**Table 1**:Chemical Composition and Mechanical Properties of API 5L X65 and API 5L X56 steel pipe

|  |  |  |
| --- | --- | --- |
| **Steel Grade** | **API 5L X65 PSL 1** | **API 5L X56 PSL 1** |
| **Key Parameters** | **Compositional Analysis (%)** | **Compositional Analysis (%)** |
| Cmax | 0.28 | 0.28 |
| Mnmax | 1.40 | 1.40 |
| Pmax | 0.03 | 0.03 |
| Smax | 0.03 | 0.03 |
| Silicon (Si) | ≤ 0.45 | ≤ 0.45 |
| Copper (Cu) | ≤ 0,50 | ≤ 0,50 |
| Nickel (Ni): | ≤ 0,50 | ≤ 0,50 |
| Molybdenum (Mo) | ≤ 0.15% | ≤ 0.15% |
| Niobium (Nb)+Vanadium (V)+Titanium (Ti) | Total less than or equal to 0,15 % | Total less than or equal to 0,15 % |
| Yield Strength (Mpa) minimum | 450 | 360 |
| Tensile Strength (Mpa) minimum | 453 | 460 |

**Table 2:** Gravimetric analysis for API 5L X65 and API 5L X56 Steel (MS) in 0.5 M HCl, without and with different Yellow Bush Extract Concentration

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Immersion Time (Hr)** | **Steel Grade** | **Yellow Bush Concentration (ppm)** | **Weight Loss (g)** | **General Corrosion (g/cm2Hr)** | **Average General Corrosion Rate (g/cm2Hr)** | **EI (%)** |
| 2 | API 5L X65 | Blank | 1.75E-02 | 7.01E-04 | 1.12E-04 |  |
| 2 | API 5L X56 | Blank | 5.10E-03 | 4.78E-04 |
| 2 | API 5L X65 | 20 | 2.08E-02 | 5.68E-04 | 7.15E-04 | 36% |
| 2 | API 5L X56 | 20 | 1.06E-02 | 4.25E-04 |
| 2 | API 5L X65 | 40 | 1.48E-02 | 3.81E-04 | 6.88E-04 | 38% |
| 2 | API 5L X56 | 40 | 7.10E-03 | 2.43E-04 |
| 2 | API 5L X65 | 60 | 5.90E-02 | 1.25E-03 | 5.20E-03 | 53% |
| 2 | API 5L X56 | 60 | 3.22E-02 | 1.15E-03 |
| 18 | API 5L X65 | Blank | 2.31E-01 | 8.34E-04 | 2.87E-04 |  |
| 18 | API 5L X56 | Blank | 6.29E-02 | 2.60E-04 |
| 18 | API 5L X65 | 20 | 1.02E-01 | 3.89E-04 | 6.74E-05 | 41% |
| 18 | API 5L X56 | 20 | 5.96E-02 | 2.54E-04 |
| 18 | API 5L X65 | 40 | 7.52E-02 | 2.68E-04 | 7.40E-05 | 65% |
| 18 | API 5L X56 | 40 | 2.81E-02 | 1.20E-04 |
| 18 | API 5L X65 | 60 | 7.96E-02 | 2.83E-04 | 5.53E-05 | 58% |
| 18 | API 5L X56 | 60 | 4.55E-02 | 1.73E-04 |
| 24 | API 5L X65 | Blank | 3.61E-01 | 9.65E-04 | 3.03E-04 |  |
| 24 | API 5L X56 | Blank | 1.16E-01 | 3.58E-04 |
| 24 | API 5L X65 | 20 | 8.52E-02 | 2.28E-04 | 4.93E-05 | 73% |
| 24 | API 5L X56 | 20 | 4.21E-02 | 1.29E-04 |
| 24 | API 5L X65 | 40 | 8.03E-02 | 2.14E-04 | 7.07E-05 | 78% |
| 24 | API 5L X56 | 40 | 2.56E-02 | 7.30E-05 |
| 24 | API 5L X65 | 60 | 6.91E-02 | 1.82E-04 | 1.45E-05 | 75% |
| 24 | API 5L X56 | 60 | 4.59E-02 | 2.00E-04 |

**Table 3:**Electrochemical parameters of impedance for MS (API 5L X65) in 0.5 M HCl without (blank) and with different Yellow Bush Extracts concentration

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Yellow Bush (ppm)** | **Rs(Ωcm2)** | **Rct(Ωcm2)** | **n** | **Cdl (Fcm-2)** | **IE (%)** |
| Blank | 0.54 | 8.91 | 0.74 | 1.182E-01 |  |
| 20 | 0.99 | 10.19 | 0.74 | 2.027E-01 | 13% |
| 30 | 0.20 | 10.58 | 0.79 | 1.451E+00 | 16% |
| 40 | 0.23 | 20.68 | 0.79 | 2.221E-01 | 57% |
| 50 | 0.58 | 17.27 | 0.75 | 2.738E-01 | 48% |
| 60 | 1.73 | 23.33 | 0.73 | 1.896E-01 | 62% |

**Table 4:**Quantum Chemical Parameters (QCP)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameters** |  | **1,5,9-Undecatriene-2,6,10-trimethyl-(Z)** | **Terpineol** | **Hexadecanoic acid, methyl ester** |
| E HOMO (eV) |  | -5.707 | -5.729 | -7.210 |
| E LUMO (eV) |  | -0.716 | -0.182 | -0.500 |
| ΔEgap (eV) |  | 4.991 | 5.547 | 6.710 |
| I(eV) |  | 5.707 | 5.729 | 7.210 |
| A(eV) |  | 0.716 | 0.182 | 0.500 |
| η (eV) |  | 2.496 | 2.774 | 3.355 |
| σ (eV) |  | 0.401 | 0.361 | 0.298 |
| χ (eV) |  | 3.212 | 2.956 | 3.855 |
| µ(eV) |  | -3.212 | -2.956 | -3.855 |
| ω(eV) |  | 2.066 | 1.575 | 2.215 |
| ΔE Back (eV) |  | -0.624 | -0.693 | -0.839 |
| (ΔN) (eV) |  | 1.403 | 1.262 | 1.043 |

**Table 5:**HOMO, LUMO and Iron Fermi Level Gap Analysis

|  |  |  |
| --- | --- | --- |
| **Phytochemical** | **ELUMO (eV)** | **ΔE= (LUMO - (-5.177 eV))** |
| **1,5,9-Undecatriene-2,6,10-trimethyl-, (Z)** | - 0.716 | 4.461 |
| **Hexadecanoic Acid, Methyl Ester** | - 0.500 | 4.677 |
| **Terpineol** | - 0.182 | 4.995 |
| **Phytochemical** | **EHOMO (eV)** | **ΔE= (-5.177 eV – (HOMO))** |
| **1,5,9-Undecatriene-2,6,10-trimethyl-, (Z)** | - 5.707 | 0.530 |
| **Terpineol** | - 5.729 | 0.552 |
| **Hexadecanoic Acid, Methyl Ester** | - 7.21 | 2.033 |

**Table 6:**MC Outputs and Descriptors for the Adsorption Locator Module with the Lowest Adsorption Configurations of Terpineol ( Values of all Energy terms are given in kcal/mol).

ETotal: Total Energy; Eads: Adsorption Energy; R.A.E: Rigid Adsorption Energy; Deformation Energy: Edef

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Structures** | **ETotal** | **Eads** | **R.A. E** | **Edef** | **Terpineol: dEad/dNi** | **Water: dEad/dNi** | **HCl: dEad/dNi** |
| Terpineol | -36.27 |  |  |  |  |  |  |
| Water | 11.68 |  |  |  |  |  |  |
| HCl | 0.60 |  |  |  |  |  |  |
| Fe (1 1 0) - 195 | -343.11 | -426.59 | -303.01 | -123.58 | -100.92 | -23.78 | -14.88 |
| Fe (1 1 0) - 196 | -342.84 | -426.33 | -302.20 | -124.13 | -97.05 | -22.94 | -15.28 |
| Fe (1 1 0) - 197 | -342.24 | -425.72 | -301.19 | -124.53 | -94.56 | -23.23 | -15.52 |
| Fe (1 1 0) - 198 | -341.19 | -424.68 | -301.52 | -123.15 | -98.36 | -24.77 | -15.56 |
| Fe (1 1 0) - 199 | -340.98 | -424.46 | -300.37 | -124.10 | -92.08 | -24.03 | -14.78 |
| Fe (1 1 0) - 200 | -340.43 | -423.92 | -299.08 | -124.84 | -97.84 | -24.14 | -14.89 |
| Fe (1 1 0) - 201 | -340.00 | -423.49 | -299.46 | -124.03 | -98.63 | -23.55 | -15.76 |
| Fe (1 1 0) - 202 | -335.27 | -418.75 | -295.34 | -123.41 | -101.09 | -23.81 | -14.78 |

**Table 7:**MC Outputs and Descriptors for the Adsorption Locator Module with the Lowest Adsorption Configurations of 1,5,9-Undecatriene-2,6,10-trimethyl (Z). (The values of all energy terms are given in kcal/mol.)

Terpineol (TPL); hexadecanoic acid-methyl ester (HMS); 1,5,9-Undecatriene- 2,6,10-trimethyl-, (Z)); (159 U).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Structures** | **ETotal** | **Eads** | **R.A. E** | **Edef** | **159 U dEad/dNi** | **H2O: dEad/dNi** | **HCl: dEad/dNi** |
| 159 U | -23.75 |  |  |  |  |  |  |
| H2O | 11.68 |  |  |  |  |  |  |
| HCl | 0.60 |  |  |  |  |  |  |
| Fe (1 1 0) - 169 | -364.37 | -460.38 | -337.64 | -122.73 | -130.79 | -23.34 | -15.35 |
| Fe (1 1 0) - 170 | -363.80 | -459.81 | -341.01 | -118.79 | -126.33 | -25.01 | -16.00 |
| Fe (1 1 0) - 171 | -363.37 | -459.37 | -336.03 | -123.34 | -125.73 | -23.11 | -15.70 |
| Fe (1 1 0) - 172 | -362.08 | -458.08 | -336.15 | -121.93 | -131.88 | -23.84 | -15.37 |
| Fe (1 1 0) - 173 | -361.08 | -457.08 | -334.97 | -122.11 | -128.56 | -24.11 | -14.74 |
| Fe (1 1 0) - 174 | -356.27 | -452.28 | -329.09 | -123.19 | -129.03 | -23.31 | -15.96 |
| Fe (1 1 0) - 175 | -353.26 | -449.27 | -326.43 | -122.83 | -127.09 | -23.74 | -15.90 |
| Fe (1 1 0) - 176 | -346.47 | -442.47 | -320.73 | -121.75 | -115.88 | -24.02 | -14.68 |

**Table 8:**MC Outputs and Descriptors for the Adsorption Locator Module with the Lowest Adsorption Configurations for Hexadecanoic acid and methyl ester. (The values of all energy terms are given in kcal/mol.)

Terpineol (TPL); hexadecanoic acid-methyl ester (HMS); 1,5,9-Undecatriene- 2,6,10-trimethyl-, (Z)); (159 U).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Structures** | **ETotal** | **Eads** | **R.A. E** | **Edef** | **HMS: dEad/dNi** | **H2O: dEad/dNi** | **HCl: dEad/dNi** |
| HMS | -22.72 |  |  |  |  |  |  |
| H2O | 11.68 |  |  |  |  |  |  |
| HCl | 0.59 |  |  |  |  |  |  |
| Fe (1 1 0) - 194 | -420.60 | -517.64 | -396.17 | -121.47 | -180.43 | -24.50 | -15.50 |
| Fe (1 1 0) - 195 | -420.12 | -517.16 | -394.47 | -122.69 | -186.46 | -23.12 | -15.41 |
| Fe (1 1 0) - 196 | -419.09 | -516.12 | -395.77 | -120.35 | -178.80 | -24.79 | -15.82 |
| Fe (1 1 0) - 197 | -418.53 | -515.56 | -396.46 | -119.10 | -175.10 | -23.85 | -16.03 |
| Fe (1 1 0) - 198 | -416.89 | -513.93 | -391.16 | -122.77 | -172.70 | -24.39 | -15.88 |
| Fe (1 1 0) - 199 | -415.14 | -512.18 | -387.90 | -124.28 | -175.61 | -25.43 | -15.38 |
| Fe (1 1 0) - 200 | -412.42 | -509.45 | -386.38 | -123.07 | -177.75 | -24.17 | -15.28 |
| Fe (1 1 0) - 201 | -409.88 | -506.91 | -385.46 | -121.45 | -181.55 | -24.11 | -15.41 |

**Table 9:**MC Outputs and Descriptors for the Adsorption Locator Module with the Lowest Adsorption Configurations of Combined Phytochemicals (Terpineol, Hexadecanoic acid, methyl ester and 1,5,9-Undecatriene-2,6,10-trimethyl-, (Z)). (The values of all energy terms are given in kcal/mol.)

Terpineol (TPL); hexadecanoic acid, methyl ester (HMS); 1,5,9-Undecatriene-2,6,10-trimethyl-, (Z)); (159 U).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Structure** | **ETotal** | **Eads** | **R.A. E** | **Edef** | **TPL: dEad/dNi** | **HMS: dEad/dNi** | **159 U: dEad/dNi** | **HCl: dEad/dNi** | **H20: dEad/dNi** |
| TPL | -36.27 |  |  |  |  |  |  |  |  |
| HMS | -22.71 |  |  |  |  |  |  |  |  |
| 159 U | -23.75 |  |  |  |  |  |  |  |  |
| HCl | 0.60 |  |  |  |  |  |  |  |  |
| H2O | 11.68 |  |  |  |  |  |  |  |  |
| Fe (110) 259 | -697.73 | -734.75 | -607.89 | -126.86 | -96.78 | -186.98 | -127.71 | -15.10 | -23.30 |
| Fe (110) 260 | -697.14 | -734.16 | -609.31 | -124.86 | -95.36 | -180.67 | -134.99 | -15.01 | -24.00 |
| Fe (110) 261 | -695.16 | -732.18 | -602.16 | -130.02 | -93.76 | -187.18 | -136.97 | -16.34 | -24.01 |
| Fe (110) 262 | -692.16 | -729.18 | -599.52 | -129.66 | -88.87 | -177.82 | -137.66 | -15.24 | -23.85 |

**Table 10:**GC-MS Analysis t for Yellow Bush Leave

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Yellow Bush** | | | | | | |
| PK | RT | Area Pct | Library/ID | Ref | CAS | Qual |
| 1 | 5.1912 | 0.7134 | Silane, trichlorodocosyl- | 254469 | 007325-84-0 | 27 |
| 2 | 5.7104 | 0.9848 | Methyl-2-O-methyl.alpha.d-glucopyranoside | 72945 | 015064-82-1 | 50 |
| 3 | 7.2814 | 2.3097 | Decane | 19650 | 000124-18-5 | 78 |
| 4 | 7.3385 | 2.4777 | Undecane | 29357 | 001120-21-4 | 78 |
| 5 | 7.9739 | 2.4646 | Octanoic acid, methyl ester | 31295 | 000111-11-5 | 83 |
| 6 | 9.8526 | 1.4867 | Oxalic acid, isobutyl nonyl ester | 132408 | 1000309-37-4 | 64 |
| 7 | 9.9361 | 12.1382 | Terpineol | 27454 | 1000411-59-6 | 90 |
| 8 | 10.644 | 0.344 | 2-(Hydroxymethyl)norbornadiene | 10168 | 067583-61-3 | 43 |
| 9 | 11.3929 | 0.7262 | 2(1H)-Quinolinethione, 4-methyl- | 43799 | 004437-65-4 | 38 |
| 10 | 13.3033 | 2.4695 | 3-(4-Hydroxyphenyl)propionitrile | 23200 | 017362-17-3 | 47 |
| 11 | 14.1169 | 1.0694 | Phytol | 155849 | 000150-86-7 | 47 |
| 12 | 15.2244 | 1.5632 | Undecane, 2-methyl- | 39987 | 007045-71-8 | 72 |
| 13 | 18.5193 | 2.5939 | Methyl 6-methyloctanoate | 41251 | 005129-62-4 | 64 |
| 14 | 20.3323 | 1.3202 | Undecane | 29355 | 001120-21-4 | 59 |
| 15 | 23.3682 | 1.687 | Tridecanoic acid, methyl ester | 91455 | 001731-88-0 | 53 |
| 16 | 24.8933 | 0.3177 | Thiophene, tetrahydro- | 2106 | 000110-01-0 | 25 |
| 17 | 27.7972 | 15.3353 | Hexadecanoic acid, methyl ester | 130821 | 000112-39-0 | 97 |
| 18 | 28.6941 | 1.4851 | Phthalic acid, butyl undecyl ester | 224935 | 1000308-91-2 | 64 |
| 19 | 29.1359 | 0.2613 | Octan-2-one, 3,6-dimethyl- | 29220 | 118452-32-7 | 35 |
| 20 | 29.1878 | 1.8738 | Octanoic acid, ethyl ester | 41270 | 000106-32-1 | 38 |
| 21 | 31.2359 | 3.0215 | 9,12-Octadecadienoyl chloride, (Z,Z)- | 157778 | 007459-33-8 | 80 |
| 22 | 31.3458 | 7.729 | 9-Octadecenoic acid (Z)-, methyl ester | 155751 | 000112-62-9 | 68 |
| 23 | 31.4693 | 3.2865 | 13-Octadecenal, (Z)- | 126830 | 058594-45-9 | 52 |
| 24 | 31.6267 | 1.0104 | 1-Dodecanol, 2-methyl-, (S)- | 65252 | 057289-26-6 | 30 |
| 25 | 31.8367 | 6.2501 | Methyl stearate | 157880 | 000112-61-8 | 95 |
| 26 | 32.6216 | 1.5787 | 3-Propylglutaric acid | 43328 | 004165-98-4 | 38 |
| 27 | 33.097 | 1.6446 | Oxirane, tetradecyl- | 102576 | 007320-37-8 | 35 |
| 28 | 35.5532 | 0.9064 | cis-9,10-Epoxyoctadecan-1-ol | 144292 | 013980-12-6 | 30 |
| 29 | 35.977 | 0.611 | Cyclopentanol, 1-(1-methylene-2-propenyl)- | 18066 | 078158-11-9 | 60 |
| 30 | 37.1296 | 0.2598 | Hexadecanal | 102563 | 000629-80-1 | 46 |
| 31 | 37.1545 | 0.2008 | 6-Nitroundec-5-ene | 64169 | 1000192-40-3 | 35 |
| 32 | 37.2095 | 0.2837 | Z-2-Octadecen-1-ol | 128811 | 1000131-11-0 | 49 |
| 33 | 37.2371 | 0.1127 | cis-11-Hexadecenal | 100562 | 053939-28-9 | 49 |
| 34 | 37.2797 | 0.4281 | Pentanoic acid, 10-undecenyl ester | 115375 | 1000159-93-4 | 49 |
| 35 | 37.3771 | 0.9778 | (E)-6-Methylhept-4-en-1-ol | 12872 | 855901-81-4 | 30 |
| 36 | 37.4244 | 0.1678 | Oleic Acid | 142070 | 000112-80-1 | 41 |
| 37 | 37.4684 | 0.3414 | Trichloroacetic acid, undec-10-enyl ester | 172442 | 1000280-51-3 | 52 |
| 38 | 37.4918 | 0.3092 | Heptadecanoic acid, heptadecyl ester | 267418 | 036617-50-2 | 58 |
| 39 | 37.6282 | 0.8009 | Propyl tetradecyl ether | 117560 | 1000406-27-8 | 30 |
| 40 | 37.6786 | 0.3048 | Octadecanal | 128800 | 000638-66-4 | 49 |
| 41 | 37.7041 | 0.1497 | 17-Pentatriacontene | 265112 | 006971-40-0 | 41 |
| 42 | 37.7417 | 0.2667 | Tetradecanal | 76506 | 000124-25-4 | 64 |
| 43 | 37.7951 | 0.2348 | Heptadecanoic acid, heptadecyl ester | 267418 | 036617-50-2 | 70 |
| 44 | 37.8474 | 0.1914 | Propyl tetradecyl ether | 117560 | 1000406-27-8 | 43 |
| 45 | 37.8913 | 0.1815 | Hexadecyl propyl ether | 144422 | 1000406-27-9 | 49 |
| 46 | 37.9159 | 0.1412 | Propyl tetradecyl ether | 117560 | 1000406-27-8 | 49 |
| 47 | 37.9937 | 0.564 | Heptadecanoic acid, heptadecyl ester | 267418 | 036617-50-2 | 55 |
| 48 | 38.0458 | 0.4059 | cis-5-Dodecenoic acid | 63236 | 002430-94-6 | 53 |
| 49 | 38.1374 | 0.69 | Heptadecanal | 115508 | 1000376-70-0 | 72 |
| 50 | 38.3043 | 0.9163 | Heptadecanoic acid, heptadecyl ester | 267418 | 036617-50-2 | 53 |
| 51 | 38.522 | 12.4115 | 1,5,9-Undecatriene, 2,6,10-trimethyl-, (Z)- | 57864 | 062951-96-6 | 86 |