

Electronic Supplementary Information (ESI)

Bond stretch isomerism in Be_3^{2-} driven by Renner-Teller effect

Manoswita Homray^{1,2}, Sukanta Mondal^{2,3}, Anirban Misra^{1*} and P. K. Chattaraj^{2,4*}

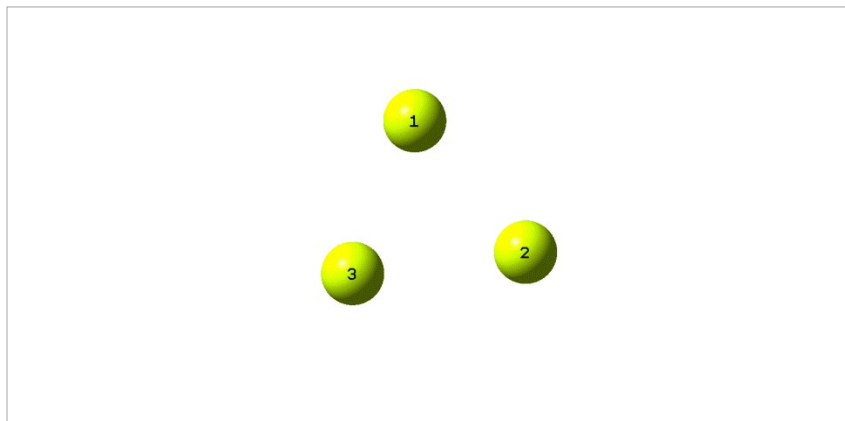
¹*Department of Chemistry, University of North Bengal, Raja Rammohunpur, Darjeeling, 734013, West Bengal, India, e-mail: anirbanmisra@yahoo.com, e-mail: manosweet.homray96@gmail.com Telephone: +91-9434228745*

²*Department of Chemistry and Center for Theoretical Studies, Indian Institute of Technology Kharagpur, Kharagpur 721302, West Bengal, India. e-mail: pkc@chem.iitkgp.ac.in, Telephone: +91-3222-283304, Fax: +91-3222-255303*

³*Department of Educational Science, Assam University, Silchar, Assam-788011, India, e-mail: sukanta.mondal@aus.ac.in, sukanta.mail13@gmail.com, Telephone: +91-7797951118*

⁴*Department of Chemistry, Indian Institute of Technology Bombay, Powai-400076, Mumbai, India*

Vid.S1. Graphics interchange format video of the isomerization process.



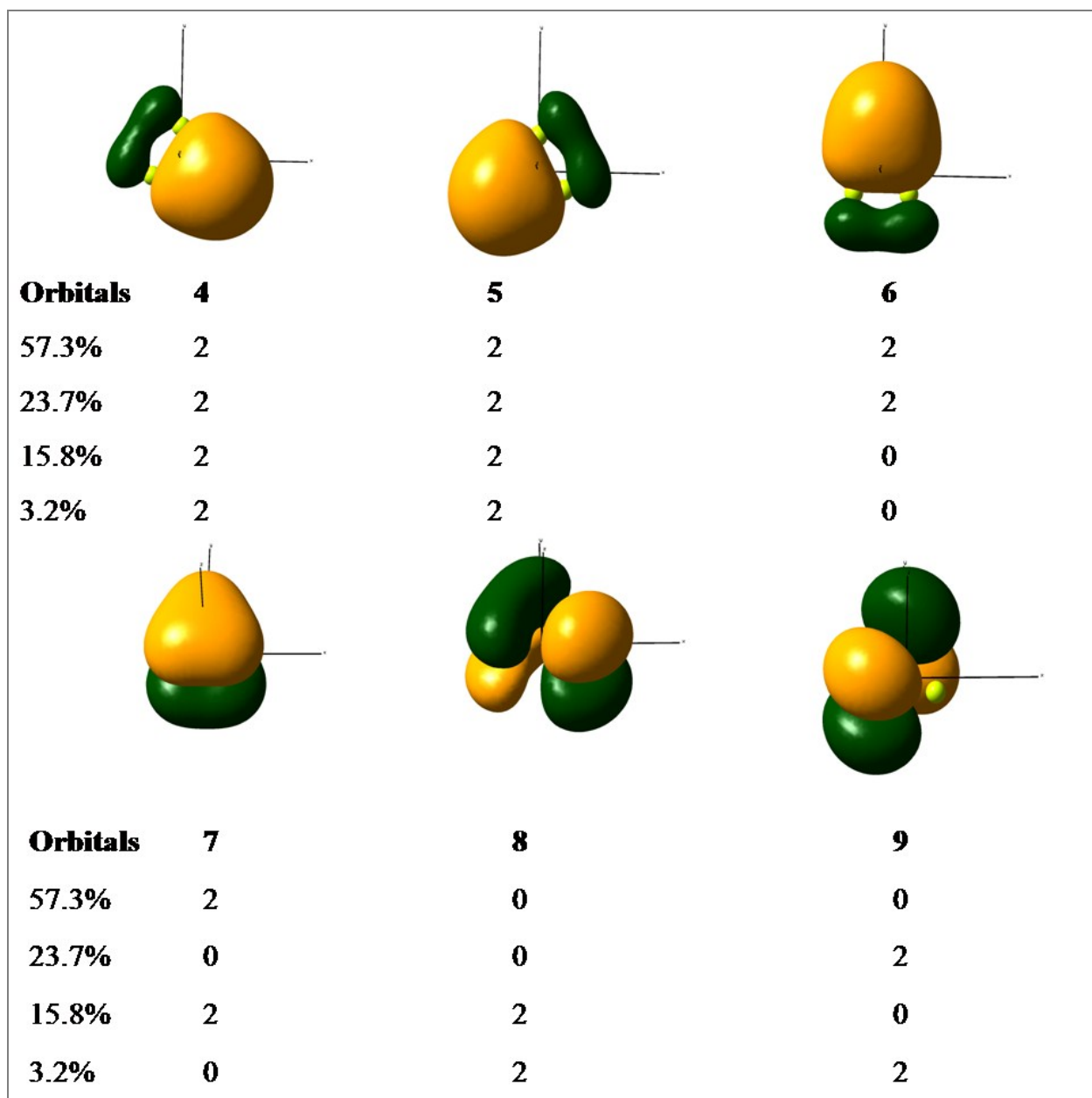


Fig. S1 The orbital set used to construct the active space in CASSCF (8,6) method along with the percentages of leading configurations in wavefunctions.

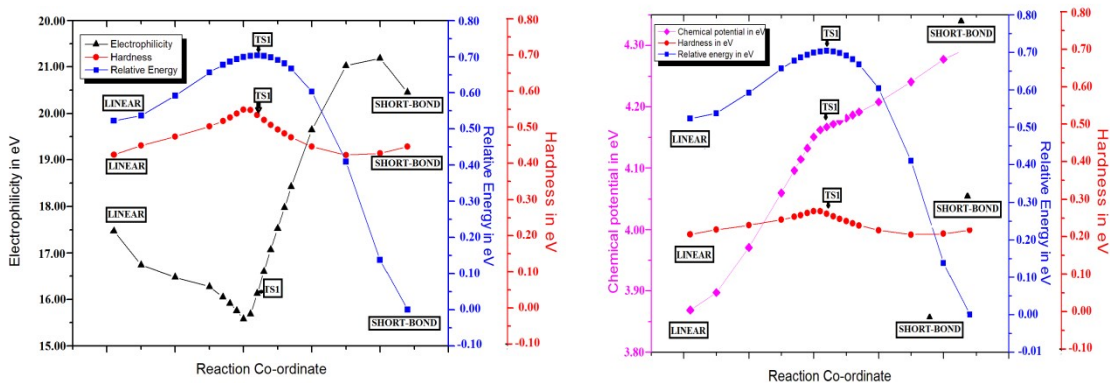


Fig. S2 Variation of hardness, electrophilicity, relative energy and chemical potential along the isomerization path from linear to short-bond via TS1.

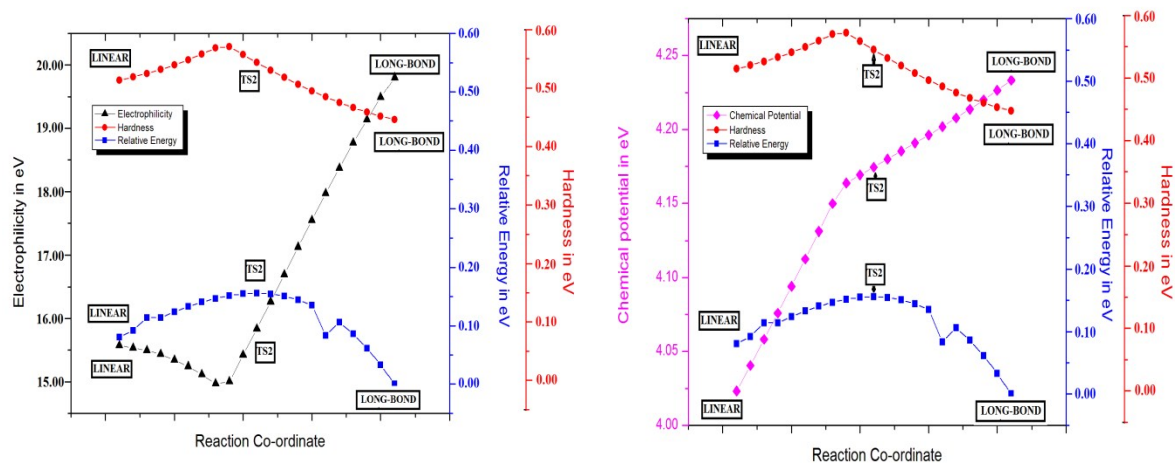


Fig. S3 Variation of hardness, electrophilicity, relative energy and chemical potential along the isomerization path from linear to long-bond via TS2.