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Solid–liquid equilibria of biphenyl binary systems

Issam Boudouh [a], Ismahane Djemai [b], Juan Antonio González [c], Djamel Barkat [a]

[a] Département de chimie industrielle, Université de Mohamed Khider, BP 145 RP, Biskra 07000, Algeria
[b] I.G.C.H.A, Université Hadj Lakhdar, Batna 05000, Algeria
[c] G.E.T.E.F., Grupo Especializado en Termodinámica de Equilibrio entre Fases, Departamento de Física Aplicada, Facultad de Ciencias, Universidad de Valladolid, E-47071, Valladolid, Spain

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ABSTRACT

Solid–liquid equilibrium temperatures, obtained by means of a differential scanning calorimetry (DSC) technique, are reported for biphenyl + *n*-C_{21}, or + *n*-C_{31}, or + *n*-C_{41} systems. Biphenyl + alkane, or + heterocyclic compound (diphenyl ether, dibenzofuran, indole, diphenylamine, 1-octadecanol or octadecanoic acid) have been investigated using DISQUAC and the ideal solubility model. This model provides good results for alkane solutions whose components which largely differ in size. Interactional effects are relevant in solutions with heptane, octadecane or mixtures involving dibenzofuran, indole, 1-octadecanol or octadecanoic acid.

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1. Introduction

In the fields of chemistry, biochemistry, or material science, aromatic–aromatic interactions are very relevant when evaluating the properties of many systems. Usually, such interactions occur between parts of complex molecules. Thus, the stabilization of the tertiary structure of proteins has been ascribed to the mentioned aromatic–aromatic interactions [1]. These interactions are also present in mixtures containing polycyclic aromatic hydrocarbons (PAHs), molecules which can be considered as built by blocks of benzene. They are typically found in crude oil, coal heavy petroleum products or lubricants and in many processes such chemical transformations of crude oil or incomplete combustion of hydrocarbon fuels. On the other hand, PAHs are environmental pollutants and present mutagenic and carcinogenic activities [2–4] and it is necessary to determine their solubility in different media, air, particulates or soil. The investigation of mixtures involving a PAH and a long chain alkane is needed as they play an important role in the flocculation and deposition of asphaltenes [5,6], a very important problem during the exploitation, transport and storage of crude oil. In addition, these solutions are precursors of the complex systems encountered in fluid reservoirs, and their study is also convenient as a first step for the investigation of mixtures containing heteroaromatic compounds, present in large amounts in coal tar and coal liquids. Biphenyl is an interesting compound. For example, it is part of the active group in the antibiotic oritavancin, used for skin infections. Due to its stability and inertness, biphenyl is also employed as heat-storage material [7], and the eutectic mixture diphenyl ether + biphenyl is used as heat transfer agent [8].

In this work, we provide solid–liquid equilibrium (SLE) temperatures, determined by means of a differential scanning calorimetry (DSC) technique, for biphenyl + *n*-C_{21}, or + *n*-C_{31}, or + *n*-C_{41} systems, which are also treated using the group contribution model DISQUAC [9]. Systems containing benzene, toluene, alkylbenzenes [10] or PAHs such as naphthalene, phenanthrene, anthracene or pyrene [11] and *n*-alkanes have been previously investigated in terms of this theory. Here, we have also developed a DISQUAC study of the biphenyl + *n*-C_7 [12], or + *n*-C_{18} [13] or + *n*-C_{22} [14], or + *n*-C_{24} [15], or + *n*-C_{26} [16] or + *n*-C_{28} [15] mixtures using the SLE data available in the literature. In addition, this DISQUAC treatment is extended to some binary systems containing biphenyl and a polycyclic compound such as diphenyl ether [7,17] or dibenzofuran [14,18] or indole [17,19], or diphenylamine [20], or 1-octadecanol [21], or octadecanoic acid [21].

2. Experimental

2.1. Materials

All the chemicals were used as delivered without further purification. Table 1 provides information about the source and purity of the compounds. Table 2 lists physical properties measured in this work, together with literature data, of biphenyl and *n*-alkanes: T_m, melting temperature, ΔH_m molar enthalpy of fusion, ΔC_{pm}, change of the molar heat capacity during the melting process of the compound, T_{tr}, transition temperature and ΔH_{tr}, the molar enthalpy of transition. These

E-mail address: jagl@termo.uva.es (J.A. González).

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Table 1
Sample description.

Chemical	CAS number	M[a]/gmol^{-1}	Source	Purity[b]
Biphenyl	92-52-4	154.211	Acros	>0.98
n-C_{21}	629-94-7	296.574	Alfa Aesar	>0.98
n-C_{31}	630-04-6	436.839	Fluka	≥0.99
n-C_{41}	7194-87-8	577.105	Fluka	≥0.99

[a] Molar mass.
[b] In mass fraction.

properties are in globally fair agreement with values from the literature (Table 2).

2.2. Procedure and experimental results

Biphenyl and n-alkanes are completely miscible in the liquid state. Experimental methodology was followed as described in the literature [22–24]. For each binary system, the mixture was heated under constant agitation until complete melting of the least volatile compound and the sample was heated very slowly inside a glass cell. After melting, the cell was immersed rapidly in a liquid nitrogen bath to obtain a homogeneous solid mixture. Then, a small amount of solid (5 to 10 mg) was sealed in the aluminium pan of the DSC (204F1 Phoenix ASC). The instrument was calibrated using 99.99% pure Indium (T_m = 429.70 K; ΔH_m = 28.45 J · g^{-1}). The solubility measurements were carried out under an inert atmosphere (20 ml · min^{-1}). The heating rate was fixed at 0.8 K min^{-1}. The accuracy of the temperature measurements is ±0.1 K and the corresponding reproducibility is ±0.3 K. The accuracy of the mole fraction is 0.0005.

Results for the solid–liquid equilibrium temperatures are given in Table 3. No data have been encountered in literature for comparison.

3. DISQUAC model

3.1. Main features

The main features of the model are presented briefly. (i) DISQUAC is a group contribution model based on the rigid lattice theory developed by Guggenheim [25]. (ii) The total molecular volumes, r_i, surfaces, q_i, and the molecular surface fractions, α_i, of the compounds present in the mixture are calculated additively on the basis of the group volumes R_G and surfaces Q_G recommended by Bondi [26]. As volume and surface units, the volume R_{CH4} and surface Q_{CH4} of methane are taken arbitrarily [27]. The geometrical parameters for the groups referred to in this work

Table 2
Physical properties of pure compounds: melting temperature, T_m, enthalpy of fusion, ΔH_m; heat capacity change at the melting point, ΔC_{pm}; transition temperature, T_{tr} and enthalpy of the transition, ΔH_{tr}.

Compound	T_m/K	ΔH_m/kJ · mol^{-1}	ΔC_{pm}/kJ · mol^{-1}	T_{tr}/K	ΔH_{tr}/kJ · mol^{-1}
Biphenyl	341.4	18.78	36.3[a]		
	342.10[b]	18.53[b]			
	342.1[c]	18.57[c]			
	341.62[d]				
	340.69[e]				
n-C_{18}	301.25[d]	61.71[f]	71.2[g]		
n-C_{21}	312.5	48.26	−100[h]	304.40	16.15
	313.2[i]	47.7[i]		304.4[i]	16.6[i]
	313.00[j]	46.6[j]			
n-C_{22}	316.95[k]	39.76[l]	58.5[l]	316.15[l]	36.35[l]
n-C_{24}	323.8[m]	54.90[l]	66.6[l]	321.25[n]	31.30[n]
n-C_{26}	329.21[e]	68.34[e]	78.3[l]	326.40[e]	36.72[e]
n-C_{28}	334.7[m]	66.52[l]	118.9[l]	331.15[l]	33.66[l]
n-C_{31}	341.3	81.86		334.70	27.53
	340[i]	73.3[i]		335.2[i]	36.6[i]
n-C_{41}	355.1	176.17			
	354.8[i]	149.2[i]			
	357.45[n]	134.5[n]			
Diphenyl ether	300.13[b]	17.05[b]			
Dibenzofuran	355.70[o]	18.35[o]	9.6[o]		
Indole	326.26[p]	10.9[p]			
Diphenylamine	326[q]	17.86[r]			
1-octadecanol	331.2[s]	47.2[t]			
Octadecanoic acid	339.3[s]	61.21[u]			

[a] [44]
[b] Ref [7].
[c] [45].
[d] [13].
[e] [16].
[f] [46].
[g] [47].
[h] From linear extrapolation of data for odd- and even-numbered n-alkanes in [47].
[i] [48].
[j] [49].
[k] [14].
[l] [50].
[m] [15].
[n] [51].
[o] [18].
[p] [19].
[q] [20].
[r] [52].
[s] [21].
[t] Calculated from differences between ΔH_m and ΔH_{tr} given in [53,54].
[u] [55].

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