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Q-SAR Synthesis of Titans Based on Survey Results

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ABSTRACT

Having reviewed and acquired all of the synthesis methods of the specified compound, a new model encompassing; finding applications of the compound and naturally available compounds of the desired functions, evaluation and study of the physicochemical characteristics of the found natural chemicals using PASS software and, theoretical design of structural homologues of the natural compounds and evaluating their properties using PASS software was developed. The results acquired from the software were cross-checked using different software and the results verified by 5 analytical softwares to find.Using this model allows the study of natural sources compounds of desired characteristics and applications as well as designing other suitable homologs for synthesis. a group of compounds studied by using this model, was malodorants emitted by skaunks (as a naturalmaterial). The comparison of the characteristics was performed using the PASS software and thecross checking was carried out using the Q-SAR method using Dragon, Codessa, Stepwise, GA and MLR software. 84 homologs of thietane, which is emitted by skunks were sorted out based on the order of importance and priority with respect to negative Pa≤20 and positive Pa≥80.The first seven compounds were:1) 2-Methyl Thietane 2) 2-Ethyl Thietane 3) 2-Propyl Thietane4) 2,4-Diethyl Thietane 5) 2-Butyl Thietane 6) 2,3,4-Triethyl Thietane7) 2,2,4-Triethyl ThietaneCompounds 1, 5, 6 and 7 were among homologs of thietane and compounds 2, 3, and 4 were of the bad smelling compounds of skunk. All the studies were based on the characteristics of thietane with regard to security and military applications. To study the safety application of thietane, all steps were also performed for the compounds present in natural gas (13 thiol and thioether derivatives). Next, a comparison was made between the 13 compounds and the first 7 thietane derivatives. The results revealed the top 7 titan derivatives were better with respect to less toxicity and better characteristics. Comparing the statistical tables also confirmed the priority of the thietane derivatives. 2-Methyl Thietane and 2-Ethyl Thietane (one of the compounds in the bad smell of skunk) were synthesized. To this end, all the methods of preparing the compounds were studied and summarized in a table. The SN2 nucleophilic substitution using 1, 3-dibromoalkanes and Na2S was chosen. The high yield, simplicity of steps, accessibility of the ingredients and the reaction speed were among the reasons for choosing the method. The synthesis of the compounds was verified using IR, MS, 1HNMR,and CNMR.

I. INTRODUCTION

Aromatic compounds with a structure made of acarbon atom and atleast one other element classified as the Heterocycle.Usually in Heterocycle structures instead of some carbon atoms, Hydrogenelements, many of important sulfur's Heterocycle cores placed in acircular systemwhich you can see in picture No.1:

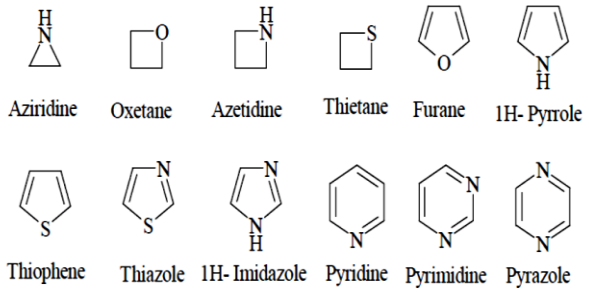
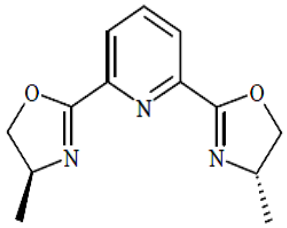


Figure 1 Some of theheterocycle compounds

Most of the discovered organic compounds at least have a one Hetero cycle part. Heterocyclecompounds have many usages such as medicine effectiveness, lucidation, andanti-lucidation oxidative and etc...well-known medicines such asAntibiotics, relaxants,anticancer,anti aids and etc... which they atleast have a one Heterocyclepart.

In addition,Heterocycle compoundswhich areintermediator in organic synthesis have anIncreasing use.Due tocirculating structure,heterocyclecompounds can enter in many synthesis levels or at a favorite level for releasing active groups.

Many of Heterocycle compounds asligand have been used for metals Refinement. But designing them with increasing processhas aguide to special usage. For exampleHeterocycle compoundsare using as active light ligand for being metalIntermediator and complexes as the catalyst inasymmetric synthesis reactions.



2,6-Bis(4-methyl-4,5-dihydro-ozazol-2-yl)-Pyridine

Figure 2Heterocycle with active light ligand

Heterocycle compoundshave distributed widely in nature. Some of theplants have Heterocycle compounds. Some of these compounds have anImportant place in Organisms system, for example, we can mention "Nucleic acid" which it Derivativesfrom Pyridine and purin and they Derivative from Pourzin's loop (Hem).they corporation in a Heredity process is undeniable. Chlorophyll and Hem, Important parts of adiet are likeThiamine (B1), Riboflavin (B2),Pyridoxine (B6),Nicotinamide (B3) and Ascorbic acid which they all haveHeterocyclecompounds.

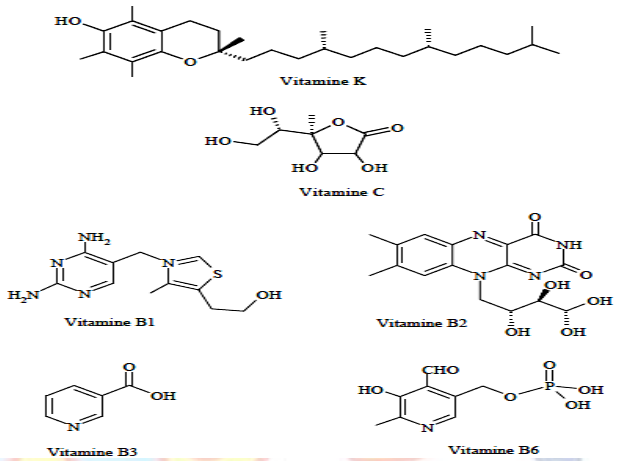


figure3 natural Heterocycle compounds

Nucleotides aremade byheterocycle which discovered and they are human's important body parts maker.

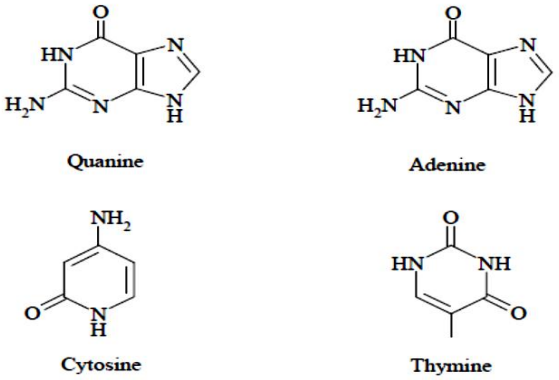


Figure 4 some of theNucleotides

In picture No.4 a few of Heterocycle compounds with sulfur Heterothemwhich has shown. Titan molecule including sulfur which contains Heterocycle with ahigh rate of importancewas in Odorous compounds and it has ahigh rate of importance for some creatures.

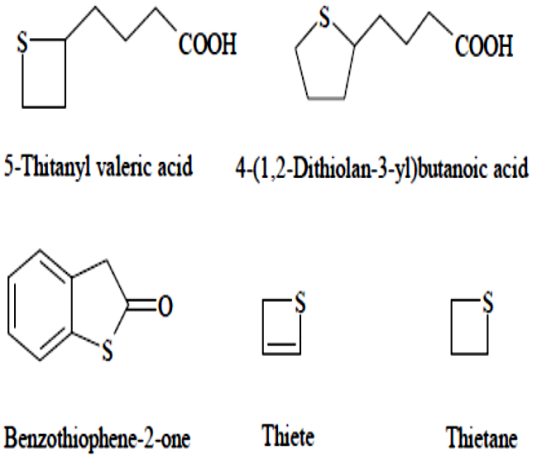


Figure 5 Heterocyclecompounds with sulfur atom

II.METHOD

1-2 material and requirement devices

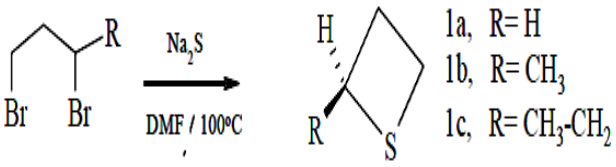
Mass spectrum has been withFINIGAN-MATT8430 Mass Spectrometerwith 20eVPotential. HNMR and CNMR spectrums with Spectrometers of Bruker DRX-500,400,250 AVANCE Respectively with1،500 and 50 MHzFrequencies are taken and spectrums of IR wave has recorded.

2-2 Chemical requirement compounds

For making titan compounds we use Sodium sulfide(Na_2S),Dimethylformamide (DMF),Dichloromethane(CH_2Cl_2),Halogenated compounds [1-3], Di Bromo Propane (BrCH2CH2CH2Br),Methanol solvent,ethanol and Acetone from Merck,Fluke, Al-Dharichcompanies prepared and they are using without more Purification.

3-2 Preparing titan (1a), 2-Methyl Titan(1b), 2-Ethyl Titan(1c)

First of all solvate Di BromoPropane(5Mm,1g) at 20milliliters DMF . while the dilutionstirredby the Magnetic stirrer. A solution of sodium sulfide (5 mM, 0.39 g) dissolved in 50 ml of DMF was added dropwise to a stirred reaction solution for 10 minutes. The reaction solution was refluxed at 100 ° C for 6 hours. The Titanproduct was then distilled into a component. Methyl Titan (1b and 2-Ethyl Titan (1c) products have also been used in similar situations). Titan, 2-Methyl Titan and 2-Ethyl Titan from sodium sulfide reaction with 1, 3-di-Bromo-propyl 1,1-di-bromobutane and 3,1-dibromo-pentane in a solvent of dimethyl are, respectively, hopeless and very good Were prepared. The factors and conditions governing the experimental reaction efficiency were studied.



Synthetic data obtained for these compounds are shown in Table 1.

1:Important Titan Synthetic Data and Its Derivatives

The product	**Yield**	**b.p(° C)**
Thietane(1a)	**%76(0/28g)**	**94**
2-methylthiettane(1b)	**%65(0/29g)**	**102**
Ethythietane(1c)	**%65(0/28g)**	**108**

Massive mass spectrometry data Three synthesized compounds Table2 is shown.

Table 2. Important data for mass spectrometry of Titan and its derivatives

	(M)+	**(M-1)+**	**(M-14)+**	**(M-28)+**	**(M-32)+**	**(M-32-14)+**
1a	74	73	60	46 (CH_2-_S)^2	42	-
1b	88	78	74	60 (CH_{3-C} H=s)$^+$	56	43 (CH_3 –CH2-CH2)$^+$
1c	102	101	-	74	71	57 ($CH_{3-CH2-CH2-}$ CH2-CH2)$^-$

III.RESULT AND DISCUSSION

The compounds of Titan (1a), and 2-Methyl Titan (1b) and 2-Ethyl Titan (1c), which were synthesized by the above method, were constructed using c NMR 1H NMR spectroscopy and mass spectrometry. Since these compounds have a very intense and penetrating smell and practically it is not possible to completely purify them in experimental environments, therefore, to ensure the synthesis of these compounds, the spectra obtained with the spectra predicted by advanced software are compared.

3.1 Investigation of the results of the Titan molecule spectroscopy (1a)

A. IR spectra of the Titan molecule;

The Titan molecule is synthesized and the pure titanium spectrum obtained by the software in Fig. 3 shows the IR spectrumgiven. As you can see, most of the Titan adsorption peaks correspond to the peaks predicted by the software for pure titan. This matching is indicated by the lines in Figure 3Has been. There is only one absorbing peak in the extracted index of your synthesized, which is due to the impurities presentIt has been synthesized in you.

B. Magnetic resonance spectrum of C NMR and Titan H NMR

The spectra obtained from the magnetic resonance of the proton and the carbon of the molecule Titan synthesized in Figures 2 to 4it has been shown.Because of the symmetry in the H-NMR spectrum, the Titan molecule (1a) appears in the methylene group protons in the form of a two-peak multiplier of 2.71 ppm and 3.13 ppm. Also,in the C-NMR spectrum, the carbon-bearing carbon radicals of Titan Figure 4 are observed in two separate couriers at 31.33 ppm and 34.93 ppm.

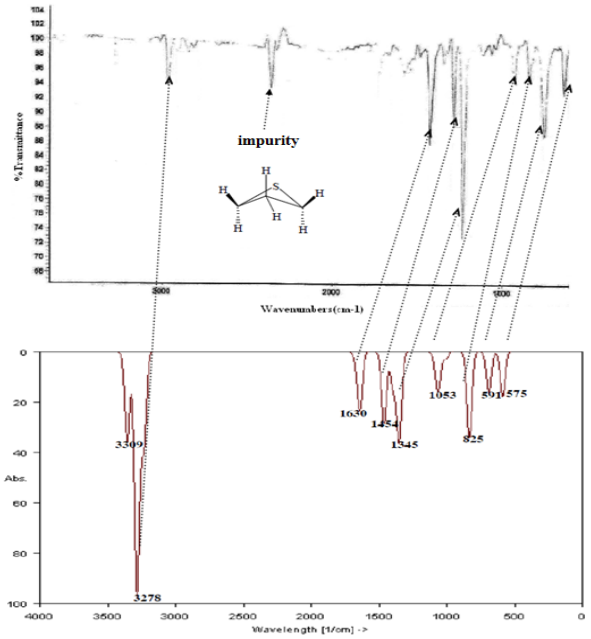


Figure 6 shows the spectrum of the synthesized Titan molecule (1a) and the spectrum obtained from the software

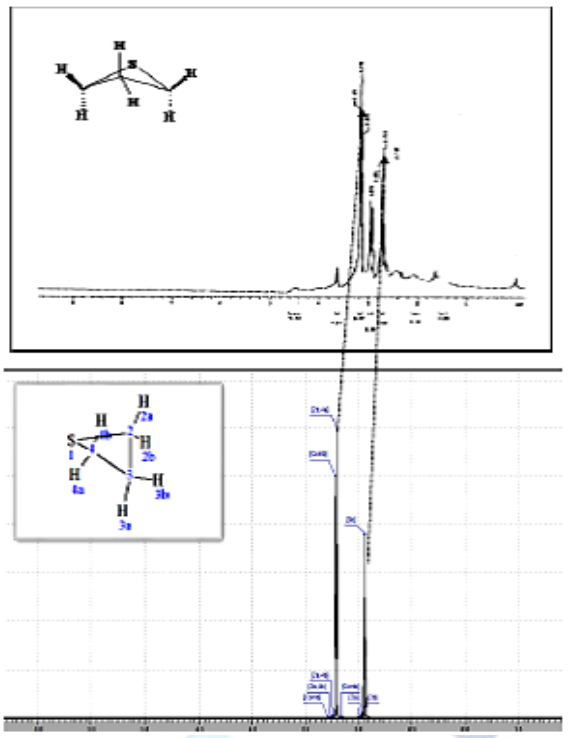


Figure 7 shows the Titanium HNMR spectra shown in Figure 3

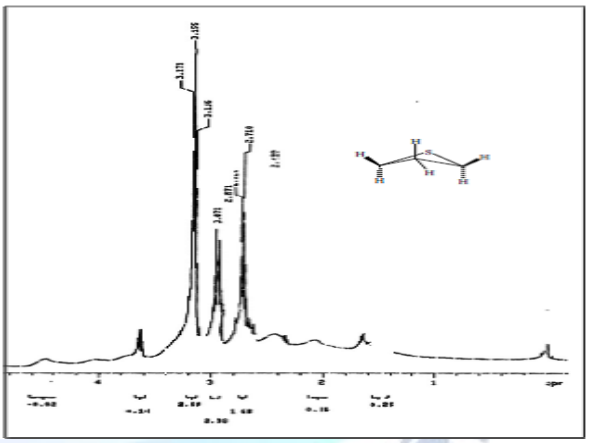


Figure 8 HNMR Spectrum Titan molecule (1a) - (in magnification mode)

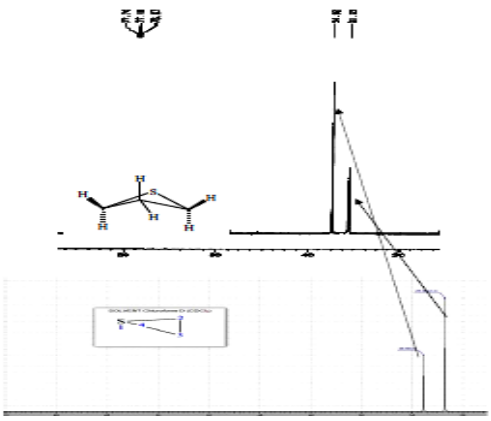


Figure 9 The CNMR Spectrum Titan molecule (1a)

The same is true when the H-NMR and C-NMR data are matched to the symmetric structure of the molecule shown in Fig 10.

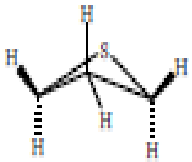


Fig 10.Structure of the Titan molecule

3.2 Mass Spectrometry of the Tangent Molecule

The mass spectrum of the synthesized molecule is shown in Fig 11. The breakdown pattern in the mass spectrometry of Figure 6 is in agreement with the structure of the molecule and the boom peak of the molecule is also visible at 74 m / z. The important components of the molecule failure are Table 2.

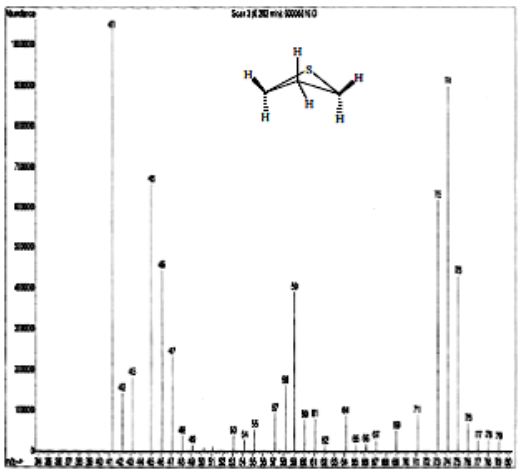


Figure 11 Mass spectrum of Titan molecule (1a)

Spectrometry results of 2-Methyl Titan molecule (1b)

A) IR spectrum of Methyl Titan (1 b)

The IR spectrum of the 2-Methyl Titan molecule is synthesized and the pure 2-Methyl Titan spectrum obtained by the software is shown in Fig. 7. As can be seen, most of the 2-Methyl Titan absorption peaks fitted with the peaks predicted by the software for pure 2-Methyl Titan. This alignment is illustrated by the lines in Figure 7.

B. Spectroscopy of the magnetic resonance of the nucleus H NMR, C NMR2-Methyl Titan

The spectra obtained from the nuclear magnetic resonance of the proton and carbon synthesized by the 2-Methyl Titan molecule are shown in Figures 8 to 10.

The 2-Methyl Titan molecule has a chiral center. In this molecule, in addition to the fragmentation between adjacent protons, the twin proton of the CH2 group also splits up because of differences in space position. Hence, expect.

It turns out that the tetra-methylene diastereotron (CH2) protons in rigid quaternary ring appear in the H-NMR spectrum of a different chemical transfer and appear as a five-peak pair.

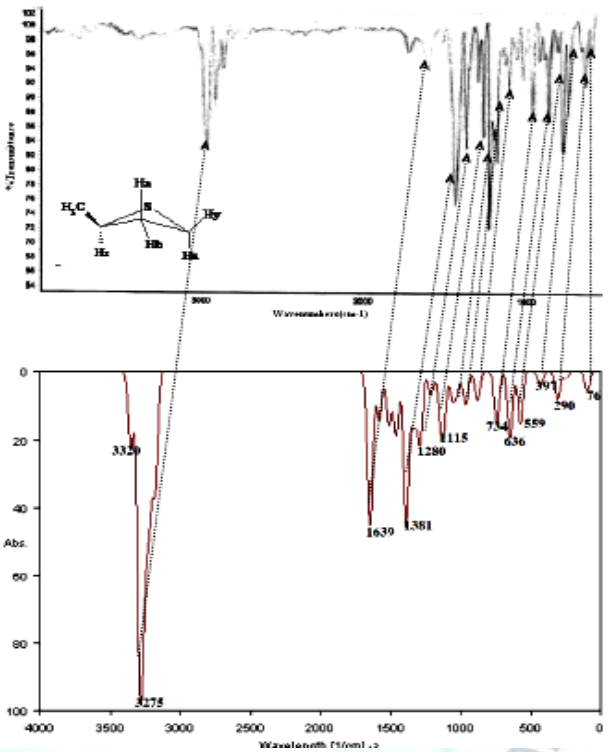


Figure . 12 is the spectrum of the 2-Methyl Titan molecule (1b) synthesized and the spectrum simulated by the software

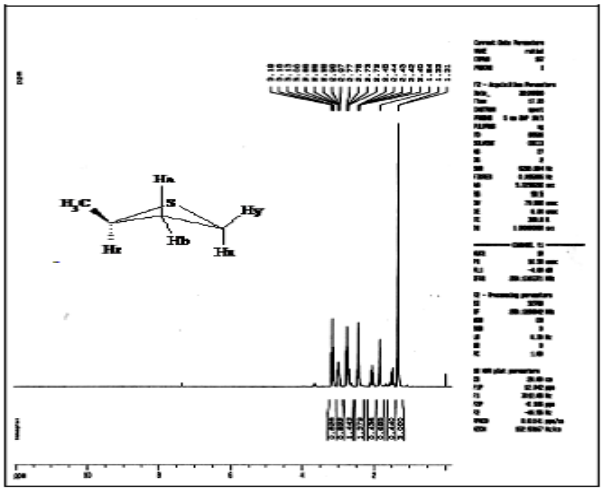


Figure 13The HNMR Spectrum of Synthesized 2-Methyl Titan (1b)

The HNMR spectrum of the 2-Methyl Titan molecule is shown in Figure. 9

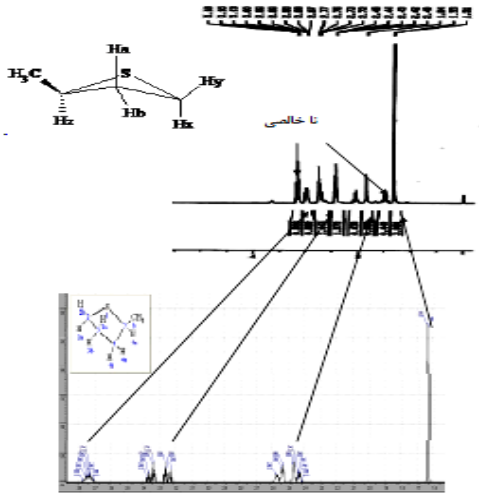


Figure 13 shows the HNMR spectrum of the 2-Methyl Titan molecule (1b) (in a magnifying state) and the HNMR spectrum of the 2-Methyl Titan molecule (1b) simulated by the software

C-Mass spectrometry of the molecule 2-Methyl Titan

The mass spectrum of the 2-methyl-titanium molecule is synthesized in Fig. 10. The breakdown pattern in the mass spectrum of the composition is in agreement with the structure of the molecule and the peak of the ion-molecule is also visible at 88 m / z. The important components of the breakdown of the 2-Methyl Titan molecule are presented in Table 2.

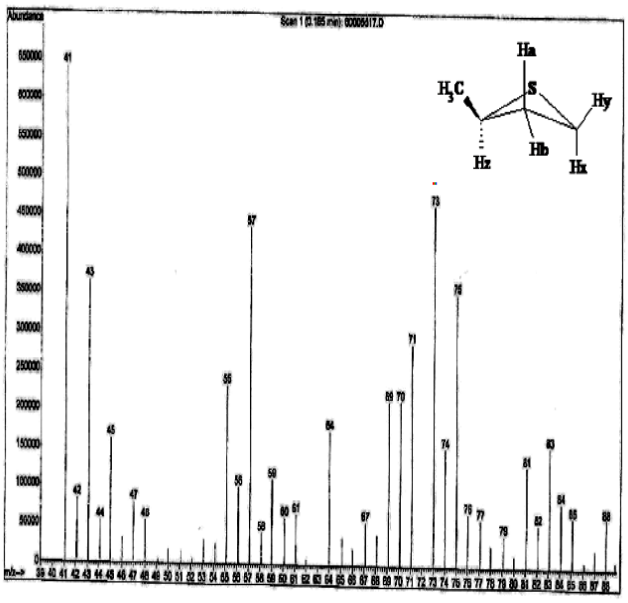


Figure 14 Mass spectrometry of 2-Methyl Titan Synthesized molecule (1 b)

Comparison of all the safety properties of thirteen compounds of thiols and tethers in domestic gas with seven preferred compounds of Titan homologs indicates that the toxic properties and Negative Pa of their compounds are significantly less than thiols And tethers. And as a result of these compounds, your compounds are better for use in domestic gas. Meanwhile, in the combination of seven Titan compounds, the first molecule (Methyl Thietane), which has been Approved by Titan homologues and the second molecule (Methy1 Thietane), which have been found to be Bad Mist Compounds and approved for security applications in the previous section, were used in household gases It is also more useful and safe than other compounds.

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