

decrease in intensity with increasing temperature until it becomes difficult to follow the spectrum beyond 410 K. Other than this intensity decrease, which is typical of organic compounds, no unusual temperature dependent anharmonicity such as a large change in the line shape, relative intensity or extremely large frequency decrease could be observed in the temperature span covered. No background luminescence was apparent in the high temperature Raman spectra excited by 514.5 nm; that is to say, no indication of dissociation to loosely associated pairs of anthracene molecules was detected either by the appearance of new Raman bands or of a fluorescence emission.

TABLE 3.—BANDS OF THE RAMAN SPECTRUM OF DIANTHRACENE- $d_{20}$  AT 296 K AND 1 bar

modes of dianthracene- $d_{20}$		corresponding modes of dianthracene	
wavenumber/cm <sup>-1</sup>	intensity <sup>a</sup>	wavenumber/cm <sup>-1</sup>	$\nu_H/\nu_D$
lattice modes			
27.4	vs	28.5	1.04
36.3	vs	37.1	1.02
51.9	vs	53.6	1.03
66.9	w	71.3	1.07
88.8	m	[91] <sup>b</sup>	1.02
98.0	s	101	1.03
105	s	110	10.5
[119]	m		
130	vs	133	1.02
135	vs	141	1.04
153	m	167	1.09
158	m	172	1.09
internal modes			
306	s	327	1.07
336	vs	361	1.07
351	w		
466	w		
558	w		
607	vw		
671	vs	711	1.06
802	vw		
803	w		
856	vs, br	885	1.03
872	w, sh	890	1.02
924	vw		
955	s		
986	m		
1117	m, sh		
1126	vs	1178	1.05
1210	m	1228	1.01
1549	vw	1582	1.02
1569	m	1603	1.02
1583	vw	1592	1.01
2184	w		
2208	w	2951	1.34
2261	m	3030	1.34
2272	vw		
2290	s	3078	1.34

<sup>a</sup> The following abbreviations have been used: s, strong; m, medium; v, very; w, weak; br, broad; sh, shoulder. <sup>b</sup> [ ] values with large uncertainty.

The pressure dependence of both the internal and the lattice modes was studied at 296 K. Table 2 also lists the values of the wavenumbers of the observed peaks at 10 kbar, while the spectrum is shown in fig. 5. Plots of wavenumber against pressure are not quite linear; therefore, only the initial slopes ( $dv/dP$ ) are tabulated

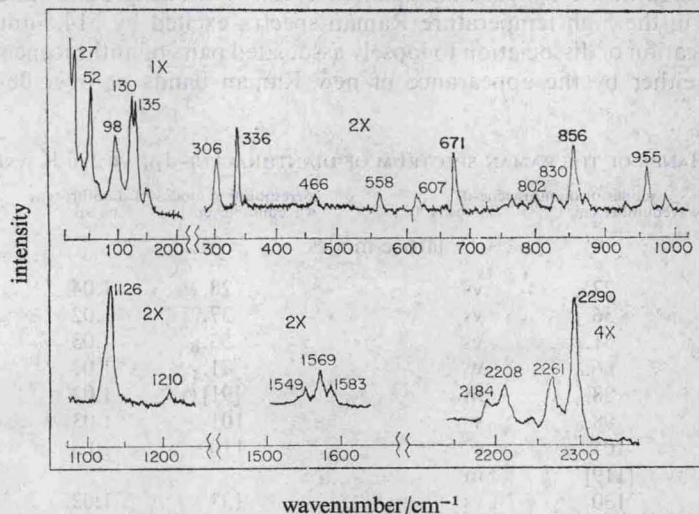


FIG. 4.—Raman spectrum of dianthracene- $d_{20}$  powder at 1 bar and 296 K.

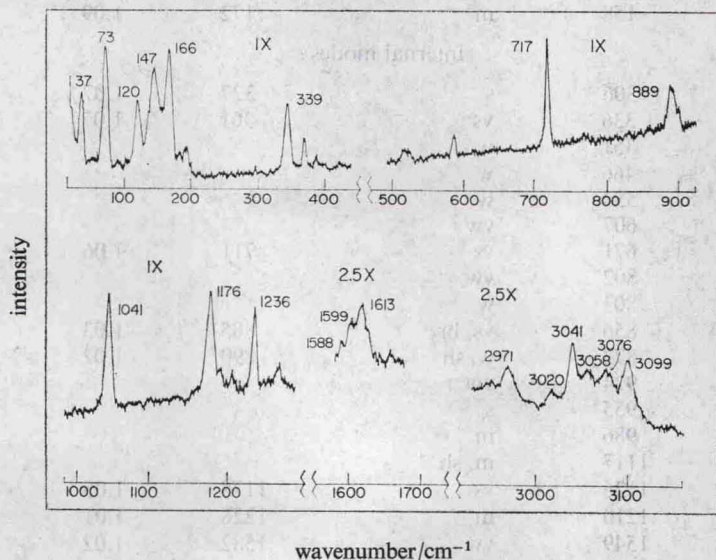


FIG. 5.—Raman spectrum of dianthracene at 10 kbar and 296 K.

(table 2). Significant qualitative changes are noted in the high pressure spectrum of the lattice phonons, with the behaviour being attributed to differing pressure dependence of the vibrational modes. Fig. 6 shows that one mode, originally at  $110\text{ cm}^{-1}$  (1 bar), separates from a mode at  $101\text{ cm}^{-1}$  (1 bar), sweeps across the peak at  $133\text{ cm}^{-1}$  (1 bar), and finally appears as a high frequency shoulder of the  $133\text{ cm}^{-1}$  peak. This implies that the modes at  $110$  and  $133\text{ cm}^{-1}$  are of different symmetry.