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Editors: Jacco van Loon, Ambra Nanni and Albert Zijlstra

Figure 1: The winning creation from the science-art competition as part of the GAPS 2021 meeting, by 12-year old Matylda Soszyńska from Poland.

Editorial

Dear Colleagues,

It is our pleasure to present you the 288^{th} issue of the AGB Newsletter. There's plenty on chemistry and dust physics including fantastic laboratory work, as well as on binary interactions and lots more.

With sadness, though, we report the death of Kees de Jager, George Wallerstein, and Peter Conti – all supergiants in our field. Their legacies and inspiration endure.

We had a great week of discussions on red (super)giants during GAPS 2021 – https://gaps2021/wixsite.com/conference where you can find the recordings as well as the entries to the science art competition – and in relation to Betelgeuse during the EAS earlier this week. Next one up is next week's Marcel Grossmann meeting's session on Betelgeuse organised by Costantino Sigismondi.

The next issue is planned to be distributed around the 1^{st} of August.

Editorially Yours,
Jacco van Loon, Ambra Nanni and Albert Zijlstra

Food for Thought

This month's thought-provoking statement is:

Are pressure-mode oscillations excited in red supergiants?

Reactions to this statement or suggestions for next month's statement can be e-mailed to astro.agbnews@keele.ac.uk (please state whether you wish to remain anonymous)

Refereed Journal Papers

Structure and dynamics of the inner nebula around the symbiotic stellar system R Aqr

V. Bujarrabal[1], *M. Agúndez*[2], *M. Gómez-Garrido*[1], *Hyosun Kim*[3], *M. Santander-García*[1], *J. Alcolea*[1], *A. Castro-Carrizo*[4] *and J. Mikołajewska*[5]

[1]Observatorio Astronómico Nacional (OAN/IGN), Spain
[2]Instituto de Física Fundamental, CSIC, Spain
[3]Korea Astronomy and Space Science Institute, South Korea
[4]Institut de Radioastronomie Millimétrique, France
[5]Nicolaus Copernicus Astronomical Center, Poland

We investigate the structure, dynamics and chemistry of the molecule-rich nebula around the stellar symbiotic system R Aqr, significantly affected by the presence of a white dwarf (WD) companion. We aim to study the effects on the circumstellar shells of the strong dynamical interaction between the AGB wind and the WD and of photodissociation by the WD UV radiation
We have obtained high-quality ALMA maps of the ^{12}CO J = 2–1, J = 3–2, and J = 6–5 lines and of ^{13}CO J = 3–2. The maps are analyzed by means of a heuristic 3D model that is able to reproduce the observations. In order to interpret such a description of the molecule-rich nebula, we have performed sophisticated calculations of hydrodynamical interaction and photoinduced chemistry.
We find that the CO-emitting gas is distributed within a relatively small region $\sim$ 1$''$.5. Its structure consists of a central dense component plus strongly disrupted outer regions, which seem to be parts of spiral arms strongly focused on the orbital plane. The structure and dynamics of those spiral arms are compatible with our hydrodynamical calculations, we argue that the observed nebula is result of the dynamical interaction between the wind and the gravitational attraction of the WD. We also find that UV emission from the hot companion efficiently photodissociates molecules except in the densest and best shielded regions, i.e. the close surroundings of the AGB star and some 'shreds' of the spiral arms, from which the detected lines come. We think that we can offer a faithful description of the distribution of nebular gas in this prototypical source, which will be a useful template to study material around other tight binary systems.

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Available from https://arxiv.org/abs/2105.07687

Multiple Stellar Evolution: a population synthesis algorithm to model the stellar, binary, and dynamical evolution of multiple-star systems

A.S. Hamers[1], *A. Rantala*[1], *P. Neunteufel*[1], *H. Preece*[1] *and P. Vynatheya*[1]

[1]Max-Planck-Institut für Astrophysik, Karl-Schwarzschild-Str. 1, 85741 Garching bei München, Germany

In recent years, observations have shown that multiple-star systems such as hierarchical triple and quadruple-star systems are common, especially among massive stars. They are potential sources of interesting astrophysical phenomena such as compact object mergers, leading to supernovae, and gravitational wave events. However, many uncertainties remain in their often complex evolution. Here, we present the population synthesis code Multiple Stellar Evolution (MSE), designed to rapidly model the stellar, binary, and dynamical evolution of multiple-star systems. MSE includes a number of new features not present in previous population synthesis codes: (1) an arbitrary number of stars, as long as the initial system is hierarchical, (2) dynamic switching between secular and direct N-body integration for efficient computation of the gravitational dynamics, (3) treatment of mass transfer in eccentric orbits, which occurs commonly in multiple-star systems, (4) a simple treatment of tidal, common-envelope, and mass transfer evolution in which the accretor is a binary instead of a single star, (5) taking into account planets within the stellar system, and

(6) including gravitational perturbations from passing field stars. MSE, written primarily in the C++ language, will be made publicly available and has few prerequisites; a convenient Python interface is provided. We give a detailed description of MSE and illustrate how to use the code in practice. We demonstrate its operation in a number of examples.

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Available from https://arxiv.org/abs/2011.04513
and from https://academic.oup.com/mnras/article-abstract/502/3/4479/6127302?redirectedFrom=fulltext

Molecular dynamics approach for predicting release temperatures of noble gases in pre-solar nanodiamonds

Alireza Aghajamali[1], *Andrey A. Shiryaev*[2] *and Nigel A. Marks*[1]

[1]Department of Physics and Astronomy, Curtin University, Perth, Australia
[2]Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Russia

Pre-solar meteoritic nanodiamond grains carry an array of isotopically distinct noble gas components and provide information on the history of nucleosynthesis, galactic mixing and the formation of the Solar system. In this paper, we develop a molecular dynamics approach to predict thermal release pattern of implanted noble gases (He and Xe) in nanodiamonds. We provide atomistic details of the unimodal temperature release distribution for He and a bimodal behavior for Xe. Intriguingly, our model shows that the thermal release process of noble gases is highly sensitive to the impact and annealing parameters as well as to position of the implanted ion in crystal lattice and morphology of the nanograin. In addition, the model elegantly explains the unimodal and bimodal patterns of noble gas release via the interstitial and substutional types of defects formed. In summary, our simulations confirm that low-energy ion-implantation is a viable way for the incorporation of noble gases into nanodiamonds and we provide explanation of experimentally observed peculiarities of gas release.

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Multi-wavelength VLTI study of the puffed-up inner rim of a circumbinary disc

Akke Corporaal[1], *Jacques Kluska*[1], *Hans Van Winckel*[1], *Dylan Bollen*[1,2,3], *Devika Kamath*[2,3] *and Michiel Min*[4]

[1]Institute of Astronomy, K.U. Leuven, Leuven, Belgium
[2]Department of Physics and Astronomy, Macquarie University, Sydney, Australia
[3]Astronomy, Astrophysics and Astrophotonics Research Centre, Macquarie University, Sydney, Australia
[4]SRON Netherlands Institute for Space Research, Utrecht, The Netherlands

The presence of stable, compact circumbinary discs of gas and dust around post-asymptotic giant branch (post-AGB) binary systems has been well established. We focus on one such system: IRAS 08544−4431. We present an interferometric multi-wavelength analysis of the circumstellar environment of IRAS 08544−4431. The aim is to constrain different contributions to the total flux in the H, K, L, and N-bands in the radial direction. The data from VLTI/PIONIER, VLTI/GRAVITY, and VLTI/MATISSE range from the near-infrared, where the post-AGB star dominates, to the mid-infrared, where the disc dominates. We fitted two geometric models to the visibility data to reproduce the circumbinary disc: a ring with a Gaussian width and a flat disc model with a temperature gradient. The flux contributions from the disc, the primary star (modelled as a point-source), and an over-resolved component are recovered along with the radial size of the emission, the temperature of the disc as a function of radius, and the spectral dependencies of the different components. The trends of all visibility data were well reproduced with the geometric models. The near-infrared data were best fitted with a Gaussian ring model while the mid-infrared data

favoured a temperature gradient model. This implies that a vertical structure is present at the disc inner rim, which we attribute to a rounded puffed-up inner rim. The N-to-K size ratio is 2.8, referring to a continuous flat source, analogues to young stellar objects. By combining optical interferometric instruments operating at different wavelengths we can resolve the complex structure of circumstellar discs and study the wavelength-dependent opacity profile. A detailed radial, vertical, and azimuthal structural analysis awaits a radiative transfer treatment in 3D to capture all non-radial complexity.

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and from https://www.aanda.org/articles/aa/full_html/2021/06/aa41154-21/aa41154-21.html

Deuterated polycyclic aromatic hydrocarbons in the interstellar medium: The C–D band strengths of multi-deuterated species

X.J. Yang[1,2], *Aigen Li*[2], *C.Y. He*[1] *and R. Glaser*[3]

[1]Department of Physics, Xiangtan University, Xiangtan 411105, China
[2]Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA
[3]Department of Chemistry, Missouri University of Science and Technology, Rolla, MO 65409, USA

Observationally, the interstellar gas-phase abundance of deuterium (D) is considerably depleted and the missing D atoms are often postulated to have been locked up into carbonaceous solids and polycyclic aromatic hydrocarbon (PAH) molecules. An accurate knowledge of the fractional amount of D (relative to H) tied up in carbon dust and PAHs has important cosmological implications since D originated exclusively from the Big Bang and the present-day D abundance, after accounting for the astration it has experienced during the Galactic evolution, provides essential clues to the primordial nucleosynthesis and the cosmological parameters. To quantitatively explore the extent to which PAHs could possibly accommodate the observed D depletion, we have previously quantum-chemically computed the infrared vibrational spectra of *mono-deuterated* PAHs and derived the mean intrinsic band strengths of the 3.3-μm C–H stretch ($A_{3.3}$) and the 4.4-μm C–D stretch ($A_{4.4}$). Here we extend our previous work to *multi-deuterated* PAH species of different deuterations, sizes and structures. We find that both the intrinsic band strengths $A_{3.3}$ and $A_{4,4}$ and their ratios $A_{4.4}/A_{3.3}$ not only show little variations among PAHs of different deuterations, sizes and structures, they are also closely similar to that of mono-deuterated PAHs. Therefore, a PAH deuteration level (i.e. the fraction of peripheral atoms attached to C atoms in the form of D) of $\sim 2.4\%$ previously estimated from the observed 4.4-μm to 3.3-μm band ratio based on the $A_{4.4}/A_{3.3}$ ratio of *mono-deuterated* PAHs is robust.

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Optical properties of elongated conducting grains

X.M. Huang[1,2], *Qi Li*[2,3], *Aigen Li*[2], *J.H. Chen*[1,2], *F.Z. Liu*[4] *and C.Y. Xiao*[5]

[1]College of Physics and Electronics, Hunan Normal University, Changsha, Hunan 410081, China
[2]Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA
[3]Hunan Key Laboratory for Stellar and Interstellar Physics and School of Physics and Optoelectronics, Xiangtan University, Hunan 411105, China
[4]College of Information Science and Engineering, Hunan Normal University, Changsha, Hunan 410081, China
[5]Department of Astronomy, Beijing Normal University, Beijing 100875, China

Extremely elongated, conducting dust particles (also known as metallic "needles" or "whiskers") are seen in carbonaceous chondrites and in samples brought back from the Itokawa asteroid. Their formation in protostellar nebulae and subsequent injection into the interstellar medium have been demonstrated, both experimentally and theoretically. Metallic needles have been suggested to explain a wide variety of astrophysical phenomena, ranging from the mid-infrared interstellar extinction at ~ 3–8μm to the thermalization of starlight to generate the cosmic microwave background. To validate (or invalidate) these suggestions, an accurate knowledge of the optics (e.g., the amplitude and

the wavelength dependence of the absorption cross sections) of metallic needles is crucial. Here we calculate the absorption cross sections of iron needles of various aspect ratios over a wide wavelength range, by exploiting the discrete dipole approximation, the most powerful technique for rigorously calculating the optics of irregular or nonspherical grains. Our calculations support the earlier findings that the antenna theory and the Rayleigh approximation, which are often taken to approximate the optical properties of metallic needles, are indeed inapplicable.

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A dusty veil shading Betelgeuse during its Great Dimming

M. Montargès[1,2], E. Cannon[2], E. Lagadec[3], A. de Koter[4,2], P. Kervella[1], J. Sanchez-Bermudez[5,6], C. Paladini[7], F. Cantalloube[5], L. Decin[2,8], P. Scicluna[7], K. Kravchenko[9], A.K. Dupree[10], S. Ridgway[11], M. Wittkowski[12], N. Anugu[13,14], R. Norris[15], G. Rau[16,17], G. Perrin[1], A. Chiavassa[3], S. Kraus[14], J.D. Monnier[18], F. Millour[3], J.-B. Le Bouquin[19,18], X. Haubois[7], B. Lopez[3], P. Stee[3] and W. Danchi[16]

[1]LESIA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Université de Paris, 5 place Jules Janssen, 92195 Meudon, France

[2]Institute of Astronomy, K.U. Leuven, Celestijnenlaan 200D B2401, 3001 Leuven, Belgium

[3]Université Côte d'Azur, Observatoire de la Côte d'Azur, CNRS, Laboratoire Lagrange, Bd. de l'Observatoire, CS 34229, 06304 Nice cedex 4, France

[4]Anton Pannekoek Institute for Astronomy, University of Amsterdam, 1090 GE, Amsterdam, The Netherlands

[5]Max Planck Institute for Astronomy, Königstuhl 17, 69117, Heidelberg, Germany

[6]Instituto de Astronomía, Universidad Nacional Autónoma de México, Apdo. Postal 70264, Ciudad de México, 04510, México

[7]European Southern Observatory, Alonso de Córdova 3107, Vitacura, Santiago, Chile

[8]School of Chemistry, University of Leeds, Leeds LS2 9JT, UK

[9]Max Planck Institute for extraterrestrial Physics, Gießenbachstraße 1, D-85748 Garching bei München, Germany

[10]Center for Astrophysics, Harvard & Smithsonian, 60 Garden Street, Cambridge, MA 02138, USA

[11]NSF's National Optical–Infrared Astronomy Research Laboratory, P.O. Box 26732, Tucson, AZ 85726-6732, USA

[12]European Southern Observatory, Karl-Schwarzschild-Str. 2, 85748, Garching bei München, Germany

[13]Steward Observatory, 933 N. Cherry Avenue, University of Arizona, Tucson, AZ, 85721, USA

[14]University of Exeter, School of Physics and Astronomy, Stocker Road, Exeter, EX4 4QL, UK

[15]Physics Department, New Mexico Institute of Mining and Technology, 801 Leroy Place, Socorro, NM 87801, USA

[16]NASA Goddard Space Flight Center, Exoplanets & Stellar Astrophysics Laboratory, Code 667, Greenbelt, MD 20771, USA

[17]Department of Physics, Catholic University of America, Washington, DC 20064, USA

[18]Department of Astronomy, University of Michigan, Ann Arbor, MI, 48109, USA

[19]Univ. Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France

Red supergiants are the most common final evolutionary stage of stars that have initial masses between 8 and 35 times that of the Sun. During this stage, which lasts roughly 100,000 years, red supergiants experience substantial mass loss. However, the mechanism for this mass loss is unknown. Mass loss may affect the evolutionary path, collapse and future supernova light curve of a red supergiant, and its ultimate fate as either a neutron star or a black hole. From November 2019 to March 2020, Betelgeuse – the second-closest red supergiant to Earth (roughly 220 parsecs, or 724 light years, away) – experienced a historic dimming of its visible brightness. Usually having an apparent magnitude between 0.1 and 1.0, its visual brightness decreased to 1.614 ± 0.008 magnitudes around 7–13 February 2020 – an event referred to as Betelgeuse's Great Dimming. Here we report high-angular-resolution observations showing that the southern hemisphere of Betelgeuse was ten times darker than usual in the visible spectrum during its Great Dimming. Observations and modelling support a scenario in which a dust clump formed recently in the vicinity of the star, owing to a local temperature decrease in a cool patch that appeared on the photosphere. The directly imaged brightness variations of Betelgeuse evolved on a timescale of weeks. Our findings suggest that a component of mass loss from red supergiants is inhomogeneous, linked to a very contrasted and rapidly changing photosphere.

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Magnetic-buoyancy-induced mixing in AGB stars: fluorine nucleosynthesis at different metallicities

Diego Vescovi[1,2,3], *Sergio Cristallo*[2,3], *Sara Palmerini*[2,4], *Carlos Abia*[2,4] *and Maurizio Busso*[5]

[1]Goethe University Frankfurt, Max-von-Laue-Straße 1, Frankfurt am Main 60438, Germany

[2]INFN, Section of Perugia, Via A. Pascoli snc, 06123 Perugia, Italy

[3]INAF, Observatory of Abruzzo, Via Mentore Maggini snc, 64100 Teramo, Italy

[4]Department of Physics and Geology, University of Perugia, via A. Pascoli snc, 06123 Perugia, Italy

[5]University of Granada, Departamento de Física Teórica y del Cosmos, 18071 Granada, Spain

Asymptotic giant branch (AGB) stars are considered to be among the most significant contributors to the fluorine budget in our Galaxy. While at close-to-solar metallicity observations and theory agree, at lower metallicities stellar models overestimate the fluorine production with respect to heavy elements. We present ^{19}F nucleosynthesis results for a set of AGB models with different masses and metallicities in which magnetic buoyancy acts as the driving process for the formation of the ^{13}C neutron source (the so-called ^{13}C pocket). We find that ^{19}F is mainly produced as a result of nucleosynthesis involving secondary ^{14}N during convective thermal pulses, with a negligible contribution from the ^{14}N present in the ^{13}C pocket region. A large ^{19}F production is thus prevented, resulting in lower fluorine surface abundances. As a consequence, AGB stellar models with magnetic-buoyancy-induced mixing at the base of the convective envelope well agree with available fluorine spectroscopic measurements at both low and close-to-solar metallicity.

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The electron-capture origin of supernova 2018zd

Daichi Hiramatsu[1,2], *D. Andrew Howell*[1,2], *Schuyler D. Van Dyk*[3], *Jared A. Goldberg*[2], *Keiichi Maeda*[4,5], *Takashi J. Moriya*[6,7], *Nozomu Tominaga*[5,6,8], *Ken'ichi Nomoto*[5], *Griffin Hosseinzadeh*[9], *Iair Arcavi*[10,11], *Curtis McCully*[1,2], *Jamison Burke*[1,2], *K. Azalee Bostroem*[12], *Stefano Valenti*[12], *Yize Dong*[12], *Peter J. Brown*[13], *Jennifer E. Andrews*[14], *Christopher Bilinski*[14], *G. Grant Williams*[14,15], *Paul S. Smith*[14], *Nathan Smith*[14], *David J. Sand*[14], *Gagandeep S. Anand*[16,17], *Chengyuan Xu*[18], *Alexei V. Filippenko*[19,20], *Melina C. Bersten*[5,21,22], *Gastón Folatelli*[5,21,22], *Patrick L. Kelly*[23], *Toshihide Noguchi*[24] *and Koichi Itagaki*[25]

[1]Las Cumbres Observatory, 6740 Cortona Drive, Suite 102, Goleta, CA 93117-5575, USA

[2]Department of Physics, University of California, Santa Barbara, CA 93106-9530, USA

[3]Caltech/Spitzer Science Center, Caltech/IPAC, Mailcode 100-22, Pasadena, CA 91125, USA

[4]Department of Astronomy, Kyoto University, Kitashirakawa-Oiwake-cho, Sakyo-ku, Kyoto 606-8502, Japan

[5]Kavli Institute for the Physics and Mathematics of the Universe (WPI), The University of Tokyo Institutes for Advanced Study, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8583, Japan

[6]National Astronomical Observatory of Japan, National Institutes of Natural Sciences, 2-21-1 Osawa, Mitaka, Tokyo 181-8588, Japan

[7]School of Physics and Astronomy, Faculty of Science, Monash University, Clayton, Victoria 3800, Australia

[8]Department of Physics, Faculty of Science and Engineering, Konan University, 8-9-1 Okamoto, Kobe, Hyogo 658-8501, Japan

[9]Center for Astrophysics – Harvard & Smithsonian, 60 Garden Street, Cambridge, MA 02138-1516, USA

[10]The School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel

[11]CIFAR Azrieli Global Scholars program, CIFAR, Toronto, Canada

[12]Department of Physics, University of California, 1 Shields Ave, Davis, CA 95616-5270, USA

[13]Mitchell Institute for Fundamental Physics and Astronomy, Texas A&M University, College Station, TX 77843, USA

[14]Steward Observatory, University of Arizona, 933 North Cherry Avenue, Tucson, AZ 85721-0065, USA

[15]MMT Observatory, P.O. Box 210065, Tucson, AZ 85721-0065, USA

[16]Infrared Processing and Analysis Center, California Institute of Technology, Pasadena, CA 91125, USA

[17]Institute for Astronomy, University of Hawai'i, 2680 Woodlawn Drive, Honolulu, HI 96822, USA

[18]Media Arts and Technology, University of California, Santa Barbara, CA 93106-6065, USA

[19]Department of Astronomy, University of California, Berkeley, CA 94720-3411, USA

[20]Miller Institute for Basic Research in Science, University of California, Berkeley, CA 94720, USA

[21]Instituto de Astrofísica de La Plata (IALP), CONICET, Argentina

[22]Facultad de Ciencias Astronómicas y Geofísicas, Universidad Nacional de La Plata, Paseo del Bosque, B1900FWA, La Plata, Argentina

[23]School of Physics and Astronomy, University of Minnesota, 116 Church Street SE, Minneapolis, MN 55455, USA

[24]Noguchi Astronomical Observatory, Katori, Chiba 287-0011, Japan

[25]Itagaki Astronomical Observatory, Yamagata, Yamagata 990-2492, Japan

In the transitional mass range ($\sim$ 8–10 solar masses) between white dwarf formation and iron core-collapse supernovæ, stars are expected to produce an electron-capture supernova. Theoretically, these progenitors are thought to be super-asymptotic giant branch stars with a degenerate O+Ne+Mg core, and electron capture onto Ne and Mg nuclei should initiate core collapse. However, no supernovæ have unequivocally been identified from an electron-capture origin, partly because of uncertainty in theoretical predictions. Here we present six indicators of electron-capture supernovæ and show that supernova 2018zd is the only known supernova having strong evidence for or consistent with all six: progenitor identification, circumstellar material, chemical composition, explosion energy, light curve, and nucleosynthesis. For supernova 2018zd, we infer a super-asymptotic giant branch progenitor based on the faint candidate in the pre-explosion images and the chemically-enriched circumstellar material revealed by the early ultraviolet colours and flash spectroscopy. The light-curve morphology and nebular emission lines can be explained by the low explosion energy and neutron-rich nucleosynthesis produced in an electron-capture supernova. This identification provides insights into the complex stellar evolution, supernova physics, cosmic nucleosynthesis, and remnant populations in the transitional mass range.

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Evolutionary models for the remnant of the merger of two carbon–oxygen core white dwarfs

Josiah Schwab[1]

[1]University of California, Santa Cruz, USA

We construct evolutionary models of the remnant of the merger of two carbon–oxygen (CO) core white dwarfs (WDs). With total masses in the range 1–2 $M_{\odot}$, these remnants may either leave behind a single massive WD or undergo a merger-induced collapse to a neutron star (NS). On the way to their final fate, these objects generally experience a ~ 10 kyr luminous giant phase, which may be extended if sufficient helium remains to set up a stable shell-burning configuration. The uncertain, but likely significant, mass loss rate during this phase influences the final remnant mass and fate (WD or NS). We find that the initial CO core composition of the WD is converted to oxygen–neon (ONe) in remnants with final masses $\gtrsim 1.05\ M_{\odot}$. This implies that the CO core / ONe core transition in single WDs formed via mergers occurs at a similar mass as in WDs descended from single stars, and thus that WD–WD mergers do not naturally provide a route to producing ultra-massive CO-core WDs. As the remnant contracts towards a compact configuration, it experiences a "bottleneck" that sets the characteristic total angular momentum that can be retained. This limit predicts single WDs formed from WD–WD mergers have rotational periods of $\approx$ 10–20 min on the WD cooling track. Similarly, it predicts remnants that collapse can form NSs with rotational periods ~ 10 ms.

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On the thermally pulsing asymptotic giant branch contribution to the light of nearby disk galaxies

Eric E. Martínez-García[1]*, Gustavo Bruzual*[2]*, Rosa A. González Lópezlira*[2] *and Lino H. Rodríguez-Merino*[3]

[1]CONACYT–Instituto Nacional de Astrofísica, Óptica y Electrónica, Luis E. Erro 1, Tonantzintla, Puebla, México
[2]Instituto de Radioastronomía y Astrofísica, UNAM, Campus Morelia, Michoacán. México
[3]Instituto Nacional de Astrofísica, Óptica y Electrónica, México

The study of the luminosity contribution from thermally pulsing asymptotic giant branch (TP-AGB) stars to the stellar populations of galaxies is crucial to determine their physical parameters (e.g., stellar mass and age). We use a sample of 84 nearby disk galaxies to explore diverse stellar population synthesis models with different luminosity contributions from TP-AGB stars. We fit the models to optical and near-infrared (NIR) photometry, on a pixel-bypixel basis. The statistics of the fits show a preference for a low-luminosity contribution (i.e. high mass-to-light ratio in the NIR) from TP-AGB stars. Nevertheless, for 30–40% of the pixels in our sample a high-luminosity contribution (hence low mass-to-light ratio in the NIR) from TP-AGB stars is favored. According to our findings, the mean TP-AGB star luminosity contribution in nearby disk galaxies may vary with Hubble type. This may be a consequence of the variation of the TP-AGB mass-loss rate with metallicity, if metal-poor stars begin losing mass earlier than metal-rich stars, because of a pre-dust wind that precedes the dust-driven wind.

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Silicon and hydrogen chemistry under laboratory conditions mimicking the atmosphere of evolved stars

Mario Accolla[1], Gonzalo Santoro[1], Pablo Merino[1,2], Lidia Martínez[1], Guillermo Tajuelo-Castilla[1], Luis Vázquez[1], Jesús M. Sobrado[3], Marcelino Agúndez[2], Miguel Jiménez-Redondo[4], Víctor J. Herrero[4], Isabel Tanarro[4], José Cernicharo[2] and José Ángel Martín-Gago[1]

[1]Instituto de Ciencia de Materiales de Madrid (ICMM, CSIC), Materials Science Factory, Group of Interdisciplinary Studies based on Nanoscopic Systems, c/ Sor Juana Inés de la Cruz 3, E-28049 Cantoblanco, Madrid, Spain

[2]Instituto de Física Fundamental (IFF, CSIC), Group of Molecular Astrophysics, c/ Serrano 123, E-28006 Madrid, Spain

[3]Centro de Astrobiología (CAB, INTA–CSIC), Crta. de Torrejón a Ajalvir km 4, E-28850, Torrejón de Ardoz, Madrid, Spain

[4]Instituto de Estructura de la Materia (IEM, CSIC), Molecular Physics Department, c/ Serrano 123, E-28006 Madrid, Spain

Silicon is present in interstellar dust grains, meteorites and asteroids, and to date 13 silicon-bearing molecules have been detected in the gas phase toward late-type stars or molecular clouds, including silane and silane derivatives. In this work, we have experimentally studied the interaction between atomic silicon and hydrogen under physical conditions mimicking those in the atmosphere of evolved stars. We have found that the chemistry of Si, H, and H_2 efficiently produces silane (SiH_4), disilane (Si_2H_6) and amorphous hydrogenated silicon (a-Si:H) grains. Silane has been definitely detected toward the carbon-rich star IRC +10°216, while disilane has not been detected in space yet. Thus, based on our results, we propose that gas-phase reactions of atomic Si with H and H_2 are a plausible source of silane in C-rich asymptotic giant branch stars, although its contribution to the total SiH_4 abundance may be low in comparison with the suggested formation route by catalytic reactions on the surface of dust grains. In addition, the produced a-Si:H dust analogs decompose into SiH_4 and Si_2H_6 at temperatures above 500 K, suggesting an additional mechanism of formation of these species in envelopes around evolved stars. We have also found that the exposure of these dust analogs to water vapor leads to the incorporation of oxygen into Si–O–Si and Si–OH groups at the expense of SiH moieties, which implies that if this kind of grain is present in the interstellar medium, it will probably be processed into silicates through the interaction with water ices covering the surface of dust grains.

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INFRA-ICE: an ultra-high vacuum experimental station for laboratory astrochemistry

Gonzalo Santoro[1], Jesús M. Sobrado[2], Guillermo Tajuelo-Castilla[1], Mario Accolla[1], Lidia Martínez[1], Jon Azpeitia[1], Koen Lauwaet[3], José Cernicharo[4], Gary J. Ellis[5] and José Ángel Martín-Gago[1]

[1]Instituto de Ciencia de Materiales de Madrid (ICMM, CSIC), Materials Science Factory, Structure of Nanoscopic Systems Group, c/Sor Juana Inés de la Cruz 3, E-28049 Cantoblanco, Madrid, Spain

[2]Centro de Astrobiolog´ía (CAB, INTA–CSIC), Crta. de Torrejón a Ajalvir km 4, E-28850 Torrejón de Ardoz, Madrid, Spain

[3]IMDEA Nanociencia, Ciudad Universitaria de Cantoblanco, E-28049 Cantoblanco, Madrid, Spain

[4]Instituto de Física Fundamental (IFF, CSIC), Group of Molecular Astrophysics, c/Serrano 123, 28006 Madrid, Spain

[5]Instituto de Ciencia y Tecnología de Polímeros (ICTP, CSIC), c/Juan de la Cierva 3, E-28006 Madrid, Spain

Laboratory astrochemistry aims at simulating, in the laboratory, some of the chemical and physical processes that operate in different regions of the universe. Amongst the diverse astrochemical problems that can be addressed in the laboratory, the evolution of cosmic dust grains in different regions of the interstellar medium (ISM) and its role in the formation of new chemical species through catalytic processes present significant interest. In particular, the dark clouds of the ISM dust grains are coated by icy mantles and it is thought that the ice–dust interaction plays a crucial role in the development of the chemical complexity observed in space. Here, we present a new ultra-high vacuum experimental station devoted to simulating the complex conditions of the coldest regions of the ISM. The INFRA-ICE machine can be operated as a standing alone setup or incorporated in a larger experimental station called Stardust, which is dedicated to simulate the formation of cosmic dust in evolved stars. As such, INFRA-ICE expands the capabilities of Stardust allowing the simulation of the complete journey of cosmic dust in space, from its formation in asymptotic giant branch stars to its processing and interaction with icy mantles in molecular clouds. To demonstrate some of the capabilities of INFRA-ICE, we present selected results on the ultraviolet photochemistry of undecane ($C_{11}H_{24}$) at 14 K. Aliphatics are part of the carbonaceous cosmic dust, and recently, aliphatics and short n-alkanes have been detected in situ in the comet 67P/Churyumov–Gerasimenko.

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