

Supporting information for:

[CuSn₅Sb₃]₂⁴⁻ as a Dual Spherical-Spherical Aromatic Heterometallic Cluster Bridged via an Antiaromatic Cu₂Sn₂ Motif

Peter L. Rodríguez-Kessler^a and Alvaro Muñoz-Castro^{b*}

^a*Centro de Investigaciones en Óptica A.C., Loma del Bosque 115, Col. Lomas del Campestre, León, Guanajuato, 37150, Mexico.*

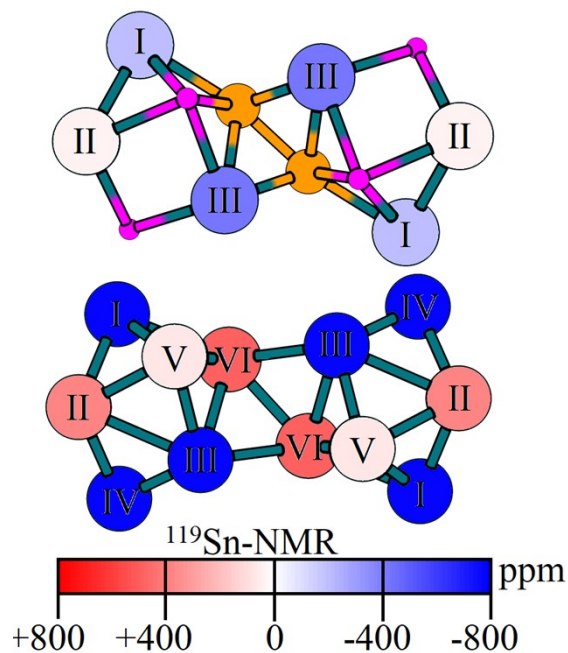
^b*Facultad de Ingeniería, Arquitectura y Diseño, Universidad San Sebastián, Bellavista 7, Santiago, 8420524, Chile.*

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Table S1. Calculated ^{119}Sn -NMR parameters in ppm, denoting a graphical representation of the different Sn-atom types in the studied cluster dimers.



$[\text{CuSn}_5\text{Sb}_3]_2^{4-}$	σ_{11}	σ_{11}	σ_{11}	σ_{iso}	$^{119}\text{Sn } \delta$
Sn I	1900.4	3457.1	3909.6	3089.0	-212.1
Sn II	1257.1	2989.4	4241.2	2829.2	47.7
Sn III	2228.8	3438.9	4169.8	3279.2	-402.2
$[\text{Sn}_{18}]^{4-}$					
Sn I	2432.6	4046.2	4675.9	3718.2	-841.3
Sn II	905.3	2646.1	3911.0	2487.5	389.5
Sn III	2853.9	3572.2	4879.3	3768.5	-891.5
Sn IV	3494.9	4237.9	5414.4	4382.4	-1505.5
Sn V	1934.5	2557.9	3654.0	2715.5	161.5
Sn VI	-816.6	2550.0	5266.9	2333.5	543.5

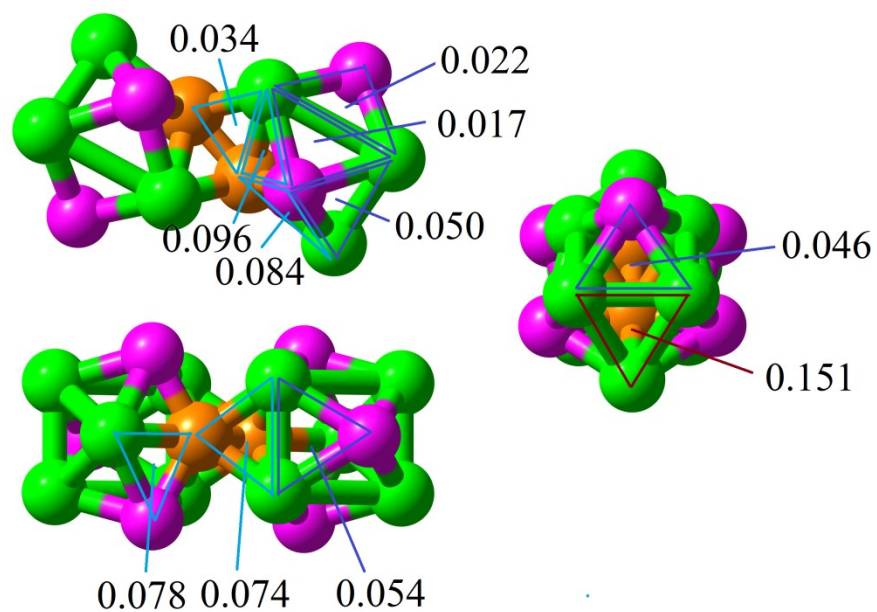


Figure S1. Calculated multicenter index for representative triangular faces of the studied $[\text{CuSn}_5\text{Sb}_3]_2^{4+}$, featuring two fused deltahedrons. Different views are showed for sake of clarity.

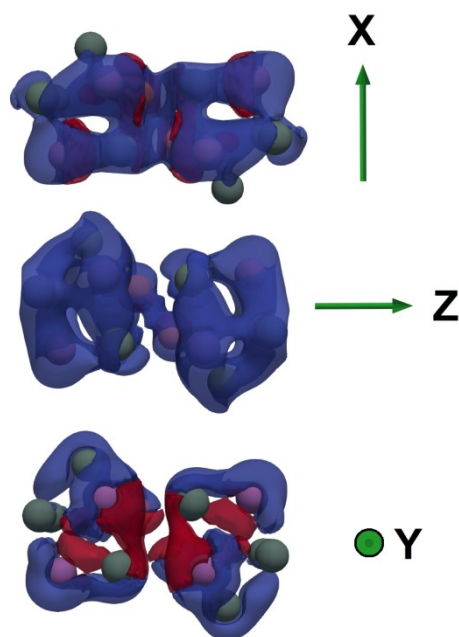


Figure S2. Calculated current density from GIMIC calculations with isosurface values of ± 0.02 nA/T, for different orientation of the applied field for $[\text{CuSn}_5\text{Sb}_3]_2^{4+}$. Blue: diatropic/ Red: Paratropic.

Gaussian09 full citation

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.