Tetrahedron Letters No. 21, pp. 768-770, 1961. Pergamon Press Ltd. Printed in Great Britain.

THE OCCURRENCE OF PHYTANE IN PETROLEUM

R.A. Dean and E.V. Whitehead
The British Petroleum Company Limited
Research Centre
Petroleum Division
Sunbury-on-Thames, Middlesex

(Received 13 October 1961; in revised form 3 November 1961)

IN the course of recent studies on the composition of petroleum, we had occasion to remove normal paraffins from petroleum distillates boiling in the range 250°-370°C by means of molecular sieve 5A. The gas liquid chromatogram obtained on a non-aromatic fraction of an Agha Jari (Iran) distillate from which normal paraffins had been removed, showed very strong peaks having retention volumes on a silicone column very close to those of n-heptadecane and n-octadecane. These peaks were superimposed on the "envelope" which is present in chromatograms of all petroleum distillate fractions boiling above about 200°C, and it was estimated from their areas that the compounds giving rise to them were present, very approximately, to the extent of 0.3 per cent weight of the crude oil. No peaks of comparable magnitude were present at the retention volumes of other n-paraffins (C_{16} and C_{19} to C_{23}). This suggested that these two compounds did not, unlike many components of petroleum, belong to a series in which adjacent members, differing by one carbon atom, are present to approximately the same extent, e.g. the n- and 2-methyl-alkanes.

Our initial postulate was that they were both C_{20} compounds based on isoprene and to substantiate this they were isolated (5 mg of each) using a combination of fractional distillation, liquid thermal diffusion and trapping from gas chromatographic columns using a polyphenyl ether and silicone oil as successive stationary phases. The higher boiling of the two compounds had an infra-red spectrum very similar to that of phytane (2:6:10:14-tetramethylhexadecane, n_D^{20} 1.4418, synthesized from commercial phytol by catalytic hydrogenation with a platinum catalyst at 20°C and 100 atm, conversion of the dihydrophytol to its p-toluene-sulphonate, and reduction of this with lithium aluminium hydride) which in turn was identical within the limits of reproducibility with that recorded by Pliva and Sörensen[1]. Differences in the spectra of the isolated and synthetic compounds were the presence of minor peaks at 8.22, 10.1, 10.98 and 11.26μ and an overall higher absorbance in the former. Mass spectra of the isolated and synthetic materials were also similar, differences being attributable to the presence of other C_{20} branched chain paraffins. These results coupled with the identity of retention volumes (isolated and synthetic respectively: 1.06, 1.06 relative to n-octadecane with silicone oil as stationary phase at 257°C; 0.89, 0.89 relative to n-octadecane with a C_{30} polyphenyl ether as stationary phase at 257°C) make it reasonably certain that the compound almost coincident with n-octadecane on the silicone column is phytane.

The mass spectrum of the material almost coincident with n-heptadecane was, however, that of a C_{19} isoparaffin, not that of a hydrogenated isoprene tetramer. Identity of its retention volumes (0.79 on silicone, 0.65 on polyphenyl ether, conditions as above) with those of 2:6:10:14-tetra-

---

[1] J. Pliva and N.A. Sörensen, Acta Chem.Scand. 4, 846 (1950).

methylpentadecane[2] (0.79 and 0.64 respectively) suggests that it may have this structure. The quantity of the two hydrocarbons isolated was insufficient to permit the determination of their optical activity, however, a determination on a phytane-containing concentrate showed no measurable activity. Further confirmation of the structures of the two compounds, data on the amount present in a number of different crude oils and a discussion of the significance of their presence in petroleum (*cf*. page 312 of ref. 3) will form the subject of a future communication.

Acknowledgement - Our thanks are due to the Chairman and Directors of The British Petroleum Company Limited for permission to publish these results.

---

[2] J.S. Sörensen and N.A. Sörensen, *Acta Chem.Scand.* *3*, 939 (1949).

[3] S.F. Birch, T.V. Cullum, R.A. Dean and D.G. Redford, *Tetrahedron* *7*, 311 (1959).