Water Ice in AGN and Starbursts

A.G.Yeghikyan*and A.L.Samsonyan†

NAS RA Byurakan Astrophysical Observatory, Byurakan 0213, Aragatzotn Province, Armenia

Abstract

Complex chemical species are easier formed in a solid phase, for example in a mixture of ices of water, carbon oxides, methane, ammonia, methanole and other, less abundant molecules. Ultraviolet photons in the range 5 - 13.6 eV and the charged particles with MeV-GeV energies serve as an energy source of reactions. Icy particles containing mentioned substances, can exist only in internal areas of the interstellar molecular clouds protected from influence of external ultraviolet radiation. However cosmic rays are capable to penetrate in clouds and to cause an irradiation of ices by means of secondary ultra-violet photons necessary for initiation of chemical reactions of complexisation. In this work a survivability of ices under harsh conditions of active galaxies is discussed. Preliminary model calculations show that abundances of ices depend not only on ionization parameters of the clouds but also on the shape of incident radiation that is on presence and level of hard ultraviolet and X-ray radiation. The last circumstance is directly related to the radiation of the accretion disk of galaxies with active nuclei and can be used to classify active galaxies, for example to distinguish starburst galaxies from those with active nuclei.

Keywords: *active galaxies, AGN, Starburst galaxies, IR spectra, water ice, UV radiation modeling, ice survivability*

1. Introduction

Water ice and polycyclic aromatic hydrocarbon (PAH) molecules are observed in the spectra of galaxies indicating the possibility of the formation of complex compounds, possibly involved in the synthesis of prebiomolecules. This is also supported by the results of laboratory experiments on the formation of heavy hydrocarbons (up to 30 carbon atoms) and amino acids due to irradiation of mixtures of ices with UV photons and energetic particles (Cottin et al., 2003), (Dworkin et al., 2004). UV radiation does not penetrate into the internal dense regions of molecular clouds, and it is in these areas that ice (ice mantle of dust particles) exists, which is believed to be responsible for the formation of very complex compounds (Tielens, 2005). The energy sources of the corresponding reactions in ices are the above-mentioned energetic particles in the MeV-GeV energy range (i.e. cosmic rays, CR), as well as the secondary UV radiation caused by them (in the range 6–13.5 eV). All of the above is true for active galaxies, where the observed ice and PAH content is directly related to the level of activity of galaxies (Yeghikyan, 2016), (Yeghikyan & Martirosyan, 2018). However, many of the details associated with the source/sources of hard radiation regulating the molecular content as well as the possibility of direct interaction between molecules and radiation, remain unclear.

The ices of the most common molecules and other carbon-containing compounds are observed in the spectra of normal galaxies in the form of characteristic bands. On the other hand, so far only absorption bands of 3.1 μm and 6.0 μm of water ice are visible in the spectra of active galaxies, for example, galaxies with starburst formation and galaxies with active nuclei (Boogert et al., 2015), (Imanishi et al., 2006), (Spoon et al., 2002). Often, absorption bands of 3.1 μm of ice appear in combination with a carbon dust absorption band of 3.4 μm and an emission band of 3.3 μm from PAH molecules.

*ayarayeg@gmail.com, Corresponding author
†anahit.sam@gmail.com

DOI: 10.52526/25792776-2019.66.2-143

Ice plays an important role in the physics and chemistry of interstellar molecular clouds, including, as already noted, the formation of many complex compounds. Moreover, the formation of very complex chemical compounds containing tens of atoms is obviously difficult in a rarefied gas medium, while it is possible in the solid phase, even at low temperatures of the order of 5-10 K. The most famous example is the polycondensation of solid methane in experiments on the irradiation of solid methane with protons with energies of the order of 10 MeV with the formation of alkanes, alkenes and PAHs containing up to 30 carbon atoms (Kaiser, 1998, Kaiser & Roessler, 1997, Kaiser et al., 1997). The formation of complex compounds under the influence of UV radiation should also be indicated: according to experimental data irradiation of a mixture of ices (like water, carbon oxides, methanol, ammonium and methane) with photons with energies of about 10 eV leads to the appearance of a polycondensate containing, for example, up to 22 carbon atoms (Cottin et al., 2003), (Dworkin et al., 2004). The complex hydrocarbons observed in the experiments (Dworkin et al., 2004) are similar to natural bitumen (a mixture of aliphatic and aromatic hydrocarbons), which, interestingly, are considered as quite adequate analogues for reproducing the photometric characteristics of comets and surfaces of some asteroids (Moroz et al., 1998). It should also be emphasized that PAH and amino acid-related compounds are also formed in the above experiments (Cottin et al., 2003), (Dworkin et al., 2004).

To calculate the UV radiation inside the clouds of the circum-nuclear regions of active galaxies where narrow emission lines (so called Narrow Line Regions - NLRs) are formed, one can use the Cloudy computer program designed to model the ionization and physical-chemical structure of gas-dust clouds and described in Ferland et al. (2013).

This article is devoted to the description of some observational data and theoretical modeling of molecular clouds of active galaxies responsible for the existence of ices. The conditions under which that is possible can be interesting not only from the point of view of the possibility of the formation of various species, which in itself is important, but also as observational criteria, to distinguish galaxies with different levels of activity especially in circum-nuclear regions. Further, the observational data (Spitzer's archive) concerning ices in active galaxies are presented in Section 2, with the optical thicknesses of the absorption lines of water ice and silicates measured by us in the spectra, which were later transformed into column densities of ice and neutral hydrogen. The calculations of the radiation field with the given NLR parameters and various external conditions were implemented using Cloudy and discussed in Section 3. The calculations of the water ice content in dust particles are described and discussed in comparison with the observations in Section 4, and the conclusion is given in section 5.

2. Observational data

In this article we selected 22 galaxies from our list of active galaxies observed by the Spitzer observatory, whose spectra contain absorption bands of water ice and silicates (Table 1, see also Fig.1). The list of galaxies is given in Table. 1, together with the coordinates and possible classification. Optical thicknesses at the 6.0 μm, and 9.7 μm bands were measured according to the scheme proposed in (Spoon et al., 2002), (see also Fig. 2). In Table 2 optical thicknesses of water ice and neutral hydrogen are converted to the column densities according to (Hagen et al., 1983),(Bohlin et al., 1978), (Roche, 1984).

After determining the optical thicknesses of the ice (6.0 mcm) and silicates (9.7 μm), the column densities of ice and neutral hydrogen can be calculated, respectively, by the relations (Hagen et al., 1983), (Roche, 1984), (Bohlin et al., 1978).

$$N(ice) = \frac{\tau(ice)}{4.2 \cdot 10^{-20} cm^2 \cdot molecules^{-1}} \tag{1}$$

$$N(H) = \tau(silicate) \cdot 3.5 \cdot 10^{22} cm^2 \tag{2}$$

Table 1: A sample of 22 galaxies from the Spitzer archive, with optical thicknesses measured by us according to (Spoon et al., 2004)

Number	Name	RA	Dec	Type	Redshift	$\tau(ice)$	$\tau(silicate)$
1	IRAS06035-7102	90.72346	71.05331	AGN	0.0795	0.721	0.407
2	IRAS06206-6315	95.25333	-63.28978	AGN	0.0924	0.688	0.464
3	UGC5101	143.96521	61.35314	AGN	0.0394	0.627	0.320
4	IRASF09414+4843	146.176	48.48778	AGN	0.0553	0.875	0.522
5	IRAS10378+1109	160.12154	10.88825	AGN	0.1363	0.531	0.567
6	IRASF13279+3401	202.56346	33.77483	AGN	0.0213	0.815	0.143
7	Mrk273	206.1755	55.88697	AGN	0.0378	0.717	0.143
8	IRAS14348-1447	219.40946	-15.00683	AGN	0.0827	0.611	0.520
9	IRAS17068+4027	257.13383	40.39117	AGN	0.179	0.686	0.571
10	IC5298	349.00279	25.55675	AGN	0.0274	0.688	0.714
11	IRAS00199-7426	5.52921	-74.16158	Comp	0.0964	0.742	0.667
12	IRASF02417-0857	41.06071	-8.73914	Comp	0.0553	0.701	0.381
13	IRASF02437+2122	41.66304	21.58622	Comp	0.0233	0.850	0.208
14	IRAS04103-2838	63.08138	-28.50678	Comp	0.1175	0.876	0.902
15	IRAS04114-5117	63.18717	-51.1595	Comp	0.1246	0.757	0.714
16	IRASF08344+5105	129.51512	50.91917	Comp	0.0967	0.807	0.636
17	IRAS10494+4424	163.09829	44.14625	Comp	0.0921	0.877	0.700
18	IRAS13469+5833	207.16762	58.31442	Comp	0.1578	0.647	0.857
19	IRAS16487+5447	252.44533	54.70983	Comp	0.1038	0.711	0.455
20	IRAS17028+5817	255.92462	58.229	Comp	0.1061	0.851	0.750
21	IRAS20087-0308	302.84942	-2.99744	Comp	0.1057	0.803	0.500
22	IRAS23230-6926	351.51487	69.17231	Comp	0.1063	0.700	0.400

Table 2: The column densities of water ice and neutral hydrogen

Number	$\tau(ice)$	$\tau(sil)$	N(ice)	N(hydrogen)	N(ice)/N(hydrogen)
1	0.721	0.407	1.72E+019	1.42E+022	0.00121
2	0.688	0.464	1.64E+019	1.63E+022	0.00101
3	0.627	0.320	1.49E+019	1.12E+022	0.00133
4	0.875	0.522	2.08E+019	1.83E+022	0.00114
5	0.531	0.567	1.26E+019	1.98E+022	0.000637
6	0.815	0.143	1.94E+019	5.00E+021	0.00388
7	0.718	0.143	1.71E+019	5.00E+021	0.00342
8	0.611	0.520	1.46E+019	1.82E+022	0.000800
9	0.686	0.571	1.63E+019	2.00E+022	0.000817
10	0.688	0.714	1.64E+019	2.50E+022	0.000655
11	0.742	0.667	1.77E+019	2.33E+022	0.000757
12	0.701	0.381	1.67E+019	1.33E+022	0.00125
13	0.850	0.208	2.02E+019	7.26E+021	0.00279
14	0.876	0.902	2.09E+019	3.16E+022	0.000661
15	0.757	0.714	1.80E+019	2.50E+022	0.000721
16	0.807	0.636	1.92E+019	2.23E+022	0.000863
17	0.877	0.700	2.09E+019	2.45E+022	0.000853
18	0.647	0.857	1.54E+019	3.00E+022	0.000514
19	0.711	0.455	1.69E+019	1.59E+022	0.00106
20	0.851	0.750	2.03E+019	2.63E+022	0.000772
21	0.803	0.500	1.91E+019	1.75E+022	0.00109
22	0.700	0.400	1.67E+019	1.40E+022	0.00119

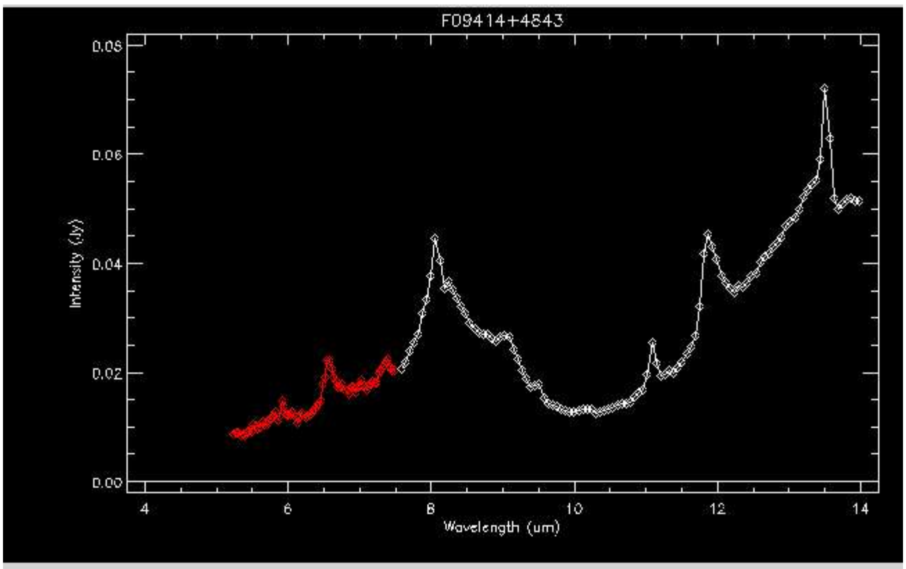

Figure 1: Absorption bands of water ice (6.0 μm) and silicates (9.7 μm) for active galaxy IRASF 0494-4843

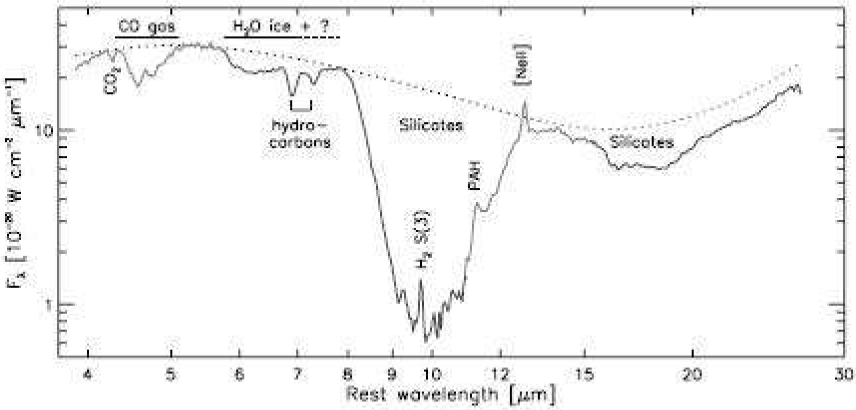

Figure 2: An example of a continuum drawing when measuring optical thicknesses according to (Spoon et al., 2004)

3. Constraining input values for column densities and ionization parameter

The data from Table 2 are analyzed in Fig.3, namely, the scattered values of N(ice) depending on N(H) values for 22 active galaxies are shown.

It turns out that the column densities of ice are between 1.3 and 2.2 (in units of 10^{19} cm^2) with N(H) values between 5 and 30 (in units of 10^{21} cm^2). The presence of ice in active galaxies, at least in the clouds of the near-nuclear regions, does not always depend on the type of activity, although it can be said that in Seyfert galaxies, ice survives worse than in galaxies with intense star formation or in merging galaxies. In this case, it is desirable to have a quantitative criterion for the survival of ice under the harsh conditions of active galaxies. It is clear that the ice content is sensitive to direct electromagnetic and corpuscular radiation, as well as to the physical parameters of the medium, for example, the gas and dust temperatures supported by these radiation. The conditions for the survival of ice can theoretically be clarified by means of numerical physicochemical models of interstellar gas-dust clouds with the correct description for the effects of radiation transfer, like in Cloudy code (see below).

First, we determine the total number of hydrogen ionizing quanta Q_H, which cause the recombination lines H_α and H_β in the gaseous nebulae of the NLR regions. In the SDSS spectra, the

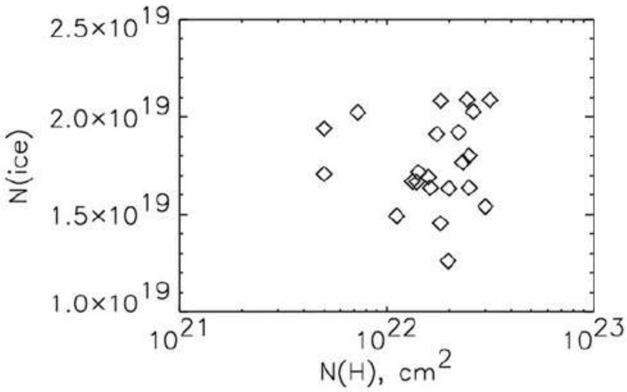

Figure 3: The N(ice) values depending on N(H) for 22 active galaxies from Table 2

$H_\alpha(6563\mathring{A})$ line is resolved from the [NII] lines 6548 and 6584 Å. In the NLR, typical velocities in the medium are of the order of 400 km/s (Netzer, 2013), then the line widths can be estimated usually as $\Delta\lambda = \lambda \cdot z = \lambda \cdot v_{ave}/c = 8.8$ Å. Other NLR parameters, characteristic sizes and concentration, were adopted, respectively, $r \sim 100$ pc, and $n_e \sim 10 \sim 10^3\ cm^3$ (Netzer, 2013). Sometimes the so-called filling factor, which characterizes the raggedness of the medium, $f \sim 0.1$ or less. Next, we use $f \sim 1$. The distance to the galaxies was estimated by the redshift, $d = c \cdot z/H$, $H = 70$ km/s/Mpc.

We use the standard photoionization model of the hydrogen cloud (a so-called case B at $T_e = 10^4$ K), in which the recombination coefficient for all levels except the first is $\alpha_B = 2.59 \cdot 10^{-13} cm^3 s^{-1}$, and the effective recombination coefficients for the H_α and H_β lines are equal to $\alpha_{eff}(H_\alpha) = 1.17 \cdot 10^{-13}$ and $\alpha_{eff}(H_\beta) = 0.301 \cdot 10^{-13}$ (in units $cm^3 s^{-1}$), respectively. Then, for Q_H we have (Osterbrock & Ferland, 2006)

$$Q_H = 4\pi d^2 \frac{F(H_\alpha)}{h\nu(H_\alpha)} \frac{\alpha_B}{\alpha_{eff}(H_\alpha)}, Q_H = 4\pi d^2 \frac{F(H_\beta)}{h\nu(H_\beta)} \frac{\alpha_B}{\alpha_{eff}(H_\beta)}. \quad (3)$$

Further, we determine the ionization parameter

$$U = \frac{Q_H}{4\pi r^2 n_H c}. \quad (4)$$

4. The radiation field inside the molecular cloud

It should be noted that only for photons with energies above 13.6 eV there are no internal sources inside the cloud, while photons in the energy range 6–13.6 eV are still emitted and are important in the processes of ionization (of some elements), thermal and photochemical balance of both gas and dust. These photons participate in many secondary processes which occur with such intensity that their contribution is obligatory when considering many problems of cloud physics and chemistry, including ice content in dust particles depending on the radius of the cloud. It is interesting to note that the absence of ices outside the clouds where the lifetime of the ice is much shorter than the characteristic time of chemical reactions that transform the ice mixtures into a stable form is due to intense UV radiation in the entire spectrum, while in the inner regions where ices are present, their content is regulated by the UV radiation field mainly at 10 eV. The only significant source of such photons inside the clouds, far from the boundary, is the process of generation of secondary radiation as a result of the excitation of hydrogen molecules by CR (protons with energies of the order of MeV and higher), with subsequent emission of photons in Layman and Werner bands predominantly at 10 eV. Details of corresponding theory for the first time were considered by (Prasad, 1983) and in subsequent publications of many authors (Ferland et al., 2013) and references therein). Also (Ferland et al., 2013) have implemented it into the Cloudy model and corresponding code.

In this case molecular clouds in the circumnuclear regions of the active galaxy are considered similar to the clouds of our Galaxy, that is interstellar gas-dust objects with a dominant H_2 content and characteristic values of concentration, size and temperatures of the order of $n_H \sim 10^3 - 10^4 cm^{-3}$, $L \sim 30pc$ and $T \sim 10 - 100K$, respectively.

Dust is of the order of less than 1/100 by mass. Dust particles with silicate or graphite cores with sizes of the order of 0.01-0.1 μm have mantles of several 0.1 μm thick, consisting of stable polymers of unknown nature and/or ices of volatile compounds, primarily water, carbon oxides, and other, less abundant molecules. The one-dimensional physicochemical model of the cloud, including the radial dependence of the flux of the electromagnetic radiation field in this work, was calculated by the CLOUDY program (Ferland et al., 2013). The model includes the full calculated ionization atomic-molecular and thermal structures of the gas and dust components, as well as the spectral distribution of the radiated energy, including several million emission lines from the radio to the gamma range.

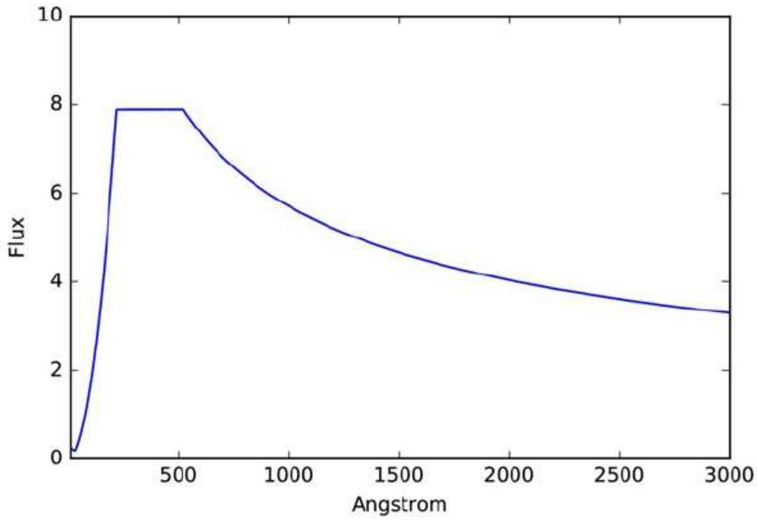

Figure 4: The hard incident radiation in the case of starbursts

The state of the medium, under the influence of external electromagnetic and particle radiation, was assumed to be stationary and homogeneous, with the initial atomic composition of a given metallicity of the first 30 elements, from hydrogen to elements of the iron group. Chemical reactions in the gas and on the surface of the dust particles lead to the kinetic equilibrium between atoms (585 with all ions) and 83 molecules, molecular ions and radicals in the gas, and, specifically, for H_2O, CO and OH species in the solid phase, that is Cloudy calculates their content not only in gas, but also in ice mantle of dust particles. In this case, the program uses the currently most accurate reaction rate coefficients and interaction cross sections between all species including interaction with radiation. It should be noted that the kinetic equations are solved for multilevel models of atoms, ions and molecules, and the effects of radiation transfer in the continuous spectrum and for the most important optically thick spectral lines are taken into account in the approximation known as *escape probability*. This approximation provides the necessary accuracy of calculations in the used static and homogeneous cloud model. Thus, a one-dimensional cloud model with the most complete consideration for all possible elementary processes, was used to calculate the radiation field and ice content along the radius using Cloudy. The cloud distance from the central source in all models was taken to be 15-20 pc, the hydrogen concentration was $10^3 - 10^4\ cm^3$, and the values of the ionization parameter U, was chosen as $lg(U) = -2, -3$ (Netzer, 2013). Hydrogen ionization rates by energetic protons with energies of several MeV and higher, $\zeta, (s^{-1})$, corresponds to the our galactic value $(lg(\zeta) = -16))$. The values of hydrogen column densities were chosen according to Fig.3.

As the longest chemical timescale of water and water ice formation is much less ($t \sim 10^9/n_H \sim 10^5 - 10^6$ years) as compared with the NLR clouds timescale of about 10^8 years (a limit following from the condition of exhaustion of the star formation gas (Stasińska et al., 2015)) one can use stationery models for description of the clouds. Thus we model clouds in steady-state conditions with constraints following from observational data.

The spectral energy distribution of radiation sources were chosen corresponding to the AGN mode of Cloudy obtained by their authors by combining available observations (Ferland et al., 2013). The intensity of the radiation was varied by changing the initial parameters presented in Table 3. The spectral distribution of the radiation incident on the cloud is shown in Fig. 4.

5. On the survivability of ices in the interstellar clouds of active galaxies

Now we turn to the question of the sensitivity of the water ice content to the spectral shape of radiation incident on the cloud.

Ices are sensitive to the presence of direct irradiation by electromagnetic and corpuscular radiation, as well as to the values of the medium parameters determined by these radiations, for example, by the temperature of gas and dust.

Now we present results of our calculated models (Table 3).

Table 3: The calculated column densities of water ice for some models

Model	lg(r_0)	lg(n)	lg(U)	N(H)	N(ice)
1	19.65	4	-3	3.00E+23	1.00E+20
2	19.65	4	-2	3.00E+23	1.10E+19
3	20.48	3	-2	1.00E+22	2.00E+19
4	20.48	3	-2	9.00E+22	1.20E-01

As we see, the ice content depends on the value of the ionization parameter, and is inversely proportional to its value, as was shown in (Yeghikyan, 2016). It should be noted that first 2 models correspond to the concentration 10^4 cm^{-3} and have hydrogen column densities larger than in Fig. 3. Models 3,4 have the concentration of 10^3 cm^{-3} and smaller hydrogen column densities in accordance with Fig.3.

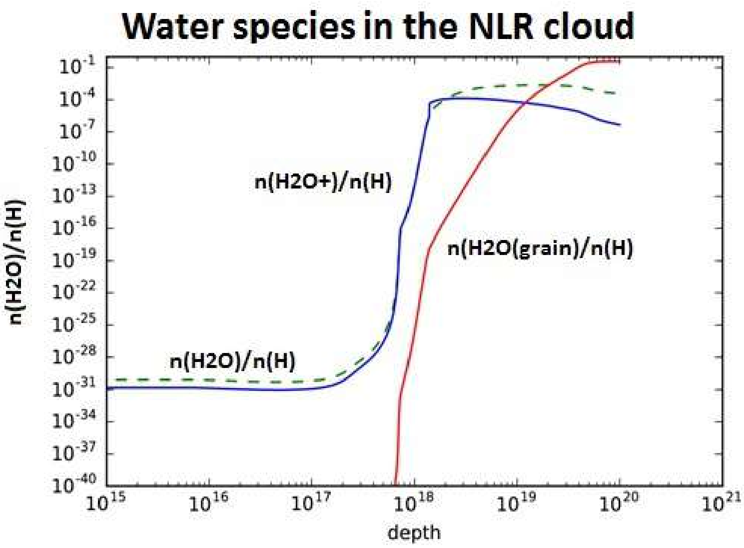

Figure 5: Water ice and related abundances in model 3

It should be underlined that there is a strong difference between shapes of incident radiation for starburst galaxies and AGN. In the case of starbursts it is due to the total amount of thermal radiation of massive and hot stars while AGN have a contribution in the hard part of the spectrum because of an accretion disk radiation. Now we will increase the contribution of hard UV and X-ray radiation as shown in Fig. 6. Results are shown in Table 3.

The hardening of the incident radiation intensity similar to that observed in typical AGN is described (in Cloudy) by

$$I_\nu = \nu^{\alpha_{UV}} exp(-h\nu/kT_{BB}) exp(-kT_{IR}/h\nu) + a\nu^{\alpha_X}, \quad (5)$$

where $\alpha_{UV} = -0.5$ is the low-energy slope of the continuum at $\approx 1Ryd$ (so-called Big Bump component), $T_{BB} = 1.5 \cdot 10^5 K$ - the temperature of the bump. Also the shape of spectral distribution is regulated by non-thermal parameters, related with UV and X-ray parts, namely by $\alpha_{0X} = -1.4$ and $\alpha_X = -1$, where the 1-st parameter is the X-ray to UV ratio and the 2-nd parameter is the slope of the X-ray component.

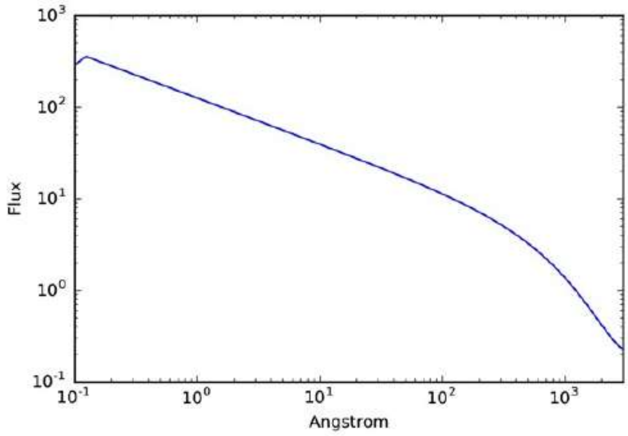

Figure 6: The hard incident radiation from AGN

The calculation results are presented in Table 3 which shows the column densities of water ices for different models. First 2 models are adopted from (Yeghikyan, 2016) and just supported observed column densities of starbursts for typical parameters of circumnuclear clouds. Models 3 and 4 are slightly different and influenced by two type of incident radiation like starburst (model 3) and AGN (model 4). One can easily seen that radiation from the accretion disk of the AGN is enough to completely disrupt water ice wherever it is in the cloud. Also intensity of X-ray and UV part of the incident spectrum should be about 100 times larger then that of in the starburst case.

6. Conclusion

Earlier we have shown (Yeghikyan, 2016) that ices in active galaxies regardless of type of galaxy (starburst or AGN) could not survive if cosmic ray fluxes are about 1000 times larger than in the Galaxy. Now we show that if the X-ray and UV fluxes are about 100 times larger which is typical for AGNs as compared with starbursts water ice is completely absent and could not be observed.In the case of starbursts the incident radiation is much softer and ices are present and even may be close to the observed values. But in Table 1 we have typical AGN or composite galaxies and ices are observed. These are preliminary model calculations and such analysis should be carried out for all other galaxies from Table 1 to be ready for further statistical considerations.

References

Bohlin R. C., Savage B. D., Drake J. F., 1978, ApJ, 224, 132

Boogert A. C. A., Gerakines P. A., Whittet D. C. B., 2015, ARA&A, 53, 541

Cottin H., Moore M. H., Bénilan Y., 2003, ApJ, 590, 874

Dworkin J. P., Seb Gillette J., Bernstein M. P., Sandford S. A., Allamandola L. J., Elsila J. E., Ryan McGlothlin D., Zare R. N., 2004, Advances in Space Research, 33, 67

Ferland G. J., et al., 2013, RMXAA, 49, 137

Hagen W., Tielens A. G. G. M., Greenberg J. M., 1983, AAS, 51, 389

Imanishi M., Dudley C. C., Maloney P. R., 2006, , 637, 114

Kaiser R. Roessler K., 1998, ApJ, 503, 959

Kaiser R. I., Roessler K., 1997, ApJ, 475, 144

Kaiser R. I., Eich G., Gabrysch A., Roessler K., 1997, ApJ, 484, 487

Moroz L. V., Arnold G., Korochantsev A. V., Wäsch R., 1998, Icarus, 134, 253

Netzer H., 2013, "The Physics and Evolution of Active Galactic Nuclei", Cambridge, UK: Cambridge University Press

Osterbrock D. E., Ferland G. J., 2006, "Astrophysics of gaseous nebulae and active galactic nuclei", CA: University Science Books

Prasad S. Tarafdar S., 1983, Astrophys. J., 267, 603

Roche H. Aitken D., 1984, MNRAS, 208, 481

Spoon H. W. W., Keane J. V., Tielens A. G. G. M., Lutz D., Moorwood A. F. M., Laurent O., 2002, A&A, 385, 1022

Spoon H. W. W., et al., 2004, ApJS, 154, 184

Stasińska G., Costa-Duarte M. V., Vale Asari N., Cid Fernandes R., Sodré L., 2015, MNRAS, 449, 559

Tielens A. G. G. M., 2005, "The Physics and Chemistry of the Interstellar Medium", ISBN 0521826349. Cambridge, UK: Cambridge University Press

Yeghikyan A., 2016, ASP Conf. Ser., 505, 144

Yeghikyan A., Martirosyan J., 2018, Communications of the Byurakan Astrophysical Observatory, 65, 303

Acknowledgements

The authors acknowledge the partial support of this work from Ambartsumian research award in 2019