Supporting information

New insights on the decomposition mechanism of Molybdenum DialkyldiThioCarbamate (MoDTC): A Raman spectroscopic study

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Figure S 1. Raman spectra obtained from different regions of the tribopair wear scars after tests with 0.5 wt% MoDTC at 20°C. (a) Ball wear scar (b) disc wear scar.

Figure S 2. Raman spectra obtained from the tribopair wear scars after tests with 0.5 wt% MoDTC at 40°C. (a) Ball wear scar (b) Disc wear scar.
Figure S 3. Raman spectra obtained from the tribopair wear scars after tests with 0.5 wt% MoDTC at 60°C. (a) Ball wear scar (b) Disc wear scar

Figure S 4. Raman spectra from the tribopair wear scars after tests with 0.5 wt% at 100°C. (a) Ball wear scar (b) disc wear scar
Figure S 5. Raman spectra obtained from the tribopair wear scars after tests with 0.1 wt% MoDTC at 60°C. (a) Ball wear scar (b) disc wear scar

Figure S 6. Raman spectra obtained from the tribopair wear scars after tests with 0.5 wt% MoDTC at 60°C. (a) Ball wear scar (b) disc wear scar
**Figure S 7.** Raman spectra obtained from the tribopair wears scar generated with 0.9 wt% MoDTC at 60°C. (a) Ball wear scar (b) disc wear scar

**Figure S 8.** Raman spectra obtained from the tribopair wear scars after tests at 0.98 GPa. (a) Ball wear scar (b) disc wear scar
Figure S 9. Raman spectra obtained from tribopair wear scars after tests at 2.12 GPa at 60°C. (a) Ball wear scar (b) disc wear scar

Figure S 10. Raman spectra of Group III mineral oil used as the base oil and MoDTC additive concentrate
Figure S 11. Raman spectra of pure microcrystalline powders

Figure S 12. Examples of Raman spectra obtained outside wear scars. In most regions no Raman peaks were observed. In some regions, Fe$_3$O$_4$ peak $\sim$670 cm$^{-1}$ was observed
**Figure S 13.** Raman spectrum obtained from Fe$_3$O$_4$ deposits after heating 1 wt% MoDTC lubricant containing 5 wt% Fe$_3$O$_4$ at 100°C for 1h

**Table S1.** Bond dissociation energy for bonds in MoDTC

<table>
<thead>
<tr>
<th>Bond type</th>
<th>Bond dissociation energy (kJ mol$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo-S</td>
<td>450</td>
</tr>
<tr>
<td>Mo=O</td>
<td>420</td>
</tr>
<tr>
<td>C-H</td>
<td>410</td>
</tr>
<tr>
<td>C-C</td>
<td>350</td>
</tr>
<tr>
<td>C-N</td>
<td>300</td>
</tr>
<tr>
<td>C-S</td>
<td>260</td>
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