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Radiative cooling in collisionally ionized and photoionized plasmas

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ABSTRACT

We discuss recent improvements in the calculation of the radiative cooling in both collisionally ionized and photoionized plasmas. We are extending the spectral simulation code `CLOUDY` so that as much as possible of the underlying atomic data are taken from external data bases, some created by others and some developed by the `CLOUDY` team. This paper focuses on recent changes in the treatment of many stages of ionization of iron, and discusses its extensions to other elements. The H- and He-like ions are treated in the isoelectronic approach described previously. Fe II is a special case treated with a large model atom. Here we focus on Fe III through Fe XXIV, ions which are important contributors to the radiative cooling of hot ($T \sim 10^5$ – 10^7 K) plasmas and for X-ray spectroscopy. We use the Chianti atomic data base to greatly expand the number of transitions in the cooling function. Chianti only includes lines that have atomic data computed by sophisticated methods. This limits the line list to lower excitation, longer wavelength, transitions. We had previously included lines from the Opacity Project data base, which tends to include higher energy, shorter wavelength, transitions. These were combined with various forms of the ‘g-bar’ approximation, a highly approximate method of estimating collision rates. For several iron ions the two data bases are almost entirely complementary. We adopt a hybrid approach in which we use Chianti where possible, supplemented by lines from the Opacity Project for shorter wavelength transitions. The total cooling including the lightest 30 elements differs from some previous calculations by significant amounts.

Key words: atomic data – plasmas – methods: numerical.

1 INTRODUCTION

This paper describes recent advances in the treatment of cooling in the spectral simulation code `CLOUDY`. A companion paper in preparation by Williams et al. determines the emission spectrum of a non-equilibrium cooling and recombining plasma where the physics is largely driven by radiative cooling.

`CLOUDY` performs, as its primary goal, a full simulation of the microphysics of a non-equilibrium gas. As described in the last major review (Ferland et al. 1998), the code is designed to incorporate the essential microphysics of gas between the molecular and fully ionized limits, with densities between the local thermodynamic equilibrium and the low-density limit, and with temperatures between the current cosmic microwave background and 10^{10} K. Osterbrock & Ferland (2006, hereafter AGN3) provide many details of this

physics. Our approach is to treat the microphysics in great detail, using basic cross-sections and transition rates where possible, to do exactly what nature does under this broad range of conditions.

The atomic/molecular data base is the essential difficulty in producing a full simulation of a non-equilibrium gas. Atomic data, like the underlying quantum mechanics, are complex due to the idiosyncrasies that are characteristic of each molecule or ion. Through much of its history we have added physical processes to the code as special cases, each treated individually. A large model of the Fe II atom was developed by Katya Verner as part of her PhD thesis (Verner et al. 1999), while Gargi Shaw did a complete model of the hydrogen molecule as part of her PhD thesis (Shaw et al. 2005). Ryan Porter developed a unified treatment of the He-like isosequence (Porter et al. 2005; Porter & Ferland 2007) and extended it to include the H-like sequence (Luridiana et al. 2009) as part of his thesis.

Additional contributors to the emission spectrum and cooling were added on a line-by-line basis. Initially, a range of lines based

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on previous calculations of the cooling function were used (Kato 1976; Gaetz & Salpeter 1983). Additional lines were added on an ad hoc basis. Finally, all Opacity Project (Seaton 1987) permitted lines that directly connect to the ground state were added (see also Verner, Verner & Ferland 1996). The Opacity Project did not compute collision rates so the emission data were combined with various forms of the ‘g-bar’ approximation, an approximate relationship between the collision rate and other atomic parameters, to compute the emission. The current implementation uses g-bar approximations from Mewe (1972), Gaetz & Salpeter (1983) and Mewe, Gronenschild & van den Oord (1985). Additionally, level energies and line wavelengths for OP lines are uncertain by roughly 15 per cent, although these energies can be improved by comparing with experiments, as was done by Verner et al. (1996). The new improvements are described next.

2 CALCULATIONS

We have updated CLOUDY to use iron lines from the Chianti¹ data base (Dere et al. 1997; Landi et al. 2012) version 7. Of the astrophysically abundant elements, iron is the one with the richest spectrum and an element which has been an emphasis for the Chianti project. CLOUDY will now make use of the experimentally measured lines from the Chianti data base for Fe IV through Fe XXIV. The Chianti implementations of Fe XXV and Fe XXVI, He- and H-like iron, are not used because we treat these using the isoelectronic approach described in Porter et al. (2005), Porter & Ferland (2007) and Luridiana et al. (2009). The special case of Fe II continues to be treated with the Verner model atom.

In situations where Chianti has provided transitions without collision strengths, the g-bar approximation from Mewe (1972) is used. The transitions are estimated to be allowed or forbidden based on the value of their oscillator strength (gf). Transitions where $gf \geq 1 \times 10^{-8}$ are classified as allowed and all others are forbidden. After classification, the appropriate g-bar approximation equation is used.

In addition to the Chianti data base lines for Fe IV through Fe XXIV, we added Fe III lines from the Kurucz Atomic Database (Kurucz 2009). The Kurucz lines, like the Opacity Project lines, lack collisional data so we use the g-bar approximation. We will use the Chianti and Kurucz data where they are available since they have more accurate energies. We supplement these with Opacity Project lines that come from levels that have higher excitation than those in Chianti and Kurucz. This implementation, called the Hybrid configuration, gives CLOUDY the greatest accuracy and wavelength coverage.

In the remainder of this section, we outline our approach and compute cooling functions for collisionally ionized and photoionized plasmas. We find surprisingly good agreement with older calculations, and with others based on a detailed incorporation of the atomic physics, but not with several recent studies.

A calculation of the gas cooling involves several steps. First, the ionization or chemical state of the gas must be determined. This distribution is then used to compute the cooling, the rate that collisions convert kinetic energy into light. The following sections give details concerning these calculations.

¹ Chianti is a collaborative project involving the NRL (USA), the Universities of Florence (Italy) and Cambridge (UK), and George Mason University (USA).

2.1 The ionization balance

This paper is limited to atomic and ionic cooling, and so is limited to temperatures greater than 10^4 K. A calculation of the ionization balance involves rates for collisional ionization and photoionization, and various recombination processes. These are described in the following subsections.

2.1.1 Collisional ionization

CLOUDY has used the collisional ionization rate coefficients tabulated by Voronov (1997) since the publication of that paper. More recently, Dere (2007) presented a new compilation which is largely in excellent agreement with Voronov (1997). The Dere (2007) recommendations originated with experiments from different sources and theoretical calculations using the flexible atomic code (FAC) described in Gu (2002). The collisional ionization rate coefficients of Dere (2007) and Voronov (1997) only differ significantly for about half a dozen ions. We provide options which will allow CLOUDY to use either set of rates.

We have implemented these data in the following way in our default calculation. The Dere (2007) coefficients are provided in a discrete format for selected temperatures which do not span the temperature range needed by CLOUDY. Voronov (1997) provides continuous functions which are valid for any temperature, going to the appropriate low and high temperature limits. We scaled the Voronov (1997) rates to the values of Dere (2007). For each species, the scale factor is the ratio of the Dere (2007) to Voronov (1997) rates at the centre of the temperature range where the ion abundance peaks. These scaling coefficients are typically within 10 per cent of unity. This is now the default for CLOUDY.

2.1.2 Photoionization

The photoionization cross-section data base remains unchanged from Ferland et al. (1998).

2.1.3 Recombination coefficients

We updated CLOUDY with the latest radiative (RR) and dielectronic recombination (DR) rate coefficients from Badnell’s web site² (Badnell et al. 2003; Badnell 2006). The update to the DR rate coefficients includes recent data for the argon-like isoelectronic sequence (Nikolić et al. 2010) and Abdel-Naby et al. (2012) for the aluminium-like sequence. We use an ion-specific ‘mean’ value for species which are not covered by the Badnell data base, as was described by Ali et al. (1991).

2.2 Temperatures of peak abundance for photoionization and collisional ionization

Our goal is to simulate both photoionized and collisionally ionized plasmas for a wide range of chemical abundances and energy sources. There are two limiting cases that are considered in much of the active literature. In the photoionization case, the gas is irradiated by an external energy source and the equations of thermal and ionization equilibrium are solved (AGN3). The gas kinetic temperature will depend on both the spectral energy distribution (SED)

² <http://amdpp.phys.strath.ac.uk/tamoc/DATA/>

and the composition, being higher for harder SEDs or lower abundances. The ionization distribution is set by the balance between photoionization and recombination rates, and is not directly set by the kinetic temperature. Similarly, the cooling is not a unique function of the temperature in this case. In the collisional ionization case the gas kinetic temperature is often specified, having been set by physics external to the problem, although it would be possible to specify a heating rate and determine the temperature. The ionization distribution is set by the balance between collisional ionization and recombination rates. The ionization and cooling are directly determined by the temperature in this collisional case.

The temperature at which a particular ion reaches its peak abundance is different for these two cases. We computed a series of models using solar abundances and a density of 1 cm^{-3} . Given these assumptions the gas ionization, for an optically thin cell, depends on the gas temperature in the collisional case, and on the intensity of light striking the gas in the photoionization case. The ‘ionization parameter’, a way of specifying the intensity of the radiation field, was varied in the photoionization case and the Mathews & Ferland (1987) SED of a typical active galactic nucleus was used. In the collisional case, the kinetic temperature was varied and the ionization balance determined. The temperature at which each successive iron ion peaked was then determined and is plotted in Fig. 1. Fig. 1 shows that for a given iron ion, the temperature of peak abundance is significantly higher when collisions rather than photons dominate ionizations.

This has two effects on the calculation of the gas cooling. In the collisional ionization case, the gas kinetic temperature is not much lower than the ionization energy of the ion. This means that very highly excited levels can be populated by thermal collisions. In the photoionization case the temperature is significantly lower, meaning that the cooling will be dominated by a few lower levels. This affects our strategy in optimizing our selection of the number of levels to include in atomic models.

2.3 Line cooling

2.3.1 CLOUDY Hybrid

We have long included all resonance lines in the TopBase Opacity Project data base (Seaton 1987), with collision strengths determined

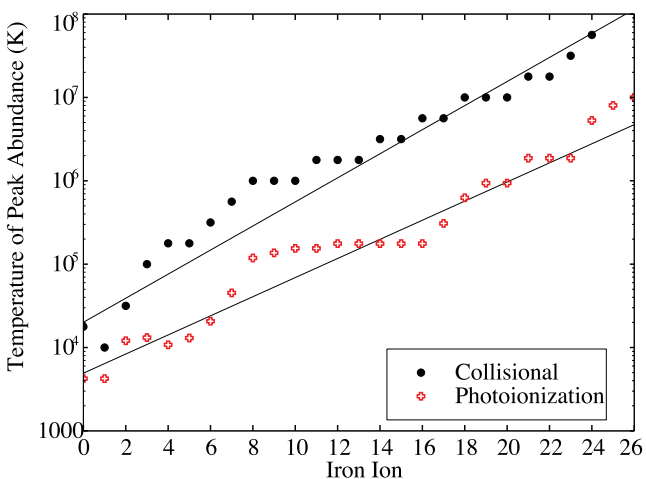


Figure 1. Temperature of peak abundance per iron ion for the collisional ionization and photoionization cases. The gas is cooler in photoionization equilibrium, which affects the strategy used to compute the cooling rate.

from highly approximate g-bar approximations. Adding the Chianti data base lines into CLOUDY required a decision about how to integrate these data bases since some Opacity Project lines may exist within Chianti. The emission spectra for the iron ions we include are shown in Fig. 2 and in the online material (Appendix A2). These show that the Opacity Project lines tend to occur at wavelengths shorter than the Chianti lines. Chianti only includes lines which have collision strengths computed with sophisticated methods, and only for transitions with the lower level in the ground term (we use the g-bar approximation for subordinate lines). The Opacity Project line data often extend to higher excitation levels. We use the Chianti data for all lines it includes, and supplement these with higher excitation Opacity Project data using the g-bar approximation. We refer to this as the Hybrid scheme.

Fig. 2 illustrates how the Opacity Project and Chianti data are blended to give the Hybrid spectrum for one ion stage (the online material shows all ions). Although all calculations are done with CLOUDY, we use different parts of the atomic data base to compare spectra. The top panel, labelled C10, shows the combination of the internal data and the Opacity Project data that were part of C10, the last major release of CLOUDY. The Chianti spectrum (middle panel) shows only lines included in that data base, and contains more lines than Opacity Project (C10) at 1000 Å and longer. The C10 spectrum, largely lines in the Opacity Project, has quite a few lines between 100 and 1000 Å that are missing from the Chianti spectrum. The Hybrid spectrum (lower panel) is the blending of these two spectra as described previously, containing both the Chianti and the Opacity Project lines. The Hybrid configuration will be the default in the next major release of CLOUDY.

The addition of the Opacity Project data to Chianti has little effect on the cooling in the photoionization case where kT is relatively lower than the ionization potential. It does increase the cooling in the collisional case where kT approaches the ionization potential and even Rydberg levels can be excited.

2.3.2 The Kurucz data base

CLOUDY uses a large model of the Fe II emission (Verner et al. 1999) and the H- and He-like ions are treated in the isoelectronic approach described previously. Fe IV through Fe XXIV come from Chianti as described in Section 2.3.1. The only missing iron ion is Fe^{2+} . To fill that void, we added data from the Kurucz data base (Kurucz & Bell 1995) for that ion. This gives energy levels and transition probabilities, but does not contain collision strengths. Collision strengths for the lowest 14 levels of Fe III are given by Zhang (1996). For the many higher levels we use the g-bar approximation as we did for the Opacity Project. We combine the Zhang (1996) and Kurucz data with the Opacity Project data using the Hybrid scheme described above.

2.4 Iron cooling

As a test we computed a collisional ionization cooling curve for a pure iron plasma using the three different available data bases. The results are shown in Fig. 3. The green dashed line is the latest release of CLOUDY, known as C10. This uses only our internal data base and the Opacity Project and does not contain any data from Chianti or Kurucz. The red dotted line, labelled Chianti+, uses Chianti and Kurucz data, but not the Opacity Project. The Hybrid configuration contains Chianti, the Opacity Project and our Kurucz additions.

All three configurations have good agreement at the temperature extremes. Between 4×10^4 and 2×10^5 K, the Hybrid configuration

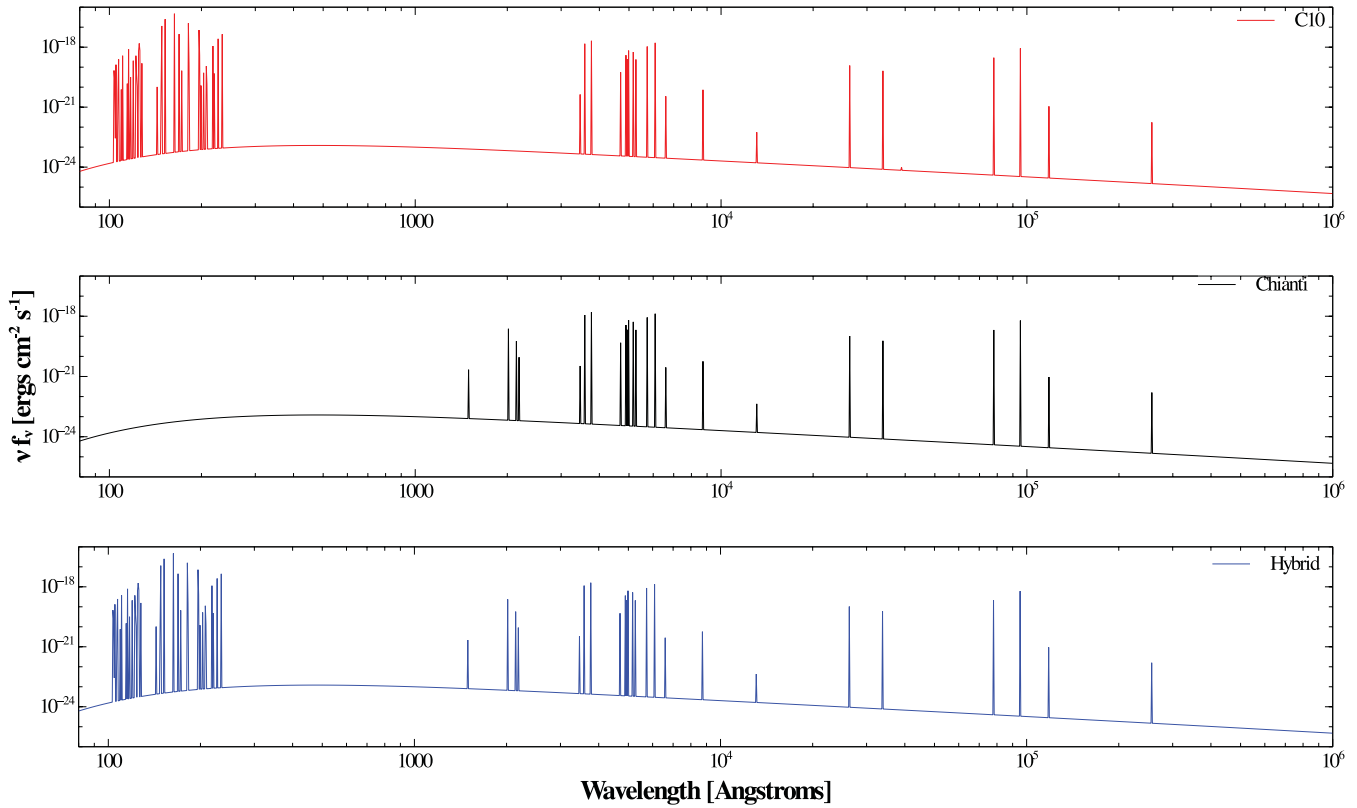


Figure 2. Plots of Fe VII spectra for a collisionally ionized gas under three different CLOUDY configurations: Opacity Project with the CLOUDY internal data base (labelled as C10), Chianti only and our new default Hybrid configuration (Chianti + Opacity Project). Spectra for other iron ions considered in this paper are shown in the online material.

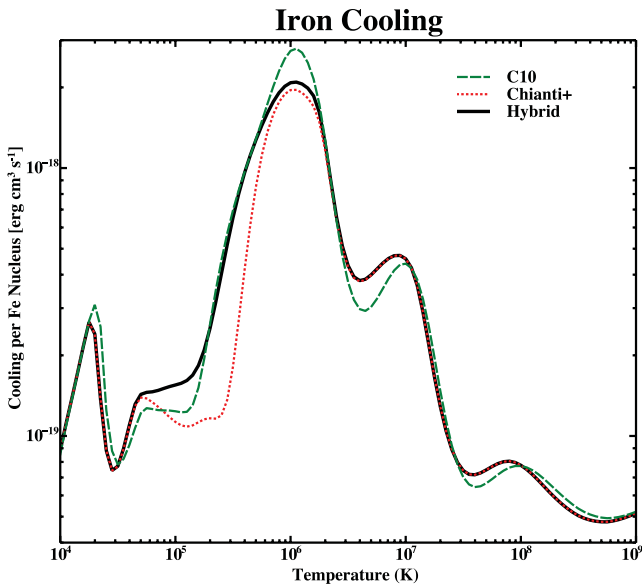


Figure 3. Comparison of the iron cooling per nucleus between the ‘C10’ internal data base (the green dashed line), ‘Chianti+’ (Chianti + Kurucz, the red dotted line) and ‘Hybrid’ (Opacity Project + Chianti + Kurucz, the solid black line).

has more cooling than the other two. Hybrid has more cooling than C10 in this range because of the addition of the Fe III Kurucz data as well as Fe IV and Fe V data from Chianti. Hybrid cooling is greater than Chianti+ for this temperature range and up to 5×10^5 K because it has the additional Opacity Project lines.

The C10 cooling exceeds both Hybrid and Chianti+ around 1×10^6 K. This is because C10 used Opacity Project data, with their uncertain g-bar approximation, for many high-excitation iron lines. Chianti uses real calculations of collision strengths and the values for the strongest lines were systematically lower than the g-bar estimates, resulting in less cooling. When a particular transition appears in both data sets, the Opacity Project version is used for C10 and the Chianti version is used for both Hybrid and Chianti+. This is why Hybrid and Chianti+ show equal cooling at many temperatures.

The Hybrid and Chianti+ cooling are equal for temperatures greater than 1×10^6 K. C10 has less cooling in this range because of the additional lines in Chianti. The C10 cooling is different than the other configurations for temperatures above 3×10^7 K due to different ionization distributions, caused in turn by the updates to the recombination coefficients described in Section 2.1.3 that are not present in C10.

In the following sections, we will compare our current calculations of the cooling with those presented in previous works. We concentrate on studies which report the cooling for specific elements to remove uncertainties caused by changes in the assumed solar composition. Fig. 4 compares the cooling for a pure iron gas for our final Hybrid configuration with the cooling functions of Raymond, Cox & Smith (1976) and Schure et al. (2009). Raymond et al. (1976) is a standard by which many cooling functions are compared. Our differences from Raymond et al. (1976) are likely the result of their use of g-bar collision strengths. Raymond et al. (1976) used estimation techniques for all collision strengths of Fe I through Fe VII whereas we only use g-bar for Fe III, the Opacity Project treatment of high-excitation lines and transitions for which

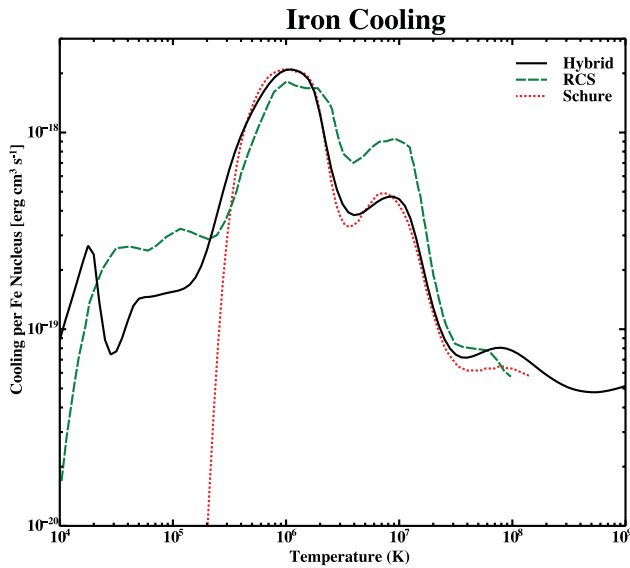


Figure 4. Comparison of the iron cooling per nucleus between the Hybrid configuration of CLOUDY, Raymond et al. (1976) and Schure et al. (2009).

Chianti provides no collision data. The agreement is surprisingly good considering the remarkable changes in the atomic data base in the time since their calculation.

Our Hybrid configuration is in good agreement with the Schure et al. (2009) curve at temperatures above 3×10^5 K. At temperatures below 3×10^5 K, the Schure et al. (2009) iron cooling drops off very quickly. Schure et al. (2009) used the package SPEX, which according to the SPEX line list, does not have iron lines at ionizations less than Fe VIII. This would explain their lack of iron cooling below 3×10^5 K. Calculations of the total cooling are compared next.

2.5 Total cooling with our three configurations

The previous sections focused on iron, the element we have expanded to include Chianti data. Here we compute the total cooling of a collisionally ionized plasma. This depends on all of the elements present, not just iron. For all species other than iron, we use our internal data base. Fig. 5 compares the total cooling for

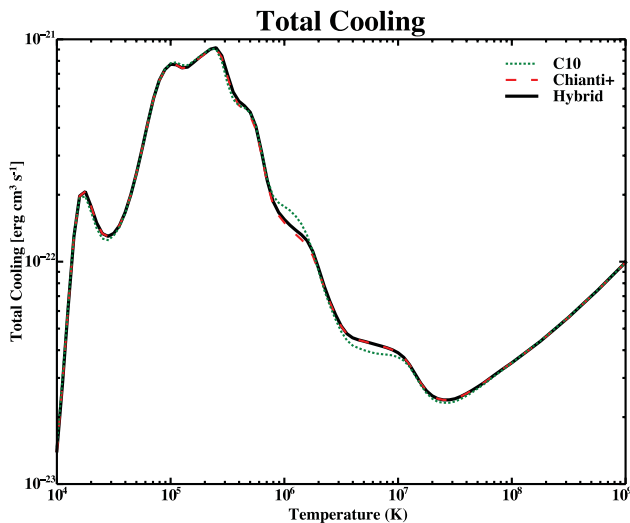


Figure 5. Comparison of the total cooling between the C10, Chianti+ and Hybrid configurations using abundances given in Raymond et al. (1976).

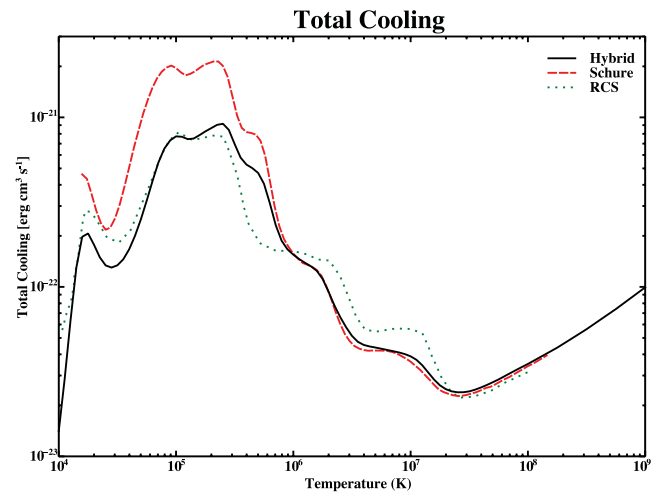


Figure 6. Comparison of the total cooling between the Hybrid configuration of CLOUDY, Raymond et al. (1976) and Schure et al. (2009) using abundances of Raymond et al. (1976).

our C10, Chianti+ and Hybrid configurations, using abundances from Raymond et al. (1976). (This composition was chosen to allow later comparisons with their paper.) The Chianti+ and Hybrid configurations give almost identical total cooling, showing that our internal data base is in good agreement with Chianti. They are also in reasonable agreement with C10. The C10 total cooling is smaller than the other configurations between 3×10^6 and 2×10^7 K. Note that the updated cooling predicts a region of instability around 6×10^6 K, while the older version predicted that this region has small regions that would have neutral thermal stability.

2.5.1 Comparison with Raymond et al. (1976) and Schure et al. (2009)

We compared the iron cooling with Raymond et al. (1976) in Section 2.4 and Fig. 4, where we found that they produced more cooling between 2×10^4 and 2×10^5 K. Fig. 6 compares the total cooling with all elements included. Their total cooling is in surprisingly good agreement with our Hybrid scheme considering the major changes in the atomic data that have occurred in the past 35 years.

Fig. 6 also shows the total cooling computed by Schure et al. (2009). We compared the iron cooling from Schure et al. (2009) in Section 2.4, and found reasonable agreement with our Hybrid configuration for higher temperatures but that their model lacked important coolants below 2×10^5 K. The significantly higher total cooling of Schure et al. (2009) around 10^5 K cannot be due to iron. Section 2.5.4 explains some possible reasons for this difference.

2.5.2 Comparison with Sutherland & Dopita (1993) and Foster et al. (2012)

Foster et al. (2012) describe the latest additions to AtomDB, an atomic data base that focuses on X-ray astronomy, and which, like Chianti and CLOUDY, pays particular attention to the atomic physics. In addition to describing all of the atomic data updated in the latest release of AtomDB, Foster et al. (2012) also provide a total cooling function based on solar abundances of Anders & Grevesse (1989). Sutherland & Dopita (1993) used MAPPINGS II to produce cooling functions between 1×10^4 and $1 \times 10^{8.5}$ K. MAPPINGS II includes calculations for 16 elements with all ion stages.

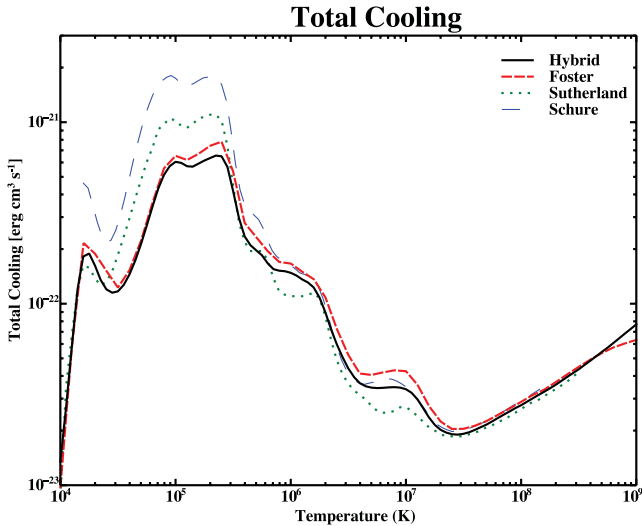


Figure 7. Comparison of the total cooling between our Hybrid configuration, Foster et al. (2012), Sutherland & Dopita (1993) and Schure et al. (2009) using abundances of Anders & Grevesse (1989).

Fig. 7 compares our Hybrid total cooling, Foster et al. (2012), Schure et al. (2009) and Sutherland & Dopita (1993), using the common solar abundances of Anders & Grevesse (1989). The four cooling functions have a similar overall shape. We agree very well with Foster et al. (2012) at all temperatures, specifically around 1×10^5 K where we differ significantly from Schure et al. (2009). However, the cooling at the peak near 1×10^5 K ranges from Hybrid to about a factor of 2 larger. The Sutherland cooling function lies roughly mid-way between our Hybrid and Schure et al. (2009). The element or elements causing the cooling difference around 2×10^5 K between CLOUDY and Schure et al. (2009) are possibly responsible for the difference with Sutherland & Dopita (1993). The differences with Schure et al. (2009) are more extreme and we concentrate on that in Section 2.5.4.

2.5.3 Comparison with Colgan et al. (2008)

Colgan et al. (2008) used the Los Alamos plasma kinetics code ATOMIC to calculate radiative losses for a specific set of abundances. They also used several programs that are part of the Los Alamos suite of atomic structure and collision codes to generate the data needed to calculate the losses. Fig. 8 compares the Hybrid total cooling function with Colgan et al. (2008). Note that the Colgan et al. (2008) plot has been converted from Watt to erg. Colgan et al. (2008) find significantly more cooling around 1×10^5 K. Colgan et al. (2008) also compared their total radiative losses with a similar calculation using data from Chianti version 6. Their Chianti 6 results are in reasonable agreement with our Hybrid cooling.

2.5.4 Differences with Schure et al. (2009)

The Schure et al. (2009) cooling curve was produced using the SPEX package using solar abundances from Anders & Grevesse (1989). They provide cooling rates for each element so that their results can be scaled to fit any set of abundances. We used these individual cooling rates to include the Schure et al. (2009) results to Figs 6, 7 and 11. Their calculation shows greater cooling than our Hybrid configuration for $T < 10^6$ K.

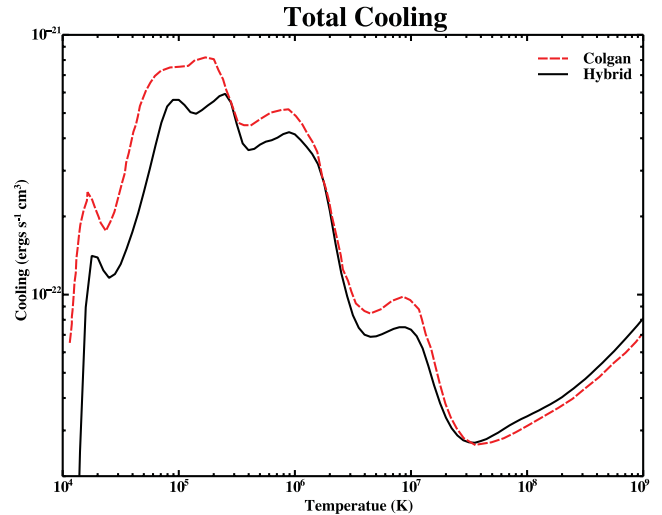


Figure 8. Comparison of the total cooling between Hybrid and Colgan et al. (2008) using the abundances of Colgan et al. (2008).

We looked into individual coolants to find the reason for this difference. It is not due to iron since the Schure et al. (2009) iron cooling is significantly less than Hybrid around 1×10^5 K in Fig. 4. CLOUDY reports that the dominant coolants around 1×10^5 K are carbon and oxygen. In the next section we examine these coolants more closely.

2.6 Carbon and oxygen cooling

The comparison presented above shows that the largest discrepancies occur around 1×10^5 K, regions where the dominant coolants are carbon and oxygen. Fig. 9 compares the carbon and oxygen cooling per nucleus for our Hybrid, Schure et al. (2009) and Chianti version 7. Our Hybrid model, which only uses our internal data base for these elements, is in good agreement with Chianti. These show that Schure et al. (2009) predict significantly higher cooling below 10^6 K, which accounts for the differences in the total cooling.

The collision strengths are most likely to be the source of the differences in the cooling. We find that the primary carbon cooling transitions at 1×10^5 K are 977 Å of C III and 1548 Å of C IV. For these transitions, CLOUDY uses collision strengths from Berrington et al. (1985) and Cochrane & McWhirter (1983), respectively. The C III 977 Å transition is the dominant coolant, contributing 56 per cent of the carbon cooling, while the C IV 1548 Å line contributes about 20 per cent.

The oxygen cooling at 2×10^5 K is dominated by the 630 Å line of O V and a multiplet of four O IV lines around 554 Å. CLOUDY uses collision strengths from Berrington et al. (1985) for 630 Å. The 554 Å transitions come from the Opacity Project which means that the collision strengths are generated using the g-bar approximation. The dominant line is O V 630 Å with 40 per cent of the oxygen cooling, while the O IV 554 Å lines account for 17 per cent of the total.

It is clear from Fig. 9 that the carbon and oxygen cooling for CLOUDY and Chianti are very similar over the entire temperature range, despite being completely independent implementations of the atomic physics. We compared the sources for the collision data as a check on its reliability. For the 977 and 1548 Å carbon transitions, Chianti uses collision strengths from Berrington et al. (1985) and Griffin, Badnell & Pindzola (2000), respectively. CLOUDY and

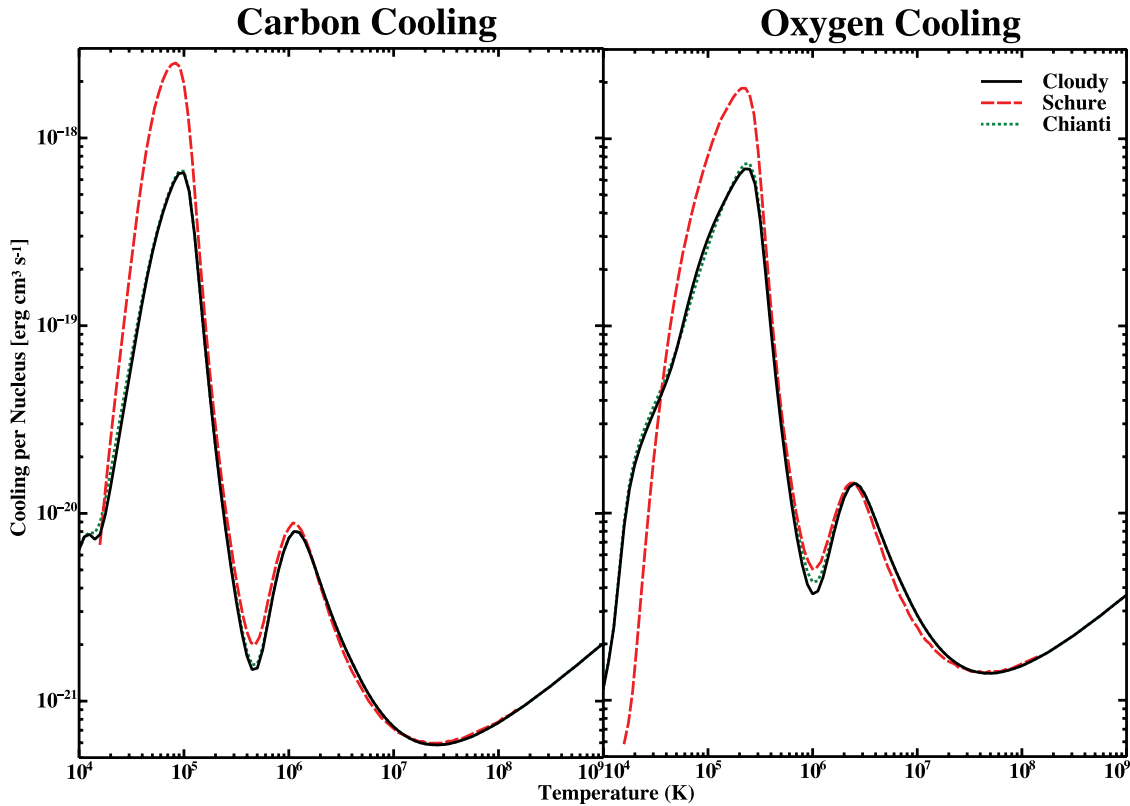


Figure 9. Comparison of the carbon cooling per nucleus (left) and the oxygen cooling per nucleus (right) for Hybrid, Schure et al. (2009) and Chianti.

Chianti use the same source for the 977 Å transition. The CLOUDY and Chianti values for the C IV 1548 Å collision strength differ by only 6 per cent.

The results are similar for the oxygen transitions. The Chianti collision strength for 630 Å is 3 per cent less than CLOUDY and comes from Berrington (private communication). The 554 Å multiplet uses \bar{g} -bar collision strengths in CLOUDY, while Chianti uses values from Zhang, Graziani & Pradhan (1994). The values of the collision strengths differ by only about 5 per cent.

The fact that Schure et al. (2009) find more cooling than CLOUDY or Chianti could be explained if they included important cooling lines which are not present in CLOUDY or Chianti. C^{2+} and O^{3+} are the dominant stages of ionization at 1×10^5 and 2×10^5 K, respectively. The collisional ionization distribution for hydrogen and helium can be found in Table 1 and for the lightest 30 elements in the online version of the table. Schure et al. (2009) used SPEX for its calculations and we were able to compare the SPEX line list to ours and with Chianti. While Chianti has significantly more transitions, there are several transitions in the SPEX line list that are not in Chianti. These transitions are in the tens or few hundreds of Angstroms in wavelength. At temperatures around 1×10^5 K, these transitions cannot contribute much cooling due to their small Boltzmann factor. This comparison suggests that the collision rates for the lines mentioned above are the source of the differences.

Unfortunately, we cannot compare our collision data with those of Schure et al. (2009), Sutherland & Dopita (1993) and Colgan et al. (2008) because they do not cite sources for, or give values of, their atomic data. They provide plots for element cooling but not a table of values. The best we can do is to say that three of the four dominant cooling lines around 1×10^5 and 2×10^5 K have two independent sources for collision strengths and that they are

Table 1. Log of the fractional ionization of hydrogen and helium. See the online version of this table which includes the 30 lightest elements and has higher temperature resolution.

T_e (K)	H ⁰	H ⁺	He ⁰	He ⁺	He ²⁺
4	0.00	-3.34	0.00	-	-
4.5	-2.56	0.00	-0.55	-0.15	-5.71
5	-4.71	0.00	-4.15	-0.95	-0.05
5.5	-5.84	0.00	-7.17	-3.35	0.00
6	-6.59	0.00	-	-4.53	0.00
6.5	-7.16	0.00	-	-5.30	0.00
7	-7.68	0.00	-	-5.89	0.00
7.5	-8.18	0.00	-	-6.43	0.00
8	-8.70	0.00	-	-6.98	0.00
8.5	-	0.00	-	-7.55	0.00
9	-	0.00	-	-8.14	0.00

in good agreement. This provides us with confidence in our atomic data as well as our cooling functions.

The iron cooling is in good agreement with the references cited above. This is the dominant coolant for higher temperatures. Differences in the carbon and oxygen cooling account for the differences we notice at lower temperatures. The last step is to compare the cooling predicted using CLOUDY's internal atomic data set to Chianti.

2.7 Comparison with the Chianti 7 cooling function

In the Hybrid implementation, we use Chianti for iron but our internal data base for other elements. Here we compare the cooling

computed using our data base with Chianti. Since we are using Chianti's iron data in CLOUDY Hybrid, we exclude iron in this comparison.

Fig. 10 shows this comparison. The Chianti calculation uses their data for all other species other than the H- and He-like isosequences where our internal models are used. Since these two calculations use independent implementations of the atomic data base, the good agreement between the cooling for all temperatures shows that these data bases are in good agreement.

2.8 Total cooling in the collisional ionization and photoionization cases

The goal of this paper is to demonstrate how recent changes to CLOUDY and the atomic data used affect the cooling of plasmas in equilibrium. These changes allow for the calculation of the spectrum of a cooling non-equilibrium plasma by Williams et al. (in preparation). Fig. 11 shows our best estimate of the total cooling for the collisional ionization and photoionization cases, using solar abundances from Grevesse et al. (2010). Appendix A provides the CLOUDY commands used to create these plots as well as a description of each command. The cooling function for the collisional case is essentially the same as the Hybrid cooling functions we have shown in previous plots but with more recent solar abundances. Note that, with these abundances, the region around 5×10^6 K is thermally stable, whereas it was marginally stable with previous abundance sets. The collisional cooling is given on a per element basis in Appendix B and a tab-delimited version is available online. Gnat & Ferland (2012) provide element-by-element cooling using the C10 version of CLOUDY. The differences between cooling plots in Gnat & Ferland (2012) and C10 in Fig. 3 are due to using different abundances.

The discussion of Fig. 1 explains how the photoionization cooling function was calculated. We used the same SED and varied the log of the ionization parameter between -6 and 3 , which is the same as in Fig. 1. The minimum temperature in the plot is 1×10^4 K, to be similar to previous figures, although the kinetic temperature goes to lower values for low ionization parameter.

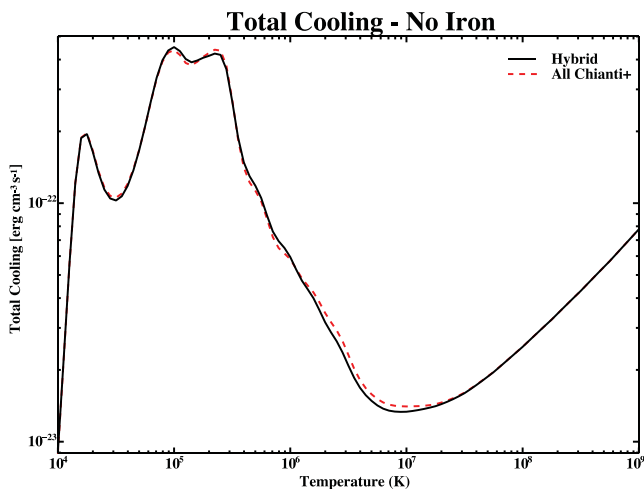


Figure 10. Comparison of the total cooling with the CLOUDY internal data base and most of Chianti version 7, labelled ‘All Chianti+’. Grevesse et al. (2010) abundances are used except that iron is not included. Other than the H- and He-like isosequences, where our treatment is used for both, these curves use fully independent implementations of the current atomic physics literature. The good agreement suggests that these implementations are complete and in accordance with one another.

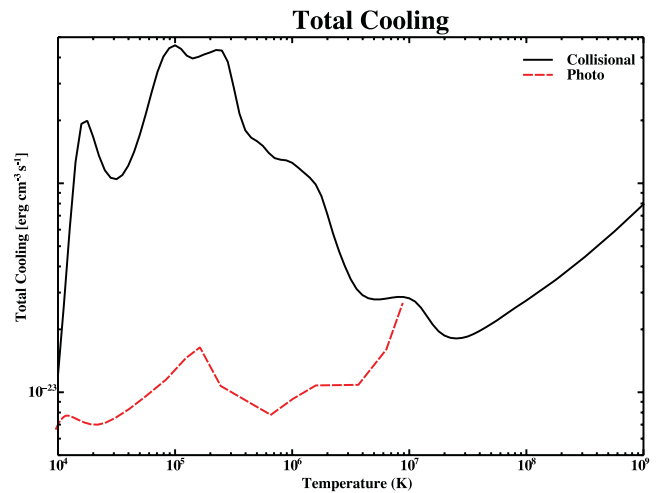


Figure 11. The total cooling for the collisional ionization and photoionization cases of Hybrid CLOUDY using solar abundances of Grevesse et al. (2010).

The cooling in the photoionization case is lower than that in the collisional case at each temperature. The gas kinetic temperature does not play a fundamental role in photoionization equilibrium because the ionization is determined by the balance between photoionization and recombination, which have only weak temperature dependences. The cooling rate in the photoionization case is determined by the heating rate, which is set by the SED (Ferland 2003; AGN3, chapter 3). The temperature is the result of the interplay between this heating and the gas composition, the so-called ‘thermostat effect’ in photoionization equilibrium (AGN3). The result is the significantly lower kinetic temperature as shown in Figs 1 and 11. This distinction will play a major role in our selection of the default number of levels used to compute the spectra in our new level trimming feature, described below.

2.9 Level trimming

In addition to the experimental iron data, CLOUDY can also use the theoretical iron data provided by Chianti. All of the tables and figures in this paper, with the exception of this section, use only experimental Chianti data with no trimming. This section is provided to describe the new capabilities of CLOUDY and does not affect any other section of this paper. Some Chianti ions which are of particular interest in the solar case have more than 300 theoretical energy levels and some have as many as 700 levels. The Kurucz data base often has thousands of levels. Solving the level populations is quite expensive due to the large number of evaluations of the emission and cooling during the solution of the equations of statistical, thermal and ionization equilibrium.

We added an option to restrict the maximum number of energy levels that are used for each species. There is a trade-off between including more levels and lines, which provides a more accurate simulation but with longer run times, versus more compact models, with fewer levels and lines and shorter compute times, but perhaps with some loss of fidelity. This section outlines how we chose the default number of levels, and shows the effects this has on predicted quantities. It is important to note that the level limiting only applies to the newly added Chianti and Kurucz data. All of the data used in C10, including Opacity Project data, are unaffected by this limiting.

Fig. 12 shows the total cooling Λ_{ALL} (top panel) using all theoretical levels in the Chianti and Kurucz data bases, and the cooling

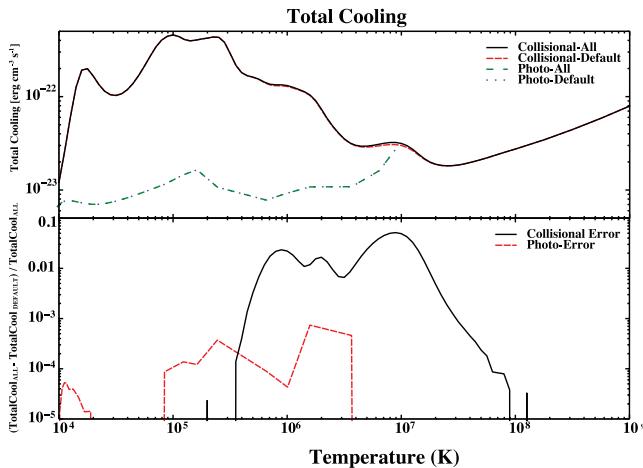


Figure 12. Total cooling using Chianti theoretical energy levels of CLOUDY Hybrid collision and photon-dominated cases using all available levels and the default numbers (top) and the associated relative difference (bottom) described in Section 2.9.

with a particular subset of these levels described below. The differences are small. The lower panel shows the relative difference between the full data base and our compact model with n levels as $(\Lambda_{\text{ALL}} - \Lambda_n) / \Lambda_{\text{ALL}}$. Plots like this one were used to decide on an optimum default limit to the number of levels n .

The kinetic temperature in a photoionized gas is lower, for a particular ionization state, than in a collisional gas (Fig. 1). As a result, for a given ion, more levels will be energetically accessible in the collisional case compared with the photoionized case. Since we will be adding more of the Chianti species in the future and since Chianti iron species have significantly more energy levels than most other species, we have a default number of levels for iron species and one for all other species. After some experiments, we settled on a default limit of 100 levels for the collisional case and 25 levels for the photoionization case for each iron species. For all other Chianti species, which will be added in the future, the default limits are 50 for collisional and 15 for photoionization. We find that these limits capture nearly all of the total cooling but requires about five times less compute time than using the full data base. This is the approximation shown in the top panel of Fig. 12. For the collisional case the limited levels produce cooling within 1 per cent of the total for most temperatures, with the worst agreement of ~ 5 per cent around 10^7 K. This peak error is mostly due to limiting Fe XIX to 100 of its 636 levels. The photoionization cooling functions are essentially identical with the smaller number of levels reproducing the total cooling within better than 0.1 per cent.

Since the accuracy required for a specific simulation may depend on particular goals, we provide a simple input option to change the number of levels. All of the plots in this paper are using the full Chianti and Kurucz data bases unless otherwise noted.

3 CONCLUSIONS

This paper outlines some improvements to the plasma simulation code CLOUDY. It will become the reference for future improvements in the atomic and molecular data base. The specific results are the following.

(i) We added much of the experimental iron data provided by Chianti version 7 (Landi et al. 2012). In addition, we added energy levels and transition probabilities from the Kurucz data base

(Kurucz 2009) for Fe III. Those Fe III data were supplemented by collision strengths using the g -bar approximation. Fe II is treated with the model described by Verner et al. (1999) and the H- and He-like ions are treated with the unified described by Porter & Ferland (2007).

(ii) The Hybrid configuration was added to expand the wavelength coverage of CLOUDY by merging the existing Opacity Project data, which we have long included, with the Chianti and Kurucz data. The Opacity Project and Kurucz data do not have corresponding collision rates, and we have used the g -bar approximation to include them.

(iii) We updated CLOUDY with the latest recombination coefficients from the Badnell web site, including Nikolić et al. (2010) and Abdel-Naby et al. (2012). We updated CLOUDY's collisional ionization rate coefficients to those given in Dere (2007), although these are very similar to the rates of Voronov (1997) which we have used soon after the publication of that paper. The ionization distributions shown in this paper are based on these updates.

(iv) We added an option to limit the number of energy levels that will be used for a particular simulation in order to reduce run time without sacrificing accuracy. This reproduces the results of the full data bases to within much better than 5 per cent but with five times shorter run times. It is easy to change this option with user-accessible commands. This limiting was not used to generate any figures or tables in this paper except for Fig. 12, which demonstrates the accuracy of the level trimming results.

(v) Our iron cooling function created with the Hybrid mix of the Opacity Project, Chianti and Kurucz data agrees surprisingly well with that of Raymond et al. (1976) considering the remarkable changes in the atomic data base in the past 35 years. Significant differences exist with Schure et al. (2009) at temperatures below 1×10^6 K. We attribute the difference in iron cooling to missing ions (Fe VII and below) in the SPEX tool.

(vi) The total cooling also agrees with Foster et al. (2012) and when we use the full Chianti data base. We find less cooling around 1×10^5 K compared to Schure et al. (2009), Sutherland & Dopita (1993) and Colgan et al. (2008). Detailed comparisons show that differences with Schure et al. (2009) (the calculation where such comparisons are possible) are due to carbon and oxygen cooling. We compared our Hybrid configuration total cooling to the total cooling using the Chianti version 7 data for the majority of the available species and concluded that these two implementations of the atomic data literature are in good agreement. We suspect that the differences in cooling compared with Schure et al. (2009), Sutherland & Dopita (1993) and Colgan et al. (2008) are due to their atomic data, although it is not possible to track down what they used.

(vii) CLOUDY is open source and is freely available. Appendix A in the online version provides the CLOUDY input scripts needed to generate the cooling functions used in this paper.

(viii) We provide detailed ionization and cooling rates for each of the 30 elements included in the calculation in the online version.

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APPENDIX A: INPUT SCRIPTS

We have included the CLOUDY input scripts for calculating the cooling in both collisional- and photon-dominated cases. These are the

scripts used to generate Fig. 11, which assumes solar abundances. We have also provided a description of each command.

coronal 4 vary.

This command sets up a collisionally ionized gas at 1×10^4 K and varies it based on the grid command.

atom chianti hybrid 'CloudyChiantiKurucz.ini'.

This command enables Hybrid mode using all species listed in CloudyChiantiKurucz.ini.

abundances GASS10.

This command makes CLOUDY use the solar abundances from Grevesse et al. (2010).

atom feii.

This command enables the Fe II model developed by Verner et al. (1999).

grid 4 9 0.05.

This command gives the limits of what is being varied as well as the increment. For Table A1, the temperature is being varied between 1×10^4 and 1×10^9 K in 0.05 dex increments. Table A2 is varying the ionization parameter.

hden 0.

This command sets the log of the total hydrogen density. In this case, it is set to 1 cm^{-3} .

stop zone 1.

This command sets the limit to the number of zone to calculate per iteration.

set dr 0.

This command sets the log of the zone thickness in cm.

set eden 0.

This command sets the log of the electron density in cm^{-3} .

table agn.

This command sets up the incident radiation field using a continuum from Mathews & Ferland (1987).

ionization parameter -2 vary.

The ionization parameter is the dimensionless ratio of hydrogen-ionizing photon to total-hydrogen densities.

save cooling 'hybrid-coll.col' last.

This command saves the cooling agents for the last zone.

Table A1. Collision-dominated cooling of CLOUDY Hybrid using solar abundances.

```
coronal 4 vary
atom chianti hybrid 'CloudyChiantiKurucz.ini'
abundances GASS10
atom feii
grid 4 9 0.05
hden 0
stop zone 1
set dr 0
set eden 0
save cooling 'hybrid-coll.col' last no hash
```

Table A2. Photon-dominated cooling of CLOUDY Hybrid using solar abundances.

```
table agn
atom chianti hybrid 'CloudyChiantiKurucz.ini'
abundances GASS10
ionization parameter -2 vary
grid -6 3 0.25
hden 0
stop zone 1
save cooling 'hybrid-photo.col' last
```

SUPPORTING INFORMATION

Additional Supporting Information may be found in the online version of this article:

Table 1. Log of the fractional ionization of hydrogen and helium.

Figure 2. Plots of Fe VII spectra for a collisionally ionized gas under three different CLOUDY configurations: Opacity Project with the CLOUDY internal data base (labelled as C10), Chianti only and our new default Hybrid configuration (Chianti + Opacity Project).

Appendix B. Cooling by Element (<http://mnras.oxfordjournals.org/lookup/suppl/doi:10.1093/mnras/sts570/-/DC1>).

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