Supplementary information for :

IRMPD spectroscopy of gaseous protonated S-nitrosocaptopril, a biologically active, synthetic amino acid

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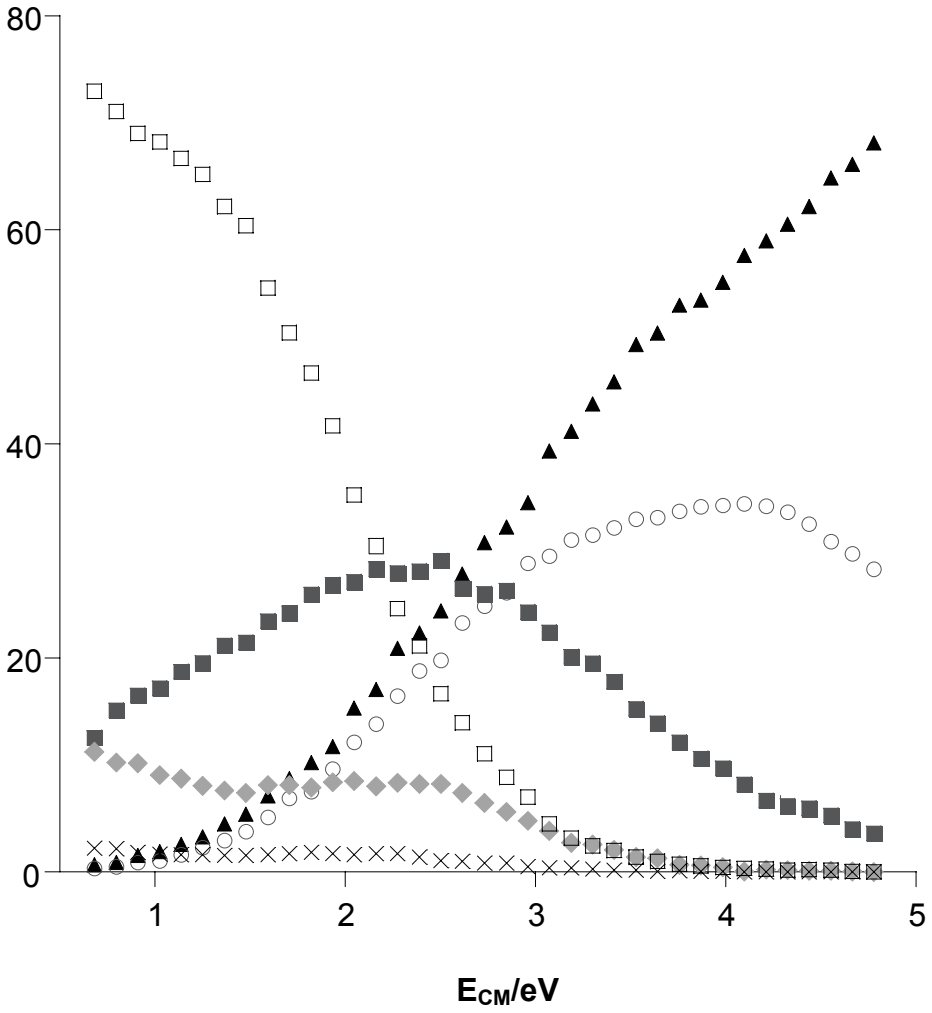
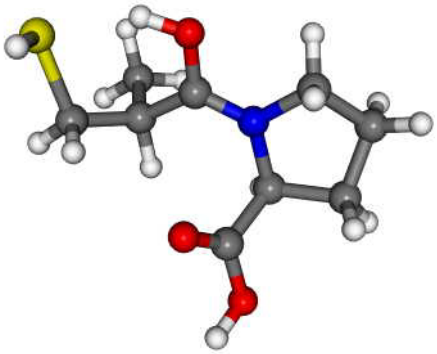
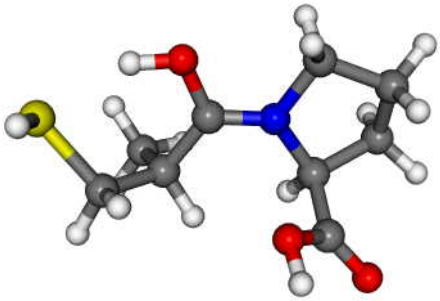


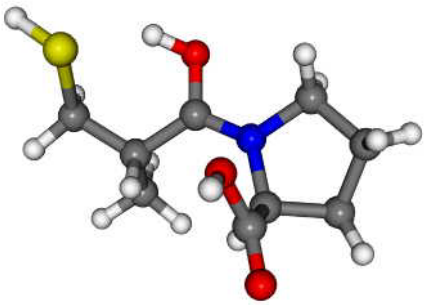
Figure S1 CID breakdown graph of mass selected $capH^+$ ions (□, m/z 218) to afford ions at m/z 200 (×), 172 (■), 116 (◆), and, at higher energies, 70 (▲) and 75 (○).



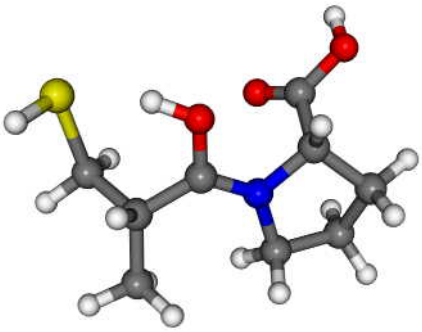
CO-T2
(2.6 kJ/mol)



CO-T3
(12.1 kJ/mol)



CO-T4
(35.0 kJ/mol)



CO-C2
(23.2 kJ/mol)

Figure S2 Optimized structures for low energy conformers of structure **CO-T1** of $capH^+$. ΔH_{rel}^0 relative values (reported in parentheses) are in kJ/mol.

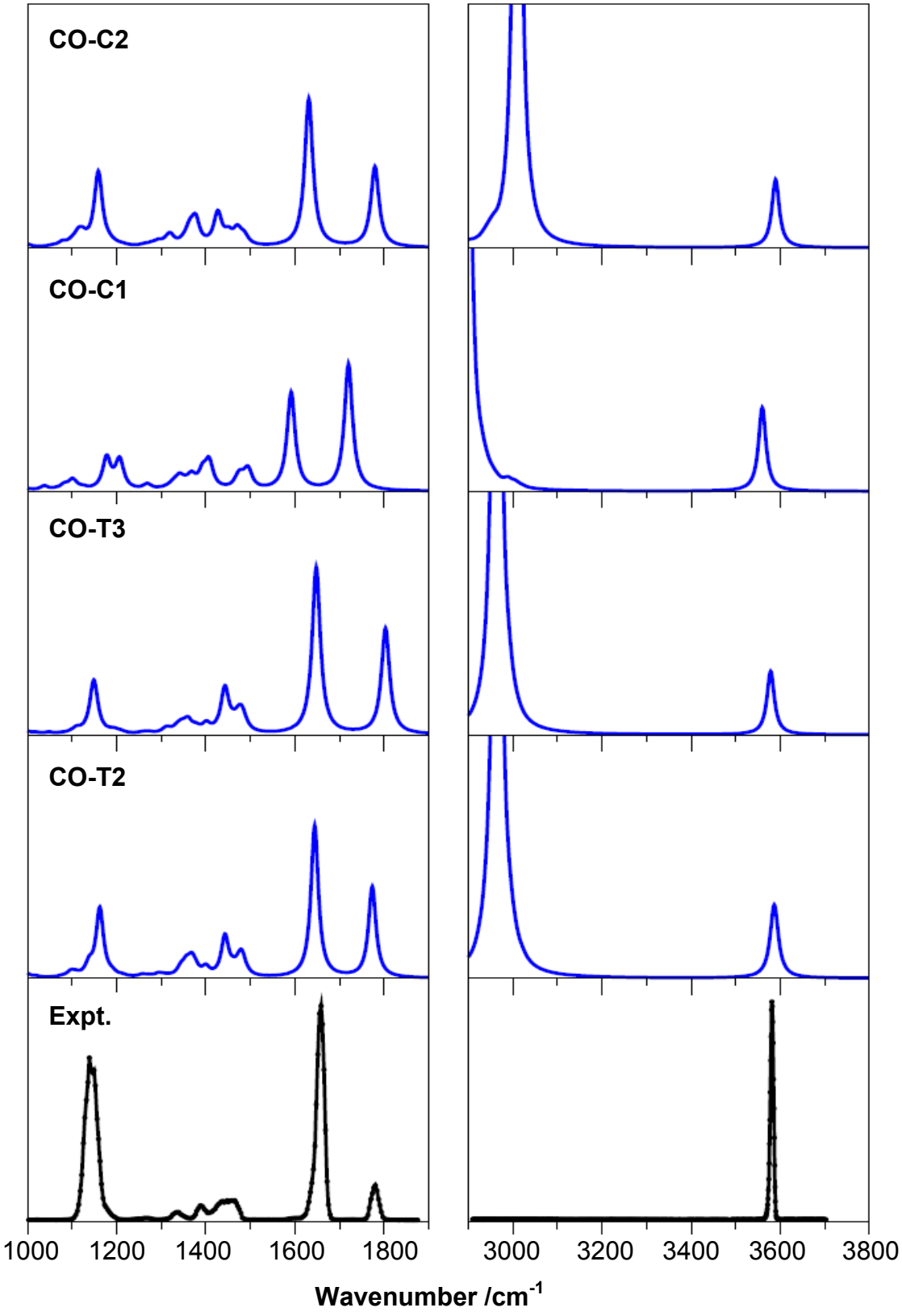


Figure S3 Experimental IRMPD spectrum of $capH^+$ (bottom) and calculated IR spectra (at the B3LYP/6-311+G** level) of structures **CO-T2**, **CO-T3, CO-C1**, **CO-C2**.

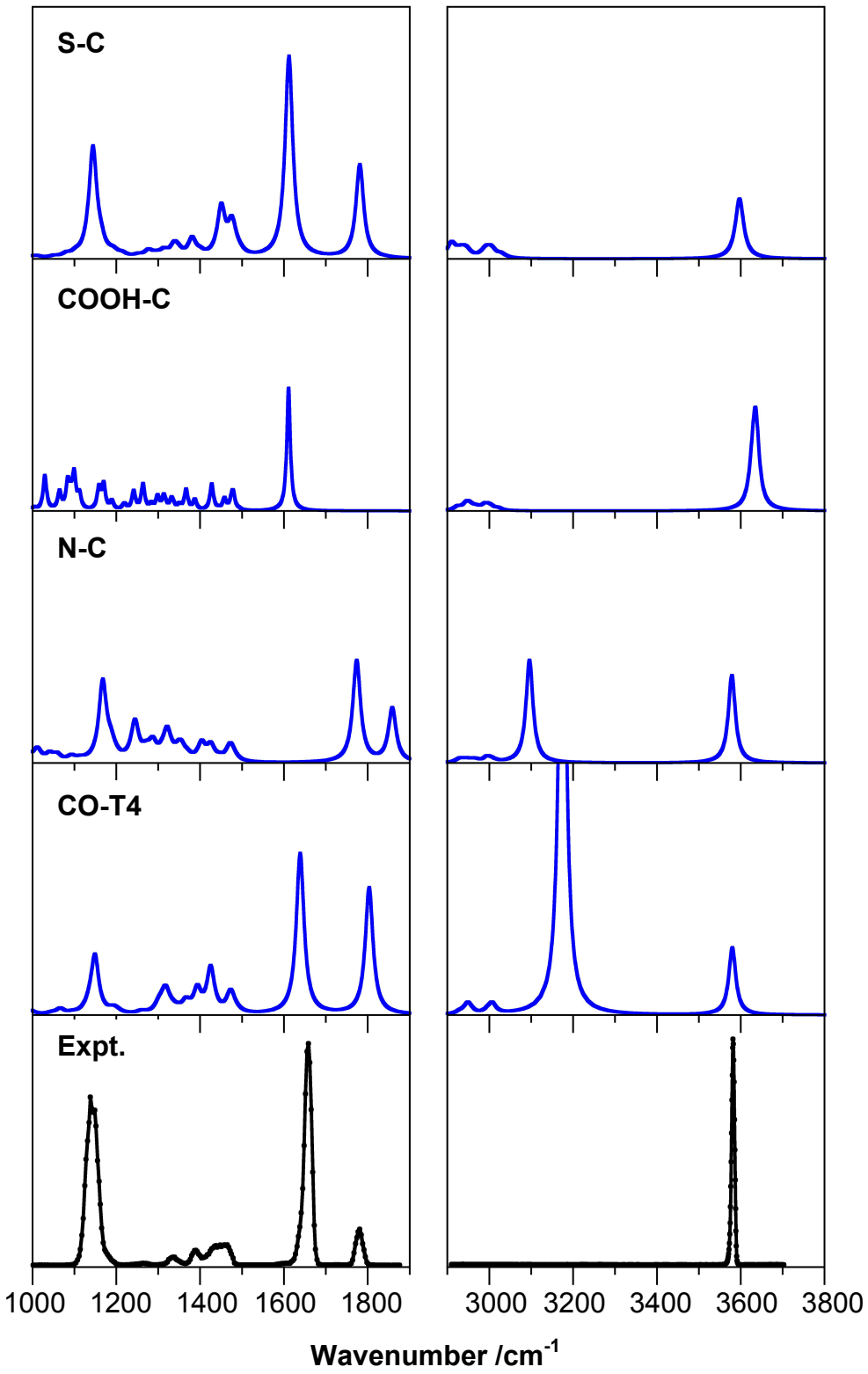


Figure S4 Experimental IRMPD spectrum of $capH^+$ (bottom) and calculated IR spectra (at the B3LYP/6-311+G** level) of structures **CO-T4**, **N-C, COOH-C, S-C**.

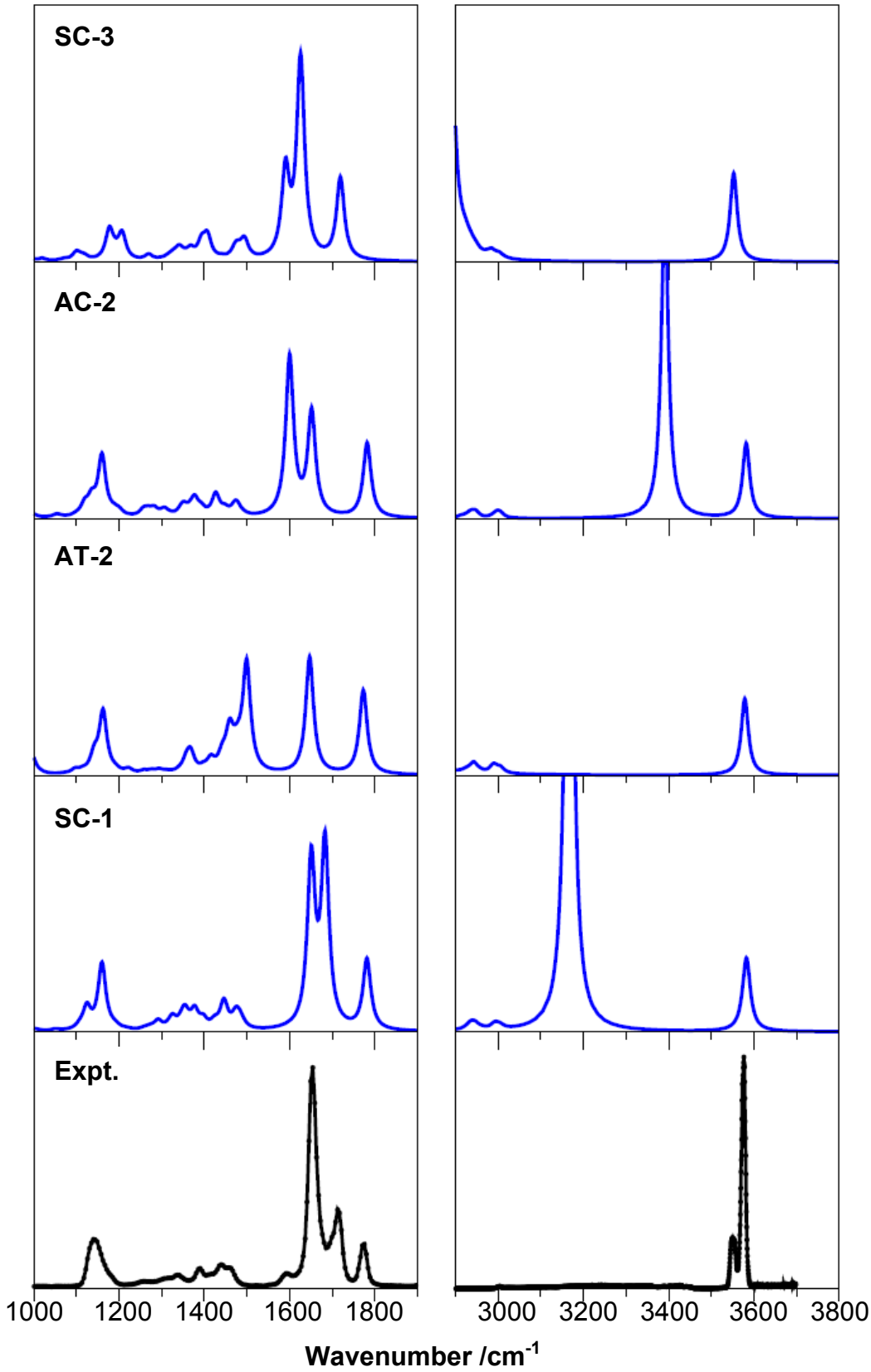


Figure S5 Experimental IRMPD spectrum of $SNOcapH^+$ (bottom) and calculated IR spectra (at the B3LYP/6-311+G** level) of isomers **SC-1**, **AT-2**, **AC-2, SC-3**.

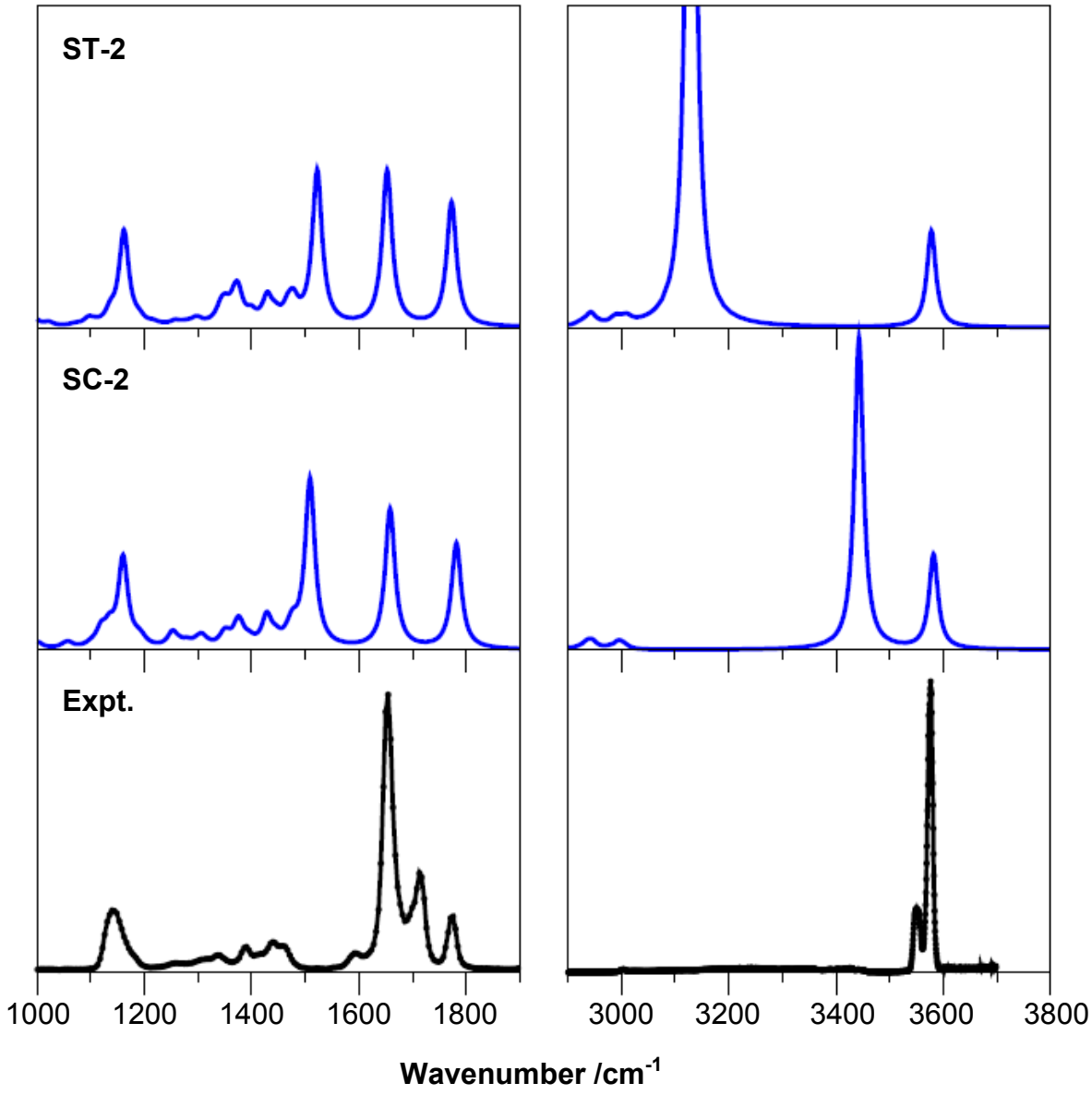


Figure S6 Experimental IRMPD spectrum of $SNOcapH^+$ (bottom) and calculated IR spectra (at the B3LYP/6-311+G** level) of isomers **SC-2**, **ST-2.**

Reference Gaussian 03, Revision C.02

Reference Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, 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, Inc., Wallingford CT, 2004.