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The UV and VUV Absorption and Reflection Spectrum of Toluene

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ABSTRACT. Low temperature absorption spectra of toluene in rare gas matrices, and its absorption and reflection spectra in pure solid phase were obtained at temperature near liquid helium temperature, in the wave length region 270-170 nm. Absolute intensity measurements in terms of the molar absorption coefficient values were made, and methyl shift in the three electronic transitions was compared with the Petrushka calculations.

In the 210 and 190 nm transitions, the absorption spectrum of toluene in the Xe matrix shows a splitting of the 0-0 line. An explanation is given, that Xe matrix may offer sufficient perturbation to remove the degeneracy of the $^1B_2$ and $^1A_1$ states which are of $^1E_{1u}$ parentage in the benzene molecule.

In previous paper (Taleb and Munro 1983) we examined the absorption spectra of C_6H_6 and C_6D_6 in rare gas matrices in the region 270-170 nm. Methyl substituted benzene, on the other hand, is of interest for three major reasons:

i) Because of the symmetry breaking effects (reduction of molecular symmetry to C_{2v}), the pure electronic and the vibrationally induced components are allowed for both the states which have $^1E_{2g}$ and $^1B_{1u}$ parentage in the benzene molecule.

ii) Methyl substitution of the benzene molecule is expected to show a splitting of the electronic degeneracy in the (π-π^*) S_3 excited state which is of the $^1E_{1u}$ parentage due to the pseudo Jahn-Teller coupling effect.

iii) Although spectral shift and intensity distribution of benzene substituents were studied thoroughly in solutions (Petrushka 1961 and Stevenson 1964), matrix isolation studies present more accurate data since molecules under study are relatively well isolated, *i.e.* effect of solvent-solute interactions are reduced to a minimum.

The two photon spectra of toluene and other benzene substituents (Goodman and Rava 1981) have shown that the intensity distribution among bands corresponding to different totally symmetric vibrations is quite different from that in the one photon absorption spectrum. The allowed part of the toluene two-photon spectrum, for example, is much stronger than in fluorobenzene, and that the halobenzene intensity ordering is Br > Cl > F, in contrast with results found for one-photon spectra (Taleb and Al-Mashat 1981).

Experimental

The experimental apparatus and techniques used were described previously (Taleb and Munro 1983). A McPherson 225 monochromator and a hydrogen filled discharge lamp were used. Gas mixture of spectrograde toluene/rare gas were prepared in a certain ratio in a special manifold before introduction into the vacuum chamber where the cold LiF or sapphire window is situated. The thickness of the deposited film was measured accurately utilizing an interferometric technique.

Solid thin films of the pure toluene were prepared and deposited in a similar manner, but with different deposition, annealing, and recording temperatures.

Results and Discussion

The 260 nm or $^1B_2 \leftarrow {}^1A_1$ Transition

In rare gas matrices

Figure 1 shows the absorption spectra of 20 μm films of toluene in Ar, Kr, and Xe matrices. The molar ratio M/A $\simeq$ 200 and the films were deposited and recorded at 20 K. Table 1 lists the position of the vibronic bands observed in the three matrices and their suggested assignments. The ground state energies of the vibrational fundamental are given in the same table (in brackets). The absorption spectra of toluene in the three rare gases are similar except that the Kr matrix produces the sharpest structure - similar to the case of benzene. The spectra recorded reveal a number of interesting features:

(i) The first strong line (line widths are 40, 30, 50 cm^{-1} in Ar, Kr, and Xe matrices respectively) is assigned to the 0-0 electronic origin. Although a splitting has been reported (Katz *et al.* 1971) in this line and its associated vibronic transitions, this has not been confirmed (within the limits of the resolution employed) by the spectra of Fig. 1. That is to say, the site splitting of ~ 80 cm^{-1} which is observed in the absorption spectra of benzene-rare gas matrices in the $^1B_{2u}$ state, is not observed in toluene. If such a splitting does exist it is characterised by a spacing $\leqslant 20$ cm^{-1} which is our experimental limit of resolution. In their study of the gas-phase spectrum Ginsburg *et al.* (1946) reported a doublet (separation $\simeq 3$ cm^{-1}) with the stronger band at 37477 cm^{-1}.

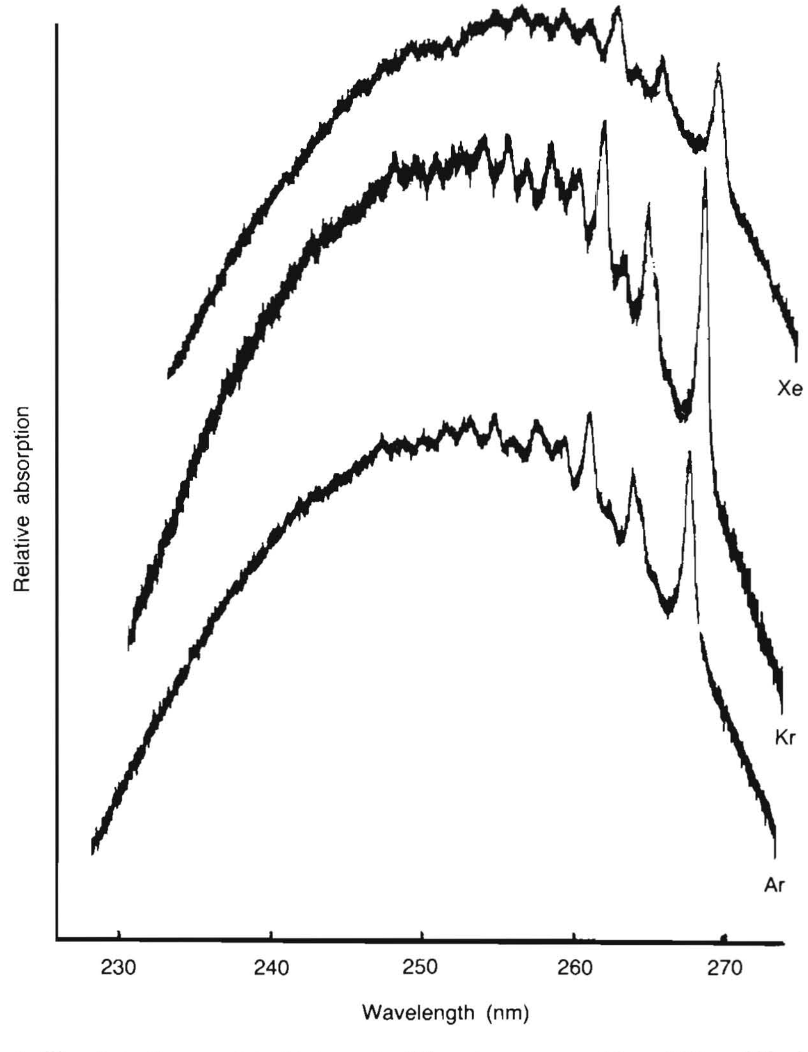

Fig. 1. The absorption spectra of toluene in different rare gas matrices. M/A ~ 200, deposition and recording at 20 K.

Table 1. The $^1B_2 \leftarrow {}^1A_1$ absorption spectrum of toluene in different rare gas matrices, M/A = 200. Deposition and recording at 20 K.

Ar Matrix			Kr Matrix			Xe Matrix			$(\nu-\nu00)\mathrm{cm}^{-1}$	Assignment
λ nm	$\nu\mathrm{cm}^{-1}$	ε	λ nm	$\nu\mathrm{cm}^{-1}$	ε	λ nm	$\nu\mathrm{cm}^{-1}$	ε	$A\bar{\nu}$	
267.3	37410	270	268.4	37260	350	269.3	37130	210	–	(0–0)
265.0	740	90	266.1	580	120	267.2	430	80	310	(0–0) + $\nu_{14(b_2)}$ [$340\mathrm{cm}^{-1}$ in G.S.]
264.4	820	140	265.2	710	170				430	(0–0) + ν_{18a} [$521\mathrm{cm}^{-1}$ in G.S.]
263.6	940	190	264.4	820	250	265.7	640	170	530	(0–0) + ν_{18b} [$622\mathrm{cm}^{-1}$ in G.S.]
262.0	38170	100	263.0	38020	170	264.0	880	130	750	(0–0) + $\nu_{6(a1)}$ [$785\mathrm{cm}^{-1}$ in G.S.]
260.6	370	200	261.8	200	280	262.7	38070	180	950	(0–0) + $\nu_{6(a1)}$ [$1002\mathrm{cm}^{-1}$ in G.S.]
259.0	610	130	260.1	450	180	261.0	310	170	1190	(0–0) + $\nu_{15(a1)}$ [$1210\mathrm{cm}^{-1}$ in G.S.]
										and/pr (0–0) + $\nu_{18(a)}$ + $\nu_{6(a1)}$
258.5	680	120	259.7	510	180				1260	(0–0) + $\nu_{18(b)}$ + $\nu_{7(a1)}$
257.2	880	150	258.3	710	200	259.2	580	140	1450	(0–0) + ν_{18ab} + $\nu_{2(a1)}$
255.5	39140	120	256.5	990	180	257.7	800	120	1700	(0–0) + $\nu_{6(a)}$ + $\nu_{2(a1)}$
254.5	290	140	255.5	39140	190	256.3	39020	130	1880	(0–0) + $2\nu_{2(a)}$
253.0	530	130	252.8	39700	180	254.7	39260	120	2130	(0–0) + $\nu_{2(a1)}$ + $\nu_{15(a1)}$
251.5	760	110	252.0	680	170	253.3	480	100	2370	(0–0) + $\nu_{18.ab}$ + $2\nu_{2(a1)}$
249.8	40030	100	250.5	920	170	251.5	760	90	2630	(0–0) + $3\nu_{2(a1)}$
247.3	440	100	248.0	40320	160				3050	(0–0) + $\nu_{18.ab}$ + $\nu_{6(a1)}$ + $2\nu_{2(a1)}$
246.0	650	80	246.3	600	150				3300	(0–0) + $\nu_{18,ab}$ + $3\nu_{2(a1)}$
			243.5	41070	140				3810	(0–0) + $4\nu_{2(a1)}$

G.S. = refers to ground state.

Two-photon fluorescene excitation (Vasudev and Brand 1979) and two photon ionization spectrum (Krogh - Jespersen *et al.* 1979) confirm the above results but with larger doublet splitting ($\simeq$ 8 cm^{-1}).

(ii) The fundamental vibrational frequencies and their relative intensities observed in the three solid matrices are in good agreement with the gas-phase data except that no hot bands are exhibited. In the Ar matrix the absorption spectrum is red shifted by ~ 70 cm^{-1} relative to the gas phase. The red matrix shift in going from Ar $\rightarrow$ Kr is ~ 150 cm^{-1}, and ~ 130 cm^{-1} in going from Kr $\rightarrow$ Xe matrix.

(iii) The methyl shift from toluene to benzene for the 0-0 line is 570 cm^{-1} in the Ar matrix, 620 cm^{-1} in the Kr matrix, and 630 cm^{-1} in the Xe matrix. This is consistent with Petrushka's calculations (Petrushka 1961) on the effect of chemical substitution on the center of gravity of the 260 nm band system.

(iv) Deposition at 40 K in a Kr matrix followed by measurement at 20 K did not enhance the fine structure, but merely reduced the overall intensity of the absorption band in a manner similar to that observed in C_6H_6 and C_6D_6.

Pure solid phase

Figure 2 shows the absorption spectrum for a toluene film of about 1 um thickness deposited at 4.2 K, annealed to 140 K, and recorded at 4.2 K. The spectra recorded at 4.2 K (before annealing) show a large broadening, similar to that in benzene. In general, the absorption spectrum of solid toluene reveals less structure than is found in rare gas matrices. Table 2 summarises the vibronic analysis together with the ϵ-values of the absorption lines.

The (0-0) electronic origin is blue shifted by about 40 cm^{-1} relative to that observed in Xe matrix, and is red shifted by about 90 cm^{-1} relative to Kr matrix.

The methyl shift is about 700 cm^{-1}, which is slightly larger than the corresponding values in rare gas matrices.

The 210 nm, or $^1A_1 \leftarrow {}^1A_1$ Transition

Rare gas matrices

Figure 3 shows the absorption spectra for toluene films (~ 2 μm thickness) mixed with different rare gases. In each case, the mixture of molar ration M/A $\simeq$ 200 was deposited and recorded at 20 K. In Table 3 we have listed the position and intensity (ϵ-value) of all the peaks observed. The spectra seem to be more detailed than those previously reported (Katz *et al.* 1971) and more than one vibrational mode is involved.

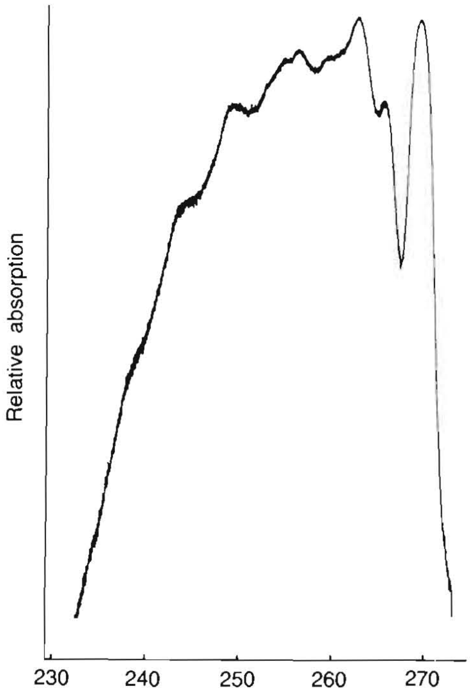

Fig. 2. The absorption spectrum of solid toluene deposited at 4.2 K, annealed to 140 K, and recorded at 4.2 K.

Table 2. The $^1B_2 \leftarrow {}^1A_1$ absorption spectrum of a solid toluene film deposition at 4.2 K, annealed to 140 K, and recorded at 4.2 K.

λ nm	νcm^{-1}	$(\nu-\nu_{00})$cm^{-1}	ε	Assignment
269.0	37170	0	400	(0−0)
265.2	37710	540	225	$(0-0) + \nu_{18b}$
262.4	38110	940	350	$(0-0) + \nu_{2(a_1)}$
260.7	38360	1190	275	$(0-0) + \nu_{15(a_1)}$
259.0	38610	1440	270	$(0-0) + \nu_{18b} + \nu_{2(a_1)}$
255.8	39090	1920	275	$(0-0) + 2\nu_{2(a)} + \nu_{15(a_1)}$
254.3	39320	2150	265	$(0-0) + \nu_{2(a_1}) + 2\nu_{15(a_1)}$
252.6	39590	2420	230	$(0-0) + \nu_{18b} + 2\nu_{2(a_1)}$
251.2	39810	2640	200	$(0-0) + \nu_{18b} + \nu_{2(a_1)} + \nu_{15(a_1)}$
249.5	40080	2910	205	$(0-0) + 3\nu_{2(a_1)}$
244.0	40980	3810	125	$(0-0) + 4\nu_{2(a_1)}$
238.5	41930	4760	75	$(0-0) + 5\nu_{2(a_1)}$

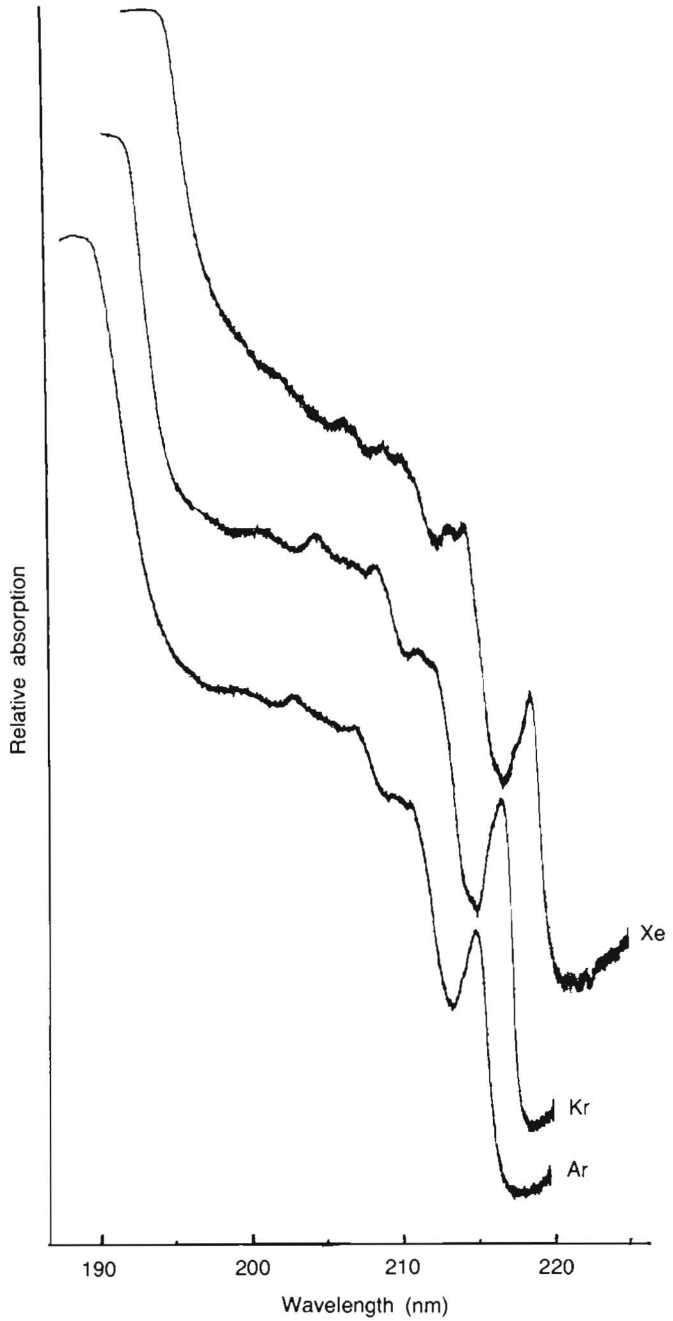

Fig. 3. The absorption spectra of toluene in different rare gas matrices. M/A ~ 200 deposition and recording at 20 K.

Table 3. The $^1A_1 \leftarrow {}^1A_1$ absorption spectrum of toluene in different rare gas matrices, M/A = 200. Deposition and recording at 20 K.

Ar Matrix			**Kr Matrix**			**Xe Matrix**			$(\nu-\nu_\infty)$cm^{-1}	**Assignment**
λ **nm**	νcm^{-1}	$\epsilon(10^2)$	λ nm	νcm^{-1}	$\epsilon(10^2)$	λ **nm**	νcm^{-1}	$\epsilon10^2)$	**Av**	
214.5	46620	40	216.0	46300	42.5	217.8	45910	37.5		(0−0)
						216.8	46130	32.0	220 ± 30	(0−0) + 220cm^{-1} (S)* and/or (0−0) + $\nu_{14}(b_1)$
212.5	47060	31.5	214.0	46730	32.5	215.7	46350	39	440	(0−0) + ν_{18a} and/or (0−0) + ε_{18b}
210.1	47600	60	211.6	47260	65	213.5	46840	55	950	(0−0) + $\nu_{2(a1)}$
209.0	850	60.5	210.5	47510	66	212.5	47060	54.5	1200	(0−0) + $\nu_{2(a1)}$ + $\nu_{14(b2)}$ and/or (0−0) + $\nu_{2(a1)}$ + (S) or (0−0) + $\nu_{15(a1)}$
			208.5	47960	69	210.5	47510	57	1630	(0−0) + $\nu_{18a,b}$ + $\nu_{2(a1)}$ + $\nu_{14(b2)}$ and/or (0−0) $\nu_{2(a1)}$ + $\nu_{6(a1)}$
206.0	48450	65	207.5	48190	71	209.5	47730	58	1880	(0−0) + $2\nu_{2(a1)}$
205.0	780	65	206.3	470	70.5	208.3	48010	59	2140	(0−0) + $\nu_{2(a1)}$ + $\nu_{15(a1)}$ and/or (0−0) + $2\nu_{2(a1)}$ + (S) or (0−0) + $2\nu_{2(a1)}$ + $\nu_{14}(b_2)$
204.0	49020	65	205.3	48710	70.5	205.5			2400	(0−0) + $\nu_{2(a1)}$ + $2\nu_{6(a1)}$ and/or (0−0) + $\nu_{2(a1)}$ + $2\nu_{14(b2)}$
202.3	430	66	203.7	49090	72	205.5	48660	60	2780	(0−0) + $3\nu_{2(a1)}$
198.7	50330	66	200.0	50000	71.5	201.5	49630	60	3710	(0−0) + $4\nu_{2(a1)}$
195.2	51230	67	196.4	920	72.5				4620	(0−0) + $5\nu_{2(a1)}$

∗ (S) refers to pseudo Jahn-Teller splitting and / or site splitting.

The first strong line on the low energy side of this transition is assigned to the 0-0 electronic origin (Potts 1955). Its line width is 300 cm^{-1} in Xe matrix and 350, 400 cm^{-1} in Kr and Ar matrices respectively. The analysis of these spectra reveals a totally symmetric $\nu_2(a_1)$ progression built on the pure electronic origin. In addition, the false origin corresponding to the ν_{18} vibration could also be identified.

The Xe matrix seems to show "Shpolskii type" structure for the toluene molecule in this region of the absorption spectrum. A shoulder is clearly identified in this matrix 240 ± 30 cm^{-1} to the high energy side of the 0-0 line. This may suggest that a third vibrational mode of the $\nu_{14}(b_2)$ type (340 cm^{-1} in the ground state) is involved. Another possible suggestion is that this shoulder could be caused by a splitting in the 0-0 electronic origin because of a pseudo-Jahn-Teller (P.J.T) effect. We would expect this to be amenable to experimental observation upon methyl or other chemical substitution in the benzene molecule (Hobey 1965). A similar splitting was observed in the rest of the progression built upon the $\nu_2(a_1)$ vibrational mode. A third possibility is that splitting could be due to "site splitting" caused by the different trapping sites which have been suggested (Katz *et al.* 1971) for the first single transition. It is possible, as in the case of benzene, that more than one mechanism is involved and in the present work it is difficult to make an unambiguous identification because of the diffuseness of the vibronic bands.

The matrix shift in going from the Xe matrix to the Kr matrix is ~ 400 cm^{-1}, and is ~ 320 cm^{-1} in going from a Kr to Ar matrix. These values are not very different from the corresponding shifts for benzene (300, 320 cm^{-1}). The methyl shifts (toluene relative to benzene) for its (0-0) + ν_{18} line are: 1410, 1440, 1490 cm^{-1} in Ar, Kr, and Xe matrices respectively. This is again consistent with Petrushka's calculations (Petrushka 1961).

Pure solid phase

In Figure 4 we present the absorption and reflection spectra of a 10 nm thick film of toluene deposited at 4.2 K, annealed to 140 K, and recorded at 4.2 K. Table 4 lists the position of all peaks observed together with their suggested assignments. The totally symmetric $\nu_2(a_1)$ progression built upon the pure electronic origin is dominant. In addition, two other vibrational modes ν_{18}, ν_{15} were identified. The 0-0 line in the pure solid is red shifted by ~ 700 cm^{-1} relative to that in Xe matrix, whilst the methyl shift for the same line is 1290 cm^{-1}.

The reflection spectrum of solid toluene was also recorded. The position of the reflection maxima do not seem to correspond with the absorption maxima (since the reflection coefficient is a function of the optical constants n, K while the absorption coefficient is a function of K only). The latter are blue shifted by about 200 cm^{-1}, while it was 40 cm^{-1} for benzene in the same region.

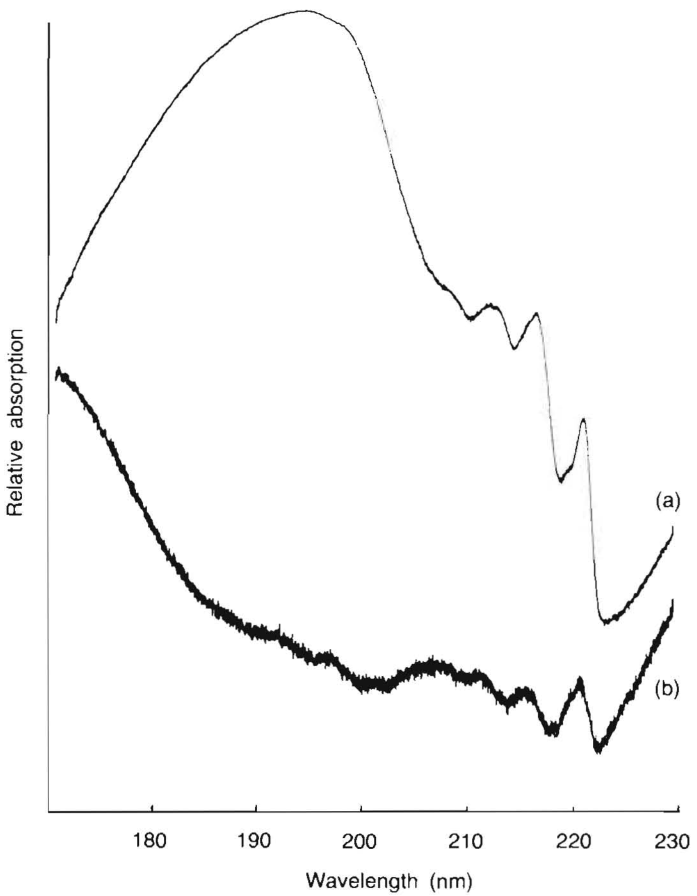

Fig. 4. Absorption (a) and reflection (b) spectra of solid toluene, deposited at 4.2 K, annealed to 140 K and recorded at 4.2 K.

Table 4. The $^1A_1 \leftarrow {}^1A_1$ absorption spectrum of a solid toluene deposition at 4.2 K, annealed to 140 K, and measured at 4.2 K.

λ nm	νcm^{-1}	$(\nu-\nu_\infty)$cm^{-1}	ϵ	Assignment
221.2	45210		5000	(0−0)
219.2	45620	410	3800	$(0-0) + \nu_{18a}$
216.7	46150	940	7700	$(0-0) + \nu_{2(a1)}$
215.7	360	1150	7250	$(0-0) + \nu_{15(a1)}$
212.5	47060	1850	7800	$(0-0) + 2\nu_{2(a1)}$
208.3	48010	2800	8000	$(0-0) + 3\nu_{2(a1)}$

The 190 nm Transition (Equivalent to $^1E_{1u} \leftarrow {}^1A_{1g}$ in Benzene)

The absorption spectrum of toluene in this region is rather diffuse compared with the corresponding transition in benzene. Figure 5 shows the absorption spectra of films ~ 0.5 μm thick in Ar, Kr, and Xe matrices. The molar ratio M/A is ~ 200 and the film in each case was deposited and recorded at 20 K. Films prepared separately at 30, 40, 50 K with Ar, Kr, and Xe matrices were cooled to 20 K and showed an overall reduction in their absorption intensity. Similar reductions were observed when the films were prepared and recorded at 20 K after annealing to 30, 40, and 50 K respectively. The spectra shown in Fig. 5 are more detailed than those previously reported in the Kr matrix (Katz *et al.* 1971) or in hydrocarbon glasses (Potts 1955). As was the case for the 210 nm ($^1A_1 \leftarrow {}^1A_1$) transition, the absorption spectrum of toluene in the Xe matrix shows a splitting in the 0-0 line. The Xe matrix may offer sufficient perturbation to remove the degeneracy of the $^1B_1$ and $^1A_1$ states which are of $^1E_{1u}$ parentage in the benzene molecule.

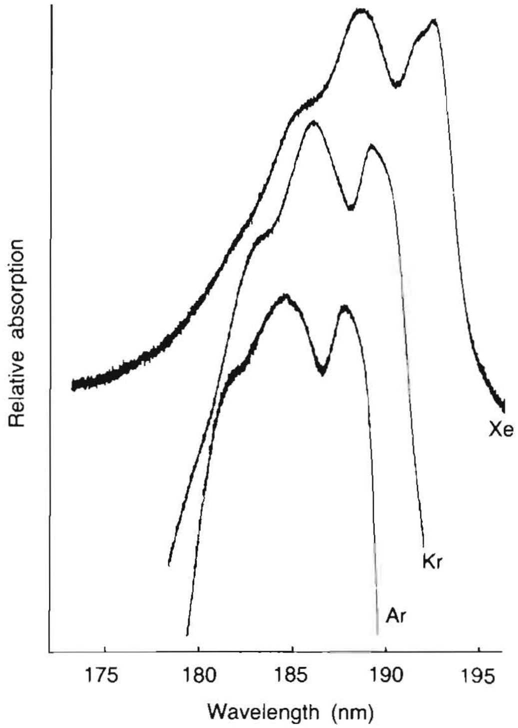

Fig. 5. The absorption spectra of toluene in different rare matrices, M/A ~ 200, deposition and recording at 20 K.

Table 5. The 190 nm absorption spectrum of toluene in different rare gases M/A = 200. Deposition and recording at 20 K.

Ar Matrix			Kr Matrix			Xe Matrix			$(\nu-\nu_\infty)\text{cm}^{-1}$	Assignment
λ nm	νcm^{-1}	$\epsilon(10^3)$	λ nm	νcm^{-1}	$\epsilon(10^3)$	λ nm	νcm^{-1}	$\epsilon(10^3)$	Av.	
187.9	53220	50	189.5	52770	52.5	193.0	51810	47.5		(0−0)
						192.2	52030	45	220	(0−0) + 220 cm^{-1} (S)*
184.7	54140	52	186.3	53680	56	189.4	52800	49.5	930	(0−0) + $\nu_{2(a1)}$
181.7	55040	35	183.2	54590	36	186.2	53710	33	2 × 930	(0−0) + $2\nu_{2(a1)}$
178.7	55960	26	180.1	55520	26	183.0	54640	22	3 × 930	(0−0) + $3\nu_{2(a1)}$

∗ (S) refers to (J.T. splitting).

Methyl substitution of the benzene molecule is expected to show a splitting of the electronic degeneracy in the $\pi-\pi^*$ excited states (due to the Jahn-Teller coupling effects) of those systems which are of E_{1u} parentage. Hobey's calculation (1965) on the ground state of negative ions of substituted benzenes lead to the conclusion that pseudo-Jahn-Teller coupling effects tend to reduce the initial electronic splitting. Thus, for toluene $d = 708\ cm^{-1}$ and $\triangle E = 470\ cm^{-1}$ (where d refers to the initial splitting, $\triangle E$ corresponds to the level spacing). The experimental level splitting in the excited state of toluene ($220 \pm 50\ cm^{-1}$) differs by a factor of approximately two from this expected value of $\triangle E$.

Katz *et al.* (1971) were not able to see this effect in toluene, simply because they used a Kr matrix only. In previous paper (Taleb and Munro 1983) we showed that Kr matrix offered a "Shpolskii type" solvent (matrix) to the benzene molecule and a similar splitting was observed in the corresponding region.

The main feature of the spectra shown in Fig. 5 is that $\nu(a_1)$ totally symmetric vibrational mode is the prominent one. The line width of the 0-0 line in the three matrices is about twice that of the corresponding lines in benzene (*i.e.* $1000 \pm 100\ cm^{-1}$).

The intensity ratio of the lines observed is similar to that recorded for benzene. Table 5 lists the positions and ϵ-values for the vibronic bands observed, together with the suggested assignments.

The matrix shift for the 0-0 line in going from the Ar to the Kr matrix is $\sim 450\ cm^{-1}$ whilst it is $\sim 960\ cm^{-1}$ in going from Kr to Xe. That is to say, the Kr → Xe matrix shift is larger than that from Ar → Kr by a factor of two. The $^1E_{1u}$ state in benzene has been shown to behave in a similar fashion. However, in the $^1B_{1u}$, $^1B_{2u}$ states in benzene and the corresponding states in toluene, the matrix shifts in going from Ar → Kr or Kr → Xe matrices both are of approximately the same order of magnitude.

The methyl shift (for the 0-0 line) is $\sim 1040, 1050, 1300\ cm^{-1}$ in Ar, Kr, and Xe matrices respectively. This is again consistent with Petrushka's calculations (Petrushka 1961).

In the pure solid phase, the absorption spectrum of toluene (see Fig. 4) is diffuse in the region of the 190 nm transition. The reflection spectrum (same fig.) shows more structured features, and four maximum reflection peaks are observed at 202.6, 200.5, 196, and 190 nm. These peaks do not necessarily correspond to vibronic bands in this region since we are not able to relate the absorption and reflection peaks in the 210 nm band system.

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طيف امتصاص وإنعكاس فوق البنفسجية وفوق البنفسجية المفرغة لجزيئة التلوين

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درس طيف امتصاص التلوين في درجات حرارية منخفضة عند انجماد الغازات النادرة. كما درس طيف الإمتصاص والإنعكاس للحالة الصلبة النقية عند درجات حرارية قريبة من درجة الهيليوم السائل وفي منطقة الطول الموجي ٢٧٠ ـ ١٧٠ نانوميتر.

لقد أجريت قياسات الشدة المطلقة بدلالة قيم معامل الإضمحلال المولي، وكذلك قورنت نتائج الإنحراف الطيفي المتسبب عن مجموعة المثيل مع الحسابات النظرية لبتروشكا.

وقد تبين أنه عند الانتقالين ٢١٠ و ١٩٠ نانوميتر فإن طيف إمتصاص التلوين عند انجماد الزينون يظهر إنقساماً في الخط O—O، وقد فسر ذلك على أساس أنه عند انجماد الزينون يتوفر نوعٌ من الاضطراب لإزالة التفكك لكل من الحالتين ${}^1B_2$ و ${}^1A_1$، اللتين هما من أصل ${}^{u}{}_{1}{}^{E}$ بالنسبة لجزيئة البنزين.