Electronic Supplementary Information (ESI)

Understanding the thermal dehydroclorination reaction of 1-chlorohexane. Revealing the driving bonding pattern at the planar catalytic reaction center

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Contents

S1. Full details for reference 39

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, 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, N. Rega, J. M. Millam, M. Klene, J. E. Knox, 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, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision C.01, (2010) Gaussian, Inc., Wallingford CT.

S2. Cartesian coordinates of the transition structure of the thermal dehalogenation of 1-chlorohexane calculated at the DFT M05-2X/6-311+G(d, p) level of theory.

H	-3.390300450	-1.0319563483	1.3732501353
C	-3.329065595	-1.1553404882	0.2908633027
H	-2.797681885	-2.0862103496	0.0898226456
H	-4.343290147	-1.2554682009	-0.094101591
C	-2.606417439	0.0262865393	-0.3487867394
H	-3.157940681	0.949462367	0.151978541
H	-2.581652657	-0.1003737575	-1.4336667597
C	-1.177290386	0.1715799909	0.1679464991
H	-0.612097291	-0.7364237258	-0.0619828211
H	-1.206698162	0.2647009914	1.2577471652
C	-0.476904468	1.3837223644	-0.441418706
H	-0.969838627	2.301023032	-0.1089697367
H	-0.583699809	1.353293782	-1.5274214902
C	0.9992576513	1.4861500454	-0.112208402
H	1.5547247411	2.3132013157	-0.5397567644
H	1.5717685651	0.4796745713	-0.5567879288
C	1.5893886511	0.8376519042	0.9715279868
H	1.0482742507	0.1267924158	1.5754739173
H	2.5981145646	1.0703595132	1.2747123418
Cl	2.522266179	-1.1854509623	-0.2499475137

S3. A video file (MP4 format) presenting the change of the electron localization function (ELF) pattern of bonding at the reaction center along the IRC path of the thermal dehalogenation of 1-chlorohexane calculated at the DFT M05-2X/6-311+G(d, p) level of theory, is available for further examination as Electronic Supplementary Information. The video presents colour-filled maps of ELF for configurations in the interval defined between the points -50 to +20 along the representative energy barrier (i.e., regions a-g). This information can be used for didactical purposes in studying in detail the two stages one step mechanism that we propose as a proper way of interpretation this polar reaction process in the gas phase. The ELF values (0 to 1) are mapped on a Red-Green-Blue colour scale indicated on the left of each frame.