J. Andersen (ed.), Reports on Astronomy, Vol. XXIVA, 1–20.
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COMMISSION 14: ATOMIC AND MOLECULAR DATA[1]

(DONNEES ATOMIQUES ET MOLECULAIRES)

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In recognition of its special interdisciplinary character, IAU Commission 14 is linked directly to the Executive Committee. The Commission's role is to inform the astronomical community of new developments in the diverse fields of research which involve atoms and molecules. Conversely it endeavours to sensitize the research community active in those fields to the specific needs of astronomy, especially concerning basic data and modeling tools. More generally, Commision 14 tries to foster long term relations and collaborations between the two communities and, when necessary, to alert funding authorities to the specific needs of ground and space based astronomy for specific atomic and molecular data.

This report is one of the main contributions of Commission 14 to the information of the astronomical community. Several meetings concerned, at least in part, with the need and availability of atomic and molecular data for astrophysics were also sponsored or co-sponsored. In the last triennium, Commission 14 cosponsored IAU Symposium 194 "Astrochemistry: From Molecular Cloud to Planetary Systems" held in Sogwipo (Korea) from Aug. 23 to 27, 1999 and organized by Commission 34. A Joint Discussion: JD1 on "Atomic and Molecular Data for Astrophysics, New Developments, Case Studies and Future Needs" has been planned for the XXIVth IAU General Assembly in Manchester (Aug. 7-19, 2000) and cosponsored by Commissions 15, 16, 29, 34, 36, 40 and 44. Several other Joint Discussions to be held at the Manchester General Assembly are co-sponsored by this commission.

The present report comprises six sections established by the specialized Working Groups of Commission 14. It is made available on the Commission 14 Website:
`http://ww.obspm.fr/IAU14`
and its mirror `http://cfa-www.harvard.edu/amp/iau14`.

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[1] Committee of the Executive Committee.

6. WORKING GROUP 6: MOLECULAR REACTIONS ON SOLID SURFACES

PRESIDENT: S. LEACH

There has been continuing and increasing recognition of the astrophysical importance of interstellar, interplanetary and cometary dust and their function as sources or catalysts of cosmochemical reactions. A new interesting field where gas-surface reactions may play a role is exobiology. Various types of dust particles in diverse astrophysical situations can act as mediators of reactions between erstwhile gaseous atomic and molecular species, as low temperature matrix traps for gas phase species, and as sources of atoms and molecules ejected into the surrounding medium by temperature mediated outgassing, through violent shocks or through energy impulses resulting from exothermic reactions in the solid phase. The understanding of these processes is aided by appropriate laboratory studies and simulations, and goes hand-in-hand with new observations of interstellar, interplanetary and cometary materials made possible by recent new satellite and ground-based telescope devices. In particular, the Infrared Space Observatory (ISO) has provided much new observational evidence of the role of gas-surface interactions in astrophysical media. The interest of surface science scientists has been aroused in these astrophysical problems and some effort has been put into providing them, via review articles, workshops and meetings, with the the basic information as to the nature of the observations and problems concerning astrophysical gas-surface interactions. There are now quite a few laboratory studies directed towards the chemical aspects of those molecular reactions on solid surfaces relevant to astrophysical problems and observations, in particular the formation of H_2 by reaction of hydrogen atoms on interstellar grains. The present report is non-exhaustive; the division into sections may appear somewhat arbitrary but it represents a coarse-grained sorting of the information. Basic references to surface science studies and techniques were given in earlier Reports. Since the last Report there have been much development and use of scanning probe microscopies such as scanning tunneling microscopy and atomic force microscopy for the elucidation of surface structures both in clean environments and in gaseous and liquid environments (Binnig et al., 1982; Suto et al., 1996; Hamers et al., 1997; Cyr et al., 1996). One application area that is bound to have repercussions in astrophysical research on gas-surface interactions concerns chemical catalysis on a nanometer scale. An example is a study of the reaction of H_2 on carbonaceous material (McIntyre et al., 1994).

6.1. Reviews and Meetings

(i) *The role of dust in the formation of stars.* Proc. ESO Workshop, Garching, 11-14 Sept. 1995. Eds. H.U.Kufl, R.Siebenmorgen, ESO Astrophys.Symp., Springer, Berlin (1996).

(ii) *Physics, chemistry, and dynamics of interplanetary dust.* Proc. 150th Colloq. I.A.U., Gainsville, Florida, 14-18 August 1995. Eds. B.A.S.Gustafson, M.S.Hanner. Astron. Soc. Pac. Conf. Ser., 104 (1996).

(iii) *Life Sciences: complex organics in space.* Proc. F3.2 Symp.COSPAR Commission F, COSPAR meeting at Birmingham, UK, 14-21 July 1996. Eds.F.Raulin, J.M.Greenberg, Adv. Space Res. 19, N 7 (1997).

(iv) *From stardust to planetesimals.* Main lectures, Astron.Soc.Pac.Conf.Ser. 122 (1997). Contributed papers. Conference Santa Clara 24-26 June, 1996, Eds. M.E.Kress, A. G. G. M. Tielens, Y.J. Pendleton, NASA-CP-3343 (1996).

(v) *Volatiles in the Earth and solar system* Proc.Conf., Pasadena, September 1994. Ed. K.A.Farley, AIP Conf.Proc. 341 (1995).

(vi) *Astrophysical implications of the laboratory study of presolar materials.* Proc.Conf. St.Louis, 31 October-2 November 1996. AIPConf.Proc. 402 (1997).

(vii) *Molecules in astrophysics: probes and processes.* Proc. 178th Symp. IAU, Leiden, 1-5 July 1996. Ed. E.F.van Dishoek, IAU Symp. 178 (1997).

(viii) *Astronomcal and biochemical origins and the search for life in the universe.* Proc. 5th Int.Conf. Bioastronomy, Capri 1-5 July 1996, Eds. C.B.Cosmovici, S.Bowyer, D.Wertheimer, IAU Colloq. 161, Editrici Compositori, Bologna (1997).

(ix) *Dust and molecules in evolved stars.* Proc. Internat.Workshop, Manchester, 24-27 March, 1997. Eds. I.Cherchneff, T.J.Millar, Astrophys.Space Sci. 251 (1997).

(x) *Chemistry and physics of molecules and grains in space.* Faraday Disc., 109 (1998).

6.2. Studies of Dust grain properties and models

Observational constraints on dust models (Mathis et al., 1996 a,b); optical and magnetic properties of dust grains (Draine, 1996); composition of interstellar grains and ices (Sandford, 1996); chemical role of cosmic dust (Williams et al., 1996); nature of silicate core of grains (Greenberg et al., 1996); formation of H_2 by H-atom reaction with grain surfaces (Duley, 1996a; Biham et al., 1998); deuterium fractionation on grain surfaces (Rodgers et al., 1996; Tielens, 1997); formation of oxygen and nitrogen hydrides on grains (Wagenblast et al., 1996); gas-grain interactions in protostellar infall (Rawlings, 1996); sputtering of atmospheric gases by cosmic dust (Pavlov, et al., 1996); dust halo of Io (Ip, 1996); alignment of grains through interaction with gases (Lazarian, et al., 1996); catalytic models of H_2S on grains (Turner, 1996); CO_2 in icy grain mantles (Grtler et al., 1996; Graauw et al., 1996; Whittet et al., 1998); grain shattering in shocks (Jones et al., 1996); generation and recombination of free radicals in dust grains (Goldanskii et al., 1996); solid-state IR features as indicators of interstellar gas-grain interactions (d'Hendecourt et al., 1996a); gas-grain chemistry implications of ISO observations (van Dishoek, 1998); grain-surface recombination of HCO+ (Aikawa et al., 1998); inorganic dust formation in astrophysical environments (Gail et al., 1998); catalysis by dust grains in the solar nebula (Kress et al., 1997); role of grains in formation of complex molecules in interstellar molecular clouds (Tielens et al., 1997); detection organic matter in interstellar grains (Pendleton, 1997); grain-grain collisions (Caselli et al., 1997); dust grain size distributions (O'Donnell et al., 1997); cometary gas-dust atmospheres (Kolesnichenko et al., 1997); propagation and survival of interstellar grains (Jones et al., 1997); possible role of interstellar grains in formation of aminoacids (Sorrell, 1997); rate equations for gas-grain reactions (Caselli et al., 1998); depletion test of dust grain models (Sofia, 1997); lifecycle of interstellar dust (Jones, 1997).

6.3. Astrophysical observations

Comparisons of organic materials in interstellar dust and the Murchison meteorite, (Pendleton, 1995); Dust in the diffuse ISM (Bernard et al., 1996); composition and state of icy surfaces in outer solar system (Brown et al., 1997); nitrogen in ices (Whittet et al., 1996); IR spectrum of Galactic center and the composition of interstellar dust (Tielens et al., 1996); formation of methane on grains (Boogert et al., 1996); possible formation of HNCO and other molecules via surface reactions in Sgr B2 envelope and in star-forming complexes (Kuan et al., 1996; Mehrger et al., 1996); H_2 observations in the LMC and relation to formation on grains (Gunderson et al., 1998); overview of interstellar dust grains (Henning, 1997).

6.4. Laboratory studies and astrophysical modelling of carbonaceous materials

UV spectroscopy of matrix-isolated amorphous carbon particles (Schnaiter et al., 1996); simulation UV processing of HAC grains (Mennella et al., 1996); laboratory studies of PAHs, fullerenes and linear carbon chains in an astrophysical context (Leach, 1995); plasma processing of PAHs (Wdowiak, et al., 1995); laboratory experiments on small carbon grain analogues of cosmic dust (Mennella et al., 1995); theory of molecule - solid transition in astrophysical dust formation (Patzer et al., 1995); laboratory production of carbon grains, including those containing C_{60}, in an arc discharge in the presence of oxygen (Saito et al., 1995); comparison of solid-state carbonaceous models of cosmic dust (Papoular et al., 1996);

thermal effects in carbonaceous dust, (Duley, 1996); carbon grains produced in partially hydrogenated atmospheres (Blanco et al., 1996); interaction of H atoms with carbon surfaces as energy source for excitation of the UIR bands (Guillois et al., 1998); formation of carbon particles in cosmic environments (Frenklach et al., 1997).

6.5. Astrophysical ices: laboratory studies and astrophysical observations

Ion irradiation of astrophysical ices (Strazzulla et al., 1995; Strazzulla et al., 1997); UV photolysis of solid methanol (Schutte et al., 1995); UV photodesorption from water ice (Westley et al., 1995); Surface features on interstellar ice (McCoustra et al., 1996); condensation dynamics of cometary ice analogs (Patnaik et al., 1996); infrared spectroscopic properties of isolated water ice and its possible detection on grains (Ehrenfreund et al., 1996a); UV processing of interstellar ice analogs (Gerakines et al., 1996); production of cometary ice tholins (McDonald et al., 1996); enrichment of CO/N_2 by trapping in amorphous ice, and implications concerning comet P/Halley (Notesco et al., 1996); light flash and ionization from hypervelocity impacts on ice (Burchell et al., 1996); thermal properties of cometary ices and sublimation residua including organics (Kmle et al., 1996); laboratory database of solid CO and CO_2 (Ehrenfreund et al., 1996b); sputtering of ices in the outer solar system (Johnson, 1996); molecular cloud sources with H_2O ice bands (Brooke et al., 1996); spectropolarimetry of ice features (Hough et al., 1996); observation of solid formaldehyde (Schutte et al., 1996); observation of ozone trapped in surface ice of Ganymede (Noll et al., 1996); CH_4 and its ices in Pluto and Triton (Stansberry et al., 1996); interstellar ices in comet Hyakutake (Irvine et al., 1996); water ice around protostar AFGI 2136 IRS 1 (Kastner et al., 1996); ISO view of interstellar ices, including implications of gas-grain chemistry, and related laboratory studies (Whittet et al., 1996; d'Hendecourt et al., 1996b; Boogert et al., 1997; Whittet et al., 1997; Dartois et al., 1998; Jourdain de Muizon et al., 1998; Ehrenfreund et al., 1998a), processing of methanol-rich ices (Chiar et al., 1996); apolar ices (Elsila et al., 1997; Ehrenfreund et al., 1998b); development of icy planetesimals (Stepinski et al., 1997); nature and evolution of interstellar ices (Chiar, 1997); heterogeneous reactions on inorganic oxide and water ice surfaces (Choi et al., 1997); IR ice band absorption in YSOs (Graham, 1998); ices in molecular cloud cores (Teixeira et al., 1998).

6.6. Interplanetary dust particles, micrometeorites and meteorites

Carbonates in Martian meteorite ALH84001 (Hutchins et al., 1997); dust particles in atmospheres of terrestrial planets and their role in prebiotic chemistry (Basiuk et al., 1996); particles in Jupiter's atmosphere from impacts of comet P/Shoemaker-Levy 9 (West, 1996); origin of presolar diamonds in meteoritic grains (Verchovsky et al., 1998); mineralogical changes in IDPs resulting from atmospheric entry heating (Keller et al., 1996).

6.7. Other relevant topics

Laboratory studies concerning oxygen in ice on Ganymede (Vidal et al., 1997); HCN polymers from impact of comet P/Shoemaker-Levy 9 on Jupiter (Matthews, 1997); role of comets, meteorites and planetesimals in formation of inner planet atmospheres (Owen et al., 1996; McKay et al., 1996); state of SO2 on surface of Io (Becker et al., 1997); ejection of SO2 from Io (Bishop et al., 1997); surface composition of Charon (Wright et al., 1997); transport of volatile molecules through cometary nuclei (Clemett et al., 1998); processing of cometary grains at nucleus surface (Guez et al., 1997); CO outgassing from comet Hale-Bopp (Lunine, 1997); solid-state greenhouse effect on icy Galilean satellites (Vidal et al., 1997); models of comet nuclei (Klinger et al., 1996; Benkhoffet al., 1996); possible relic biogenic activity in martian meteorite ALH84001 and some related issues (McKay et al., 1996; Becker et al., 1997; Bishop et al., 1997; Wright et al., 1997; Clemett et al., 1998); nucleation in Titan's lower atmosphere (Guez et al., 1997); physics and chemistry of the solar nebula (Lunine, 1997); organic degradation under simulated Martian conditions (Stoker et al., 1997).

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