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Supplementary Materials

Effects of Temperature on Enantiomerization Energy and Distribution of Isomers in the Chiral Cu_{13} Cluster

Cesar Castillo-Quevedo [1], Carlos Emiliano Buelna-Garcia [2,3], Edgar Paredes-Sotelo [2], Eduardo Robles-Chaparro [4], Edgar Zamora-Gonzalez [5], Martha Fabiola Martin-del-Campo-Solis [1], Jesus Manuel Quiroz-Castillo [2], Teresa del-Castillo-Castro [2], Gerardo Martínez-Guajardo [6], Aned de-Leon-Flores [4], Manuel Cortez-Valadez [7], Filiberto Ortiz-Chi [8], Tulio Gaxiola [9], Santos Jesus Castillo [7], Alejandro Vásquez-Espinal [10], Sudip Pan [11] and Jose Luis Cabellos [7,*]

[1] Departamento de Fundamentos del Conocimiento, Centro Universitario del Norte, Universidad de Guadalajara, Carretera Federal No. 23, Km. 191, C.P., Colotlán 46200, Jalisco, Mexico; castillo.quevedo@cunorte.udg.mx (C.C.-Q.); mfmartindelcampo@cunorte.udg.mx (M.F.M.-d.-C.-S.)
[2] Departamento de Investigación en Polímeros y Materiales, Edificio 3G, Universidad de Sonora, Hermosillo 83000, Sonora, Mexico; a209205768@unison.mx (C.E.B.-G.); a213216667@unison.mx (E.P.-S.); jesus.quiroz@unison.mx (J.M.Q.-C.); teresa.delcastillo@unison.mx (T.d.-C.-C.)
[3] Organización Científica y Tecnológica del Desierto, Hermosillo 83150, Sonora, Mexico
[4] Departamento de Ciencias Químico Biologicas, Edificio 5A, Universidad de Sonora, Hermosillo 83000, Sonora, Mexico; a214201767@unison.mx (E.R.-C.); aned.deleon@unison.mx (A.-d.L.-F.)
[5] Departamento de Bienestar y Desarrollo Sustentable, Centro Universitario del Norte, Universidad de Guadalajara, Carretera Federal No. 23, Km. 191, C.P., Colotlán 46200, Jalisco, Mexico; edgar.zamora@cunorte.udg.mx
[6] Unidad Académica de Ciencias Químicas, Área de Ciencias de la Salud, Universidad Autónomade Zacatecas, Km. 6 carretera Zacatecas-Guadalajara s/n, Ejido La Escondida C. P., Zacatecas 98160, Zac, Mexico; germtzguajardo@uaz.edu.mx
[7] Departamento de Investigación en Física, Edificio 3M, Universidad de Sonora, Hermosillo 83000, Sonora, Mexico; jose.cortez@unison.mx (M.C.-V.); santos.castillo@unison.mx (S.J.C.)
[8] CONACYT-Universidad Juárez Autónoma de Tabasco, Centro de Investigación de Ciencia y Tecnología Aplicada de Tabasco, Cunduacán 86690, Tabasco, Mexico; fortiz@conacyt.mx
[9] Facultad de Ciencias Físico-Matemáticas de la Universidad Autónoma de Sinaloa, Sinaloa 80010, Mexico; tuliogax@uas.edu.mx
[10] Computational and Theoretical Chemistry Group Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello, Republica 498, Santiago 8370035, Chile; a.vasquezespinal@uandresbello.edu
[11] Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, Marburg 35032; pans@chemie.uni-marburg.de
* Correspondence: jose.cabellos@unison.mx

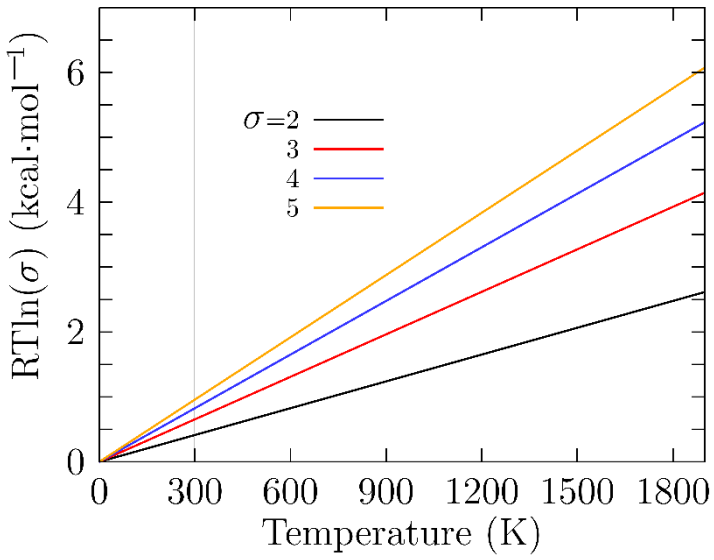

Figure S1. (Color online) shows the RTlnσ factor as a function of temperature and for different symmetry numbers. For our optimized low-energy isomers with C_2 symmetry, the symmetry number is 2, so the Gibbs free energy at 298.15 K with and without symmetry will differ by 0.41 kcal/mol regardless of the DFT method.

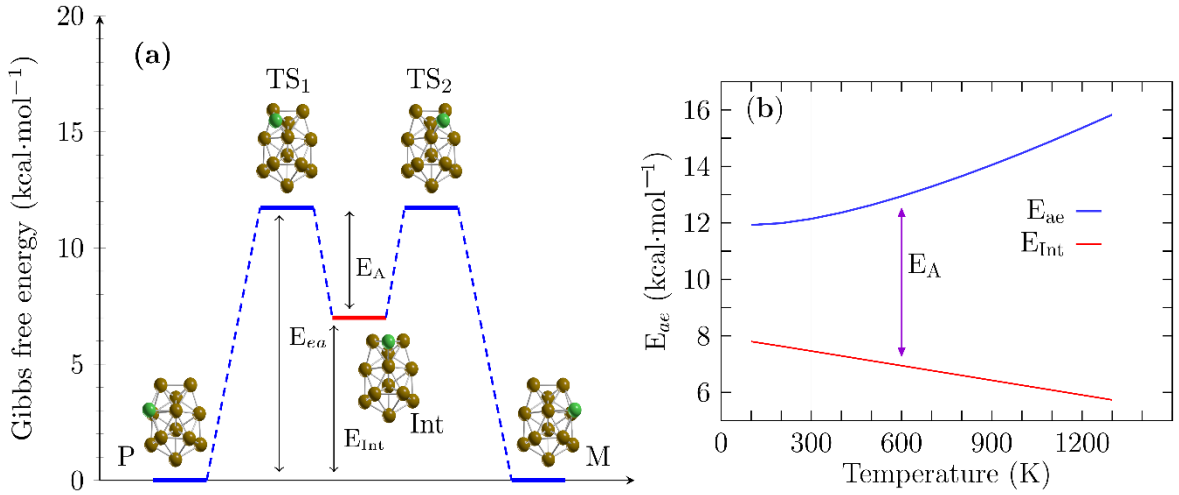

Figure S2a. (Color online) Figure (a) shows the energy profile of a chemical reaction (route A) with two symmetric transition states (TS1, TS2) and one intermediate (Int) for the interconversion between the lowest energy P and M enantiomers.

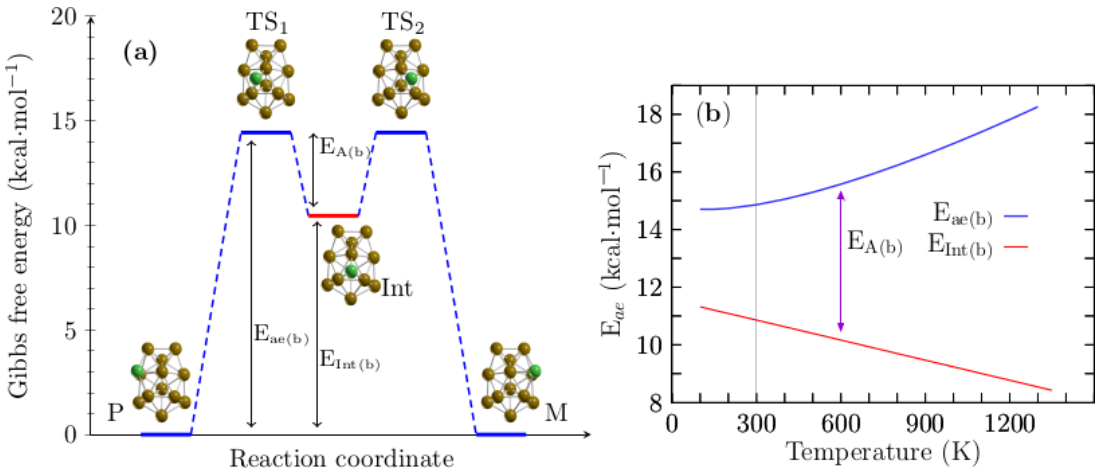

Figure S2b. (Color online) Figure (a) shows the energy profile of a chemical reaction (route B) with two symmetric transition states (TS1, TS2) and one intermediate (Int) for the interconversion between the lowest energy P and M enantiomers.

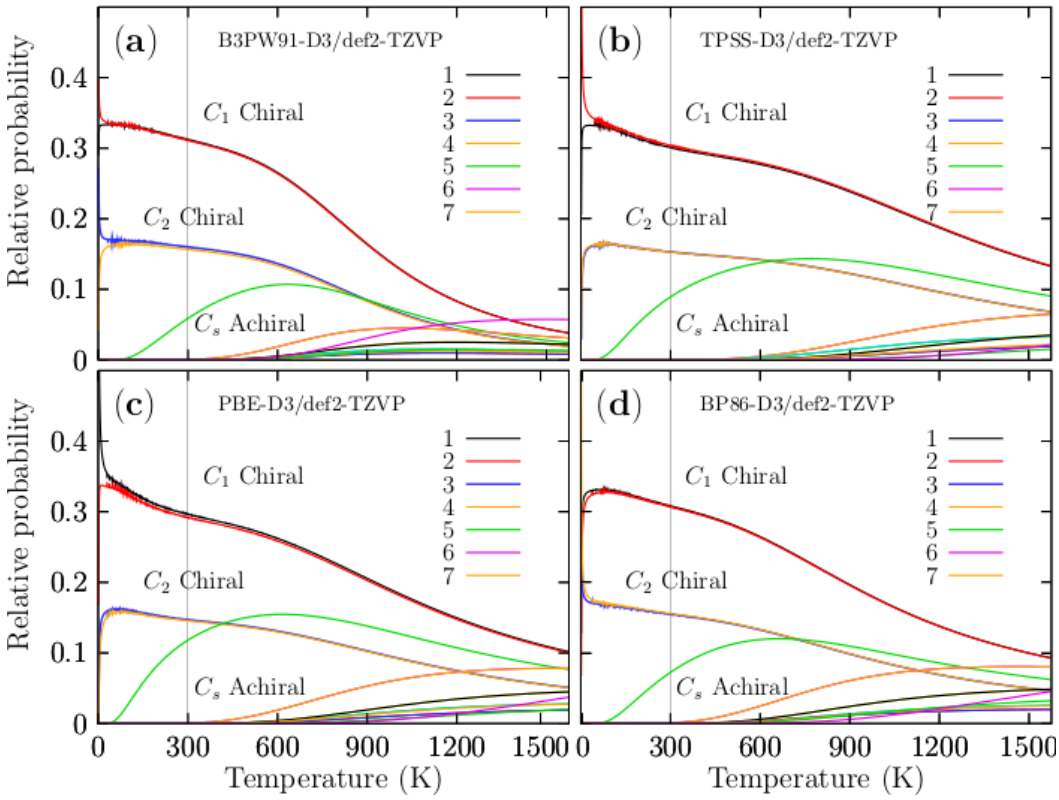

Figure S3. (Color online) Probability of occurrence or thermal population for all isomers at temperatures ranging from 20 to 1500 K computed with DFT functionals: (a) B3PW91; (b) TPSS; (c) PBE; (d) BP86. The influence of functional over the thermal population is not significant. The red and black solid lines depict the probability occurrence of the putative chiral global minimum with symmetry C_1 and strongly dominate at room temperature. The bulk melting temperature of copper is 1358 K; thus, our results below this temperature are consistent and describe correctly the Cu_{13} system.

XYZ atomic coordinates

13

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Cu 1.307754000000 0.817211000000 1.506707000000

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