Supplementary Information

(Figures S1-S4 and Complete Gaussian Reference)

Chalcogenidobis(ene–1,2–dithiolate)molybdenum(IV) Complexes (Chalcogenide E = S, Se): Probing Mo≡E and Ene–1,2–dithiolate Substituent Effects on Geometric and Electronic Structure

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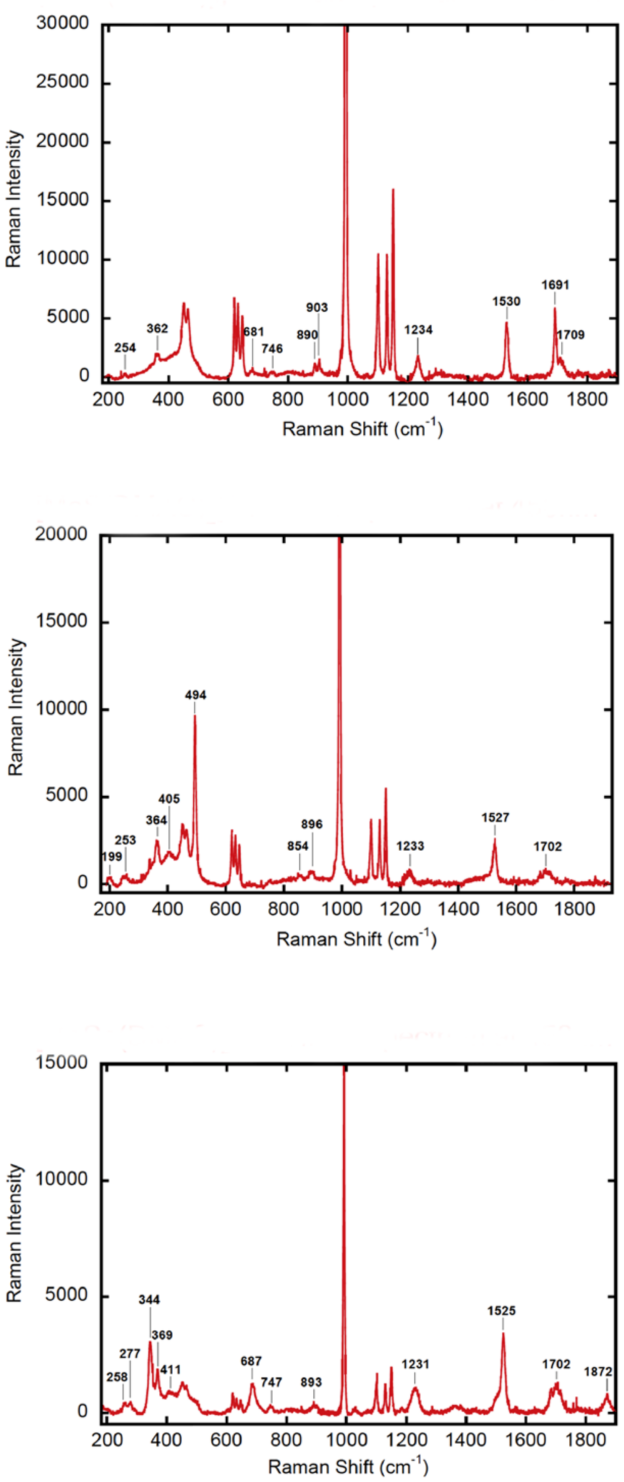

Fig. S1 Solid State resonance Raman spectra collected at 458nm for **MoOL**$^{\mathbf{COOMe}}$ (above), **MoSL**$^{\mathbf{COOMe}}$ (middle), and **MoSeL**$^{\mathbf{COOMe}}$ (bottom).

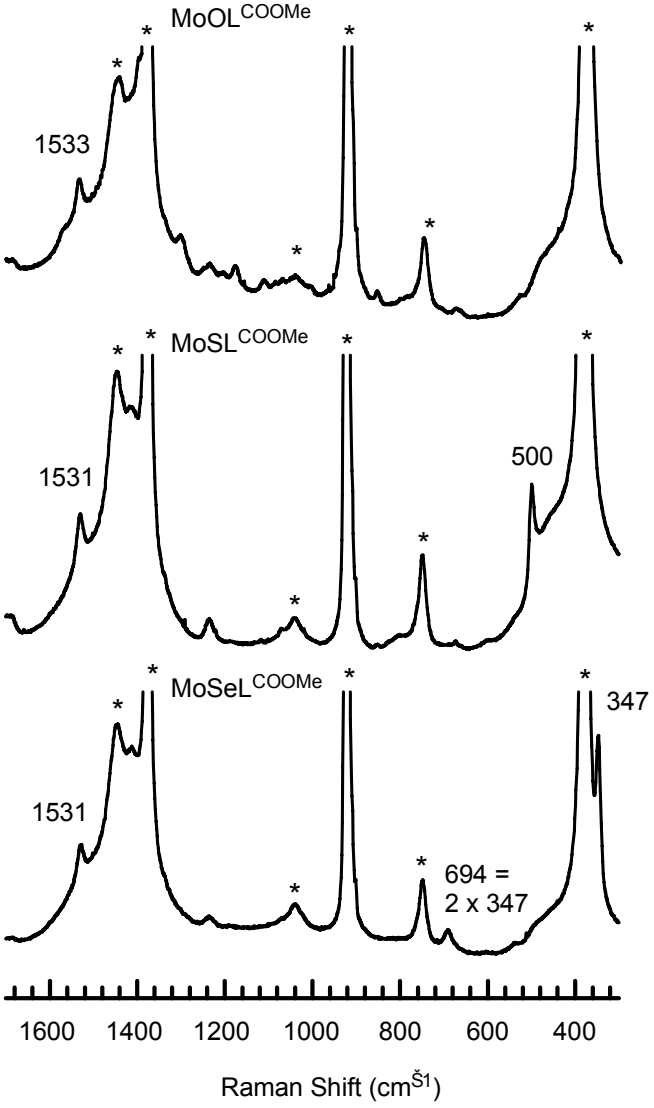

Fig. S2 resonance Raman spectra of **MoOL^{COOMe}** (above), **MoSL^{COOMe}** (middle), and **MoSeL^{COOMe}** (bottom) in CH_3CN using Ar ion laser with excitation at 488 nm (asterisks indicate solvent peaks).

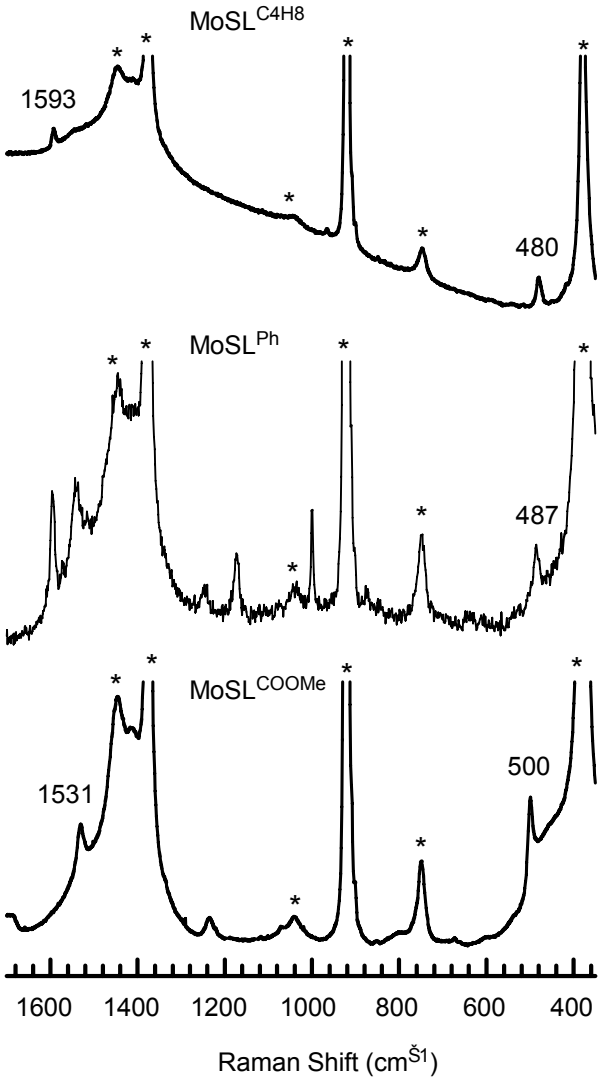

Fig. S3 resonance Raman spectra of **MoSL^{C4H8}** (above), **MoSL^{Ph}** (middle), and **MoSL^{COOMe}** (bottom) in CH_3CN using Ar ion laser with excitation at 488 nm (asterisks indicate solvent peaks).

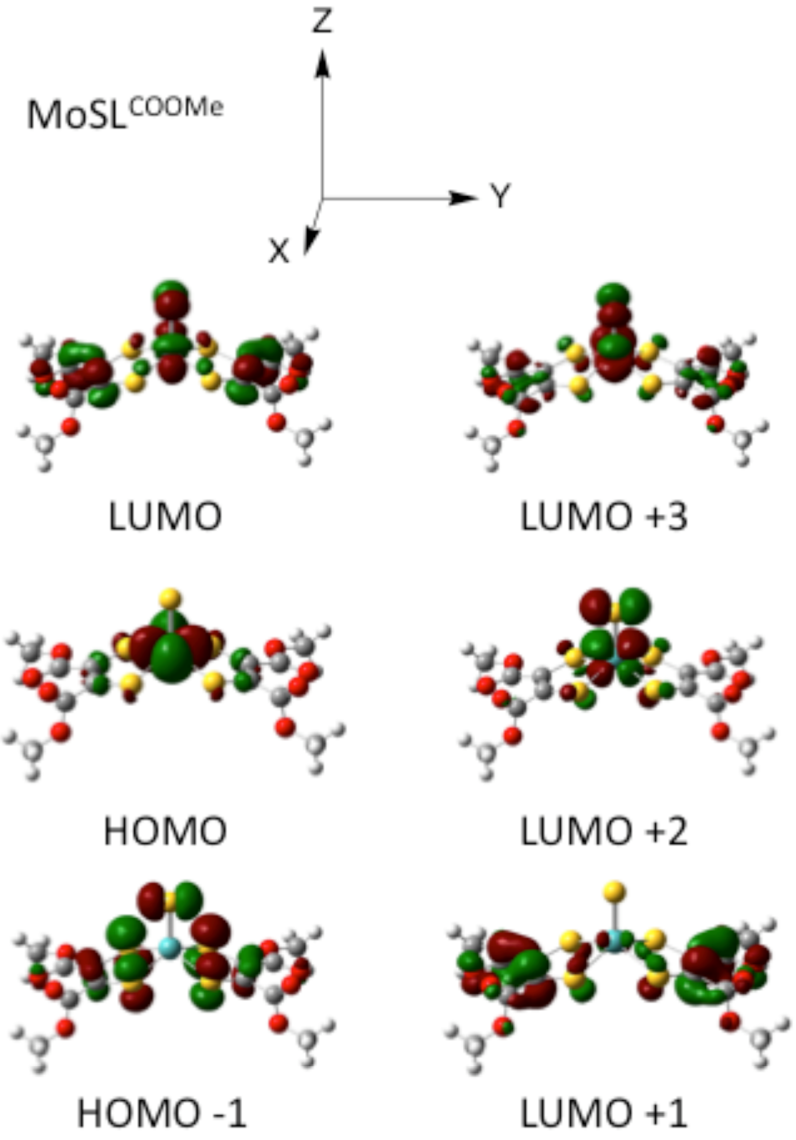

Fig. S4 Frontier Kohn-Sham molecular orbitals for **MoSL^{COOMe}**.

Gaussian Reference

M. J. Frisch, G. W. T., H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople *Gaussian 03, Revision C.02*, Gaussian, Inc.: Wallingford CT, 2004.