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## GAS CHROMATOGRAPHIC STUDY OF THE ANALYSIS AND ELUTION MECHANISM OF HYDROGEN SULPHIDE, CARBONYL SULPHIDE AND LIGHT MERCAPTANS IN PETROLEUM GASES

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### SUMMARY

Qualitative and quantitative analyses of sulphur compounds in petroleum gases were studied by a simple gas chromatographic technique. A column with a high loading (30%) of Triton X-305 on Diatomite CQ and a flame photometric detector were used to determine COS, H<sub>2</sub>S, SO<sub>2</sub>, CS<sub>2</sub> and C<sub>1</sub>-C<sub>4</sub> mercaptans in the presence of hydrocarbon gases. Chemical abstraction of H<sub>2</sub>S with acidic CdCl<sub>2</sub> was used prior to the analysis of gases containing high percentages of H<sub>2</sub>S. The simple one-column technique used gave good results and concentrations down to 0.2 ppm of sulphur gases could be determined. The elution order of H<sub>2</sub>S, COS and *n*-propyl and *tert*-butyl mercaptan on different stationary phases in this work and as reported in the literature was studied. It was found that the geometry, dipole moment, electron polarizability and interaction distance of the molecule and the nature of the stationary phase affect the elution order.

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### INTRODUCTION

The presence of trace sulphur compounds, such as COS, CS<sub>2</sub> and C<sub>1</sub>-C<sub>4</sub> mercaptans, in petroleum gases has an adverse effect on the amine sweetening processes and can cause corrosion problems in certain units and towers. Therefore there is a need for a simple method for the qualitative and quantitative evaluation of individual sulphur compounds in different petroleum gas streams. The presence of high concentrations of H<sub>2</sub>S in some sour gases would obviously complicate the analysis.

A literature survey indicated that there have been various attempts to analyse samples containing some or most of these sulphur compounds with or without the presence of gaseous hydrocarbons<sup>1-23</sup>. In these attempts, more than one column, capillary columns, valve switching and/or modifications to the gas chromatograph were employed in order to simplify the analyses. Triton X-305 at a level of 10% on Chromosorb G with and without 0.5% phosphoric acid packed in 6- and 12-m flexible FEB columns has been used to determine sulphur compounds present in raw grain spirit<sup>15</sup>.

However, the determination of H<sub>2</sub>S, COS, SO<sub>2</sub>, CS<sub>2</sub>, C<sub>1</sub>-C<sub>4</sub> mercaptans and

hydrocarbons in petroleum gases using one column has not been reported. In previous work<sup>24</sup> we studied the analysis of SO<sub>2</sub>, COS, H<sub>2</sub>S, CS<sub>2</sub> and C<sub>1</sub>-C<sub>4</sub> mercaptans using 5% DC-QF1 on Porapak QS, but quantitation of some mercaptans was not possible owing to interference by co-eluted hydrocarbons on flame photometric detection as a result of the quenching effect<sup>20</sup>.

This paper reports the possibility of using simple techniques and one column packed with a high loading of Triton X-305 on Diatomite CQ for the qualitative and quantitative analysis of sulphur compounds in petroleum gas streams at levels down to 0.2 ppm. The mechanism of the elution orders of H<sub>2</sub>S-COS and *tert.*-butyl-*n*-propyl mercaptans on different stationary phases is discussed.

## EXPERIMENTAL

A Pye Unicam (U.K.) Model 304 gas chromatograph fitted with flame-photometric, flame-ionization and thermal conductivity detectors was used. The column end was linked to a 1:1:1 three-way splitter to connect it to each detector. A Model PM8252 dual-pen recorder (Pye Unicam) and a Model SP4100 computing integrator (Spectra-Physics, U.S.A.) were used. All syringes employed were of the gas-tight type (Hamilton, Switzerland) and ranged in volume from 0.1 to 1000 ml. Gas sampling bulbs with a septum port (Altech, U.S.A.) were employed together with a 10-l PTFE calibration kit (Houston Atlas, U.S.A.). Helium of 99.996% purity (Air Products, U.K.) was used as the carrier gas. Nitrogen of 99.996% purity (Airco, U.S.A.) was used in preparing gas mixtures.

A Model 856/825 R-d H<sub>2</sub>S/total sulphur analyser (Houston Atlas) was used. Standard gas samples were obtained from E. Merck (F.R.G.). Pure mercaptans were purchased from Fluka (Switzerland). Hydrocarbons and standard mixtures of hydrocarbons of similar composition to those of natural gas and stream gases were obtained from Phillips Petroleum (U.S.A.).

The column was made of stainless steel (180 × 0.4 cm I.D.) and was cleaned thoroughly and packed with 30% Triton X-305 (Supelco, U.S.A.) on Diatomite CQ (80-100 mesh) (Pye Unicam). The column was conditioned overnight at 200°C with a helium purge.

Standard gases of different concentrations were prepared using the calibration kit and sample bulbs by diluting the required gas with pure nitrogen. The prepared samples gave very good accuracy when they were cross-checked using the H<sub>2</sub>S/total sulphur analyser. Petroleum gas samples were obtained from Kirkuk Sulphur Sweetening Plant and all analyses were made within 1 h after sample collection to minimize losses that could arise owing to the nature of sulphur compounds.

## RESULTS AND DISCUSSION

### *Analytical aspects*

The analyst will face two main difficulties when quantitation of trace sulphur compounds in a petroleum gas stream is required. First, of hydrocarbons that might co-elute with sulphur gases may be present. This will affect the excitation energy of the flame photometric detector and reduce its signal<sup>23,25</sup>. Second, if H<sub>2</sub>S is present at high concentrations, then many sulphur compounds will overlap with the H<sub>2</sub>S peak or its tail.

TABLE I

ELUTION SEQUENCE OF SULPHUR COMPOUNDS WITH THEIR RETENTION TIMES ON 30% TRITON X-305

Temperature, 60°C, held for 7 min, then programmed to 86°C at 4°C/min. Flow-rate (He), 20 ml/min. Flame-photometric detector.

Compound	Retention time (min)	Compound	Retention time (min)
COS	1.40	<i>iso</i> -C <sub>3</sub> H <sub>7</sub> SH	10.32
H <sub>2</sub> S	2.25	<i>tert.</i> -C <sub>4</sub> H <sub>9</sub> SH	
<i>n</i> -Hexane	4.13	<i>n</i> -C <sub>3</sub> H <sub>7</sub> SH	14.44
CH <sub>3</sub> SH	5.57	<i>sec.</i> -C <sub>4</sub> H <sub>9</sub> SH	16.81
C <sub>2</sub> H <sub>5</sub> SH	8.73	<i>iso</i> -C <sub>4</sub> H <sub>9</sub> SH	18.25
		<i>n</i> -C <sub>4</sub> H <sub>9</sub> SH	22.96

The column and experimental conditions used in this work could overcome these difficulties as C<sub>1</sub>-C<sub>6</sub> hydrocarbons were eluted before methylmercaptan (see Table I). Therefore, trace amounts of C<sub>7</sub><sup>+</sup> hydrocarbons would not interfere with the flame-photometric detector signal in the determination of mercaptans<sup>26</sup>.

As shown in Fig. 1, COS was eluted before H<sub>2</sub>S and the column used could

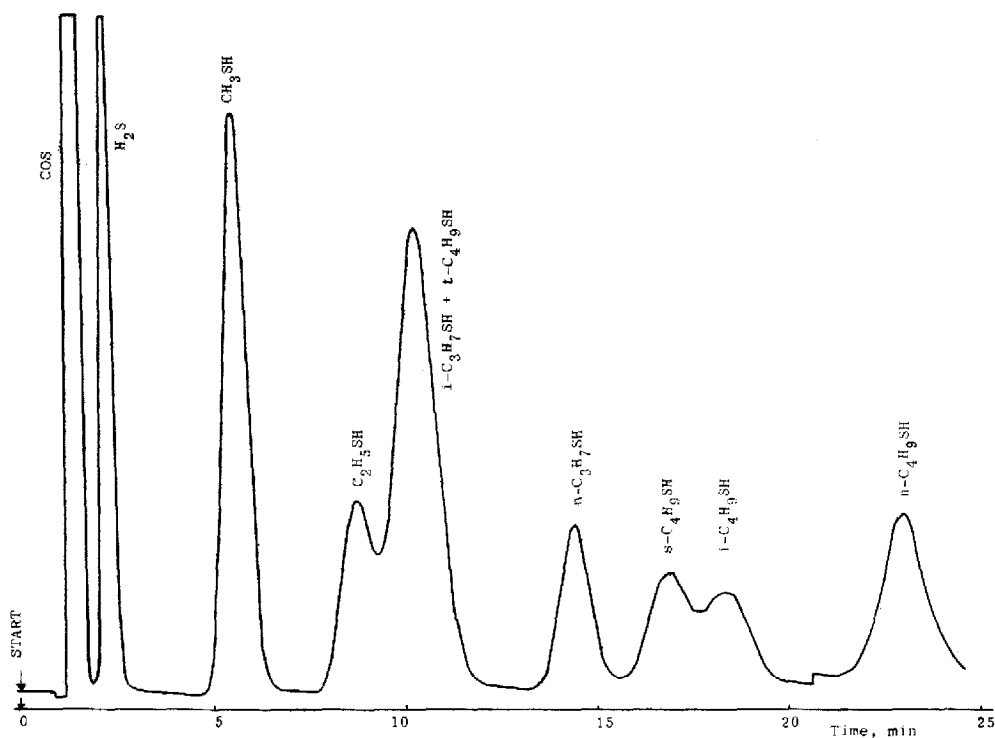


Fig. 1. Separation of some sulphur compounds on 30% Triton X-305 on Diatomite CQ. Column temperature: initial, 60°C, held for 7 min, then programmed to 86°C at 4°C/min. Carrier gas, He; flow-rate, 20 ml/min.

analyse COS, H<sub>2</sub>S and C<sub>1</sub>-C<sub>4</sub> mercaptans in one run when H<sub>2</sub>S was present at concentrations of  $\leq 0.3\%$  (v/v) and under the following experimental conditions: initial column temperature, 60°C (hold for 7 min); final column temperature, 86°C; programming rate, 4°C/min; injector temperature, 200°C; flame-photometric detector temperature, 220°C; and flow-rate of carrier gas (He), 20 ml/min.

For samples containing high concentrations of H<sub>2</sub>S (up to 15%, v/v), the analysis could be carried out as follows: (1) COS was determined directly with the present column; (2) H<sub>2</sub>S and hydrocarbons were determined using Porapak Q and a thermal conductivity detector (see Table II for the analysis conditions)<sup>24</sup>; (3) mercaptans were determined after treatment of the gas sample with 10% CdCl<sub>2</sub> in 0.01 N HCl to remove H<sub>2</sub>S only as CdS<sup>27</sup>. The decrease in the concentration of each mercaptan as a result of this treatment was taken into account by running the same procedure three times with several concentrations of each standard mercaptan under study and constructing calibration graphs between log (peak area) before and after the treatment<sup>24</sup>. Fig. 2 shows an example of these graphs for CH<sub>3</sub>SH. All analyses were carried out on the present column and the areas obtained for the mercaptan peaks in the sample after the treatment were corrected using the corresponding calibration graphs, then the concentrations were deduced.

TABLE II

GAS CHROMATOGRAPHIC CONDITIONS FOR THE SEPARATION OF H<sub>2</sub>S, CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O AND C<sub>1</sub>-C<sub>7</sub> HYDROCARBONS IN PETROLEUM GAS STREAMS

Column	180 × 0.2 cm I.D., glass
Packing	Porapak Q, 100-120 mesh size
Carrier gas	He, 30 ml/min.
Column temperature	Initial 40°C, hold 1 min then programmed to 170°C at 15°C/min.
Injector temperature	220°C
Detector	Thermal conductivity
Detector temperature	250°C
Filament temperature	280°C
Detector current	190 mA
Sample loop	1 ml
Analysis time	19 min

Trace amounts of COS, H<sub>2</sub>S, CH<sub>3</sub>SH, CS<sub>2</sub> and SO<sub>2</sub> could be determined in petroleum gas streams and some gases from the sulphur sweetening plant using isothermal temperature conditions (75°C) (see Fig. 3). Quantitative data obtained from the above analyses for sulphur compounds were compared with those from the H<sub>2</sub>S/total sulphur analyser and proved to be reliable for daily routine analyses.

Calculations of all concentrations were made using calibration graphs for each gas, taking into account the change in the detector response with concentration and type of sulphur gas<sup>22</sup>. The range of concentrations of mercaptans studied was between 100 and 0.2 ppm. The reproducibility of the method was found by running each standard mercaptan at concentrations of 2, 20 and 100 ppm four times and the results showed that the reproducibility of the method was  $\pm 3.5\%$  of the absolute tested concentrations. Table III shows typical gas chromatographic results for two gas samples. The maximum standard deviation of the data was 4.2% of the amount

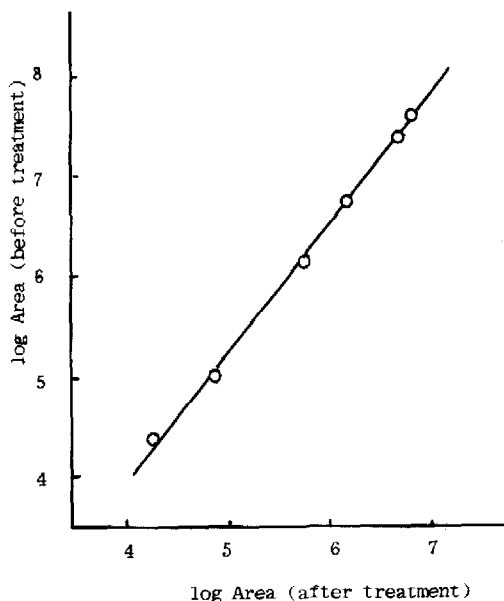


Fig. 2. Logarithmic plot of areas of CH<sub>3</sub>SH peaks before and after treatment with acidic CdCl<sub>2</sub>. Range of mercaptan concentrations: 0.8–3.2 ppm. Analyses on 30% Triton X-305 on Diatomite CQ.

present. This method has been used for routine analyses for 16 months and proved to be efficient.

#### *Elution mechanism*

It was interesting to note from the literature survey and this work that H<sub>2</sub>S–COS and *n*-propyl-*tert*-butyl mercaptans change their order of elution depending on the type of stationary phase used. These stationary phases could be classified into two groups, A and B, according to the elution sequence of the above compounds, as shown in Table IV. Calculated electron polarizabilities and molar volumes in addition to some important physical properties of the sulphur compounds studies are given in Table V.

In order to account for the elution mechanism of H<sub>2</sub>S and COS on the stationary phases given in Table IV, one should recall that the COS molecule is planar (COS angle 180°) with a cloud of  $\pi$ -electrons around it due to C=O and C=S double bonds. In contrast, the H<sub>2</sub>S molecule is V-shaped (HSH angle 93.3°)<sup>41</sup>, has no  $\pi$ -electrons, is smaller than COS, has a lower electron polarizability than COS and has a higher dipole moment than COS (see Table V).

The stationary phases on which COS eluted before H<sub>2</sub>S have inorganic supports, mainly silica gel, which were either used as such or coated with a high loading of a “polar” stationary phase. According to the Kiselev classification<sup>42</sup>, these phases are Type II and III adsorbents on which the interactions of adsorbates are “specific” molecular interactions. Therefore, the shape and dipoles of H<sub>2</sub>S molecules play an important role in facilitating a shorter interaction distance (compared with COS

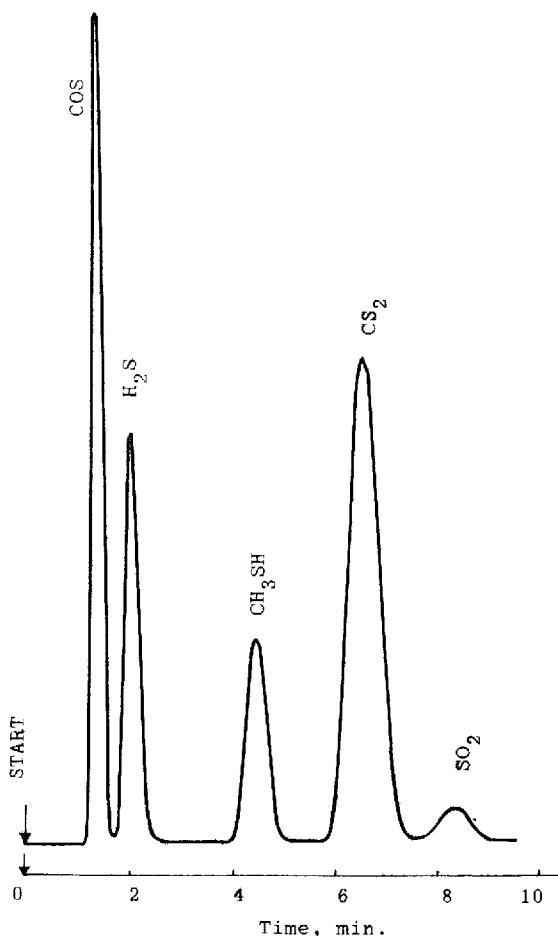


Fig. 3. Isothermal separation of some sulphur gases at 75°C on 30% Triton X-305 on Diatomite CQ. Carrier gas, He; flow-rate, 20 ml/min; flame-photometric detector.

molecules as discussed below) with the active sites on the surface of the adsorbents of this type, hence increasing the interaction energy. The smaller the interaction distance between the adsorbent and adsorbate, the greater is the interaction energy involved in the process of adsorption. More details can be found in a previous paper<sup>4,3</sup>. However, the interaction distance would obviously be larger for COS molecules because they are more bulky, have a lower dipole moment, have no hydrogen sites and have a  $\pi$ -electron cloud. These factors would cause the adsorption configuration of the COS molecule to be further from the surface than H<sub>2</sub>S, yielding a smaller energy of interaction. Therefore, on such surfaces, H<sub>2</sub>S will be retained longer than COS.

On the other hand, the stationary phases on which COS eluted after H<sub>2</sub>S are characterized by being either non-polar carbon black or a porous organic polymer matrix with a high surface area. The adsorbent-adsorbate interactions on carbon black, classified as a Type I adsorbent, are non-specific and in this instance the ge-

TABLE III

TYPICAL GAS CHROMATOGRAPHIC RESULTS FOR SULPHUR COMPOUNDS IN TWO PETROLEUM GAS STREAMS ON 30% TRITON X-305

Conditions as in text.

Compound	Gas stream A (ppm)					Gas stream B (ppm)				
	1	2	3	Average	R.S.D. (%)*	1	2	3	Average	R.S.D. (%)*
COS	<0.2	<0.2	<0.2	<0.2	—	9.21	9.50	9.61	9.44	2.2
H <sub>2</sub> S	3.08	3.14	3.26	3.16	2.9	8.09**	8.20**	7.65**	7.98**	3.6**
CH <sub>3</sub> SH	1.14	1.14	1.20	1.16	3.0	17.8	18.3	18.5	18.2	2.0
C <sub>2</sub> H <sub>5</sub> SH	0.60	0.64	0.62	0.62	3.2	10.4	9.80	10.2	10.1	3.0
<i>iso</i> -C <sub>3</sub> H <sub>7</sub> SH <i>tert</i> -C <sub>4</sub> H <sub>9</sub> SH	0.71	0.72	0.67	0.70	3.8	3.83	3.86	3.71	3.80	2.1
<i>n</i> -C <sub>3</sub> H <sub>7</sub> SH	0.70	0.72	0.68	0.70	2.9	3.80	3.69	3.60	3.70	2.7
<i>sec</i> -C <sub>4</sub> H <sub>9</sub> SH	0.47	0.49	0.45	0.47	4.2	3.06	3.22	3.01	3.10	3.5
<i>iso</i> -C <sub>4</sub> H <sub>9</sub> SH	0.36	0.38	0.36	0.37	3.1	1.93	1.88	1.89	1.90	1.4
<i>n</i> -C <sub>4</sub> H <sub>9</sub> SH	0.29	0.29	0.31	0.30	3.8	0.94	0.88	0.87	0.90	4.2

\* Relative standard deviation.

\*\* % (v/v).

TABLE IV

CLASSIFICATION OF STATIONARY PHASES ACCORDING TO THE ELUTION ORDER OF H<sub>2</sub>S-COS AND *n*-PROPYL-*tert*-BUTYLMERCAPTANS

Group A		Group B	
<i>H</i> <sub>2</sub> S elutes before COS	Ref.	COS elutes before <i>H</i> <sub>2</sub> S	Ref.
Carbon molecular sieve	28	Activated silica gel	34
Porapak Q	18, 29	Deactigel (treated silica gel)	6
Porapak PS (acetone washed)	30	Tracor special silica gel	23
Treated Porapak QS (Supelpak-S)	17, 31	Chromosil 310/330 (treated silica gel)	31
Tenax GC	32	Chromosorb 104	33
Chromosorb 101, 102, 103, 105, 106, 107, 108	33	30% Triton X-305 on Diatomite CQ	This work
Porapak N, P, Q, QS, R, S, T	33		
5% QF-1 on Porapak QS	24		
<i>n</i> -Propyl- elutes before <i>tert</i> -butyl-SH		<i>tert</i> -Butyl- elutes before <i>n</i> -propyl-SH	
5% QF-1 on Porapak QS	24	30% TCP on Chromosorb W AW	14
		40% DNP on firebrick	35
		28.6% DDP on firebrick	36
		10% TCP-TCEP-H <sub>3</sub> PO <sub>4</sub> on Chromosorb W HMDS	25
		30% Triton X-305 on Diatomite CQ	This work

TABLE V  
SOME IMPORTANT PHYSICAL PROPERTIES OF THE SULPHUR COMPOUNDS STUDIED

Compound	Mol. wt. (g/mol) <sup>37</sup>	B.p. (°C) <sup>37</sup>	Molar volume* (cm <sup>3</sup> /mol)	Dipole moment (D) <sup>38</sup>	$\alpha_E$ (cm <sup>3</sup> × 10 <sup>24</sup> ) <sup>**</sup>
H <sub>2</sub> S	34.08	-60.7	-***	0.97	3.797 <sup>§</sup>
COS	60.07	-50.2	-***	0.71	5.549 <sup>§</sup>
<i>n</i> -Propyl mercaptan	76.17	67	90.56	1.55	9.428
<i>tert.</i> -Butyl mercaptan	90.19	64	112.71	1.67	11.387

\* Calculated as the ratio of relative molecular mass to density at 20°C.

\*\* Electron polarizability, calculated from  $\alpha_E = [(n^2 - 1)/(n^2 + 2)] \cdot 3M/4\pi N\rho$  (ref. 39), where  $n$  = refractive index;  $M$  = molecular weight;  $N$  = Avogadro's number; and  $\rho$  = density.

\*\*\* Not calculated.

§ Ref. 40.

ometry of the adsorbate molecule, the orientation, general polarizability and number of electrons or the magnetic susceptibility of its force centres are important<sup>42</sup>. Moreover, most styrene-divinylbenzene porous polymers are classified as weakly specific Type III adsorbents<sup>44</sup> with no active or polar sites where non-specific interactions take place to a greater extent. Therefore, COS molecules, which have a higher electron polarizability than H<sub>2</sub>S molecules, would undergo stronger interactions with the surface of carbon black and porous organic polymers, aided by its planar structure, and hence are retained longer. Conversely, Chromosorb 104, which contains polar acrylonitrile functional groups, was classified as strongly specific Type III adsorbent<sup>44,45</sup>. The dipole-dipole interactions on this phase were predominant, and therefore the elution order of COS and H<sub>2</sub>S was reversed in comparison with other porous polymers.

The elution mechanism of *tert.*-butyl and *n*-propyl mercaptans can be realized from the fact that the *n*-propyl mercaptan molecule has a planar structure and is smaller in volume than *tert.*-butylmercaptan. On "polar" or specific stationary phases such as 30% TCP and 30% Triton X-305, the dipolar interactions were stronger for *n*-propyl mercaptan molecules owing to their ability to have closer and more frequent contacts, effecting greater retention, relative to *tert.*-butyl mercaptan molecules, which could suffer from partial geometric hindrance. The elution order was reversed on 5% QF-1 on Porapak QS owing to the predominant effect of the weakly specific surface of the porous polymer, which has a large surface area that could not be hidden by a small percentage coating of QF-1. Therefore, the electron polarizability of *tert.*-butyl mercaptan became more effective than the other parameters and resulted in stronger retention forces than with *n*-propyl mercaptan.

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