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THEORETICAL VIBRATIONAL SPECTRA COMPARED TO THE EXPERIMENT AND THE ANOMERIC EFFECT IN 2-CHLORO-1,3,2-DIOXAPHOSPHORINANE-2-OXIDE, -SULFIDE, AND -SELENIDE. II. VIBRATIONAL SPECTRA AND ASSIGNMENTS

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2-Chloro-1,3,2-dioxaphosphorinane-2-oxide, -sulfide, and -selenide are studied with the help of DFT/B3LYP and several *ab initio* methods using a 6-311G** basis set. However, due to rather large relative energies of higher conformers in all three cases, the conformational equilibrium mixture contains more than 95 % (see the preceding paper in this Journal) of the lowest *chair*-equatorial conformer (this indicates that the P=X bond is in the equatorial position), so we do not find any conformer bands in the experimental spectra and calculate our theoretical ones for the assignment only from the *chair*-equatorial conformer. The vibrational infrared and Raman spectra were calculated and are in fair agreement with their experimental counterparts. Potential energy distribution calculations are performed, and the theoretical modes where an experimental counterpart could be found to symmetry coordinates are assigned.

Keywords: vibrational spectra, 2-chloro-1,3,2-dioxaphosphorinane-2-oxide, -sulfide, and -selenide, DFT/B3LYP, 6-311G** basis set.

We are very much interested in the structural and spectroscopic (vibrational infrared (IR) and Raman) spectra of five- and six-membered heterocycles containing oxygen, sulfur, and/or phosphorus atoms. The details of our previous studies and the other literature data [1—22] are described in our preceding paper, so we refer the reader to our previous paper for them.

AB INITIO, DFT AND PED (POTENTIAL ENERGY DISTRIBUTION) CALCULATIONS

The Gaussian98 program [23] running on an IBM RS/6000 model S85 Unix server was used to carry out DFT/B3LYP and MP2 calculations using a 6-311G** basis set. We optimized the possible stationary structures (see our previous paper for details).

In order to obtain vibrational spectra, we used the Gaussian98 program that uses the harmonic approximation for the calculation of frequencies, scattering activities, depolarization factors, IR intensities, and normal modes. We converted these informations into plots of theoretical IR and Raman spectra following the formalism given in [24]. The experimental spectra in the form of observed wavenumbers and relative intensities are given in [17, 18], and we compared our theoretical spectral information to those. To assign the symmetry coordinates to normal modes, we used a program written by one of us (WF; see [24] for the formalism in some detail), which performs potential energy distribution (PED) calculations following Wilson et al. [25]. The program allows the use of an overcomplete set of internal coordinates for defining the symmetry coordinates that are easier to set up with the help of some redundant internal coordinates. However, the program detects which of the internal coordinates are actually redundant and deletes them both from the internal and the symmetry coordinate lists before calculating to what percentage any given symmetry coordinate takes part in the potential energies of the normal modes. These results allow us to assign completely the normal modes to the

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symmetry coordinates involved, also in the cases of large amounts of mixing of different symmetry coordinates in the same normal mode. Our assignment and even the symmetries of some of normal modes differ from those given in [17, 18], but we are convinced that our results are more reliable because they are based on DFT and PED calculations rather than on a simple force-field calculation and widely assumed geometries, as in [17, 18].

EQUILIBRIUM MIXTURE

The result of our calculations is that for all three molecules the most stable conformer is the *chair*-equatorial (equatorial refers to the position of the P=X bond) one, with the next higher *chair*-axial conformer being more than 2 kcal/mol higher in energy (according to our DFT calculations); only in MP2 for the selenide it is only 1.3 kcal/mol higher in energy. Therefore only for these two conformers and with DFT we showed that they are global minima on the potential energy hypersurface by a frequency calculation (harmonic approximation) to be sure that all vibrational frequencies are real. The relative free energies (273.15 K, 1 atm) of the *chair*-axial conformers are 2.66 kcal/mol for the oxide, 2.08 kcal/mol for the sulfide, and 2.01 kcal/mol for the selenide (DFT). Thus, in a conformational equilibrium mixture of these two conformers, there would be 98.9 % of the *chair*-equatorial conformer for the oxide, 97.1 % for the sulfide, and 96.8 % for the selenide. This agrees with the experimental results [17, 18], where no vibrational spectral lines of increasing intensity with increasing temperature could be found, and thus it was concluded that there exists no conformational equilibrium mixture. So, in the spectra calculations, we used the *chair*-equatorial conformer alone.

VIBRATIONAL INFRARED (IR) AND RAMAN SPECTRA AND ASSIGNMENTS

The overcomplete set of used internal coordinates are given in Table 3, while the symmetry coordinates are listed in Table 4 of our preceding paper. Note that our program removes automatically redundant internal coordinates from both sets of coordinates. The most obvious result from our PED calculations is that just as in the five-membered system, ring puckering (symmetry coordinates S_{19} and S_{20}) and ring twisting (S_{36}) are in all three molecules completely decoupled, as it should be, because they belong to different irreducible representations. This indicates that also in this case no pseudorotational movement exists because that would require a coupling between twisting and puckering. In the case of the oxide (Table 1), the puckering coordinates contribute to the vibration with the lowest wavenumber, i.e. 102 cm^{-1} , with 36 % S_{20} and 13 % S_{19} .

Further, S_{20} mixes into the mode at 253 cm^{-1} to 31 % and into that at 325 cm^{-1} to 15 %. The puckering also shows up at 377 cm^{-1} to 29 % S_{19} and at 582 cm^{-1} to 13 % S_{20} . None of those lines has very large intensities in both spectra (IR and Raman). On the other hand ring twisting appears at 152 cm^{-1} to 67 % and at 284 cm^{-1} to 31 % in both cases mixed with PXCl twisting. As in the case of the sulfide (Table 1), the puckering coordinates contribute again to the vibration with the lowest wavenumber, i.e. 102 cm^{-1} , with 50 % S_{20} and 14 % S_{19} .

Further, both puckering coordinates mix into the mode at 294 cm^{-1} to 33 % S_{20} and 20 % S_{19} while in that at 362 cm^{-1} only S_{19} of the puckering coordinates appears to 39 %. Again none of those lines has very large intensities in both spectra (IR and Raman). On the other hand ring twisting appears at 148 cm^{-1} to 52 %, at 224 cm^{-1} to 17 % and at 302 cm^{-1} to 27 % in all cases mixed with PXCl wag and twist. In the selenide (Table 1), the two puckering coordinates appear together at 100 cm^{-1} to 59 % S_{20} and 12 % S_{19} and at 290 cm^{-1} to 24 % S_{20} and 11 % S_{19} . At 295 cm^{-1} S_{20} shows up, but only to 15 %, while at 362 cm^{-1} S_{19} appears with 49 %. Apart from the 295 cm^{-1} mode in the Raman spectrum, they all have again fairly low intensities. Twisting appears at 138 cm^{-1} to 50 %, at 191 cm^{-1} to 23 %, and at 300 cm^{-1} to 26 %, mostly heavily mixed with PXCl wag and twist.

As the tables show, almost all wavenumbers in the experimental spectra are reproduced by our DFT spectra to an accuracy of better than 10 % error. Only the lowest wavenumber (not observed in the oxide) has larger errors in the wavenumbers, of 17 % in the sulfide and of 25 % in the selenide. The reason for such large errors is obviously that the spectra are calculated in the harmonic approximation, while the high contribution of ring puckering leads to large anharmonicities due to its double

Table 1

Symmetry species, s , theoretical wavenumbers, k (cm^{-1}), experimental wavenumbers, k_e (cm^{-1}) [17], error percentage, e (%), infrared intensities, I ($\text{km}\cdot\text{mol}^{-1}$), Raman activities A ($\text{\AA}^4\cdot\text{amu}^{-1}$), depolarization ratios ρ , as calculated with the DFT/B3LYP method in a 6-311G** basis set, and the potential energy distribution among the symmetry coordinates, PED (only those larger than 10% are given), calculated with our program for chair-equatorial 2-chloro-1,3,2-dioxaphosphorinane-2-oxide (liquid Raman data from [17]; no.-s in brackets are relative intensities), 2-chloro-1,3,2-dioxaphosphorinane-2-sulfide (liquid Raman data from [17]; no.-s in brackets are relative intensities), and 2-chloro-1,3,2-dioxaphosphorinane-2-selenide (liquid infrared data from [18]). Note that only theoretical lines with experimental counterparts are listed

s	k	k_e	e	I	A	ρ	PED
1	2	3	4	5	6	7	8
<i>chair-equatorial 2-chloro-1,3,2-dioxaphosphorinane-2-oxide</i>							
A'	253	269 (3)	5.9	2.5	2.1	0.69	56% S_{16} , 31% S_{20}
A''	284	298 (1)	4.7	0.0	0.8	0.75	63% S_{31} , 31% S_{36}
A'	325	341 (2)	4.7	0.1	2.9	0.45	39% S_{19} , 22% S_{16} , 15% S_{20} , 11% S_6 , 10% S_{17}
A''	341	355 (sh)	3.9	6.9	0.6	0.75	69% S_{30} , 23% S_{35}
A'	377	403 (6)	6.5	1.1	7.1	0.34	48% S_6 , 29% S_{19} , 12% S_{17}
A'	432	442 (5)	2.3	3.4	2.9	0.75	63% S_{21} , 19% S_{17}
A'	523	555 (5)	5.8	210.0	6.8	0.04	38% S_6 , 32% S_{17}
A'	582	590 (0)	1.4	16.9	0.3	0.72	43% S_{18} , 26% S_{15} , 13% S_{20} , 11% S_{11}
A'	738	754(10)	2.1	97.8	17.5	0.07	74% S_9 , 14% S_8
A''	811	825 (0)	1.7	123.4	0.1	0.75	66% S_{34} , 17% S_{33}
A'	867	878 (1)	1.3	26.4	2.7	0.43	69% S_8 , 10% S_9
A'	943	935 (1)	1.1	69.5	2.8	0.35	32% S_{18} , 26% S_7 , 24% S_{15} , 11% S_{11}
A''	970	976 (0)	0.6	69.5	2.2	0.75	32% S_{33} , 31% S_{32} , 13% S_{34}
A''	1051	1042 (1)	0.9	1.2	2.2	0.75	62% S_{32} , 20% S_{33} , 14% S_{28}
A'	1085	1060 (sh)	2.4	294.8	5.5	0.74	67% S_7 , 14% S_{15}
A'	1154	1141 (1)	1.1	8.0	1.1	0.32	70% S_{11} , 14% S_{15}
A''	1249	1239 (1)	0.8	0.7	0.6	0.75	39% S_{29} , 35% S_{27} , 18% S_{25}
A''	1257	1280 (1)	1.8	18.0	9.0	0.75	36% S_{27} , 32% S_{29}
A'	1306	1305 (2)	0.1	3.3	9.6	0.73	92% S_{13}
A''	1404	1430 (1)	1.8	2.5	1.4	0.75	49% S_{26} , 21% S_{28} , 14% S_{29}
A'	1417	1468 (1)	3.5	1.5	3.5	0.54	94% S_{12}
A'	1469	1481 (1)	0.8	8.4	8.4	0.74	98% S_{14}
A'	3045	2913 (1)	4.5	10.2	115.5	0.15	99% S_4
A'	3063	2939 (1)	4.2	17.0	178.6	0.10	84% S_2 , 12% S_3
A''	3064	2965 (1)	3.3	21.4	20.6	0.75	97% S_{23}
A'	3089	2984 (1)	3.5	18.1	104.3	0.35	81% S_3 , 15% S_2
A''	3115	3015 (1)	3.3	6.9	67.7	0.75	97% S_{22}
<i>chair-equatorial 2-chloro-1,3,2-dioxaphosphorinane-2-sulfide</i>							
A'	102	123 (1)	17.1	3.0	1.3	0.75	50% S_{20} , 19% S_{18} , 18% S_{17} , 14% S_{19}
A''	148	163 (1)	9.2	0.5	1.9	0.75	52% S_{36} , 45% S_{31}
A'	192	205 (7)	6.3	2.7	7.6	0.72	91% S_{16}
A''	224	235 (2)	4.7	0.0	2.9	0.75	39% S_{30} , 30% S_{31} , 17% S_{36} , 11% S_{34}
A''	302	311 (2)	2.9	2.1	1.4	0.75	50% S_{30} , 27% S_{36} , 22% S_{31}
A'	362	381 (6)	5.2	4.7	9.2	0.25	39% S_6 , 39% S_{19} , 14% S_{21}

Table 1 (continued)

1	2	3	4	5	6	7	8
A'	388	399 (5)	2.8	6.5	8.4	0.48	34% S ₂₁ , 31% S ₁₇ , 19% S ₅
A''	424	422 (1)	0.5	9.1	2.5	0.75	86% S ₃₅
A'	459	495 (6)	7.3	127.4	9.3	0.02	42% S ₆ , 25% S ₂₁
A'	566	574 (0)	1.4	30.3	1.1	0.27	45% S ₁₈ , 26% S ₁₅
A'	672	687 (10)	2.2	133.8	25.0	0.11	33% S ₉ , 27% S ₅ , 12% S ₈ , 10% S ₁₇
A'	797	794 (1)	0.4	49.8	4.0	0.32	51% S ₉ , 33% S ₅
A'	875	835 (0)	4.8	83.1	3.8	0.17	75% S ₈
A''	898	885 (1)	1.5	8.7	0.2	0.75	60% S ₂₅ , 12% S ₃₃ , 11% S ₂₇
A'	951	941 (0)	1.1	213.9	2.5	0.75	31% S ₁₈ , 24% S ₇ , 23% S ₁₅
A''	953	959 (0)	0.6	60.8	0.6	0.75	37% S ₃₂ , 23% S ₃₃ , 14% S ₃₄ , 12% S ₂₅
A''	1047	1025 (1)	2.1	0.8	3.6	0.75	55% S ₃₂ , 24% S ₃₃ , 17% S ₂₈
A'	1071	1038 (1)	3.2	491.5	16.8	0.55	67% S ₇ , 15% S ₁₅
A'	1151	1136 (0)	1.3	5.9	1.0	0.33	70% S ₁₁ , 15% S ₁₅
A''	1246	1218 (0)	2.3	0.1	0.4	0.75	47% S ₂₇ , 27% S ₂₉ , 20% S ₂₅
A''	1255	1235 (1)	1.6	17.3	9.3	0.75	45% S ₂₉ , 23% S ₂₇
A'	1303	1275 (1)	2.2	2.8	10.6	0.74	93% S ₁₃
A''	1402	1426 (1)	1.7	1.7	1.4	0.75	43% S ₂₆ , 25% S ₂₈ , 14% S ₂₉
A'	1411	1463 (1)	3.6	10.5	1.8	0.73	96% S ₁₂
A'	1470	1475 (1)	0.3	8.2	9.6	0.74	98% S ₁₄
A'	3045	2903 (0)	4.9	11.5	124.9	0.16	99% S ₄
A''	3066	2934 (1)	4.5	22.3	30.5	0.75	97% S ₂₃
A'	3089	2958 (0)	4.4	20.4	121.2	0.32	81% S ₃ , 16% S ₂
A''	3118	2974 (1)	4.8	6.1	70.6	0.75	97% S ₂₂
A'	3121	3006 (1)	3.8	21.5	83.5	0.46	91% S ₁
A'	100	133(w)	24.8	3.4	1.5	0.75	59% S ₂₀ , 22% S ₁₇ , 12% S ₁₉
<i>chair-equatorial 2-chloro-1,3,2-dioxaphosphorinane-2-selenide</i>							
A''	138	152(w) ^a	9.2	0.9	1.5	0.75	50% S ₃₆ , 50% S ₃₁
A'	157	170(s)	7.6	2.6	5.1	0.67	93% S ₁₆
A''	191	205(w)	6.8	0.1	1.4	0.75	50% S ₃₀ , 23% S ₃₆ , 16% S ₃₁
A'	295	305(s)	3.3	4.4	13.1	0.15	33% S ₅ , 26% S ₂₁ , 17% S ₆ , 15% S ₂₀
A''	300	310(s)	3.2	1.7	1.0	0.75	43% S ₃₀ , 30% S ₃₁ , 26% S ₃₆
A'	362	385(m)	6.0	3.4	5.4	0.37	49% S ₁₉ , 32% S ₆
A''	422	420(m)	0.5	7.3	2.0	0.75	89% S ₃₅
A'	445	480(s)	7.3	89.3	8.1	0.04	43% S ₂₁ , 37% S ₆
A'	547	545(w)	0.4	99.9	0.7	0.26	20% S ₁₈ , 18% S ₁₅ , 14% S ₅ , 12% S ₁₇
A'	624	633(s)	1.4	114.3	6.3	0.13	31% S ₁₈ , 18% S ₅ , 14% S ₁₇
A'	755	760(w)	0.7	50.2	16.0	0.13	72% S ₉ , 13% S ₅
A''	774	792(m)	2.3	80.7	0.8	0.75	66% S ₃₄ , 22% S ₃₃
A'	869	875(s)	0.7	91.7	3.5	0.22	77% S ₈
A''	897	890(w)	0.8	13.0	0.1	0.75	59% S ₂₅ , 14% S ₃₃
A''	943	930(s)	1.4	49.3	0.4	0.75	37% S ₃₂ , 19% S ₃₃ , 16% S ₃₄ , 15% S ₂₅
A'	947	1030(s)	8.1	203.5	3.1	0.73	36% S ₁₈ , 30% S ₇ , 21% S ₁₅ , 10% S ₁₁
A''	1047	947(m)	10.6	0.5	3.9	0.75	52% S ₃₂ , 26% S ₃₃ , 17% S ₂₈
A'	1063	1055(s)	0.8	440.6	18.6	0.54	61% S ₇ , 20% S ₁₅

Table 1 (continued)

1	2	3	4	5	6	7	8
A'	1151	1132(w)	1.7	12.2	1.2	0.36	70% S ₁₁ , 12% S ₁₅
A''	1238	1231(w)	0.6	0.4	0.7	0.75	40% S ₂₇ , 35% S ₂₉ , 16% S ₂₅
A''	1258	1270(w)	1.0	17.1	8.7	0.75	36% S ₂₉ , 31% S ₂₇
A'	1303	1374(w) ^a	5.2	5.7	10.5	0.75	92% S ₁₃
A''	1381	1380(w) ^a	0.1	0.3	0.1	0.75	46% S ₂₆ , 41% S ₂₈
A''	1402	1420(w)	1.3	1.3	1.3	0.75	43% S ₂₆ , 25% S ₂₈ , 15% S ₂₉
A'	1410	1458(w)	3.3	13.1	1.5	0.73	96% S ₁₂
A'	1471	1473(w)	0.1	8.1	9.8	0.74	98% S ₁₄
A'	3045	2905(w)	4.8	14.2	164.9	0.11	97% S ₄
A'	3051	2935(w)	4.0	23.7	116.0	0.14	73% S ₂ , 17% S ₁
A'	3092	2970(w)	4.1	21.7	94.5	0.44	90% S ₃ , 10% S ₂
A'	3132	3005(w)	4.2	13.2	141.5	0.25	81% S ₁ , 16% S ₂

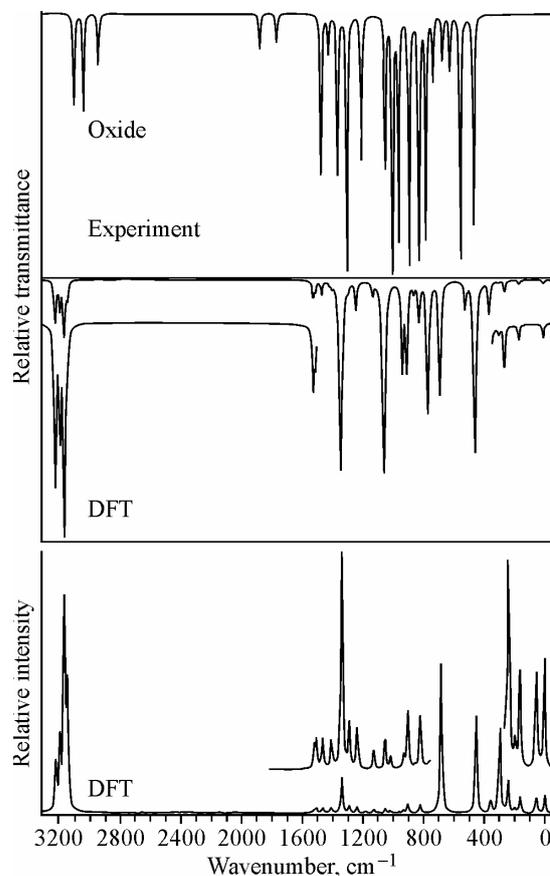
^a Crystal IR data from [18].

minimum (*chair*-equatorial and *chair*-axial) potential. Relatively large intensities in the Raman spectrum of the sulfide occur at 295 cm⁻¹ which is P=X (highly polarizable) stretch to 33 %, and at 755 cm⁻¹ and 1063 cm⁻¹ that are mainly ring breathing and ring deformation. In the sulfide ring, breathing has the largest intensity in the Raman spectrum at 672 cm⁻¹. The same is true for the oxide at 738 cm⁻¹. In the IR spectrum, the largest intensities in the oxide occur at 523 cm⁻¹ (P—Cl stretch and PXCl rock), at 811 cm⁻¹ (ring deformation), at 1085 cm⁻¹ (ring deformation), and at 1350 cm⁻¹ (P=X stretch). In the IR spectrum of the sulfide, the largest intensities occur at 459 cm⁻¹ (P—Cl stretch), at 672 cm⁻¹ (ring breathing, highly mixed), at 951 cm⁻¹ (ring deformation), and at 1071 cm⁻¹ (ring deformation). Since S and Se are less electronegative than O, the P=X stretch does not have a very high intensity in the IR spectra of the sulfide and selenide. Finally, in the IR spectrum of the selenide, large intensities occur at 445 cm⁻¹ (P—Cl stretch), at 624 cm⁻¹ (ring deformation, highly mixed), at 947 cm⁻¹ (ring deformation, highly mixed), and at 1063 cm⁻¹ (ring deformation).

Fig. 1 shows a replot of the experimental IR spectrum of the oxide together with our calculated infrared and Raman spectra.

Obviously, there appears to be a rather fair agreement between experiment and theory, although the relative intensities, apart from the most intense bands, seem to be somewhat underestimated in the

Fig. 1. Experimental (upper panel) and theoretical (central panel) vibrational infrared and theoretical Raman spectra (lower panel) of *chair*-equatorial 2-chloro-1,3,2-dioxaphosphorinane-2-oxide, as calculated by the DFT/B3LYP method in a 6-311G** basis set (since according to total energy the equilibrium mixture would contain 98.9 % equatorial conformer, only that one was calculated)



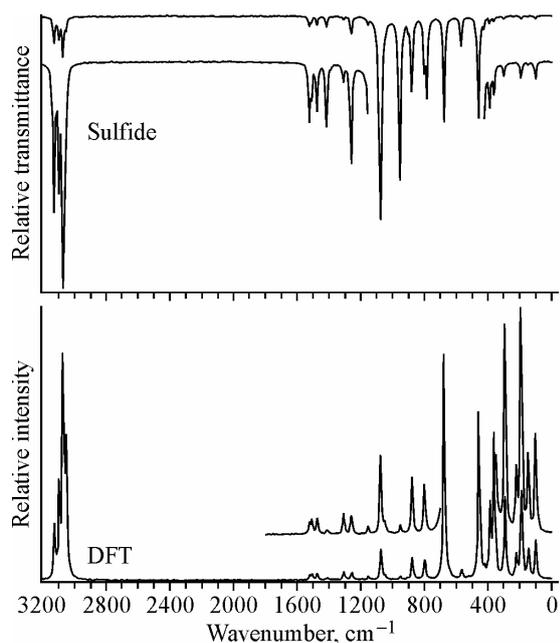


Fig. 2. Theoretical vibrational infrared (upper panel) and Raman (lower panel) spectrum of *chair*-equatorial 2-chloro-1,3,2-dioxaphosphorinane-2-sulfide, as calculated with the DFT/B3LYP method in a 6-311G** basis set (since according to total energy the equilibrium mixture would contain 97.1 % equatorial conformer, only that one was calculated)

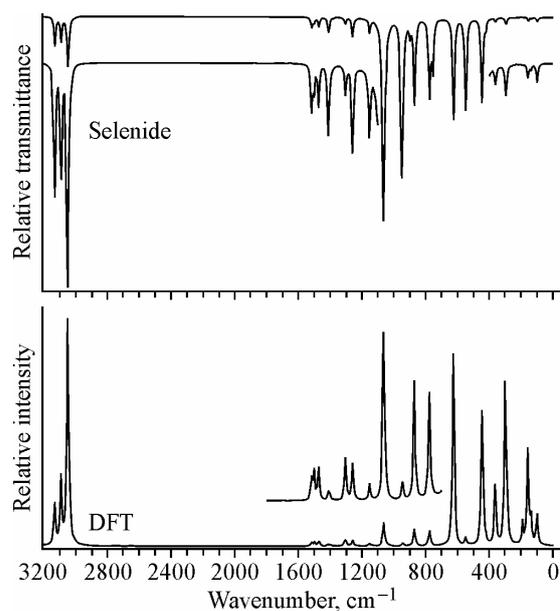


Fig. 3. Theoretical vibrational infrared (upper panel) and Raman (lower panel) spectrum of *chair*-equatorial 2-chloro-1,3,2-dioxaphosphorinane-2-selenide, as calculated with the DFT/B3LYP method in a 6-311G** basis set (since according to total energy the equilibrium mixture would contain 96.8 % equatorial conformer, only that one was calculated)

theoretical spectrum, while the most intense seven bands are reproduced rather well. Because of the agreement between the experiment and calculation shown in the tables, we expect that our calculated Raman spectrum of the oxide (Fig. 1) and the calculated IR and Raman spectra of the sulfide (Fig. 2) and the selenide (Fig. 3) should be rather good predictions: at least the line positions and intensities (given only qualitatively in the literature) should be in fair agreement.

CONCLUSIONS

Phosphorinanes turned out to be good examples to study the effects of going down in a period of the periodic table. The anomeric effect decreases when going from O to S to Se in a P=X bond, with the P atom and two neighboring oxygens in a six-membered ring. According to the PED, in all three molecules, there occurs no pseudorotational motion, and the conformation equilibrium mixture contains almost only the *chair*-equatorial conformer (to more than 95 %) in agreement with variable-temperature vibrational spectroscopy [17, 18]. Our calculated spectra are in fair agreement with the experimental ones, and the results of our PED calculations were used to assign all calculated bands to symmetry coordinates.

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