

## Scientific publications by Prof. Nadia Balucani

219 publications in ISI journals + 26 other publications (August 23, 2022)

### ISI-WOS PUBLICATIONS

219. G Vanuzzo, D Marchione, L Mancini, P Liang, G Pannacci, P Recio, Y Tan, M Rosi, D Skouteris, P Casavecchia, N Balucani. The Reaction N(2D) + CH<sub>2</sub>CHCN (Vinyl Cyanide): A Combined Crossed Molecular Beams and Theoretical Study and Implications for the Atmosphere of Titan. *The Journal of Physical Chemistry A*, in press (2022).
218. C Vastel, F Alves, C Ceccarelli, M Bouvier, I Jimenez-Serra, T Sakai, P Caselli, L Evans, F Fontani, R Le Gal, CJ Chandler, B Svoboda, L Maud, C Codella, N Sakai, A Lopez-Sepulcre, G Moellenbrock, Y Aikawa, N Balucani, E Bianchi, G Busquet, E Caux, S Charnley, N Cuello, M De Simone, F Dulieu, A Duran, D Fedele, S Feng, L Francis, T Hama, T Hanawa, E Herbst, T Hirota, M Imai, A Isella, D Johnstone, B Lefloch, L Loinard, M Maureira, NM Murillo, S Mercimek, S Mori, F Menard, A Miotello, R Nakatani, H Nomura, Y Oba, S Ohashi, Y Okoda, J Ospina-Zamudio, Y Oya, JE Pineda, L Podio, A Rimola, D Segura Cox, Y Shirley, L Testi, S Viti, N Watanabe, Y Watanabe, A Witzel, C Xue, Y Zhang, B Zhao, S Yamamoto. Hot methanol in the [BHB2007] 11 protobinary system: hot corino versus shock origin?: FAUST V. *Astronomy & Astrophysics*, in press (2022).  
<https://arxiv.org/abs/2206.10176>
217. C Cavallotti, A Della Libera, C-W Zhou, P Recio, A Caracciolo, N Balucani, P Casavecchia. Crossed-beam and theoretical studies of multichannel nonadiabatic reactions: branching fractions and role of intersystem crossing for O (3P)+ 1, 3-butadiene. *Faraday Discussions*, in press, 2022; doi: 10.1039/D2FD00037G208.
- 216 M Rosi, P Casavecchia, N Balucani, P Recio, A Caracciolo, D Skouteris, C Cavallotti. Lecture Notes in Computer Science, 13378 (2022) 260–269; doi: 10.1007/978-3-031-10562-3\_19
- 215 G Vanuzzo, A Giusti, M Rosi, P. Casavecchia, N Balucani. Theoretical Study of the Reaction O(3P) + 1,2-Butadiene. *Lecture Notes in Computer Science*, 13382 (2022) 249–263; doi: 10.1007/978-3-031-10592-0\_19
214. L Mancini, M Trinari, E Valenca Ferreira de Aragao, M Rosi, N Balucani. The S<sup>+</sup>(<sup>4</sup>S)+SiH<sub>2</sub>(<sup>1</sup>A<sub>1</sub>) Reaction: Toward the Synthesis of Interstellar SiS. *Lecture Notes in Computer Science*, 13378 (2022) 233–245; doi: 10.1007/978-3-031-10562-3\_17
213. M Imai, Y Oya, B Svoboda, H Baobab Liu, B Lefloch, S Viti, Y Zhang, C Ceccarelli, C Codella, C J Chandler, N Sakai, Y Aikawa, F O Alves, N Balucani, E Bianchi, M Bouvier, G Busquet, P Caselli, E Caux, S Charnley, S Choudhury, N Cuello, M De Simone, F Dulieu, A Durán, L Evans, C Favre, D Fedele, S Feng, F Fontani, L Francis, T Hama, T Hanawa, E Herbst, S Hirano, T Hirota, A Isella, I Jimenez-Serra, D Johnstone, C Kahane, R Le Gal, L Loinard, A López-Sepulcre, L T Maud, M J Maureira, F Menard, S Mercimek, A Miotello, G Moellenbrock, S Mori, N M Murillo, R Nakatani, H Nomura, Y Oba, R O'Donoghue, S Ohashi, Y Okoda, J Ospina-Zamudio, J Pineda, L Podio, A Rimola, T Sakai, D Segura-Cox, Y Shirley, V Taquet, L Testi, C Vastel, N Watanabe, Y Watanabe, A Witzel, C Xue, B Zhao, S Yamamoto. Chemical and Physical Characterization of the Isolated Protostellar Source CB68: FAUST IV. *The Astrophysical Journal*, 934 (2022) 70; doi: 10.3847/1538-4357/ac77e7

212. D Marchione, L Mancini, P Liang, G Vanuzzo, F Pirani, D Skouteris, M Rosi, P Casavecchia, N Balucani. Unsaturated Dinitriles Formation Routes in Extraterrestrial Environments: A Combined Experimental and Theoretical Investigation of the Reaction between Cyano Radicals and Cyanoethene (C<sub>2</sub>H<sub>3</sub>CN). *The Journal of Physical Chemistry A* 126 (2022) 3569-3582; doi: <https://doi.org/10.1021/acs.jpca.2c01802>
211. E. Bianchi, C. Ceccarelli, C. Codella, A. López-Sepulcre, S. Yamamoto, N. Balucani, P. Caselli, L. Podio, R. Neri, R. Bachiller, C. Favre, F. Fontani, B. Lefloch, N. Sakai, D. Segura-Cox SOLIS XV. CH<sub>3</sub>CN deuteration in the SVS13-A Class I hot corino. *Astronomy and Astrophysics*, 662 (2022) A103; doi: <https://doi.org/10.1051/0004-6361/202141893>
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209. A Rimola, N Balucani, C Ceccarelli, P Ugliengo. Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. *International Journal of Molecular Sciences* 23 (2022) 4252; doi: <https://doi.org/10.3390/ijms23084252>
208. J Perrero, J Enrique-Romero, B Martínez-Bachs, C Ceccarelli, N Balucani, P Ugliengo, A Rimola Non-energetic Formation of Ethanol via CCH Reaction with Interstellar H<sub>2</sub>O Ices. A Computational Chemistry Study *ACS Earth Space Chemistry*, 6 (2022) 496; doi: 10.1021/acsearthspacechem.1c00369
207. S Ohashi, C Codella, N Sakai, C J Chandler, C Ceccarelli, F Alves, D Fedele, T Hanawa, A Durán, C Favre, A López-Sepulcre, L Loinard, S Mercimek, N M Murillo, L Podio, Y Zhang, Y Aikawa, N Balucani, E Bianchi, M Bouvier, G Busquet, P Caselli, E Caux, S Charnley, S Choudhury, N Cuello, M De Simone, F Dulieu, L Evans, S Feng, F Fontani, L Francis, T Hama, E Herbst, S Hirano, T. Hirota, M Imai, A Isella, I Jimenez-Serra, D Johnstone, C Kahane, R Le Gal, B Lefloch, L T Maud, M Jose Maureira, F Menard, A Miotello, G Moellenbrock, S Mori, R Nakatani, H Nomura, Y Oba, R O'Donoghue, Y Okoda, J Ospina-Zamudio, Y Oya, J Pineda, A Rimola, T Sakai, D Segura-Cox, Y Shirley, B Svoboda, V Taquet, L Testi, C Vastel, S Viti, N Watanabe, Y Watanabe, A Witzel, C Xue, B Zhao, S Yamamoto *The Astrophysical Journal*, 927 (2022) 54; doi: 10.3847/1538-4357/ac4cae
206. S Pantaleone, M Corno, A Rimola, N Balucani, P Ugliengo Water Interaction with Fe<sub>2</sub>NiP Schreibersite (110) Surface: a Quantum Mechanical Atomistic Perspective *The Journal of Physical Chemistry C* 126 (2022), 2243-2252; DOI: 10.1021/acs.jpcc.1c09947
205. J Enrique-Romero, A Rimola, C Ceccarelli, P Ugliengo, N Balucani, D Skouteris Quantum mechanical simulations of the radical-radical chemistry on icy surfaces *The Astrophysical Journal Supplement Series*, 259 (2022) 39; doi: 10.3847/1538-4365/ac480e
204. A Remijan, C Xue, L Margulès, A Belloche, RA Motiyenko, J Carder, C Codella, N Balucani, CL Brogan, C Ceccarelli, TR Hunter, A Maris, S Melandri, M Siebert, BA McGuire Expanding the

submillimeter wave spectroscopy and astronomical search for thioacetamide ( $\text{CH}_3\text{CSNH}_2$ ) in the ISM *Astronomy and Astrophysics*, 658 (2022) A85; <https://doi.org/10.1051/0004-6361/202142504>

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200. G Vanuzzo, A Caracciolo, T K Minton, N Balucani, P Casavecchia, C de Falco, A Baggioli, C Cavallotti Crossed-Beam and Theoretical Studies of the  $\text{O}(3\text{P}, 1\text{D}) + \text{Benzene}$  Reactions: Primary Products, Branching Fractions, and Role of Intersystem Crossing. *The Journal of Physical Chemistry*, 125 (2021) 8434–8453, doi: 10.1021/acs.jpca.1c06913

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191. A. Rimola, C. Ceccarelli, N. Balucani, P. Ugliengo. Interaction of HCO+ cations with interstellar negative grains. Quantum chemical investigation and astrophysical implications. *Frontiers in Astronomy and Space Sciences* 8 (2021) 655405; <https://doi.org/10.3389/fspas.2021.655405>.
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174. M. De Simone, C. Codella , C. Ceccarelli, A. López-Sepulcre, A. Witzel, R. Neri, **N. Balucani**, P. Caselli, C. Favre, F. Fontani, B. Lefloch, J. Ospina-Zamudio, J. E. Pineda, and V. Taquet Seeds of Life in Space (SOLIS) X. Interstellar complex organic molecules in the NGC 1333 IRAS 4A outflows Astronomy & Astrophysics, 640 (2020) A75, DOI: 10.1051/0004-6361/201937004
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