ₃	0.13	— 0.34	0.46	0.0343	0.0432	0.060	0.067	0.0346	0.0550	0.068	0.091
BrReO ₃	0.13	— 0.32	0.33	0.0343	0.0382	0.061	0.066	0.0346	0.0571	0.070	0.099
SPO ₃ ³⁻	0.61	— 0.67	0.35	0.0401	0.0439	0.057	0.059	0.0405	0.0479	0.061	0.067
HPO ₃ ²⁻	0.72	— 0.62	0.77	0.0392	0.0862	0.058	0.109	0.0395	0.0862	0.063	0.109
HPO ₃ ²⁻	0.57	— 0.64	0.53	0.0386	0.0414	0.056	0.060	0.0389	0.0423	0.060	0.067
HOPO ₃ ²⁻	0.60	— 0.66	0.54	0.0394	0.0409	0.056	0.060	0.0398	0.0415	0.059	0.067
SSO ₃ ²⁻	0.58	— 0.66	0.35	0.0387	0.0429	0.056	0.059	0.0390	0.0467	0.059	0.069
HSO ₃ ⁻	0.71	— 0.61	0.77	0.0373	0.0812	0.055	0.103	0.0375	0.0812	0.059	0.104
FSO ₃ ⁻	0.56	— 0.63	0.50	0.0363	0.0416	0.053	0.058	0.0364	0.0426	0.055	0.064
ClSO ₃ ⁻	0.57	— 0.66	0.33	0.0373	0.0440	0.055	0.066	0.0375	0.0485	0.058	0.087
HOSO ₃ ⁻	0.59	— 0.66	0.53	0.0374	0.0405	0.053	0.058	0.0377	0.0411	0.056	0.063
HOSeO ₃ ⁻	0.30	— 0.43	0.60	0.0376	0.0400	0.061	0.064	0.0381	0.0411	0.068	0.074
SReO ₃ ⁻	0.13	— 0.33	0.51	0.0357	0.0351	0.063	0.062	0.0360	0.0384	0.074	0.077
FCrO ₃ ⁻	0.38	— 0.48	0.57	0.0384	0.0433	0.063	0.069	0.0389	0.0454	0.071	0.086
ClCrO ₃ ⁻	0.37	— 0.49	0.35	0.0384	0.0426	0.063	0.069	0.0388	0.0485	0.072	0.093
NOSO ₃ ⁻	0.14	— 0.31	0.73	0.0360	0.0356	0.061	0.065	0.0366	0.0359	0.069	0.076
FCIO ₃	0.52	— 0.60	0.49	0.0354	0.0431	0.053	0.053	0.0356	0.0446	0.056	0.065
HOClO ₃	0.54	— 0.62	0.51	0.0365	0.0439	0.054	0.059	0.0367	0.0452	0.056	0.065
FSiH ₃	0.06	— 0.33	0.35	0.0888	0.0404	0.150	0.117	0.0888	0.0409	0.151	0.119
ClSiH ₃	0.06	— 0.32	0.30	0.0888	0.0431	0.150	0.125	0.0888	0.0461	0.151	0.128
BrSiH ₃	0.06	— 0.32	0.28	0.0888	0.0422	0.150	0.127	0.0888	0.0476	0.151	0.132
ISiH ₃	0.06	— 0.31	0.27	0.0887	0.0435	0.151	0.132	0.0887	0.0516	0.152	0.139
HSiF ₃	0.63	— 0.62	0.86	0.0397	0.0865	0.063	0.115	0.0402	0.0865	0.075	0.117
HSiCl ₃	0.98	— 0.74	0.70	0.0432	0.0876	0.062	0.125	0.0464	0.0876	0.090	0.129
HSiBr ₃	0.99	— 0.85	0.82	0.0421	0.0880	0.053	0.127	0.0476	0.0880	0.094	0.134
FSiCl ₃	0.70	—	—	0.0395	0.0407	0.062	0.062	0.0416	0.0413	0.092	0.078
BrSiCl ₃	0.70	—	—	0.0429	0.0433	0.066	0.053	0.0460	0.0502	0.106	0.077
	0.73	—	—	0.0430	0.0433	0.059	0.059	0.0460	0.0502	0.082	0.097
ClSiBr ₃	0.85	—	—	0.0419	0.0437	0.054	0.056	0.0477	0.0471	0.100	0.084
ISiCl ₃	0.70	—	—	0.0435	0.0429	0.069	0.052	0.0467	0.0510	0.115	0.078
ClSiI ₃	0.89	—	—	0.0437	0.0443	0.051	0.059	0.0528	0.0480	0.112	0.099
ISiBr ₃	0.83	—	—	0.0414	0.0487	0.057	0.049	0.0463	0.0648	0.118	0.087
	0.84	—	—	0.0414	0.0487	0.050	0.055	0.0463	0.0648	0.087	0.114
FGeH ₃	0.02	— 0.31	0.35	0.0893	0.0401	0.154	0.122	0.0893	0.0415	0.156	0.125
ClGeH ₃	0.02	— 0.30	0.31	0.0893	0.0407	0.154	0.128	0.0893	0.0464	0.156	0.134
BrGeH ₃	0.02	— 0.30	0.29	0.0894	0.0379	0.155	0.128	0.0894	0.0477	0.156	0.134
IGeH ₃	0.02	— 0.30	0.28	0.0895	0.0380	0.155	0.134	0.0895	0.0517	0.157	0.143
HGeCl ₃	0.46	— 0.56	0.99	0.0405	0.0886	0.066	0.130	0.0461	0.0886	0.102	0.137
HGeBr ₃	0.66	— 0.71	0.99	0.0376	0.0895	0.056	0.132	0.0476	0.0895	0.109	0.142
ClGeBr ₃	0.69	—	—	0.0376	0.0411	0.057	0.060	0.0477	0.0472	0.111	0.099
BrSnCl ₃	0.32	—	—	0.0400	0.0356	0.076	0.062	0.0468	0.0468	0.146	0.107
ClSnBr ₃	0.55	—	—	0.0361	0.0406	0.061	0.063	0.0481	0.0480	0.132	0.104
BrTiCl ₃	0.55	—	—	0.0417	0.0395	0.073	0.062	0.0464	0.0478	0.133	0.104
ClTiBr ₃	0.75	—	—	0.0391	0.0424	0.059	0.063	0.0472	0.0476	0.122	0.109

Table 3. Coriolis coupling constants of the type $E \times E$ and mean amplitudes of vibration (in Å); where the ζ_{55} and ζ_{66} values are not given these cannot be calculated with enough accuracy. In these cases the $u_{Y...Y}$ and $u_{Y...Z}$ are also not very accurate (see text).

ZXY ₂	$T = 0$				$T = 298.2^\circ$			
	u_{X-Y}	u_{X-Z}	$u_{Y...Y}$	$u_{Y...Z}$	u_{X-Y}	u_{X-Z}	$u_{Y...Y}$	$u_{Y...Z}$
OCH ₂	0.0805	0.0377	0.121	0.096	0.0805	0.0377	0.121	0.096
OCD ₂	0.0686	0.0375	0.100	0.082	0.0686	0.0375	0.100	0.083
HCO ₂ ⁻	0.0408	0.0802	0.048	0.096	0.0409	0.0802	0.049	0.096
DCO ₂ ⁻	0.0407	0.0683	0.048	0.083	0.0408	0.0683	0.049	0.083
OCO ₂ ²⁻	0.0421	0.0451	0.047	0.050	0.0422	0.0454	0.048	0.051
(unident.)								
OCO ₂ ²⁻	0.0446	0.0400	0.049	0.050	0.0448	0.0401	0.050	0.051
(bident.)								
OCF ₂	0.0434	0.0362	0.051	0.048	0.0436	0.0362	0.053	0.050
OClCl ₂	0.0480	0.0368	0.054	0.052	0.0498	0.0369	0.068	0.058
OCB ₂	0.0474	0.0367	0.046	0.052	0.0506	0.0368	0.071	0.062
SCF ₂	0.0453	0.0383	0.053	0.049	0.0457	0.0385	0.056	0.053
SClCl ₂	0.0491	0.0416	0.059	0.052	0.0509	0.0420	0.083	0.065
FCIF ₂	0.0466	0.0435	0.070	0.059	0.0493	0.0450	0.085	0.064
FBrF ₂	0.0438	0.0412	0.071	0.059	0.0468	0.0432	0.088	0.066
HONO ₂	0.0389	0.0463	0.048	0.052	0.0390	0.0469	0.049	0.054
DONO ₂	0.0391	0.0458	0.047	0.053	0.0391	0.0463	0.048	0.055
(CH ₃)NO ₂	0.0393	0.0473	0.048	0.057	0.0394	0.0478	0.049	0.060
FNO ₂	0.0379	0.0472	0.052	0.055	0.0380	0.0481	0.055	0.059
ClNO ₂	0.0387	0.0425	0.053	0.055	0.0388	0.0434	0.056	0.063

Table 4. Mean amplitudes of vibration (in Å).