Table 1. Crystal data and structure refinement for Moris-38new.

<table>
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<tr>
<th>Identification code</th>
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<tr>
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<td>C13 H22 O5 Si</td>
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<tr>
<td>Formula weight</td>
<td>286.40</td>
</tr>
<tr>
<td>Temperature</td>
<td>293(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system, space group</td>
<td>Monoclinic, P 21/c</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>a = 9.148(2) Å, alpha = 90 deg.</td>
</tr>
<tr>
<td></td>
<td>b = 12.189(2) Å, beta = 94.32(2) deg.</td>
</tr>
<tr>
<td></td>
<td>c = 13.7676(3) Å, gamma = 90 deg.</td>
</tr>
<tr>
<td>Volume</td>
<td>1530.8(4) Å³</td>
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<tr>
<td>Z, Calculated density</td>
<td>4, 1.243 Mg/m³</td>
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<tr>
<td>Absorption coefficient</td>
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<tr>
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<tr>
<td>Theta range for data collection</td>
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<tr>
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<tr>
<td>Reflections collected / unique</td>
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<tr>
<td>Completeness to theta = 25.07</td>
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<tr>
<td>Absorption correction</td>
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<tr>
<td>Refinement method</td>
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<td>Data / restraints / parameters</td>
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<tr>
<td>R indices (all data)</td>
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<td>0.178 and -0.193 e.Å⁻³</td>
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Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for Moris-38new. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

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<th>U(eq)</th>
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Table 3. Bond lengths [Å] and angles [deg] for Moris-38new.

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<tr>
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<td>C(2)-H(2B)</td>
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Page 2
Si - C(1) - H(1B)  109.5
H(1A) - C(1) - H(1B)  109.5
Si - C(1) - H(1C)  109.5
H(1A) - C(1) - H(1C)  109.5
Si - C(2) - H(2A)  109.5
Si - C(2) - H(2B)  109.5
H(2A) - C(2) - H(2B)  109.5
Si - C(3) - H(3A)  109.5
Si - C(3) - H(3B)  109.5
H(3A) - C(3) - H(3B)  109.5
Si - C(3) - H(3C)  109.5
H(3A) - C(3) - H(3C)  109.5
H(3B) - C(3) - H(3C)  109.5
C(5) - O(4) - Si  130.8(16)
O(4) - C(5) - O(13)  111.0(17)
O(4) - C(5) - C(14)  118.5(2)
O(13) - C(5) - C(14)  109.2(19)
O(4) - C(5) - C(6)  113.8(2)
O(13) - C(5) - C(6)  113.8(19)
C(14) - C(5) - C(6)  88.88(17)
O(8) - C(6) - C(7)  106.0(2)
O(8) - C(6) - C(18)  110.0(2)
C(7) - C(6) - C(18)  121.0(2)
O(8) - C(6) - C(5)  111.1(2)
C(7) - C(6) - C(5)  119.3(2)
C(18) - C(6) - C(5)  88.6(2)
C(6) - C(7) - H(7A)  109.5
C(6) - C(7) - H(7B)  109.5
H(7A) - C(7) - H(7B)  109.5
H(7A) - C(7) - H(7C)  109.5
H(7B) - C(7) - H(7C)  109.5
C(9) - O(8) - C(6)  120.64(19)
O(10) - C(9) - O(8)  118.1(2)
O(10) - C(9) - C(11)  124.6(3)
O(8) - C(9) - C(11)  117.1(2)
O(13) - C(11) - C(12)  108.5(18)
O(13) - C(11) - C(9)  106.4(19)
C(12) - C(11) - C(9)  110.9(2)
O(13) - C(11) - C(15)  104.28(17)
C(12) - C(11) - C(15)  117.0(2)
C(9) - C(11) - C(15)  109.13(19)
C(11) - C(12) - H(12A)  109.5
C(11) - C(12) - H(12B)  109.5
C(12) - C(11) - H(12C)  109.5
C(12) - C(11) - H(12C)  109.5
C(11) - C(12) - H(12B)  109.5
C(11) - C(12) - H(12C)  109.5
C(11) - C(12) - H(12C)  109.5
C(5) - O(13) - C(11)  103.75(15)
C(15) - C(14) - C(18)  115.9(2)
C(15) - C(14) - C(5)  102.9(2)
C(18) - C(14) - C(5)  88.6(2)
C(15) - C(14) - H(14)  109.5(13)
C(18) - C(14) - H(14)  118.8(13)
C(5) - C(14) - H(14)  119.1(11)
O(17) - C(15) - C(16)  111.1(19)
O(17) - C(15) - C(14)  109.8(2)
C(16) - C(15) - C(14)  110.3(2)
O(17) - C(15) - C(11)  110.20(18)
C(16) - C(15) - C(11)  112.3(2)
C(14) - C(15) - C(11)  102.81(19)
C(15) - C(16) - H(16A)  109.5
C(15) - C(16) - H(16B)  109.5
H(16A) - C(16) - H(16B)  109.5
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å² x 10³) for Moris-38new.
The anisotropic displacement factor exponent takes the form:
-2 \pi^2 \left[ h^2 a^*^2 U_{11} + \ldots + 2 h k a^* b^* U_{12} \right]

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<th>U33</th>
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Table 5. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å² x 10³) for Moris-38new.

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<td>108</td>
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<tr>
<td>H(16C)</td>
<td>6907</td>
<td>2442</td>
<td>696</td>
<td>108</td>
</tr>
<tr>
<td>H(14)</td>
<td>8270(20)</td>
<td>2538(18)</td>
<td>2387(15)</td>
<td>53(7)</td>
</tr>
<tr>
<td>H(17)</td>
<td>10260(30)</td>
<td>1370(20)</td>
<td>514(18)</td>
<td>68(10)</td>
</tr>
<tr>
<td>H(18A)</td>
<td>10520(30)</td>
<td>1098(19)</td>
<td>2749(17)</td>
<td>78(8)</td>
</tr>
<tr>
<td>H(18B)</td>
<td>9720(20)</td>
<td>1394(17)</td>
<td>3630(16)</td>
<td>49(8)</td>
</tr>
</tbody>
</table>
You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.
Please wait while processing....

Datablock: I

Wavelength=0.71073
(C=13.7676(3
gamma=90

C-C = 0.0034 A
(b=12.189(2
(a=9.148(2
(beta=94.32(2
(alpha=90
K 293

Reported
(4)1530.8
P 21/c

Calculated
(4)1530.8
P 21/c

Space group

Hall group-P 2ybc-

Moietiy formula-C13 H22 O5 Si

Sum formula-C13 H22 O5 Si

Mr-286.40

Dx,g cm-3-1.243

Z4

Mu (mm-1-0.166

F000616.0

F000'616.64

h,k,lmax10,14,16

Nref27102698

Tmin,Tmax0.951,0.990

Correction method= Not given

Theta(max)= 25.070

Data completeness= 0.996

wr2(reflections)= 0.0800(2698)

R(reflections)= 0.0418(1353)

Npar= 188

S = 0.846

The following ALERTS were generated. Each ALERT has the format .test-name_ALERT_alert-type_alert-level.
.Click on the hyperlinks for more details of the test.

Alert level C

MoieityFormula Not GivenPLAT048_ALERT_1_C

No '_symmetry_space_group_name_Hall' GivenPLAT125_ALERT_4_C

Check Low Ueq as Compared to Neighbors for SiPLAT242_ALERT_2_C

U(iso) H18B Smaller than U(eq) C18 by ... 0.01 PLAT245_ALERT_2_C

Alert level G

Check the Reported _cell_measurement_temperature 293 KPLAT199_ALERT_1_G

Check the Reported _diffrn_ambient_temperature 293 KPLAT200_ALERT_1_G

The Model has Chirality at C5 (Verify) ... SPLAT793_ALERT_4_G

The Model has Chirality at C6 (Verify) ... SPLAT793_ALERT_4_G

The Model has Chirality at C11 (Verify) ... SPLAT793_ALERT_4_G

The Model has Chirality at C14 (Verify) ... SPLAT793_ALERT_4_G

The Model has Chirality at C15 (Verify) ... RPLAT793_ALERT_4_G
**ALERT level A** = Most likely a serious problem - resolve or explain 0
**ALERT level B** = A potentially serious problem, consider carefully 0
**ALERT level C** = Check. Ensure it is not caused by an omission or oversight 4
**ALERT level G** = General information/check it is not something unexpected 7

**ALERT type 1** CIF construction/syntax error, inconsistent or missing data 3
**ALERT type 2** Indicator that the structure model may be wrong or deficient 2
**ALERT type 3** Indicator that the structure quality may be low 0
**ALERT type 4** Improvement, methodology, query or suggestion 6
**ALERT type 5** Informative message, check 0