

Chemistry

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- [1] Jean Brocas, Francis Buekenhout, and Michel Dehon, *Enantiomeric labelling of reaction graphs*, J. Chem. Inf. Comput. Sci. (1998), no. 38, 798–810.
- [2] A. Brown, A. B. McCoy, B. J. Braams, Z. Jin, and J. M. Bowman, *Quantum and classical studies of vibrational motion of CH₅⁺ on a global potential energy surface obtained from a novel ab initio direct dynamics approach*, J. Chem. Phys. **121** (2004), 4105–4116.
- [3] Chao Chen, Benjamin C. Shepler, Bastiaan J. Braams, and Joel M. Bowman, *Quasiclassical trajectory calculations of the OH + NO₂ association reaction on a global potential energy surface*, J. Chem. Phys **127** (2007), no. 104310, 11 pages.
- [4] S. Fritzsche, *Application of point-group symmetries in chemistry and physics: A computer-algebraic approach*, Int. J. Quantum. Chem. **106** (2006), 98–129.
- [5] Modjtaba Ghorbani and Ali Reza Ashrafi, *Counting the number of hetero fullerenes*, Journal of Computational and Theoretical Nanoscience **3** (2006), no. 5, 803–810.
- [6] Xinchuan Huang, Bastiaan J. Braams, and Joel M. Bowman, *Ab initio potential energy and dipole moment surfaces for H₅O₂⁺*, J. Chem. Phys **122** (2005), no. 044308, 12 pages.
- [7] K. Kutnar, A. Malnič, and Dragan Marušič, *Chirality of toroidal molecular graphs*, J. Chem. Inf. Model. **45** (2005), no. 6, 1527–1535. MR MR1687732
- [8] Amit R. Sharma, Bastiaan J. Braams, Stuart Carter, Benjamin C. Shepler, and Joel M. Bowman, *Full-dimensional ab initio potential energy surface and vibrational configuration interaction calculations for vinyl*, J. Chem. Phys **130** (2009), no. 174301, 9 pages.
- [9] Amit R. Sharma, J. Wu, B. J. Braams, S. Carter, R. Schneider, B. Shepler, and J. M. Bowman, *Potential energy surfaces and MULTIMODE vibrational analysis of C₂H₃⁺*, J Chem Phys. **125** (2006), 224306.

- [10] Yimin Wang, Bastiaan J. Braams, Joel M. Bowman, Stuart Carter, and D. P. Tew, *Full-dimensional quantum calculations of ground-state tunneling splitting of malonaldehyde using an accurate ab initio potential energy surface*, J. Chem. Phys **128** (2008), no. 224314, 9 pages.
- [11] Yimin Wang, Stuart Carter, Bastiaan J. Braams, and Joel M. Bowman, *Multimode quantum calculations of intramolecular vibrational energies of the water dimer and trimer using ab initio-based potential energy surfaces*, J. Chem. Phys **128** (2008), no. 071101, 5 pages.
- [12] Yimin Wang, Benjamin C. Shepler, Bastiaan J. Braams, and Joel M. Bowman, *Full-dimensional, ab initio potential energy and dipole moment surfaces for water*, J. Chem. Phys **131** (2009), no. 054511, 8 pages.
- [13] Peng Zhang, Satoshi Maeda, Keiji Morokuma, and Bastiaan J. Braams, *Photochemical reactions of the low-lying excited states of formaldehyde: T1/S0 intersystem crossings, characteristics of the S1 and T1 potential energy surfaces, and a global T1 potential energy surface*, J. Chem. Phys **130** (2009), no. 114304, 10 pages.