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Vibrational spectroscopy and theoretical studies of the potential energy surface of the first excited triplet state of the phenol group. The potential energy surface of the ground state and the first excited triplet state of the phenol group has been investigated at the coupled cluster singles and doubles level, in conjunction with the aug-cc-pVQZ basis set. Then, the new predicted potential energy surface has been used to characterize the first triplet state of phenol and to perform explicit calculations of high-frequency out-of-plane bending motion. The theoretical results show that this motion has a large contribution, compared to phenol's ground state. Potential energy curves in the PES of the first triplet state are predicted to be localized in the region where the ground state is non-stable. This state exhibits a large anharmonicity due to interaction with the first singlet and triplet states of phenol.

The present invention relates to a composition of matter for use in lubricating oils. More particularly, the present invention relates to a composition of matter comprised of a molybdenum dithiocarbamate-coated iron or aluminum barstock. Bar stock used in the crankcase of internal combustion engines is subjected to severe mechanical and thermal stresses. On the one hand, the crankcase is subjected to the high temperature and pressure conditions present in the engine compartment during operation. On the other hand, the crankcase undergoes the substantial thermal and mechanical stresses present in the

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