Relationship between chemical composition and pyrolysis behaviour
of a medium temperature pitch (or Lurgi-gasifier pitch)

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Abstract.

This paper studies the chemical composition and pyrolysis behaviour of a medium temperature pitch produced in the Sasol-Lurgi coal gasification process. The results are compared to a commercial petroleum pitch and a commercial binder coal-tar pitch. The SASOL pitch had a high content in oxygen, mainly forming phenols, which make it very reactive at temperatures between 410-430°C, temperatures at which the commercial pitches do not react in a great extent. Despite the high reactivity shown by the SASOL pitch, anisotropic structures, of peculiar shapes, where developed on pyrolysis. Also noticeable is the low polyaromatic hydrocarbons (PAH) content of this pitch, which is of significant interest from a safety and environmental point of view. On the light of these results, possible applications for the SASOL pitch are pointed out.

Key words.- Medium temperature pitch, chemical composition, thermal analysis, mesophase
1. Introduction

Pitches are one of the most important precursors to carbon. Different to resins, pitches normally have a high carbon yield and are capable of developing graphitisable carbons on pyrolysis [1, 2]. However, pitches differ significantly in chemical composition depending on their origin. This in turn determines their behaviour during pyrolysis and the characteristics of the resultant materials [3]. The most common coal-based pitches are the so-called binder and impregnating pitches, currently used for the preparation of anodes and electrodes for the aluminium and steel industry respectively [4]. Other applications include the preparation of high value-added carbon materials, such as fibres and composites, with applications in racing cars, aeronautics and aerospace, among others. However, for this kind of applications commercial pitches need to be pre-treated in order to improve some of their properties, such as increasing their carbon yield, retaining at the same time a relatively high fluidity [5, 6].

In the last few years, there has been an increasing interest for the use of pitch-based carbon materials in energy applications (Li-ion batteries and super-capacitors) [7-9]. The great variety of carbon materials that can be prepared, by tailoring their structure through an adequate selection of the precursor and/or the processing conditions, makes it possible to achieve high efficiency for Li insertion or high storage capacity. In this context, it would be of great interest to search on the potential of other pitches rather than the traditional binder and impregnating coal-tar pitches, which may have an additional value. Medium temperature pitches are produced by distillation of tars generated as by-products of the Lurgi coal gasification process. In the Sasol process, the distillate tars are converted to transport
fuels via hydrogenation whereas the pitch residue is converted via delayed coking to carbon; the coker gas oil being blended with the distillate tars. The testing of the medium temperature pitches as precursors of new carbon materials is of great interest both from a scientific and a commercial point of view. The former because it would enrich the knowledge on the behaviour of their components on pyrolysis and their effect on the structure of the final carbons, and the latter because it would widen the applications of these pitches.

The aim of this paper is to get a deeper knowledge on the composition and pyrolysis behaviour of a Lurgi medium temperature pitch and to envisage its potential as carbon precursor. A commercial binder coal-tar pitch and a commercial petroleum pitch (A240) have been used as a reference, in order to compare their properties and behaviour.

2. Experimental

2.1. Raw materials

A medium temperature pitch, produced by distillation of a tar from the Lurgi gasification process by SASOL, has been used in this study and will be referred to as SASOL. Two other commercial pitches, a coal-tar pitch (CTP or BINDER) supplied by Nalonchem and petroleum pitch Ashland A-240 (PP or ASHLAND) were also studied for comparative purposes. The main characteristics of these pitches are summarised in Table 1.
2.2. Characterisation of raw materials

2.2.1 Softening point. Mettler softening point (SP) of the different pitches was measured using a Mettler Toledo FP90 following the ASTM D3104 standard procedure. A small cup (with pierced bottom) was filled with approximately 0.5 g of pitch. The cup was placed in the Mettler furnace and preheated to 20°C below the expected SP. Subsequently, the oven temperature was increased at a rate of 2°C min\(^{-1}\) until a drop of pitch flowed through the hole, which characterised the softening temperature of the pitch.

2.2.2. Solubility. The solubility in toluene was determined using a standard procedure. Two grams of samples, < 0.4 mm particle diameter, and 100 mL toluene were placed in a 500 mL flask. The solution was heated to boiling point, and maintained under reflux for 30 min. Filtering was performed with a No. 4 porous ceramic plate. The residue was washed with hot toluene and acetone for complete removal of the toluene soluble.

The procedure used to determine pitch solubility in N-methyl–2-pyrrolidone (NMP) was similar to that presented above. One gram per sample and 25 mL of NMP were placed in a 100 mL flask. The solution was then heated to boiling point and maintained under reflux for 30 min. The residue was washed with hot NMP, toluene and acetone for complete NMP removal.

2.2.3. Elemental analysis. Carbon, hydrogen, sulphur and nitrogen contents were determined using a LECO-CHNS-932 microanalyser. Oxygen content was obtained using a LECO-TF-900 furnace coupled to the same microanalyser.
2.2.4. *Infrared spectroscopy*. The aromaticity indices of the different samples were calculated from their infrared spectra. The spectra were obtained in a Nicolet Magna IR-560 spectrometer, using the diffuse reflectance (DRIFT) accessory COLLECTOR and a MCT-A detector refrigerated with liquid nitrogen. Solid samples (0.2 mm particle diameter) were placed in a 0.10 g holder. 64 scans (2 cm\(^{-1}\) resolution) per sample were registered between 4000 and 600 cm\(^{-1}\). Aromaticity indices were calculated from the spectra following a procedure described by Guillén et al. [10].

2.2.5. *Optical microscopy*. Optical microscopy examination under polarized light was carried out on samples embedded in an epoxy resin and polished. The microscope was equipped with an adjustable ocular (10 X), an oil immersion objective (50 X) and a 1-wave retarder plate. Micrographs of the most representative features were taken using a Leica DC100 digital camera.

2.2.6. *Gas chromatography*. Gas chromatography was performed on 25 mg of sample dissolved in 2 mL toluene. Tridecane, N-icosane and triacontane were used as internal standards. Analyses were performed in an HP chromatograph fitted with a HP-1 capillary column (crosslinked methyl siloxane column) and a FID detector. 1 μL of sample was injected in splitless mode and the oven temperature increased from 50°C to 280°C at 4°C/min\(^{-1}\). Hydrogen was used as the carrier gas at a flow rate of 35 mL min\(^{-1}\). The injector temperature was 315°C and detector one was 300°C. The toxicity of the pitches was evaluated in terms of the PAH concentration and benzo[a]pyrene equivalents in the samples, following the procedure established elsewhere [11, 12].
2.2.7. *Size exclusion chromatography.* Size exclusion chromatography (SEC) was carried out using a 30 cm long, 7.5 mm o.d. polystyrene-polydivinylbenzene column (Mixed-D, 5 mm particle size; Polymer Laboratories). All pitches were run at 80°C with NMP at a flow rate of 0.5 mL min\(^{-1}\). Detection was carried out at different wavelengths using a Perkin-Elmer LC250 variable wavelength UV-absorption detector and a diode array detector. The eluent was pumped using a Perkin-Elmer isocratic pump with a maximum pressure of 14 MPa.

2.2.8. *Phenols extraction.* One gram of the SASOL pitch was dissolved in 200 mL toluene. 200 mL of a 10 % NaOH solutions were added to form the phenolates from phenols in the pitch. The organic phase and the aqueous phase, which contained the phenolates, were separated in a decantation funnel. Phenols were restored in the aqueous phase by adding concentrated HCl to the solution until pH=3. Toluene was added to the solution and the phenols were finally extracted in the organic phase. The two fractions obtained, the phenols enriched one and the residual pitch, were characterised by IR and size exclusion chromatography. Phenols were sililated with hexamethyldisilazane maintaining the mixture under reflux for an hour. Sililation was required in order to block the alcohol groups in order to be able to perform gas chromatography analysis without damaging the column.

2.2.9. *Thermogravimetry.* The thermal behaviour of the different pitches was studied from the weight loss curves (TG) and the curves of the first derivative of the weight loss with respect to time (DTG). TG and DTG analyses were performed in a TA Instruments SDT 2960 thermal analyser on 10 mg of sample (particle diameter \(< 0.4\)
mm). The temperature was increased up to 1000°C at a heating rate of 10°C min⁻¹ under a nitrogen flow of 95 mL min⁻¹.

2.3. Pitch pyrolysis behaviour

Pitch pyrolysis behaviour was studied by treating the pitches at 410, 420 and 430°C respectively for 3 h, under a dynamic nitrogen pressure of 1 MPa and a flow of 40 L h⁻¹. Treatments were performed with 12 g of sample in Pyrex tubes that were placed in an autoclave with an internal volume of 2 L. The bottom part of the tubes (approximately 5 cm) are embedded in a steel block to ensure temperature uniformity throughout the sample. After completing the treatment, reactions were quenched by releasing the pressure before cooling down in order to release the volatile matter. The tubes were cut longitudinally into two halves. One halve was embedded in epoxy resin, ground and polished for optical microscopy examination. The other halve was characterised in the same way as described above. Samples were labelled SASOL-1, SASOL-2 and SASOL-3 for the treatments at 410, 420 and 430°C respectively, and in a similar way for the other two pitches.

3. Results and discussion

3.1. Characterisation of pitches

As received pitches were ground <0.4 mm particle size and characterised following the procedures described in the experimental section. The main properties of these pitches are summarised in Table 1. The softening point of the SASOL pitch (74°C) is the lowest of the three pitches. The toluene insoluble content is low compared to the coal-tar pitch but slightly higher than the petroleum pitch. At the same time, the SASOL and petroleum pitch are completely soluble in NMP, while
the coal-tar pitch has around 16 wt. % NMPI, this being related with the primary quinoline insolubles present in the binder pitch. The hydrogen content is also the highest for the SASOL pitch while the aromaticity index is the lowest. This indicates that this pitch has a high aliphatic content, even higher than the petroleum pitch. But the most striking characteristic of this pitch is the high oxygen content, 7.49 wt. %. In view of these results, a high reactivity of this pitch could be expected, which may hinder the development of anisotropy in this pitch during pyrolysis. The results obtained also indicate that the SASOL pitch has similar properties to low temperature pitches, i.e. high oxygen content and low aromaticity [13].

Infrared spectroscopy of the samples was performed in order to obtain information about the functional groups present in the samples. Different to the other two pitches, the SASOL pitch shows a wide band at 3500 cm\(^{-1}\), related to the presence of phenolic groups or carboxylic acids (Figure 1). After extraction of the phenols, the remaining pitch did not show this band (Figure 2). Moreover, the fraction containing the phenols shows a strong band at around 1200 cm\(^{-1}\), due to C-O bonding stretching that is not present in the residue. This corroborates that the main oxygenated groups present in the SASOL pitch are phenols, as it is also the case in low temperature pitches [13, 14].

Gas chromatography was used to evaluate the relative amount of different polyaromatic hydrocarbons, with different degrees of potential toxicology, present in the different pitches. There is an increasing demand for these determinations due to environmental and safety regulations. The results obtained are summarised in Table 2. The coal-tar pitch has the highest content in the PAH studied, followed by the
SASOL pitch, while the petroleum pitch has the lowest content. However, when the benzo(a)pyrene equivalents are estimated, the SASOL pitch has about the same content as the petroleum pitch, which is significantly lower than in the coal-tar pitch. The results obtained can also be expressed in terms of the total content in PAHs of different toxicity (low, medium and high) (Figure 3). The results show that the SASOL pitch has about the same content in low toxicity PAHs as the coal-tar pitch, while the petroleum pitch has the lowest content in this type of compounds. When PAHs of higher toxicity are evaluated, the differences between the three pitches increase, the coal-tar pitch having the highest content (5.45 %), followed by the SASOL pitch having around half of that content (1.95 %) and finally the petroleum pitch with just an 0.72 %. However, when the most toxic compounds are evaluated, the SASOL pitch has slightly less content than the petroleum pitch (0.95 vs 0.98 %), while the coal-tar pitch has the highest content (2.93 %), as could be expected. These results indicate that the SASOL pitch has a significant lower toxicity than the binder coal-tar pitch, it being similar to that of the petroleum pitch, which is a great advantage to the use of SASOL pitch in some applications, as restrictions to toxic PAHs emissions are rapidly increasing.

Size exclusion chromatograms of the pitches are shown in Figure 4. From the two peaks that are normally observed in the chromatographic region, the one that elutes at shorter times is related with larger size compounds, but also contains those with functional groups [13]. This peak is more intense in the SASOL pitch and also its intensity is higher than the one at longer retention times. This was corroborated by analysing the fractionated SASOL pitch (Figure 5). The results show that in the chromatographic region, the fraction containing the phenols elutes at shorter times
than the pitch residue, where phenols were extracted. The profile of both curves together perfectly matches the curve corresponding to the whole pitch. Additionally, pure compounds were analysed by SEC in order to compare their retention times with the peaks observed in the pitches. Toluene, phenol and cresol elute at longer retention times than the phenolic fraction of the SASOL pitch, which indicates that the phenols of this pitch are of higher molecular weight than the compounds analysed.

The thermogravimetric analysis of the SASOL pitch (Figure 6) indicated that this pitch has a low carbon yield (10 wt. %) at atmospheric pressure. This is due to the high amount of light compounds. The temperature of initial weight loss is also low, around 125°C, as compared to the binder and petroleum pitches which initiate weight loss at around 200°C. The presence of light compounds is also reflected in the DTG results (Figure 6b), where the SASOL pitch shows a wide band due to distillation centered at 300°C. In fact, the SASOL pitch losses about 60 % of its weight below the 350°C. By contrast, the petroleum pitch losses most of its weight between 350°C and 550°C, while the binder pitch is in between them. These results suggest that the use of pressure will be required for the conversion of the SASOL pitch into carbons.

It should be born in mind that the SASOL pitch is a soft pitch, which softening point has not been increased to fit user’s requirements, as it is common practice in the commercial petroleum and coal tar pitches. Therefore, the initial properties of the SASOL pitch could be improved by an additional treatment prior to
supply. In this way, the softening point, insoluble content and carbon yield, for example, would be increased.

3.2. Pitch pyrolysis behaviour

Pyrolysis of the three pitches was performed at temperatures of 410, 420 and 430°C for 3 h and under 1 MPa pressure in order to avoid excessive distillation of the SASOL pitch components. Some of the main properties of the pyrolysis products are summarised in Table 3. Under the pressure conditions used, the carbon yield from the SASOL pitch was continuously lower than that obtained from the binder pitch and petroleum pitch. The yield for the former was usually between 70-80 wt- % whereas that for the latter between 90-98 wt. %. The softening point for the Sasol pitch increased significantly after pyrolysis and it was higher than for the other two pitches. After treatment at 430°C, the softening point could not be measured by the Mettler procedure as it was higher than 350°C. The insoluble content also increased significantly. This behaviour could be due to the high content of functional groups present in this pitch, which leads to a high reactivity. The C/H ratio also increased significantly for the SASOL pitch with increasing pyrolysis temperature (from 1.58 to 1.85) whereas for the other two pitches the change was not significant. These results suggest that at the temperatures studied the SASOL pitch has significantly higher reactivity than the other two pitches. The significant decrease in oxygen content observed for the SASOL pitch indicates that the oxygenated compounds are lighter and distil during the treatments or they are more prone to reaction and oxygen containing molecules are removed as decomposition products. On the other hand, the oxygen content in the other two pitches did not change significantly, indicating that the oxygenated compounds present are less reactive and/or less volatile.
After pyrolysis of the SASOL pitch at 410°C (SASOL-1), some mesophase spheres are developed (Figure 7 a). These spheres are very small as compared to those developed in the petroleum and the coal-tar pitch (Figure 7 b and 7 c). In addition, the spheres in the SASOL sample tend to be in clusters, while very small mesophase spheres are dispersed in the continuous isotropic phase. The formation of clusters could be due to several reasons. First, it could be that the mesophase easily binds together but the internal viscosity of the spheres is high and makes it difficult to coalesce to form a new spherical form. It could also be that the reaction medium is relatively turbulent, so promoting the mobility and contact between the spheres. The formation of gas bubbles would support the turbulent medium. On the other hand, the mesophase spheres present in the petroleum pitch are big and dispersed in the isotropic phase, not in clusters. In the binder pitch, the presence of primary quinoline insolubles determines the development of mesophase. Large mesophase spheres surrounded by quinoline insolubles are observed, the shape of the spheres being more irregular.

After pyrolysis at 420°C, the mesophase spheres in the SASOL sample have coalesced, to a greater extent than in the other two pitches (Figure 8). This is more evident in the sample at the bottom of the tube (Figure 8 a-bottom). At the top (Figure 8 a-top), the spheres are smaller and do not form clusters. This seems to indicate that the clusters of mesophase spheres initially formed, and which probably correspond to the more reactive fractions of the pitch, have deposited at the bottom of the tube. In the petroleum pitch, the mesophase spheres have also sedimented at the bottom of the tube, but in this case, the spheres have not coalesced. The
behaviour of the binder pitch is different, few single mesophase spheres are observed, and anisotropic structures are associated to the quinoline insolubles, forming aggregates. No sedimentation was observed in this sample.

After treatment at 430°C (Figure 9), the situation in the petroleum and coal-tar pitch is similar to that observed at 420°C. However in the SASOL (Figure 9 a) pitch significant amount of coalesced mesophase is observed. The anisotropic regions exhibit unusual structures derived from the clusters formed initially. Their texture decreases from the bottom to the top of the tube. These results are quite significant because one would not expect this highly reactive pitch to develop such anisotropic structures. Also noticeable is the peculiar anisotropic structures developed, which have not been observed in other systems.

The unusual characteristics shown by the SASOL material make it a unique pitch among current commercial pitches. Some of the properties displayed by this pitch may limit its use in traditional applications. However, due to these same peculiarities it may be possible to use it in other emerging fields where carbon materials can play an important role. It is worth remarking its relatively low content in toxic PAHs, especially if benzo(a)pyrene equivalents are considered. But what really makes the SASOL pitch different from the other two pitches studied is its high oxygen content, which makes the reactivity of this pitch to be high at relatively low temperatures. Despite this high reactivity, the SASOL pitch is able to generate anisotropic structures on pyrolysis, as previously described. Possible applications for this pitch could be found as precursors of carbon materials for different energy storage systems such as Li-ion batteries or supercapacitors. In the case of
supercapacitors, it has been recently proven that the presence of functional groups that alter the surface chemistry of the carbon material could have a positive influence on the charge capacity of the electrodes [14]. In addition, the SASOL pitch could also be used in applications similar to those of low temperature pitches, like wood protection or agricultural uses.

4. Conclusions

The SASOL pitch is different to other commercial pitches in that it has a significant aliphatic content and specially an extremely high oxygen content. This oxygen is mainly in the form of phenols, as confirmed by the fractionation sequence used followed by infrared analysis of the fractions obtained. There is also an important content in light compounds, as reflected by the low carbon yield and weight loss bands due to distillation as observed by thermogravimetric analysis. However, light compounds could be removed, thus increasing the carbon yield by means of a treatment prior to supply, as it is common practice with commercial coal-tar and petroleum pitches.

The SASOL pitch has a relatively low PAHs content, especially those compounds with higher toxicity. This is a great advantage of this pitch in comparison with coal-tar pitches, which applications are increasingly being limited by safety and environmental regulations.
On pyrolysis at temperatures between 410–430°C, the SASOL pitch was found to be highly reactive, when compared to commercial petroleum and coal-tar pitches. The softening point, insoluble content in toluene and NMP increased significantly after the treatments. Despite this high reactivity, anisotropic structures were developed, these having a peculiar and unique shape.

The unusual characteristics shown by the SASOL pitch suggest a significant potential of this pitch in emerging applications such as precursor of carbon materials for different energy storage systems i.e. Li-ion batteries or supercapacitors.

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References


<table>
<thead>
<tr>
<th>Pitches</th>
<th>SP</th>
<th>TI</th>
<th>NMPI</th>
<th>C</th>
<th>H</th>
<th>N</th>
<th>S</th>
<th>O</th>
<th>C/H</th>
<th>Iar</th>
</tr>
</thead>
<tbody>
<tr>
<td>SASOL</td>
<td>74</td>
<td>5.28</td>
<td>0</td>
<td>84.62</td>
<td>5.84</td>
<td>1.65</td>
<td>0.40</td>
<td>7.49</td>
<td>1.21</td>
<td>0.25</td>
</tr>
<tr>
<td>ASHLAND</td>
<td>127</td>
<td>3.36</td>
<td>0</td>
<td>91.99</td>
<td>5.05</td>
<td>0.20</td>
<td>1.54</td>
<td>1.22</td>
<td>1.52</td>
<td>0.37</td>
</tr>
<tr>
<td>BINDER</td>
<td>115</td>
<td>33.59</td>
<td>16.12</td>
<td>93.12</td>
<td>3.88</td>
<td>0.99</td>
<td>0.47</td>
<td>1.54</td>
<td>2.00</td>
<td>0.50</td>
</tr>
</tbody>
</table>

SP, Mettler softening point (°C)  
TI, toluene insoluble content (wt. %)  
NMPI, N-methyl-2-pyrrolidone insoluble content (wt. %)  
C, carbon content (wt. %)  
H, hydrogen content (wt. %)  
N, nitrogen content (wt. %)  
S, sulfur content (wt. %)  
O, oxygen content (wt. %)  
C/H, atomic ratio  
Iar, aromaticity index
Table 2: PAHs evaluation and benzo(a)pyrene equivalent in the pitches.

<table>
<thead>
<tr>
<th>Compound</th>
<th>RTI</th>
<th>SASOL</th>
<th>COAL-TAR</th>
<th>ASHLAND</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naphthalene (L)</td>
<td>0</td>
<td>0.0436</td>
<td>0.0085</td>
<td>0</td>
</tr>
<tr>
<td>Acenaphthylene (L)</td>
<td>0</td>
<td>0.0109</td>
<td>0.0011</td>
<td>0</td>
</tr>
<tr>
<td>Acenaphtene (L)</td>
<td>0</td>
<td>0.0427</td>
<td>0.1780</td>
<td>0</td>
</tr>
<tr>
<td>Fluorene (L)</td>
<td>0</td>
<td>0.1826</td>
<td>0.0545</td>
<td>0.0049</td>
</tr>
<tr>
<td>Phenanthrene (L)</td>
<td>0</td>
<td>0.3568</td>
<td>0.3599</td>
<td>0.0466</td>
</tr>
<tr>
<td>Anthracene (L)</td>
<td>0</td>
<td>0.2342</td>
<td>0.0766</td>
<td>0.0142</td>
</tr>
<tr>
<td>Fluoranthene (M)</td>
<td>0.034</td>
<td>0.4990</td>
<td>0.7557</td>
<td>0.0789</td>
</tr>
<tr>
<td>Pyrene (L)</td>
<td>0</td>
<td>0.3617</td>
<td>0.6269</td>
<td>0.2482</td>
</tr>
<tr>
<td>Benzo(a)fluorene (L)</td>
<td>0</td>
<td>0.3773</td>
<td>0.297</td>
<td>0.0660</td>
</tr>
<tr>
<td>Benzo(b)fluorene (L)</td>
<td>0</td>
<td>0.2518</td>
<td>0.1639</td>
<td>0.0441</td>
</tr>
<tr>
<td>Benzo(a)anthracene (M)</td>
<td>0.033</td>
<td>0.3533</td>
<td>0.6836</td>
<td>0.2436</td>
</tr>
<tr>
<td>Chrysene (H)</td>
<td>0.260</td>
<td>0.1964</td>
<td>0.6732</td>
<td>0.3669</td>
</tr>
<tr>
<td>Benzo(b)fluoranthene (M)</td>
<td>0.100</td>
<td>0.3733</td>
<td>1.6064</td>
<td>0.0854</td>
</tr>
<tr>
<td>Benzo(k)fluoranthene (M)</td>
<td>0.100</td>
<td>0.0719</td>
<td>0.5394</td>
<td>0.0219</td>
</tr>
<tr>
<td>Benzo(e)pyrene (M)</td>
<td>0.050</td>
<td>0.4169</td>
<td>0.9232</td>
<td>0.2041</td>
</tr>
<tr>
<td>Benzo(a)pyrene (H)</td>
<td>1.000</td>
<td>0.3061</td>
<td>1.2414</td>
<td>0.2610</td>
</tr>
<tr>
<td>Indeno(1,2,3,-c,d)pyrene (M)</td>
<td>0.100</td>
<td>0.2409</td>
<td>0.9394</td>
<td>0.0910</td>
</tr>
<tr>
<td>Dibenzo(a,h)anthracene (H)</td>
<td>1.400</td>
<td>0.0855</td>
<td>0.2079</td>
<td>0.0480</td>
</tr>
<tr>
<td>Benzo(g,h,i)perylene (H)</td>
<td>1.000</td>
<td>0.3632</td>
<td>0.8084</td>
<td>0.3054</td>
</tr>
</tbody>
</table>

**PAH content (%)**  
4.77  
10.06  
2.13  

**B(a)P equivalents (%)**  
0.95  
2.87  
0.77

RTI, Relative toxicity index  
L, low toxicity  
M, medium toxicity  
H, high toxicity
Table 3. Main properties of samples obtained from pyrolysis of pitches.

<table>
<thead>
<tr>
<th>Pitches</th>
<th>Yield</th>
<th>SP</th>
<th>TI</th>
<th>NMPI</th>
<th>C</th>
<th>H</th>
<th>N</th>
<th>S</th>
<th>O</th>
<th>C/H</th>
<th>Iar</th>
</tr>
</thead>
<tbody>
<tr>
<td>SASOL-1</td>
<td>77.60</td>
<td>172</td>
<td>42.22</td>
<td>14.56</td>
<td>87.60</td>
<td>4.62</td>
<td>1.81</td>
<td>0.29</td>
<td>5.68</td>
<td>1.58</td>
<td>0.37</td>
</tr>
<tr>
<td>ASHLAND-1</td>
<td>96.43</td>
<td>127</td>
<td>27.58</td>
<td>8.25</td>
<td>91.43</td>
<td>4.57</td>
<td>0.21</td>
<td>1.46</td>
<td>2.33</td>
<td>1.67</td>
<td>0.41</td>
</tr>
<tr>
<td>BINDER-1</td>
<td>98.12</td>
<td>131</td>
<td>40.02</td>
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<td>33.48</td>
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<td>20.75</td>
<td>91.61</td>
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<td>32.54</td>
<td>92.02</td>
<td>3.76</td>
<td>0.96</td>
<td>0.42</td>
<td>2.84</td>
<td>2.04</td>
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</table>

SP, Mettler softening point (°C)  
TI, toluene insoluble content (wt. %)  
NMPI, N-methyl-2-pyrrolidone insoluble content (wt. %)  
C, carbon content (wt. %)  
H, hydrogen content (wt. %)  
N, nitrogen content (wt. %)  
S, sulfur content (wt. %)  
O, oxygen content (wt. %)  
C/H, atomic ratio  
Iar, aromaticity index
Figure captions

Figure 1.- Infrared spectra of pitches.

Figure 2.- Infrared spectra of SASOL pitch and its fractions.

Figure 3.- Different toxicity groups of PAHs present in the pitches.

Figure 4.- SEC chromatogram of pitches.

Figure 5.- SEC chromatogram of SASOL pitch and its fractions.

Figure 6.- a) TG curves of pitches; b) DTG curves of pitches.

Figure 7.- Optical microscopy of pitches pyrolysed at 410°C: a) SASOL; b) petroleum; c) binder pitch.

Figure 8.- Optical microscopy of pitches pyrolysed at 420°C: a) SASOL; b) petroleum; c) binder pitch.

Figure 9.- Optical microscopy of pitches pyrolysed at 430°C: a) SASOL; b) petroleum; c) binder pitch.
Figure 1

![Graph showing Kubelka-Munk values for Ashland, Coal-tar, and SASOL samples across different wavenumbers (cm⁻¹).]
Figure 2

![Graph showing Kubelka-Munk absorption spectra for SASOL, PHENOLS, and RESIDUE](image)

- **Kubelka-Munk**
- **Wavenumber (cm\(^{-1}\))**
- **SASOL**
- **PHENOLS**
- **RESIDUE**
Figure 3

The bar chart shows the content (%) of SASOL, COAL-TAR, and PETROLEUM in different groups of toxicity:

- **Low**
  - SASOL: ~1%
  - COAL-TAR: ~1%
  - PETROLEUM: ~0.5%

- **Medium**
  - SASOL: ~2%
  - COAL-TAR: ~5%
  - PETROLEUM: ~0.5%

- **High**
  - SASOL: ~2%
  - COAL-TAR: ~3%
  - PETROLEUM: ~1%
Figure 4
Figure 5

![Graph showing Sasol Phenols Residue](image-url)
Figure 8