

Ion Dissociation Dynamics of 1,2,3,4-Tetrahydronaphthalene: Tetralin as a Test Case For Hydrogenated PAHs

Malick Diedhiou,^a Brandi J. West,^a Jordy Bouwman^b and Paul M Mayer^{a,*}

^a Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa Canada K1N 6N5

^b Laboratory for Astrophysics, Leiden Observatory, Leiden University, PO box 9513, NL-2300RA Leiden, the Netherlands

*corresponding author: Paul M Mayer pmmayer@uottawa.ca, 613 562-5800 ext 6038

Supporting Information

Complete citation of reference 33

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J., Gaussian 16 rev. B.01, Wallingford, CT, 2016.

Complete citation of reference 16

Gatchell, M.; Stockett, M. H.; de Ruette, N.; Chen, T.; Giacomozzi, L.; Nascimento, R. F.; Wolf, M.; Anderson, E. K.; Delaunay, R.; Vizcaino, V.; Rousseau, P.; Adoui, L.; Huber, B. A.; Schmidt, H. T.; Zettergren, H.; Cederquist, H. Phys. Rev. A 2015, 92, 050702.

Table S1. Comparison of the experimental and OVGF/cc-pVTZ molecular orbital vertical ionization energies.

MO	Orbital Vertical IE (eV)		PS*
	TPES	OVGF	
1		18.155	0.854
2		16.489	0.854
3		15.483	0.865
4		15.709	0.876
5	15.2	14.946	0.871
6	14.5	14.643	0.89
7	14.0	14.332	0.88
8	13.5	13.706	0.875
9	13.0	13.324	0.866
10	12.8	12.959	0.882
11	12.6	12.788	0.892
12	10.0 - 12.0	12.049	0.891
13		11.884	0.906
14		11.618	0.842
15		11.032	0.899
16		10.809	0.896
17	8.9	8.735	0.891
18	8.46 ± 0.01	8.507	0.893

* Pole Strength

Figure S1. Expanded view of the iPEPICO breakdown curve with $[M-4H]^+$ clearly visible.

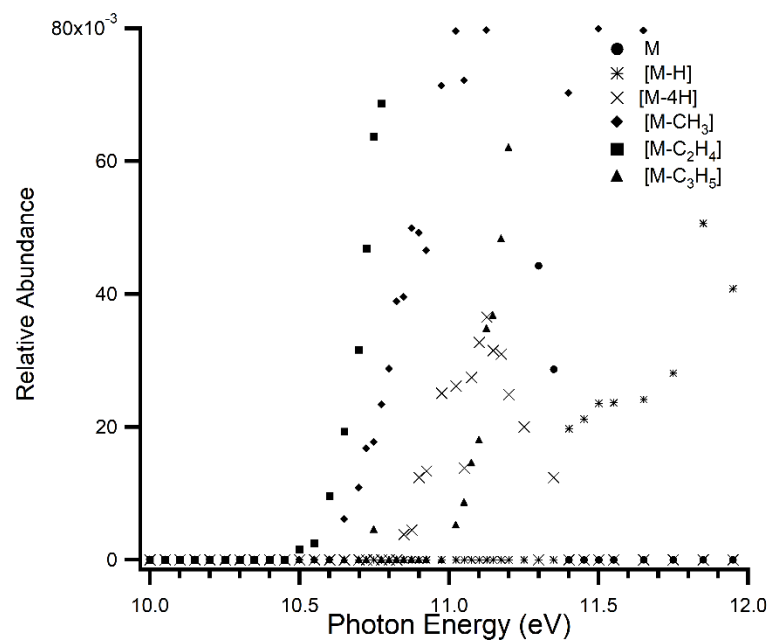


Figure S2. B3-LYP/6-31+G(d,p) key intermediates in the azulene-containing pathway to C₂H₄ loss.

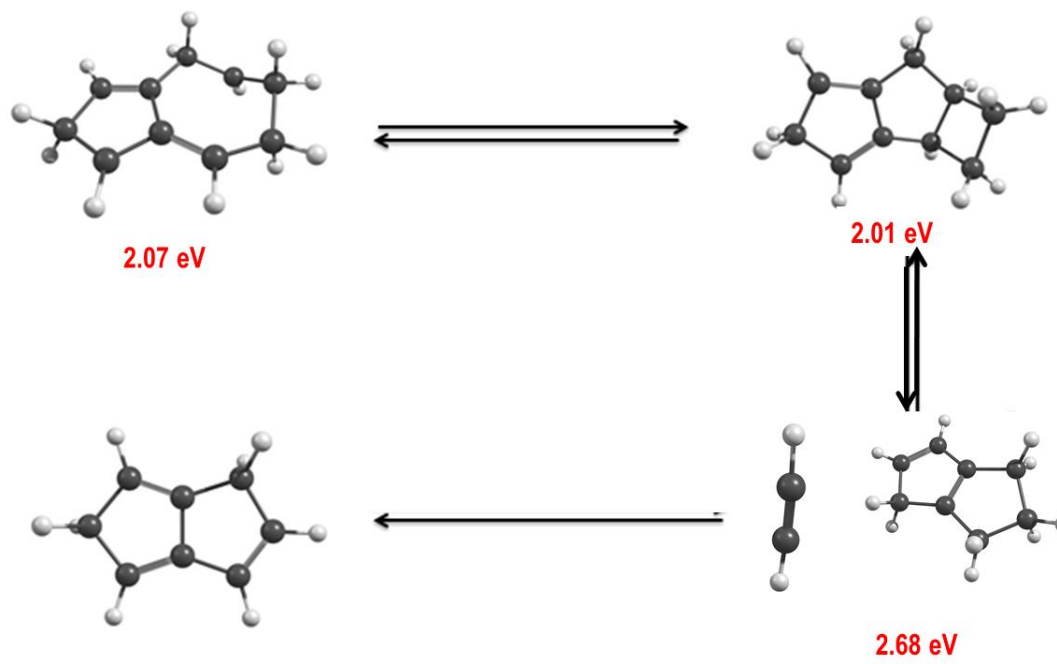


Figure S3. Potential energy scan (B3LYP/6-31G(d)) for loss of H from an sp^3 carbon atom of tetralin ions.

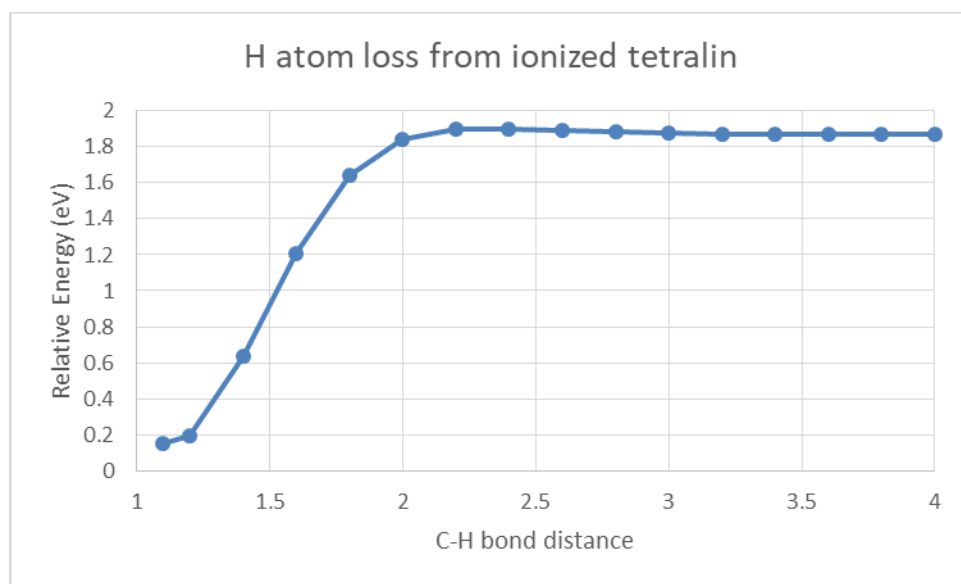


Figure S4. Molecular Orbitals

