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Phase Behavior of some Condensed Polycyclic Aromatics

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PHASE BEHAVIOR OF SOME CONDENSED POLYCYCLIC AROMATICS

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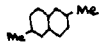
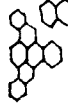
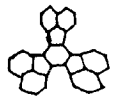
This letter reports phase behavior for 11 polycyclic aromatics. Although melting temperatures for these materials have been published elsewhere, no previous latent heat data are known to us. The experimental methods of Ref. 1 were used. Both transition temperatures and latent heats were obtained by differential scanning calorimetry (DSC). By taking appropriate precautions it was possible to study transitions at temperatures as high as 770K.

Samples were obtained from commercial sources, with one exception - ovalene.[2] No attempt at purification was made because of the limited quantities of material available (50-1000 mg). Sample purity was indicated by the DSC spectral "quality" (i.e. the sharpness of the DSC lines corresponding to first order phase transitions). For the most part, the quality was reasonably good, indicating acceptable purity of the samples. A check on purity was also provided by comparing measured melting temperatures with previously published values. In all cases but one the temperatures were comparable to or greater than literature values, confirming the adequacy of purity levels. Transition temperatures were determined from positions of maximum DSC peak height, the accepted procedure for analysis of all but very sharp peaks[1-3]. Latent heats were found by planimeter interation of peak areas, using the baseline correction of Smith[4]. Experimental uncertainties in temperature and latent heat determination are estimated to be no more than $\pm$ 0.5K and $\pm$ 1% respectively. Experimental scatter is indicated in Table I.

The transition temperatures and latent heats are listed in Table I. In addition to melting data, Table I also gives parameters for solid-solid phase transitions for two compounds - benzo (m, n, o) fluoranthene and ovalene.

TABLE I. PHASE BEHAVIOR OF 12 CONDENSED POLYCYCLIC AROMATICS

Compound	Structure	Mol. Wt.	DSC Spectral Quality[e]	Melting Data T(K)	Melting Data L(KJ/mol)	Other Transitions T(K)	Other Transitions L(KJ/mol)
1,4-dimethylnaphthalene $C_{12}H_{12}$		156.2	F	279.9±.2[a] 280.9[b]	10.6±.3[a]		
2,3-dimethylnaphthalene $C_{12}H_{12}$		156.2	G-E	378.4±.3[a] 378[b]	15.9±1.2[a]		
2,6-dimethylnaphthalene $C_{12}H_{12}$		156.2	G-E	383.9±.2[a] 383[c]	25.1±.04[a]		
benzo(m,n,o)fluoranthene $C_{18}H_{10}$		226	E	424.4±.4[a] 421[c]	11.8±.1[a]	352.7[a] 402.1[a] 402.8[a]	0.435±.02[a] 0.88 ± .04[a] 5.35 ±.08[a]
1,12-benzoperylene $C_{22}H_{12}$		276.3	G	553.0±.2[a] 545[c]	17.6±.08[a]		
o-phenylenepyrene $C_{22}H_{12}$		276.3	P-F	435[a] 436[d]	21.5[a]		
Coronene $C_{24}H_{12}$		300.4	G-E	710.5±.2[a] 711[c]	19.2±1.2[a]		
1,12-phenyleneperylene $C_{26}H_{14}$		326.4	F	541.5±.4[a] 541[d]	17.26±.8[a]		
1,2,4,5,8,9 tribenzopyrene $C_{28}H_{16}$		352	G	608[a] 604[c]	28.8[a]		
ovalene $C_{32}H_{14}$		398.5	F	770.1±.6[a] 746[d]	17.4±1.1[a]	729±1[a]	8.08±.5[a]
decacyclene $C_{36}H_{18}$		450.5	F	666[a] 660[c]	25.4±1.5[a]		

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c. Dictionary of Organic Chemistry, Oxford Press, New York (1965) (plus supplements).

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e. E = excellent, G = good, F = fair, P = poor.

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2. The author is grateful to Dr. S. Aronson for supplying the sample of ovalene.

3. Perkin-Elmer Corp., Instructions, Model DSC-2 Differential Scanning Calorimeter, Perkin-Elmer, Norwalk, CT 4-3 (1974).

4. G. W. Smith, Thermochimica Acta 21, 431 (1977).