

Data Repository Item 2006086

Table DR1

Molecular parameters for the Matinenda fluid inclusion oil, including biomarker ratios.

<i>i</i> -C ₅ / <i>n</i> -C ₅	0.84 ¥
Benzene/ <i>n</i> -C ₆	57 ¥
Toluene/ <i>n</i> -C ₇	203 ¥
Furan/ <i>n</i> -C ₆	10.1 ¥
<i>n</i> -C ₇ /methylcyclohexane	0.13 ¥
Benzene/toluene	0.96 ¥
Toluene/ <i>o</i> -xylene	15.5 ¥
Pristane/phytane	1.08 §
Pristane/ <i>n</i> -C ₁₇	0.42 §
Phytane/ <i>n</i> -C ₁₈	0.33 §
Ts/Tm	1.4
Tm/C ₂₇ β	13.7
C ₂₉ Ts/C ₂₉ αβ hopane	0.24
C ₃₀ */C ₃₀ αβ hopane	0.07
C ₂₉ 25-norhopane/C ₂₉ αβ hopane	0.12
C ₃₀ αβ/(αβ+βα) hopanes	0.95
C ₃₁ αβ 22 <i>S</i> /(22 <i>S</i> +22 <i>R</i>) hopanes	0.58
C ₃₁ : 32 : 33 : 34 : 35 αβ homohopanes	39 : 29 : 13 : 12 : 7 \$
C ₂₉ αβ hopane/C ₃₀ αβ hopane	1.2 \$
29,30-BNH/C ₃₀ αβ hopane	0.16
C ₃₀ 30-norhopane/C ₃₀ αβ hopane	0.11
Gammacerane/C ₃₀ αβ hopane	0.06
C ₂₆ /C ₂₅ tricyclic terpanes	0.99 \$
C ₂₃ tricyclic terpane/C ₃₀ αβ hopane	0.63 \$
C ₂₃ /C ₂₁ tricyclic terpanes	2.6 \$
C ₂₄ tetracyclic/C ₂₃ tricyclic terpanes	0.54 \$
(C ₁₉ +C ₂₀)/C ₂₃ tricyclic terpanes	0.34 \$
C ₃₁ 2α Me/(C ₃₁ 2α Me+C ₃₀ αβ hopane)	0.60 †
C ₃₂ 2α Me/(C ₃₂ 2α Me+C ₃₁ αβ hopanes)	0.40 †
C ₂₉ steranes/C ₂₉ αβ hopane	0.48 *
C ₂₁ sterane/C ₂₉ ααα 20 <i>R</i> sterane	2.1 P
C ₂₇ : 28 : 29 βα diasteranes	48 : 29 : 23
Norcholestane ratio (24-nor/(24-nor+27-nor))	0.34
C ₂₉ βα diasteranes/(ααα+αββ steranes)	0.67
C ₂₉ ααα steranes 20 <i>S</i> /(20 <i>S</i> +20 <i>R</i>)	0.44
C ₂₉ steranes αββ/(αββ+ααα)	0.53
C ₂₉ βα diasteranes 20 <i>S</i> /(20 <i>S</i> +20 <i>R</i>)	0.65
Methylnaphthalene ratio (2-MN/1-MN)	2.3 #
Dimethylnaphthalene ratio 1 ([2,6-+2,7-DMN]/1,5-DMN)	5.7 #
Trimethylnaphthalene ratio 2 ([2,3,6-+1,3,7-TMN]/[1,4,6-+1,3,5-+1,3,6-TMN])	0.90 #
Methylphenanthrene index (1.5*[3-MP+2-MP]/[P+9-MP+1-MP])	0.53 #
Methylphenanthrene ratio (2-MP/1-MP)	1.7 #
Dimethylphenanthrene ratio (3,5-+2,6-DMP+2,7-DMP)/ (1,3-+3,9-+2,10-+3,10-DMP+1,6-+2,9-+2,5-DMP)	0.48 #
Methylbiphenyl ratio (3-MBp/2-MBp)	3.0 #
Phenanthrene/dibenzothiophene	8.3 #
Methyldibenzothiophene ratio (4-MDBT/1-MDBT)	2.1 #

Ratios were calculated from MRM data, (m/z $M^+ \rightarrow 191, 217$ for hopanes, and steranes and diasteranes, respectively), except for ¶ (% mol fraction), ¥ (FID equivalents derived from corrected SIM runs), § (m/z 85), \$ (m/z 191), † (m/z 205), P (m/z 217), * (m/z 217 and m/z 191) and # (aromatic hydrocarbon ratios, SIM).

Methods DR1

Microthermometry of approximately 250 fluid inclusions was performed on a Linkam heating-freezing stage calibrated with synthetic fluid inclusions.

The conglomerate was fragmented into 2 mm pieces and thoroughly cleaned with hydrogen peroxide, hot chromic acid, Aqua Regia and a range of solvents of different polarity (Dutkiewicz et al., 2004; Volk et al., 2005). Rock fragments were checked repeatedly for cleanliness by gas chromatography–mass spectrometry (GC–MS) analyses of outside rinse blanks on a Hewlett Packard 5890 gas chromatograph (DB5MS, 60 m x 0.25 mm i.d, 0.25 µm film thickness) interfaced to a VG AutospecQ Ultima mass spectrometer. A system blank using exactly the same experimental conditions as the actual crushing was obtained one day earlier. An offline crushing method was used for the analysis of traces of C_{12+} hydrocarbons such as biomarkers, whereas an online crushing method (Quantum MSSV 1 Thermal Analysis System) yielded complementary information on the low molecular weight hydrocarbon distribution (Volk et al., 2005). Both on- and offline-crushing experiments were in replicate, with repeats giving similar results as reported. Peak identifications for biomarkers in single ion monitoring (SIM) runs were confirmed by metastable reaction monitoring (MRM) analyses. Low molecular weight hydrocarbon data were acquired by SIM runs, with conversion to flame ionisation detector equivalent data using response factors before data manipulation

Dutkiewicz, A., Volk, H., Ridley, J., and George, S.C., 2004, Geochemistry of oil in fluid inclusions in a middle Proterozoic igneous intrusion: implications for the source of hydrocarbons in crystalline rocks: *Organic Geochemistry*, v. 35, p. 937–957.

Volk, H., George, S.C., Dutkiewicz, A., and Ridley, J., 2005, Characterisation of fluid inclusion oil in a Mid-Proterozoic sandstone and dolerite (Roper Superbasin, Australia): *Chemical Geology*, v. 223, p. 109–135.