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Supporting Information

on

Quantum Chemical Calculation studies for interactions of antiwear lubricant additives with metal surface

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S1. Antiwear Testing

The antiwear tests were performed using Four-Ball Lubricant Tester (Stanhope-Seta, London Street, Chertsey, UK) at 1475 rpm (equivalent to a sliding speed of 567 mm/sec) using different loads for different time durations according to ASTM D4172. The wear scar diameter on the lower three balls was measured after running for 15, 30, 45, 60, 75 and 90 min respectively at 392N load.

S1.1 Experimental details

The wear scar diameter of each of the three horizontal balls was measured in two mutually perpendicular directions, one in the sliding direction (d_s) and the other perpendicular (d_p) to it using an optical microscope. Geometric mean of the two perpendicular diameters on the same ball was taken as given by the equation 1.

For each experiment arithmetic mean of the above diameter of each ball (d_1,d_2 and d_3) was taken as given by equation 2. The three stationary balls were not disturbed while taking the readings and the wear scar diameter was taken by tilting eye piece of the microscope at an angle of 70.5^0 making it perpendicular to the surface of the scar.

S1.2 Tribological Parameters

S1.2.1 Mean wear scar diameter (MWD)

$$d_1 = \sqrt{(d_s d_p)} \qquad 1$$

$$d = \frac{d_1 + d_2 + d_3}{3} \qquad 2$$

S1.2.2 Mean wear volume (MWV)

Mean wear volume, $$V = \frac{\Pi\, d_0^4}{64\, r}\{(\frac{d}{d_0})^4 - (\frac{d}{d_0})\} \quad (3)$$

Hertzian diameter, $$d_0 = 2(\frac{3\,Pr}{4E})^{\frac{1}{3}}$$

Where, $$\frac{1}{r} = \frac{1}{r_1} + \frac{1}{r_2}$$

$$\frac{1}{E^*} = \frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2}$$

Where, E^* = Resultant modulus of elasticity

v = Poissons ratio

r = Radius of steel ball

$E_1 = E_2 = 206$ GPa

$v_1 = v_2 = 0.3$

P = Actual load in Newton on each of the three horizontal balls that is 0.408 times of applied load.

S1.2.3 Wear-rate:

Mean wear volumes at different times (15, 30, 45, 60, 75 and 90 min.) for each experiment were plotted with time and a linear regression model was fitted on the points including origin to find out overall wear rate.

$$\frac{V}{l} = K\frac{P}{H}$$

V = mean wear volume

l = sliding distance ($2\pi r.N$)

K = wear coefficient

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H = hardness of steel ball (59-61 HRC)

P = applied load (0.408x392N)