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The Ultraviolet Absorption Spectra of GeO in Rare Gas Matrices

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The absorption spectra of GeO isolated in rare gas matrices have been investigated in the wavelength region 1150–3000 Å using the 2.5-GeV synchrotron in Bonn as a continuum light source. Two vibrational progressions of bands have been found in each of the matrices, in neon, argon, krypton, and xenon. These progressions are situated in the regions 2400–2700 and 1800–2100 Å. They have been analyzed as corresponding to gas-phase bands of the $A^1\Pi$–$X^1\Sigma^+$ and the $E^1\Sigma^+$–$X^1\Sigma^+$ systems, respectively. Absorption lines of matrix-isolated GeO were also found in the region 1180–1500 Å.

I. INTRODUCTION

This investigation of the absorption spectra of GeO isolated in different rare gas matrices is a contribution to our systematic study of matrix-isolated group IV monoxides (*1–4*). We have measured the absorption spectrum of GeO matrix isolated in neon, argon, krypton, and xenon between 1150 and 3000 Å. Two progressions of GeO bands were observed in each of the four matrices. The aim of the work was to investigate the influences of the different matrices on the electronic states in GeO.

The effects of guest–host interactions were studied in Ne, Ar, Kr, and Xe matrices by (i) comparing the vibrational constants for matrix-isolated GeO with those for gas-phase GeO; (ii) comparing the intensity distributions by the absorption coefficients for matrix-isolated GeO with gas-phase oscillator strengths; and (iii) determining the energy shift of the electronic states relative to gas-phase energies for GeO.

Up to now there has been only one published paper which deals with the electronic absorption spectra of matrix-isolated GeO (*5*). Meyer *et al.* reported well-resolved bands of GeO in krypton and xenon in the region 2400–2700 Å, which were classified as the $A^1\Pi$–$X^1\Sigma^+$ bands. In argon the bands were broad and structureless. Infrared absorption studies on matrix-isolated germanium oxides have been carried out by Ogden and Ricks (*6*) and by Bos *et al.* (*7*). They observed GeO in argon, krypton, and nitrogen. The vibrational frequencies for matrix-isolated GeO were found to agree well with those for gas-phase GeO.

The gas-phase spectrum of GeO has been known for a long time (*8*) but, owing to the multiplicity of Ge isotopes, no complete rotational analysis had been possible. Recently, three papers by Lagerqvist and Renhorn (*9*), Appelblad *et al.* (*10*), and Appelblad *et al.* (*11*) have appeared on the absorption spectrum of GeO in high

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resolution. Isotopically enriched germanium was used in these experiments, and the spectrum of $^{74}Ge^{16}O$ as well as $^{74}Ge^{18}O$ was photographed. This made rotational and vibrational analysis of the $A^1\Pi$–$X^1\Sigma^+$ (*9*), $E^1\Sigma^+$–$X^1\Sigma^+$ (*10*), and $F^1\Sigma^+$–$X^1\Sigma^+$ (*11*) systems possible.

In the region where the *F–X* system is situated, Appelblad *et al.* (*11*) have discovered at least three more systems. According to the molecular constants, probably all these excited states are Rydberg states. The only probable valence state in this short wavelength region was observed from a perturbation in the $F(v' = 0)$ state.

Recently, Baig and Connerade (*12*) extended the investigated region of the GeO spectrum down to 1000 Å. They found further transitions, the most intense of which are situated around 1374, 1258, and 1184 Å. The experiment was performed at low resolution and no rotational analysis could be made. The lack of progressions also made a vibrational analysis impossible.

Lagerqvist and his co-workers also photographed the absorption spectra of $^{74}Ge^{16}O$ and $^{74}Ge^{18}O$ in the wavelength region between 1220 and 1290 Å. However, the bands in this region are very broad and diffuse, probably owing to predissociation, which make a rotational analysis impossible. Even a vibrational analysis is ambigious as the bands are structureless and overlap each other severely, but it is not out of the question that there is a 0,0 GeO band around 1258 Å (*13*).

2. EXPERIMENTAL DETAILS

The experiment was performed in Bonn using the light from the 2.5-GeV synchrotron as a background source. The experimental set up was the same as that used for the SiO investigation, and has been described earlier (*2, 4*).

The GeO molecule was produced by evaporating a mixture of Ge and GeO_2 in a Al_2O_3 crucible within a tantalum tube heated to a temperature of about 900°C. The GeO beam and the rare gas were frozen simultaneously onto a LiF plate cooled by the "cold finger" of a liquid helium bath cryostat at 5.5 K. With the cryostat cold, the vacuum in the main chamber was about 1×10^{-9} Torr. The sample thicknesses varied from 50 to 100 kÅ, this being about two to four times thicker than the SiO films used in our earlier experiment (*2*). This was done because GeO has a smaller absorption coefficient than SiO.

For all measurements reported in this paper, the ratio between GeO and rare gas was about 1:100, except for xenon, where it was 1:50. The ratio for xenon was higher in order to reduce the sample thickness, the reason for this being that our preparation temperature was far from optimum (*14*). We had too low a temperature, especially for preparing good xenon samples, and lattice defects were created. For thick samples the surface is also rough and much of the incident light is scattered, making the measurements of weak lines difficult, especially at shorter wavelengths. All spectra except those for neon were taken before and after annealing. No significant changes between these measurements were observed.

3. ANALYSIS PROCEDURE

Three groups of absorption lines were observed in each matrix except for xenon, where the group at shortest wavelength could not be observed because of strong

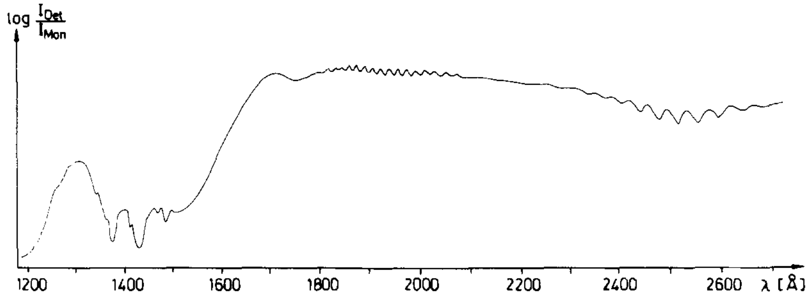

FIG. 1. The absorption spectrum of GeO in an argon matrix.

absorption by a Xe exciton line. In Fig. 1 the whole spectrum of GeO in an argon matrix is shown. The lines in the two groups at longer wavelengths could be grouped into two progressions of bands. The progressions were interpreted as corresponding to the *A–X* and *E–X* transitions in gaseous GeO.

Each measurement was performed at least twice. The wavelengths for the band lines are the averages from all measurements. The intensities of the lines were normalized relative to the most intense line in each progression.

The molecular constants for the matrix bands were calculated using a least-squares polynomial fit program.[2] The vibrational constants for the ground state were assumed to be the same as for the gas phase, based on the results obtained by Ogden and his co-workers (*6*, *7*). The polynomial (1) was fitted to the measured absorption bands ν_0 in the matrix.

$$\nu_0 = T'_e + (v' + 0.5)\omega'_e - (v' + 0.5)^2\omega'_e x'_e - 0.5\omega''_e + 0.25\omega''_e x''_e, \qquad (1)$$

where the gas-phase values ω''_e and $\omega''_e x''_e$ were taken from (*15*). The value T'_e is the energy difference between the minima of the excited state potential and the ground state potential.

In order to establish the assignment of the observed matrix transitions ν_0 relative to the gas phase, we assumed that also the intermolecular potentials of the excited states are hardly changed by the matrix. We then calculated δ^2 from the following expression for different values of vibrational quantum number v'.

$$\delta^2 = \sum [T'_{em} - T'_{eg} + (v' + 0.5)(\omega'_{em} - \omega'_{eg}) - (v' + 0.5)^2(\omega'_{em}x'_{em} - \omega'_{eg}x'_{eg})]^2, \qquad (2)$$

where m = matrix and g = gas phase. One should notice that, by changing v', the ω'_e values change but not the $\omega'_e x'_e$ values.

The less affected the intermolecular potentials are by the matrix the smaller are the δ^2's. We thus chose the numbering of v' which gave a minimum for δ^2. Differences in δ^2 for different v' numberings were only regarded as significant for an assignment when the difference between the δ^2 values was larger than the square sum, Δ^2, of the errors of the ν_0 values calculated with polynomial (1).

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[2] Program CWLT 7 by G. Newson, Harvard College Observatory, Cambridge, Mass. (1979), unpublished.

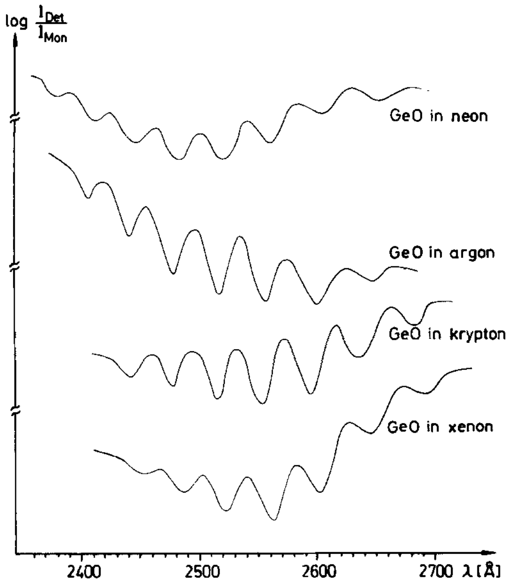

FIG. 2. The $A^1\Pi$-$X^1\Sigma^+$ system of GeO in four rare gas matrices.

4. THE *A*-*X* SYSTEM

The GeO matrix spectra between 2400 and 2700 Å are shown in Fig. 2. In all matrices the band lines are slightly asymmetric. The positions of the band lines minima are given in Table I. It also shows the relative intensities. The values for the gas-phase GeO are taken from (*9*). The estimated errors vary between 0.7 and 3.8 Å for the band lines and between 0.05 and 0.18 for the intensities. The larg-

TABLE I

The $A^1\Pi$-$X^1\Sigma^+$ System

	gas phase(9)		in neon		in argon		in krypton		in xenon	
v', v''	λ_{vac}(Å) origin	osc str	λ_{vac}(Å)	I_{rel}	λ_{vac}(Å)	I_{rel}	λ_{vac}(Å)	I_{rel}	λ_{vac}(Å)	I_{rel}
0,0	2659.96	0.25	2647	0.3	2644	0.26	2661	0.35	2689	0.28
1,0	2615.40	0.68	2601	0.6	2598.9	0.65	2616	0.73	2644	0.55
2,0	2572.80	0.98	2559.0	0.9	2556.2	0.94	2574.6	0.97	2599.6	0.91
3,0	2532.10	1.0	2520.1	1.0	2516.6	1.00	2534.0	1.00	2560.5	1.00
4,0	2493.18	0.81	2481	0.96	2479.1	0.85	2495.2	0.88	2521.5	0.84
5,0	2555.91	0.55	2443	0.8	2441.6	0.67	2458	0.61	2484	0.55
6,0	2420.17	0.33	2409	0.7	2406.3	0.42	2422	0.43	2450	0.39
7,0		0.18	2375	0.5						
8,0		0.09	2345	0.3						

est errors are for the weaker lines; the half-width value of the lines being about 3.1×10^2 cm^{-1}.

All the bands must originate from the $v'' = 0$ level of the $X^1\Sigma^+$ ground state, owing to the low temperature of the matrix. The progressions are situated in the wavelength region were the A–X bands appear in the gas phase, and the vibrational spacings $\Delta G'_{v+1/2}$ between consecutive bands agree fairly well with those of the $A^1\Pi$ state. This was why we assumed that this matrix transition corresponded to A–X.

The vibrational numbering of the bands was determined by the method described under Section 3. The result obtained was that the first band of each progression is the 0,0 band. This vibrational numbering agrees with that which would be expected on the assumption that the intensity distribution of the bands in the matrix should be the same as in the gas phase.

The molecular constants calculated from Eq. (1) and the shifts of the electronic excited matrix state relative to the gas-phase state are given in Table II. The agreement for ω'_e between gas phase and matrix lies within 2% for all the matrices. The intensity distributions of the matrix bands are compared with the oscillator strengths calculated from gas-phase constants (Table I). The agreement is seen to be rather good except for neon, where the two distributions disagree at higher v'. The values plotted for GeO in argon are shown in Fig. 3.

The progressions in krypton and xenon agree with those observed by Meyer *et al.* (*5*), except for one band line at longer wavelengths in xenon that we did not observe. They identified this additional band line as the 0,0 transition, but the molecular constants calculated with this interpretation are in bad agreement with the gas phase results (*9*).

5. THE *E*–*X* SYSTEM

The GeO matrix lines situated between 1800 and 2100 Å were interpreted as corresponding to the gas-phase E–X bands. The interpretation was based on a similar argumentation as used for the A–X bands. The E–X matrix bands are shown in Fig. 4; they appear to be symmetric. Their half-width values are around 3.0×10^2 cm^{-1}.

The wavelengths and intensities of the lines are given in Table III together with gas-phase values for band origins (*10*) and oscillator strengths. The estimated errors

TABLE II

Molecular Constants and Shifts (in cm^{-1}) for the $A^1\Pi$–$X^1\Sigma^+$ System

GeO in	T'_e	ω'_e	$\omega'_e x'_e$	$T'_e(\text{matr})-T'_e(\text{gas}) = \Delta T'_e$
gas phase	37763.1	648.8	4.02	
neon	37966(10)	650(6)	4.4(1.0)	203(10)
argon	38007(10)	647(5)	3.9(1.0)	244(10)
krypton	37762(10)	635(5)	2.4(1.0)	-1(10)
xenon	37367(10)	642(6)	5.4(1.5)	-396(10)

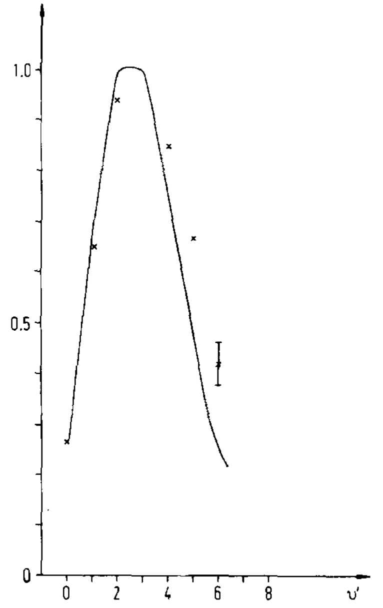

FIG. 3. Comparison between the experimental absorption coefficients of the $A^1\Pi-X^1\Sigma^+$ system of GeO in argon and the calculated oscillator strengths for the gas phase (both distributions are normalized).

vary between 0.7 and 5 Å for the band lines and between 0.04 and 0.18 for the intensities, the largest errors again being for the weaker lines.

Appelblad *et al.* (*10*) found that bands from levels with low vibrational quantum numbers, v', could not be observed in the gas phase. If the potential curves do not change too much in the matrix as compared to the gas phase, one would expect that the matrix E–X bands with low v' numbering should also be too weak to be observed.

It proved more complicated to find the vibrational numberings for the E–X bands using the procedure described under Section 3 than for the A–X bands. In order to compare matrix values with gas-phase values, we had to recalculate the vibrational constants for the gas phase without the restriction on $\omega_e'x_e'$ which Appelblad *et al.* (*10*) used. However, we also used only bands with $v' \leqslant 13$ as they did because, at higher v' values for the gas phase, the potential curve deviates greatly from the form of the Morse potential. The results derived from Eq. (2) for different v' numberings, but with $v' > 13$ bands excluded, are given in Table IV.

With the criterion that the most probable v' numbering is that for which δ^2 is a minimum, there are two possible values in the case of neon, because the differences in δ^2 are smaller than the value of Δ^2 and are therefore not significant. The choice between the two depended on the intensity distribution of the bands. Only when 5,0 is assumed to be the "first" observed band in neon and the internuclear distance is reduced by 1.5% does the relative intensity distribution for the Ne matrix E–X bands coincide with the calculated oscillator strengths (see below). There is also some ambiguity for krypton because of the very high values of Δ^2 arising from the

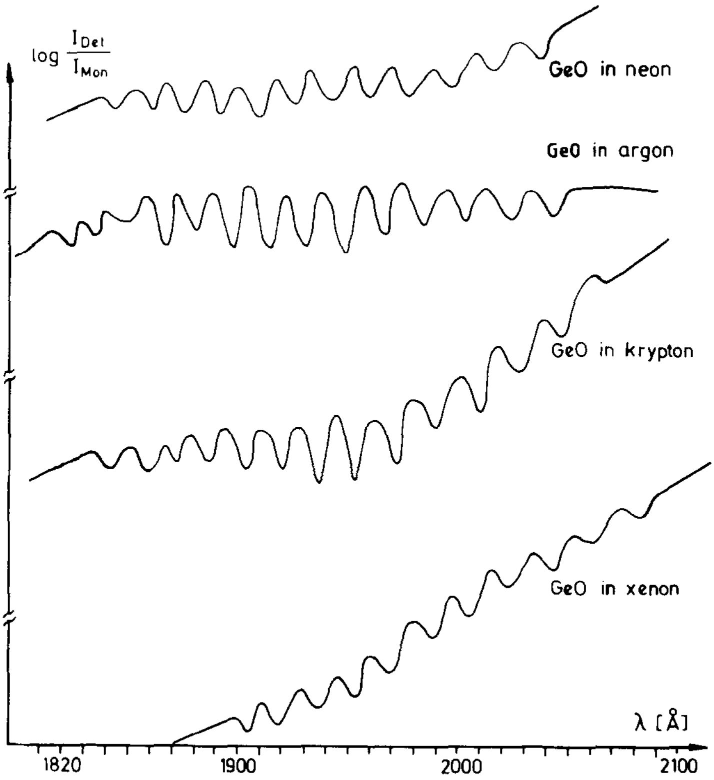

FIG. 4. The $E^1\Sigma^+$–$X^1\Sigma^+$ system of GeO in four rare gas matrices.

restriction $v' \leq 13$, that causes a Δ^2 to be dependent on only a few bands with large errors. The final decision in this case was also based upon the intensity distribution of the bands.

The "first" observed bands for GeO were thus interpreted as being the 5,0 in neon, 6,0 in argon, 6,0 in krypton, and 7,0 in xenon. The molecular constants and shifts $(T'_{em} - T'_{eg}) = \Delta T'_e$ obtained using polynomial (1) for the most probable v' numberings on the bands with $v' \leq 13$ are given in Table V.

For GeO in neon and argon we found that the polynomial fit gave very different values when all measured bands were used or only those with $v' \leq 13$. For GeO in krypton and xenon this makes little difference.

The matrix band line intensities measured were compared with oscillator strengths calculated from gas-phase constants. The rotational constants used were taken from Appelblad *et al.* (*10*) and the vibrational constants were our recalculated values. The intensity distributions in the matrix and gas phase do not correspond. This was also the case for the E–X transition in matrix-isolated SiO. As for SiO we assumed that the internuclear distances in GeO had been reduced, owing to interaction with the matrix. The reduction of r_e for Ar matrix-isolated SiO in the $E^1\Sigma^+$ state has lately been verified in theoretical work on SiO (*16*). In GeO the oscillator strengths

TABLE III

The $E^1\Sigma^+$-$X^1\Sigma^+$ System

	gas phase(10)		in neon		in argon		in krypton		in xenon	
v',v''	λ_{vac}(A) origin	osc str	λ_{vac}(A)	I_{rel}	λ_{vac}(A)	I_{rel}	λ_{vac}(A)	I_{rel}	λ_{vac}(A)	I_{rel}
5,0		0.07	2040	0.50						
6,0	2045.15	0.14	2017	0.55	2044	0.4	2066	0.4		
7,0	2024.74	0.25	1997	0.72	2023	0.6	2048	0.48	2106	0.4
8,0	2004.98	0.39	1978	0.92	2003	0.7	2029	0.60	2083	0.7
9,0	1985.87	0.55	1960	0.88	1985	0.8	2009	0.63	2062	0.8
10,0	1967.38	0.71	1942	0.93	1966.2	0.9	1988.5	0.63	2042	0.8
11,0	1949.50	0.83	1925	0.97	1948.5	1.00	1971.0	0.86	2023.1	0.86
12,0	1932.23	0.93	1908	1.00	1930.6	0.98	1953.0	1.00	2004.3	0.94
13,0	1915.56	0.99	1891	0.86	1912.6	0.85	1935.5	0.92	1987.1	1.00
14,0	1899.50	1.00	1875	0.75	1898	0.84	1920	0.65	1968.5	0.98
15,0	1884.05	0.99	1859	0.73	1881	0.72	1902	0.7	1952	0.9
16,0	1869.23	0.93	1845	0.55	1866	0.78	1886	0.4	1937	0.9
17,0	1855.09	0.86			1851	0.5	1870	0.4	1920	0.7
18,0	1841.67	0.78			1837[a]	0.4	1857[a]	0.4	1906[a]	0.6
19.0	1829.06	0.67			1823[a]	0.30	1841[a]	0.2		

a) Unaccurate line.

based on a shorter internuclear distance also gave better agreement with matrix band intensities. The two normalized distributions for the *E*–*X* transition of GeO in an Ar matrix are plotted in Fig. 5, both for the gas-phase r_e and r_e reduced by 1%. To get a good agreement we had to reduce r_e for neon by 1.5%, argon by 1%, krypton by 1%, and xenon by 0.5%.

TABLE IV

Square Sum δ^2 and Δ^2 for Different Vibrational Numberings of the *E*–*X* Bands

	GeO in							
'first' observed	neon		argon		krypton		xenon	
band	δ^2	Δ^2	δ^2	Δ^2	δ^2	Δ^2	δ^2	Δ^2
5,0	2910	1945	3686	693	2325	3219		
6,0	2640	1945	478	661	668	2784	2201	1453
7,0	7253	1781	820	823	1444	3107	438	315
8,0							1450	604

TABLE V

Molecular Constants and Shifts (in cm^{-1}) for the $E^1\Sigma^+$-$X^1\Sigma^+$ System

GeO in	'first' observed band	T'_e	ω'_e	$\omega'_e x'_e$	T'_e(matr)-T'_e(gas) =$\Delta T'_e$
gas phase		46004.6^a	543.3(0.9)^a	3.53(0.02)^a	
neon	5,0	46474(104)	592(22)	6.26(1.5)	469(140)
argon	6,0	46202 (61)	511(15)	1.98(0.9)	197(100)
krypton	6,0	45635(125)	504(31)	1.6 (1.8)	-370(160)
xenon	7,0	43902 (94)	591(21)	5.8 (1.3)	-2103(130)

a) By us recalculated values.

6. BANDS BELOW 1500 Å

In the wavelength region below 1500 Å there are several absorption bands originating from GeO. They are shown in Fig. 6. The measured lines of GeO in the various matrices are given in Table VI. The intensities of the lines are indicated only in the following way: Very strong (vs), strong (s), medium (m), or weak (w). The first three apply to thinner film measurements, where excitation and scattering

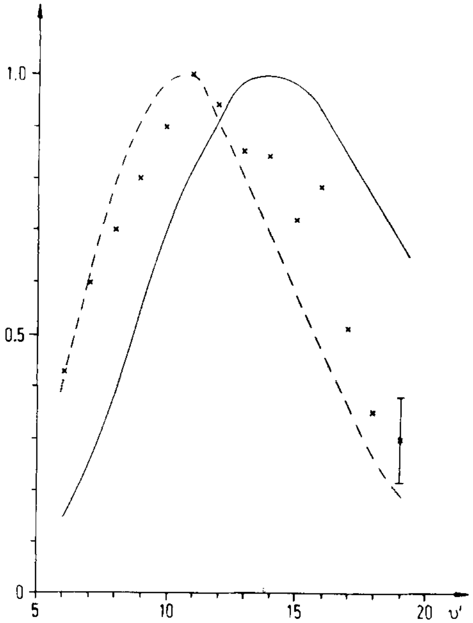

FIG. 5. Comparison between the experimental absorption coefficients of the $E^1\Sigma^+$-$X^1\Sigma^+$ system of GeO in argon and the calculated oscillator strength. ——, Calculated using the internuclear distance of the gas-phase r_e. - - -, Calculated with the internuclear distance r_e reduced by 1% (all distributions are normalized).

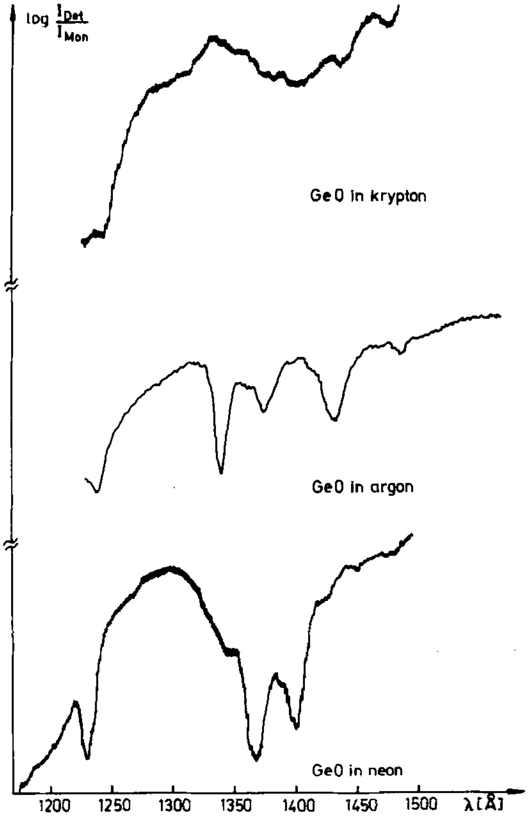

FIG. 6. Unidentified lines of GeO below 1500 Å in neon, argon, and krypton.

effects are not so pronounced. These effects are also the reason why Figs. 1 and 6 are different in appearance. The indication (w) in Table VI applies to lines seen only for thicker films. In the region between the *E–X* matrix progressions and 1500 Å, no evidence of absorption in any matrix was observed.

Although the lines below 1500 Å have the same energy width as the *A–X* and *E–X* lines, they do not form any vibrational progressions. The positions of GeO gas-phase systems in this region also differ greatly from those observed in the matrices. The reason why we believe them to be GeO is based on the following facts. The bands only appear when there is GeO in the furnace. One measurement was performed with Ge powder in the furnace, and none of the lines observed with GeO in the furnace were seen. The matrix spectrum of Ge has already been studied by Martin and Schaber (*17*), and they found some strong absorption lines at 2282 and 2377 Å which we did not observe in our experiment.

These facts, together with the knowledge that no state observed for an electronic transition has been identified as a valence state in the gas-phase GeO molecule, leads us to the conclusion that all the matrix lines below 1500 Å originate from transitions to Rydberg states. Assuming the intensity relation between the systems

TABLE VI

Known Gas-Phase Systems (*11*) and Matrix Band Lines (in Å) in the Wavelength Region 1100–1500 Å

gas phase			neon		argon		krypton	
system	v',v"	band head	line	int	line	int	line	int
		1184[a]	1231	m	1238	m	1256	w
		1258[a]	1345	m	1339	s	1376[b]	m
$J\Sigma - X^1\Sigma^+$	0,0	1376.48	1366	vs	1363	w	1404[b]	m
$F^1\Sigma^+ - X^1\Sigma^+$	0,0	1484.04	1397	m	1375	s	1416[b]	m
			1421	m	1431	s	1441	m
			1446	w	1469	w	1480	s
$I\Sigma - X^1\Sigma^+$	0,0	1511.85	1471	w	1487	m	1527	m
$H - X^1\Sigma^+$	1,0[c]	1530.18						
$G\Sigma - X^1\Sigma^+$	1,0[c]	1533.44						

a) From Ref. 12.

b) Could be one broad line with some structure.

c) The 0,0 band was not observed.

in the gas phase and the matrix to be unchanged, the lines at 1366, 1375, and 1416 Å in Ne, Ar, and Kr matrices, respectively, would correspond to the *F*–*X* gas-phase transition. This would imply a massive shift of more than 5000 cm^{-1} for the electronic excited states. However, any analysis of the matrix lines would lead to either very large shifts of electronic states, to great changes in the intensity relations, or to both.

7. CONCLUSIONS

The results of the analyses of the absorption spectrum of GeO in different rare gas matrices can be summarized as follows: (i) The trapping site of the molecule appears to be a single trapping site, as no annealing effects were observed. (ii) The energy states of GeO are shifted from higher to lower energies from Ne to Xe matrices. The shifts for Kr and Xe matrices are to lower energies compared to gas phase; the shifts for Ne and Ar to higher energies. (iii) The forms of the potential curves for the *A* and *E* states given by the vibrational constants ω_e and $\omega_e x_e$ are, to a first approximation, only slightly changed by the matrix influence on GeO. (iv) The intensity distribution of the *A*–*X* bands in each matrix is about the same as that for the gas-phase bands. For the *E*–*X* bands the intensity distribution for GeO bands in a matrix and the GeO bands in gas phase are different. This latter effect can be explained by a decrease in the internuclear distance of the molecule. (v) Absorption lines in the short-wavelength part of the investigated region were interpreted as GeO transitions to Rydberg states. (vi) The effects of the rare gas matrices on the GeO molecule are very similar to those on the SiO molecule (*2*).

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