IMPETUS: NEW CLOUDY’S RADIATIVE TABLES FOR ACCRETION ONTO A GALAXY BLACK HOLE

José M. Ramírez-Velasquez1,2, Jaime Klapp2,3, Ruslan Gabbasov4, Fidel Cruz5, and Leonardo Di G. Sigalotti1,5

1 Centro de Física, Instituto Venezolano de Investigaciones Científicas (IVIC), Apartado Postal 20632, Caracas 1020A, Venezuela
2 ABACUS-Centro de Matemáticas Aplicadas y Cómputo de Alto Rendimiento, Departamento de Matemáticas, Centro de Investigación y de Estudios Avanzados (Cinvestav-IPN), Carretera México-Toluca km. 38.5, La Marquesa, 52740 Ocoyoacac, Estado de México, Mexico
3 Departamento de Física, Instituto Nacional de Investigaciones Nucleares (ININ), Carretera México-Toluca km. 36.5, La Marquesa, 52750 Ocoyoacac, Estado de México, Mexico
4 Instituto de Ciencias Básicas e Ingenierías, Universidad Autónoma del Estado de Hidalgo (UAHEH), Ciudad Universitaria, Carretera Pachuca-Tulancingo km. 4.5 S/ N, Colonia Carboneras, Mineral de la Reforma, C.P. 42184, Hidalgo, Mexico
5 Área de Física de Procesos Irreversibles, Departamento de Ciencias Básicas, Universidad Autónoma Metropolitana-Azcapotzalco (UAM-A), Av. San Pablo 180, 02200 Mexico City, Mexico

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ABSTRACT

We present digital tables for the radiative terms that appear in the energy and momentum equations used to simulate the accretion onto supermassive black holes (SMBHs) in the centers of galaxies. Cooling and heating rates and radiative accelerations are calculated with two different Spectral Energy Distributions (SEDs). One SED is composed of an accretion disk + [X-ray]-power law, while the other is made of an accretion disk + [Corona]-bremsstrahlung with $T_k = 1.16 \times 10^8$ K, where pre-computed conditions of adiabatic expansion are included. Quantifications of different physical mechanisms at operation are presented, showing discrepancies and similarities between both SEDs in different ranges of fundamental physical parameters (i.e., ionization parameter, density, and temperature). With the recent discovery of outflows originating at sub-parsec scales, these tables may provide a useful tool for modeling gas accretion processes onto an SMBH.

Key words: accretion, accretion disks – atomic data – atomic processes – galaxies: active – methods: numerical – quasars: supermassive black holes

1. INTRODUCTION

Most of our present knowledge of the cosmos has come from application of the principles of quantum mechanics and atomic physics. For instance, the evolution of spectroscopy in every band of the electromagnetic spectrum from radio to γ-rays has allowed the study of the supernova remnants, the solar winds, the accretion onto supermassive black holes (SMBHs), and the large-scale structure of the universe in a way that we would have never imagined to be possible a century ago. Astrophysical processes that involve radiative energy transfer are calculated by the balance between heating and cooling. Analytical prescriptions for the heating and cooling rates in complex environments are only possible under certain limits. Moreover, it is well-known that they depend on the Spectral Energy Distribution (SED) used (Kallman & McCray 1982) and that stability curves also show a dependence on the SED in active galactic nuclei (e.g., Chakravorty et al. 2009, 2012).

However, the increasing computer power available today has allowed us to model complex astrophysical scenarios efficiently and at relatively low cost, including the dynamical update of the microphysics and chemistry. Non-equilibrium thermodynamics, ionization, molecular states, level populations, and kinetic temperatures of low densities environments are some of the ingredients that have no analytical counterparts and that can be calculated with highly efficient numerical algorithms.

Among the several publicly available codes for the calculation of astrophysical environments, CLOUDY (Ferland et al. 2013) and XSTAR (Kallman & Bautista 2001) have become the most popular because they treat the atomic physics at an ab-initio level. In addition, they have the ability to correctly handle a wide variety of scenarios, while predicting the spectrum of different gas geometries, including the Ultraviolet (UV) and the Infrared (IR), as well as a broad range of densities up to $10^{15}$ cm$^{-3}$ and temperatures from the cosmic microwave background (CMB) to $10^{10}$ K. The electronic structure of atoms, the photoionization cross-sections, the collisional and radiative processes between atomic levels so that the plasma behaves correctly in the low density limit and converges naturally to local thermodynamic equilibrium (LTE) either at high densities or when exposed to “quasi-real” blackbody radiation fields (Ferland et al. 1998). Moreover, collisions, line trapping, continuum lowering, and absorption of photons by continuum opacities are all included as very general processes (Rees et al. 1989). Inner-shell processes are also considered, including the radiative one (i.e., line emission after the removal of an electron; Ferland et al. 1998). On the other hand, analytical formulas for the heating and cooling rates have been widely used. For instance, previous work on accretion onto SMBHs in the centers of galaxies (active galactic nuclei, AGNs) by Proga et al. (2000), Proga & Kallman (2004), Proga (2007), and Barai et al. (2011) have made use of Blondin (1994) analytical formulas for the heating and cooling rates, which are limited to temperatures in the range $10^6 \lesssim T \lesssim 10^8$ K and ionization parameters ($\xi = L/(nHr^2)$) in the interval $1 \lesssim \log(\xi) \lesssim 5$.

In this paper, we develop a methodology and present tabulated values that account for highly detailed photoionization calculations together with the underlying microphysics to provide a platform for use in existing radiation hydrodynamics codes based either on Smoothed Particle Hydrodynamics
2. RADIATIVE COOLING AND HEATING

In numerical simulations of accretion onto a BH with either SPH (e.g., Katz et al. 1996) or standard Eulerian methods (e.g., Kurosawa & Proga 2009), it is common practice to add the net radiative heating (or cooling, depending on the sign used) rate, \( \rho \mathcal{L}(\rho, T) = \mathcal{H} - C \), into the energy equation as

\[
\frac{d}{dt} \left( \frac{e}{\rho} \right) = -\rho \nabla \cdot \mathbf{v} + \rho \mathcal{L},
\]

where \( p, \rho, e, \) and \( \mathbf{v} \) are the pressure, density, energy density, and velocity of the gas, respectively. The heating (\( \mathcal{H}[\rho, T] \)) and cooling (\( C[\rho, T] \)) rates are computed using CLOUDY 13.03 (Ferland et al. 2013). A detailed account of the techniques and atomic data can be found in the (very extended) documentation of the code, namely Hazy1, Hazy2, and Hazy3. Therefore, many of the details will not be repeated here, but rather we shall focus on describing all the input parameters and code commands in order to accurately reproduce our results. In brief, the problem reduces to have an abstract non-thermal equilibrium multidimensional unit cell (cloudy cell), which is able to return pre-computed physical conditions, that is, \( \mathcal{H}, \mathcal{C}, g_{\text{Cont}}, g_{\text{Grav}}, g_{\text{Elec}}, g_{\text{Line}} \) and \( g_{\text{Total}} \) for given values of the hydrogen number density \( n_H \), temperature \( T \), distance to the source \( r \), and incident angle \( \theta \).

In order for CLOUDY to handle the radiative transfer module, we must specify the geometry to be employed. In particular, we use the WIND geometry in which line widths and escape probabilities are evaluated either in the Sobolev or Large Velocity Gradient approximation. In this way, the effective line optical depth is

\[
\tau_{\text{eff}}(r) = \alpha_{\text{eff}}(r) \min(r, \Delta r) \left( n_l - n_{\text{exp}} \right) \left( \frac{u_{\text{th}}}{\max(u_{\text{th}}, u_{\text{exp}})} \right),
\]

where \( u_{\text{th}}\) and \( u_{\text{exp}}\) are the thermal and expansion velocities, respectively. The radius is chosen to be the minimum between the thickness of the gas slab, \( \Delta r \), and its distance from the ionizing source, \( r \), which defines an effective column density smaller than the total cloud column density when the radius is large and the expansion velocity is small. The populations of the lower and upper levels are \( n_l \) and \( n_{\text{exp}} \), while their statistical weights are \( g_l \) and \( g_{\text{exp}} \), respectively. The atomic absorption cross-section of the transition is \( \alpha_{\text{eff}}(cm^2) \). Here we set a micro-turbulence velocity \( u_{\text{turb}} = 100 \text{ km s}^{-1} \) and an initial expansion velocity of \( 100 \text{ km s}^{-1} \). The thin shell approximation is also invoked.

The input SEDs are shown in Figure 1. The total luminosity is chosen to be the typical luminosity of an AGN and is based on the accretion luminosity \( L_\eta = 2\eta G M_{\text{BH}} \dot{M}_\eta / r_{\text{Sch}} \), where \( \eta = 0.0833 \) is the accretion efficiency and \( M_\eta = 1.6 M_\odot \text{ yr}^{-1} \) (Proga 2007). For a fiducial SMBH with \( M_{\text{BH}} = 10^8 M_\odot \), the total luminosity is set to \( L = L_{\eta} = 7.5 \times 10^{43} \text{ erg s}^{-1} \). The two SEDs used are multicomponent spectra similar to the ones observed for AGNs. The first one (i.e., SED1, blue solid line) is composed of an accretion disk + [X-ray]–power law, while the second one (i.e., SED2, red solid line) is made of an accretion disk + [Corona]-bremsstrahlung, with \( T_K = 1.16 \times 10^8 \text{ K} \). The luminosity of the disk is defined as \( L_{\text{disk}} = f_{\text{disk}} L \), where \( f_{\text{disk}} = 0.95, 0.8 \), and 0.5 (see Table 1), while the luminosity of the X-ray power law is \( L_{\text{pl}} = f_{\text{pl}}^X L \), with \( f_{\text{pl}}^X = 0.05, 0.2, \) and 0.5. The energy index of the power
and log 410 = \approx 3.2 \text{ for SED1. The dark green and}

log 710 = 6.0 \text{ in order to facilitate comparison with previous work in the literature.}

In Table 1, we present a summary of the SED fractions used in the construction of the tables and refer to them as calculations I, II, III, IV, V, and VI, respectively.

Table 1: Emission Fractions of the SEDs Used for Constructing the Tables

| Calculation | Base SED | \( f_{\text{disk}} \) | \( f_{\text{X}} \) | \( T_{\text{X}} \times 10^8 (\text{K}) \) |
|-------------|----------|----------------|----------------|-----------------|
| I           | 1        | 0.95           | 0.05           | 1.79            |
| II          | 1        | 0.8            | 0.2            | 7.00            |
| III         | 1        | 0.5            | 0.5            | 18.08           |
| IV          | 2        | 0.95           | 0.05           | 1.11            |
| V           | 2        | 0.8            | 0.2            | 4.39            |
| VI          | 2        | 0.5            | 0.5            | 11.87           |

Notes.

Illuminating SED used as input for a given calculation: Base SED(1) ≡ Disk + Pl (Higginbottom et al. 2014); Base SED(2) ≡ Disk + Bremsa.

The Compton temperature depends on the ionization parameter, which changes with density and distance, with a fixed luminosity. This is \( T_{\text{X}} \) for \( n_H = 10^5 \text{ cm}^{-3} \) and \( r = 10^{16} \text{ cm} \). The entire range of \( T_{\text{X}} \) for the grid of parameters that we present in these tables can be found in their large version (see Table 2).

A photoionizing background radiation from radio to X-rays (Ostriker & Ikeuchi 1983; Ikeuchi & Ostriker 1986; Vedel et al. 1994) and the CMB have been considered, where the CMB temperature, \( T_{\text{CMB}} = T_0 (1 + z) \) (K), is taken to be \( T_0 = 2.725 \pm 0.002 \text{ K} \) (Wilkinson et al. 1987, p. 163; Mather et al. 1999).

A sample of the heating and cooling rates as determined from the tables is shown in Figure 2. The gas has a number density of \( 10^6 \text{ cm}^{-3} \). In both cases, \( C[\rho, T] \) and \( H[\rho, T] \) are calculated as functions of the temperature for two different characteristic ionization parameters: \( \log_2(\xi) = 5.88 \) and \( 1.88 \text{ [erg cm}^{-1} \text {s}^{-1}] \). For comparison, the blue and red lines display the total \( C[\rho, T] \) and \( H[\rho, T] \) for SED1. The dark green and orange lines display the total \( C[\rho, T] \) and \( H[\rho, T] \) for SED2. In Figure 3, we depict the gas equilibrium temperature predicted by \( H = C (\rho L = 0) \) as a function of the ionization parameter \( \log_2(\xi) \) for both the heating and cooling rates calculated with the disk+corona (e.g., calculations VI, with \( \theta \approx \pi/2 \)) and with the disk+X-ray power law presented in calculation III (e.g., \( \theta \approx \pi/2 \)). As stated by Kallman & McCray (1982), one of the main elements of the photoionization calculations is the SED used. For instance, we have overlaid two more calculations: one is a pure 10 keV bremsstrahlung (dotted line), which includes; (a) adiabatic cooling due to the hydrodynamic expansion of the gas, \( C_{\text{exp}} = -p D \rho + e \nabla \cdot \mathbf{v} \), and (b) Doppler shift due to the expansion. The other is a pure 10 keV bremsstrahlung (dashed-dotted line), but in this case we have relaxed the WIND model (see Equation (2)), NOwIND model, and as a consequence, adiabatic cooling and Doppler shift effects are not taken into account. As can be seen the net effect is to drop the equilibrium temperature of the gas from \( \sim 2 \times 10^7 \) to \( \sim 7 \times 10^6 \text{ K} \) in the range of photoionization parameters \( 4 \lesssim \log_2(\xi) \lesssim 7 \).

Finally, we note an increase in \( T_{\text{eq}} \) in the range \( 0 \lesssim \log_2(\xi) \lesssim 4 \), from the NOwIND bremsstrahlung model to the SED2 disk+bremsstrahlung, which is basically explained by the presence of UV and hard photons that are able to photoionize the gas and contribute with the heating rate in that range of the ionization parameters. The disk-blackbody component from the accretion disk affects the lower temperature part of the stability curve (see, for example, Chakravorty et al. 2012). The NOwIND bremsstrahlung model
being the frequency-dependent free–free expansion effects. See the text for details.

Finally, the net heating due to collisional ionization and cooling by 3-body recombination is defined as

$$G_{nk} - \Lambda_{nk} = \sum_n P_n^* n_e n_p C_{nk} n_T h v_0 (1 - b_n),$$  \hfill (12)

where $n_e$ and $n_p$ are the populations for the upper and lower levels, respectively, and the $C_{nk}$ are the collision rates. The SED1 calculated functions depicted in Figure 2 show differences in shape and magnitude for some temperature ranges compared to those obtained using SED2.

Figure 4 shows the net radiative heating ($>0$) of the system for three characteristic highly ionized plasmas with $\log_{10}(\xi) = 9.88$, 5.88, and 1.88 [erg cm s$^{-1}$] (for $n_p = 10^8$ cm$^{-3}$) usually found at sub-parsec distances from the SMBH as obtained from SED2 calculations (dashed lines) and SED1 calculations (solid lines). Important differences between both net radiative heatings are observed for two of the distances tried, which may range from 50% to factors of a few percent (as expected). A higher level of the rate for all temperatures in the net heating...
is observed for calculations VI at log_{10}(\xi) = 9.88, which leads to much warmer systems at low temperatures compared to SED1’s photoionization calculations. Farther away from the BH, at ionization parameters log_{10}(\xi) = 5.88 and in the temperature range 10^2 \lesssim T \lesssim 10^4, the heating exhibits a steeper slope due to the removal of electrons from the pool by radiative recombination. This occurs because of the large number of available transitions at these temperatures. Nevertheless, at ionization parameters log_{10}(\xi) = 1.88, \rho L shows very similar behavior.

3. RADIATIVE ACCELERATION

Along with the heating and cooling rates, we also calculate the radiative acceleration, which appears as a source term in the momentum equation

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p + \rho g + \rho g_{\text{Total}}^\text{rad}. \quad (14)$$

In the tables we report here, the radiative acceleration, \( g_{\text{Total}}^\text{rad} \) (defined as a force per unit mass), is calculated in a grid of \( \theta, r, n_H \), and \( T \) using CLOUDY 13.03. For a direct attenuated continuum, \( F_\nu \), and a density, \( \rho \), we have that

$$g_{\text{Total}}^\text{rad} = \frac{1}{\rho c} \int F_\nu \tilde{\kappa}_\nu \, d\nu + \frac{1}{\rho c} \sum_i F_i(\lambda) \kappa_i \gamma_i B_{\lambda,\nu} \text{ [cm s}^{-2}], \quad (15)$$

where \( \tilde{\kappa}_\nu \) is the effective opacity from the continuum. The acceleration includes the usual photoelectric absorption as well as the free–free, Rayleigh, and Compton processes. The integral is over the range between \( \lambda \approx 10 \) m and \( h\nu = 100 \) MeV. The second term is a summation over all lines contributing (typically \( 10^4-10^5 \) transitions). The quantity \( \kappa_i \) is the opacity of the line, \( B_{\lambda,\nu} \) is the Einstein coefficient, and \( \gamma_i \) is the escape probability toward the ionizing source (see Appendix B).

In Figures 5(a)–(c), we display the variation of the total outward acceleration (solid lines), the radiative acceleration due to continuum processes (dashed lines), and the acceleration due to spectral lines (dotted lines) with temperature for three characteristic ionization parameters: log_{10}(\xi) = (9.88, 5.88, 1.88) [erg cm s^{-1}]. We may see from Figure 5(a) that in a highly ionized plasma with log_{10}(\xi) = 9.88 (very close to the source, \( \approx 4r_{\text{Sch}} \)), the contribution is mostly due to scattering. At log_{10}(\xi) = 5.88 (\( \approx 340r_{\text{Sch}} \)), Figure 5(b) shows that the acceleration due to lines dominates up to \( \approx 10^3 \) K and then falls sharply at higher temperatures due to the contribution of continuum processes, while at log_{10}(\xi) = 1.88 (\( \approx 34, 000r_{\text{Sch}} \)), the acceleration due to spectral lines dominates over the entire range of temperatures, except for \( T \gtrsim 6 \times 10^7 \) K, as shown in Figure 5(c). The force multiplier as a function of the temperature for the above three characteristic values of \( \xi \) is displayed in Figure 5(d).

Moreover, in our calculations we assume that the contribution to \( g_{\text{Total}}^\text{rad} \) coming from the disk, depends on the radial direction (r) and the polar angle (\theta) through the incident radiation

$$F_{\text{disk}}(r, \theta) = \cos(\theta) \frac{L_{\text{disk}}}{4\pi r^2}, \quad (16)$$

while the radiative flux from the central object is isotropic

$$F_{\text{CO}}(\theta) = \frac{L_{\text{CO}}}{4\pi r^2}. \quad (17)$$

In Figure 6, we compare the radiative acceleration, \( g_{\text{Total}}^\text{rad} \), as calculated from Equation (15) (black lines) for SED1, with \( g_{\text{Total}}^\text{rad} \), given by SED2 (blue lines), both as functions of the ionization parameter for three different angles, i.e., \( \theta = 0^\circ \) (solid lines), 36^\circ (dashed lines), and 90^\circ (dotted lines). When both approaches, i.e., the calculations I-III and the calculations IV-VI, are used in the range 0 \( \lesssim \log_{10}(\xi) \lesssim 15 \) (10r_{\text{Sch}} \lesssim r \lesssim 10,000r_{\text{Sch}}), they will both influence the distribution of velocities resulting from the momentum equation in numerical simulations of the accretion onto SMBHs.

4. THE TABLES

The tables are available to the public at the following links: www.abacus.cinvestav.mx/impetus and Zenodo. They are plain ASCII files (my1Part_OUT.txt) stored in the directories simul_i_j.j, where the index i corresponds to a value of the number density (\( n_H \)) and j corresponds to a value...
of the incident angle $\theta$. For example, the sub-directory $\text{simul}_11/1$ contains the ASCII text, with 12 columns (to be explained later), of the first density ($i \equiv 1$, $n_H = 10^{-2}$ cm$^{-3}$) and first angle ($j \equiv 1$, $\theta = 0$) in our grid. Moreover, in directory $\text{simul}_{101.6}/1$, one can find the calculations for $n_H = 10^8$ cm$^{-3}$ and $\theta = \pi/2$. 

**Figure 5.** Calculated radiative accelerations for a BH of mass $M_{\text{BH}} = 10^8 M_\odot$. Panels (a), (b), and (c) show the total outward acceleration (solid lines), the acceleration due to continuum processes (dashed lines), and that due to spectral lines (dotted lines), respectively. Panel (d) shows the force multiplier ($M(t) \approx 1$: no contribution from spectral lines and $M(t) > 1$: line contribution different from zero) for three characteristic ionization parameters $\log_{10}(\xi) = 9.88, 5.88, \text{and } 1.88$ [erg cm s$^{-1}$]. In these plots we have used $\theta = 0^\circ$, SED1, $f_{\text{esc}} = 0.5$, $f_X$ = 0.5, and $n_H = 10^8$ cm$^{-3}$. 

- (a) $\log_{10}(\xi) = 9.88$
- (b) $\log_{10}(\xi) = 5.88$
- (c) $\log_{10}(\xi) = 1.88$
Each main directory is provided with an ASCII file nH_SED1_mod_11.txt, where it is easy to see the values of $i$ and $j$ corresponding to a given density and angle. Inside this file we can find:

1. Column1: Index $i$.
2. Column2: Index $j$.
3. Column3: Number density $\log_{10}(n_H)$ [in cm$^{-3}$].
4. Column4: Incident angle $\theta$ [in radians].
5. Column5: Initial radius $\log_{10}(r)$ [in cm].
6. Column6: Final radius $\log_{10}(r)$ [in cm].

We now describe in more detail the content of the ASCII file my1Part_OUT.txt. There are 12 columns inside:

1. Column1: Incident angle $\theta$ [in radians].
2. Column2: Number density $\log_{10}(n_H)$ [in cm$^{-3}$].
3. Column3: Distance from the BH $\log_{10}(r)$ [in cm].
4. Column4: Temperature $\log_{10}(T)$ [in K].

5. Column5: Total cooling rate $\frac{dE_{\text{cool}}}{dt}$ [in erg cm$^{-3}$s$^{-1}$].
6. Column6: Total heating rate $\frac{dE_{\text{heat}}}{dt}$ [in erg cm$^{-3}$s$^{-1}$].
7. Column7: Acceleration due to continuum $g_{\text{Cont}}^{\text{rad}}$ [in cm s$^{-2}$].
8. Column8: Acceleration due to gravity $g_{\text{Grav}}^{\text{rad}}$ [in cm s$^{-2}$].
9. Column9: Total outward acceleration $g_{\text{total}}^{\text{rad}}$ [in cm s$^{-2}$].
10. Column10: Acceleration due to electron scattering $g_{\text{elec}}^{\text{rad}}$ [in cm s$^{-2}$].
11. Column11: Acceleration due to spectral lines $g_{\text{Line}}^{\text{rad}}$ [in cm s$^{-2}$].
12. Column12: Force multiplier $M_f$ [dimensionless].

Two versions of the tables are made available: short and full versions. The short version contains only the my1Part_OUT.txt file, the illuminating SED at $r = 10^4$ cm (the my1cont-File_OUT_14 file), and the ionic fractions at $r = 10^6$ cm (the my1Part_OUT_frac.txt file). On average, the short versions of the Tables (e.g., SED1, $f_{\text{disk}} = 0.95$ and $f_X = 0.05$) are about ~47 MB. The full version contains the full output (my1Part_OUT.out) from CLOUDY, which is useful for exploring features related to the calculations in deeper detail. Each uncompressed directory has, on average, a size of ~32 GB. Multiplying this size by six leads to ~200 GB for the full versions of the tables. A summary of the short and full versions and their locations can be found in Table 2.

5. DISCUSSION AND CONCLUDING REMARKS

The contribution of the microphysics to the heating and cooling rates is displayed in Figure 7. For instance, at $0.32$ pc we may see from Figure 7(a) that the main contributor to the heating over the temperature range $400 \lesssim T \lesssim 8000$ K is the Unresolved Transition Array (UTA, Behar et al. 2001, Netzer 2004 and also see Ramírez et al. 2008 for an observational point of view), which accounts for $\approx 12\%–16\%$ of the heating rate. In the interval $10^4 \lesssim T \lesssim 8 \times 10^4$ K, photoionization heating of O$^+$ becomes the major contributor, providing $\approx 12\%–16\%$ of the heating. At temperatures of $10^5 \lesssim T \lesssim 3.2 \times 10^5$ K, Fe$^{+18}$ contributes with $\approx 12\%–17\%$. In these plots, the solid line denotes the main contributors, while the dotted and dashed lines depict the second and third contributors, respectively. In Figures 7(a)–(d), we see that in the temperature range $6.3 \times 10^4 \lesssim T \lesssim 3.2 \times 10^5$ K, heating by Compton processes dominates the heating, with contributions that rise up to $\approx 100\%$, close to the upper extreme of the temperature range.

Note. The main webpage of the project is http://www.abacus.cinvestav.mx/impetus. The full versions of the tables can be accessed via the project webpage, the links in the table above, or via a request to the corresponding author.
Figure 7. Main agents contributing to the heating rates as included in the tables. A complex interplay between photoelectric heating of low and high ionization species, UTA, and Compton processes can be observed. For these plots we have used a bremsstrahlung SED with $T_v = 1.16 \times 10^8$ K, in order to directly see the different physical mechanisms in operation for a gas with $n_H = 10^7$ cm$^{-3}$ at ionization parameters $\log(\xi)$: (a) 2.90, (b) 1.90, (c) 0.90, and (d) $-0.11$ [erg cm s$^{-1}$]. The main agents (solid lines) are also labeled via straight horizontal lines to denote the temperature range where they contribute. The second (dotted lines) and third (dashed lines) contributors are also displayed. The dotted–dashed lines correspond to the 100 main heating agents.
Figure 8. Main agents contributing to the cooling rates as included in the tables. A complex interplay between radiative and collisional recombination, collisional de-excitation of low and high ionization species, UTA, and free–free processes can be observed. For these plots we have used a bremsstrahlung SED with $T_x = 1.16 \times 10^8$ K, in order to directly see the different physical mechanisms at operation for a gas with $n_H = 10^6$ cm$^{-3}$ at ionization parameters $\log(\xi)$: (a) 2.90, (b) 1.90, (c) 0.90, and (d) $-0.11$ [erg cm s$^{-1}$]. The main agents (solid lines) are also indicated by straight horizontal lines to denote the temperature range where they contribute. The second (dotted lines) and third (dashed lines) contributors are also displayed. The dotted–dashed lines correspond to the 100 main cooling agents.
In general, we find a rather complex interplay between the different heating agents, where low-ionization species contribute mostly to temperatures below 10$^4$ K, highly ionized species of heavy metals (e.g., Fe$^{+17}$–Fe$^{+24}$) and intermediate-heavy metals in the form of H- and He-like (e.g., O$^{-7}$–O$^{+8}$, C$^{-4}$–C$^{+5}$) become important at temperatures in the range 10$^4$ < T < 10$^5$ K. At T > 10$^5$ K, Compton heating becomes the dominant mechanism. The dashed-dotted lines in Figures 7(a)–(d) depict the contribution of the 100 main heating agents, which clearly account for ≈100% of the total heating rate.

A similar analysis can be done for the cooling rate. In Figure 8, we depict the cooling rates as a function of the temperature at different distances from the source. We see that radiative recombination cooling by H contributes to ≈25%–74% of the total cooling rate in the temperature range 200 < T < 4 × 10$^4$ K. Cooling by H lines dominates at higher temperatures in the range 5 × 10$^4$ < T < 4 × 10$^5$ K, with a contribution to total cooling of ≈25%–74%.

Free-free cooling contributes up to ≈86% in the temperature interval between T ∼ 1.3 × 10$^3$ K and T ∼ 1.3 × 10$^5$ K, with its contribution decreasing to ≈72% at T ∼ 10$^6$ K. The second and third contributors are represented by the dotted and dashed lines, respectively, while the dashed-dotted lines depict the contribution of the 100 main cooling agents.

Although the analytical formulas given by Blondin (1994) are useful for studying cooling and heating in high-mass X-ray binary systems, they become different for simulations of gas accretion onto SMBHs in the centers of galaxies. In this work, we adopt a similar analysis for the cooling rate. In Figure 8, we depict the cooling rates as a function of the temperature at different distances from the source. We see that radiative recombination cooling by H contributes to ≈25%–74% of the total cooling rate in the temperature range 200 < T < 4 × 10$^4$ K. Cooling by H lines dominates at higher temperatures in the range 5 × 10$^4$ < T < 4 × 10$^5$ K, with a contribution to total cooling of ≈25%–74%.

Free-free cooling contributes up to ≈86% in the temperature interval between T ∼ 1.3 × 10$^3$ K and T ∼ 1.3 × 10$^5$ K, with its contribution decreasing to ≈72% at T ∼ 10$^6$ K. The second and third contributors are represented by the dotted and dashed lines, respectively, while the dashed-dotted lines depict the contribution of the 100 main cooling agents.

Below T = 10$^4$ K, SED1 and SED2 cooling rates differ by factors of a few. In fact, neutral-to-middle ionized gas contributes mostly to the total cooling below T = 10$^4$ K and can be important in the outflows (~1400 km s$^{-1}$) of N ii/ N iii$^-$–S iii/ S iii$^+$ found at ~840 pc (Chamberlain & Arav 2015), and also in closer Iron low-ionization broad absorption lines (FeLoBAL) flows (~ few thousand km s$^{-1}$) at ~7–70 pc (McGraw et al. 2015). Moreover, at log$_{10}(\xi)$ ~ 2 the SED2 computations may overestimate the equilibrium temperature up to factors of ~20 in the range 10$^5$–10$^6$ K. This may be used as a discrimination feature for simulations of SEDs in AGNs. For the heating case, however, the differences only reach factors of ~2 to ~10. We note that Compton and Coulomb heating could well be operating at temperatures between 10$^4$ and 10$^5$ K (for instance, in pre/post shocked winds in AGNs, Faucher-Giguère & Quataert 2012). In addition, pure 10 keV bremsstrahlung heating could be important at temperatures below 10$^4$ K. This may be used as a discrimination feature for simulations of SEDs in AGNs.

We further note that Vignali et al. (2015) found a gas of high velocity (~0.14c) through the identification of highly ionized species of iron (e.g., Fe XXV and Fe XXVI) in a luminous quasar at z ∼ 1.6, located at distances of ~10$^{15}$–10$^{16}$ cm. In fact, through observed high-energy features, Tombesi et al. (2015) relate low (by molecules) and high velocities (highly ionized gas) with the predicted energy-conserved wind (Faucher-Giguère & Quataert 2012), and locate this gas at ~900 r$_{sch}$, where more precise estimates of the heating and cooling are required. It is therefore clear that a quantitative analysis of the heating and cooling agents operating on these kinds of astrophysical environments is crucial for understanding the radiation hydrodynamical processes governing the accretion onto SMBHs. We have provided the files my1Part_OUT.txt and my1Part_OUT.col as part of the tables, where the default ≈10 agents are given by CLOUDY.

The interested reader may request the modified 100 agent files from the corresponding author. These tables have the potential and the flexibility to include other physical effects, like dust and/or molecules. In fact, OH 119 μm lines have been found in ultraluminous infrared galaxies using the Herschel/PACS telescope at velocities of ~1000 km s$^{-1}$ (Veilleux et al. 2013). Also, far-ultraviolet features may be present in Mrk 231 (found with the Hubble Space Telescope), with velocities of ~7000 km s$^{-1}$ (Veilleux et al. 2016). They permit more extensive exploration of the influence of the SED on photoionization calculations (see Chakravorty et al. 2009, 2012) and their impact on the energy and velocity distribution on hydrodynamical accretion processes onto SMBHs. Another branch of SED to be explored is the reflected spectrum from the accretion disk, a rich mix of radiative recombination continua, absorption edges, and fluorescent lines (García & Kallman 2010; García et al. 2011, 2013). Additionally, if produced close to the black hole, this component suffers alterations due to relativistic effects (Dauser et al. 2013; García et al. 2014). These types of SEDs may influence cooling and heating rates, as they are very sensitive to the values of the ionization parameter, temperature, and density. In astrophysical environments like the centers of AGNs, they may play an important role in high-velocity winds and the evolutionary stages of the host galaxies (as they may expel the cold gas reservoirs within 10$^6$–10$^8$ years, Sturm et al. 2011). We also have the capacity to include them in tables of radiative acceleration for SPH codes, which will be the subject of a future study. A strict comparison between theoretical models and simulations is beyond the scope of the tables presented here. At present, such simulations are under preparation.

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APPENDIX A
THE Geometrically Thin, optically THICK DISK
USED IN THE SEDs

The luminosity of a disk with dissipation $D(r)$ is

$$ L_{\text{disk}} = 2\pi \int_{r_{\text{in}}}^{\infty} D(r) r dr = \frac{1}{2} \frac{\eta GM_{\text{BH}} M}{r_{\text{D}}}, $$

(18)

which is half of the accretion luminosity $L_a = \eta M_c c^2$. If the disk is optically thick and its luminosity, $L_{\text{disk}}$, radiates as a blackbody, its temperature $T_{bb}(r)$ as a function of distance is given by

$$ T_{bb}(r) = T_{\text{id}} \left( \frac{r}{r_{\text{id}}} \right)^{-3/4} \left[ 1 - \left( \frac{r_{\text{id}}}{r} \right)^{1/2} \right]^{1/4}, $$

(20)

where

$$ T_{\text{id}} = \left( \frac{3\eta GM_{\text{BH}} M}{8\pi r_{\text{id}}^3 \sigma_{\text{SB}}} \right)^{1/4}. $$

(21)

For our SEDs we have used $M_{\text{BH}} = 10^8 M_*$, $M_* = 1.6 M_\odot$, yr$^{-1}$, and $r_{\text{id}} = 3 r_{\text{Sch}}$ ($= r_{\text{ISCO}}$ for a non-rotating SMBH). Hence, in the inner ring of the disk $T_{bb}(r_{\text{id}}) = 1.35 \times 10^5$ K, while in the outer part, i.e., for $r_{\text{id}} = 10 r_{\text{Sch}}$, the temperature would be $T_{bb}(r_{\text{id}}) = 4.50 \times 10^4$ K.

APPENDIX B
CLOUDY’S IONIC FRACTIONS

In our calculations we have included the following astrophysically relevant elements: H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, and Fe. The abundances have been taken from Grevesse et al. (2010) and we have neglected the effects of grains and molecules. Our grid of CLOUDY’s models for the calculation of the heating and cooling rates and the radiative acceleration uses the following physical parameters and resolutions: $\theta = 0...\pi/2$ with $\Delta \theta = \pi/10$; $\log_{10}(n_H) = -2...9$ [cm$^{-3}$] with $\Delta \log_{10}(n_H) = 0.1$; $\log_{10}(r)$ = 14...18 [cm] ($= 3.4 \times [1 - 10^{-4}] r_{\text{Sch}}$) with $\Delta \log_{10}(r) = 1$; and $\log_{10}(T) = 2...9$ [K] with $\Delta \log_{10}(T) = 0.1$.

To look inside the cooling/heating tables we use a conventional bisection method, where for each SPH particle (or Eulerian cell) with coordinates $(r_i, \theta_i, \phi_i)$ and density $\rho_i$, the functions $C(\rho_i, T_i)$ and $H(\rho_i, T_i)$ are linearly interpolated within the temperature interval $T_{\text{min}} \leq T_i \leq T_{\text{max}}$. Ferland et al. (2013) discuss in great detail the numerical algorithm and the atomic databases used by CLOUDY. Here we shall only describe the calculation of the level populations and refer the interested reader to Ferland et al. (2013) and the references therein for technical details.

Radiative and collisional processes contribute to the evolution of the level populations such that

$$ \frac{db_n}{dt} = \frac{db_n}{dt} \bigg|_{\text{rad}} + \frac{db_n}{dt} \bigg|_{\text{col}}, $$

(22)

where $b_n$ is the departure coefficient given by

$$ b_n = \frac{n_n}{P_n^* n_e n_{\text{ion}}}, $$

(23)

$n_n$ is the actual population of the level, $n_e$ and $n_{\text{ion}}$ are, respectively, the electron and ion number density, and $P_n^*$ is the LTE relative population density for level $n$ defined as

$$ P_n^* = \frac{n_n^*}{P_n^* n_e n_{\text{ion}}} = \frac{g_n}{g_e g_{\text{ion}}} \frac{m_n^*}{m_e m_{\text{ion}}} \frac{h^2}{2\pi m_e kT} \exp \left( \frac{\chi_n}{kT} \right). $$

(24)

Here, $g_n = 2n^2$ is the hydrogenic statistical weight of level $n$, $n_n^*$ is the LTE population of level $n$, $g_e = 2$ is the electron statistical weight, $g_{\text{ion}}$ is the ion statistical weight, which is equal to 1 or 2 for H- or He-like species, respectively, and $\chi_n$ is the ionization potential of level $n$. The other symbols are the electron mass, $m_e$, the Planck constant, $h$, and the temperature, $T$.

The collisional term in Equation (22) can be written as

$$ \frac{db_n}{dt} \bigg|_{\text{col}} = \sum_i b_i C_{ni} + \sum_u \frac{P_u^*}{P_u} b_u C_{un} $$

$$ - b_n \left[ \sum_i C_{ni} + \sum_u \frac{P_u^*}{P_u} C_{un} + C_{nk}(1 - b_n^{-1}) \right]. $$

(25)

where the summations are taken over the upper and lower levels and the $C_{ij}$ are the collisional rates in units of s$^{-1}$. The first, second, and third terms on the right side of the above equation are, respectively, the collisional excitation from the lower levels to level $n$, the collisional de-excitation to level $n$ from higher levels, and the term for destruction processes. The collisional ionization rate, $C_{nk}$, is multiplied by a factor that takes into account the effects of collisional ionization and three-body recombination.

The radiative contribution term in Equation (22) can be written as

$$ \frac{db_n}{dt} \bigg|_{\text{rad}} = \sum_i \frac{P_i^*}{P_n} b_i A_{ni} \frac{g_i}{g_n} \eta_{\text{rad}} \gamma_{ni} $$

$$ + \sum_u \frac{P_u^*}{P_n} b_u (A_{un} \beta_{un} + A_{un} \eta_{un} \gamma_{un}) $$

$$ + \eta_{\text{rad}} + \eta_{\text{Rad}} - b_n \sum_l (A_{nl} \eta_{nl} + A_{nl} \eta_{nl} \gamma_{nl}) $$

$$ + \sum_u A_{un} \frac{g_u}{g_n} \eta_{un} \gamma_{un} + 1, $$

(26)

where $A_{ij}$ is the transition probability, $\eta_{ij} \equiv J_{ij} / (2 \hbar \nu_{ij}^3 / c^2)$ is the continuum occupation number of the transition $ij$, with $J_{ij}$ being the mean intensity of the ionizing continuum at the line frequency $\nu$. The first of the two escape probabilities, $\beta$, is a two-side function, which takes into account line scattering.
Figure 9. Relative abundances of all the elements included in our calculations (H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, and Fe) as a function of temperature. For these plots we have used $\theta = 0^\circ$, SED1, $f_{\text{disk}} = 0.8$, $f_{\chi} = 0.2$, and $n_H = 10^8$ cm$^{-3}$.
and escape

\[ \beta(\tau, T) = \frac{\beta(\tau) + \beta(T - \tau)}{2}, \]  

(27)

where \( \tau \) is the optical depth of the point in question and \( T \) is the total optical depth. The escape probability, \( \gamma_j(\tau) \), accounts for the fraction of the primary continuum penetrating up to \( \tau \) and inducing transitions between level \( i \) and \( j \).

The photoionization rate, \( \Gamma_n \), from the level \( n \) that appears in Equation (26), is given by

\[ \Gamma_n = 4\pi \int_{\nu_0}^{\infty} \frac{J_\nu}{h\nu} \sigma(\nu) d\nu, \]  

(28)

and the induced recombination rate (\( \text{cm}^3 \text{s}^{-1} \)) is defined as

\[ \alpha_{\text{ind}, n} = P_n^i 4\pi \int_{\nu_0}^{\infty} \frac{J_\nu}{h\nu} \sigma(\nu) \exp\left(-\frac{h\nu}{kT}\right) d\nu. \]  

(29)

Spontaneous radiative recombination rates, \( \alpha_{\text{rad}} \), are calculated as in Badnell et al. (2003) and Badnell (2006). In summary, we have added terms that correspond to induced upward transitions from lower levels, spontaneous and induced downward transitions from higher levels, spontaneous and induced capture from the continuum to the level, and destruction of the level by radiative transitions and photoionization. The ionic emission data is taken from CHIANTI (Dere et al. 1997) and was recently revised by Landi et al. (2012). Figure 9 shows the ionic fractions for all the elements as a function of temperature. For these plots, we have chosen \( n_H = 10^8 \text{ cm}^{-3} \), \( \theta = 0^\circ \), and a distance from the source equal to \( r = 10^{16} \text{ cm} \) (SED1, \( f_{\text{disk}} = 0.8, f_X = 0.2 \)).

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