

Analysis of Anomalous Diffuse Interstellar Bands in the Spectrum of Herschel 36

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Abstract. The extraordinary DIBs observed toward Herschel 36 (Dahlstrom *et al.* 2013) have been analyzed (Oka *et al.* 2013). The analysis led us to a new way to classify the carriers of DIBs depending on whether the molecules are polar or non-polar. The pronounced Extended Tails toward Red (ETR) observed for DIBs $\lambda 5780.5$, $\lambda 5797.1$, and $\lambda 6613.6$ are explained as due to radiative excitation of high rotational levels of polar carrier molecules in an environment with high radiative temperature ~ 90 K. Other DIBs (e.g., $\lambda 5849.8$, $\lambda 6196.0$, and $\lambda 6379.3$) which do not show ETR are likely due to non-polar molecules. Model calculations taking into account the interplay of radiative and collisional effects reproduce the observed ETR using realistic molecular parameters if the radiative temperature is sufficiently high (~ 90 K). The calculation suggests that the carriers of DIBs with ETR are likely medium size molecules with 3 - 6 heavy atoms unless the radiative temperature is much higher.

Keywords. ISM: Herschel 36, ISM: lines and bands, ISM: molecules, Line Profiles, Molecular Process

1. High radiative temperature near Herschel 36

The high radiative temperature in the environment of Herschel 36 is manifest by the rotationally excited $Q(1)$ and $R(1)$ lines of CH^+ shown in Figure 1, indicating that the $J = 1$ level, 40.1 K above the $J = 0$ level, is well populated. Out of a few hundred interstellar sightlines so far observed in CH^+ absorption, this is the only one which shows these satellite lines.

The spontaneous emission $J = 1 \rightarrow 0$ has a decay time of 2.5 minutes corresponding to the critical density of $\sim 3 \times 10^6 \text{ cm}^{-3}$. In diffuse clouds where CH^+ typically resides, collisions cannot maintain CH^+ in the $J = 1$ level. We therefore obtain the high radiative temperature $T_r = 14.6$ K equal to the observed excitation temperature of CH^+ . The high T_r is probably due to far-infrared radiation from the nearby highly obscured star Herschel 36 SE (Goto *et al.* 2006).

2. The spectacular effect of high radiative temperature on some DIBs

The extraordinary DIBs toward Her 36 are compared with ordinary DIBs toward 9 Sgr in Figure 2. One is immediately struck by 3 remarkable aspects of the spectra.

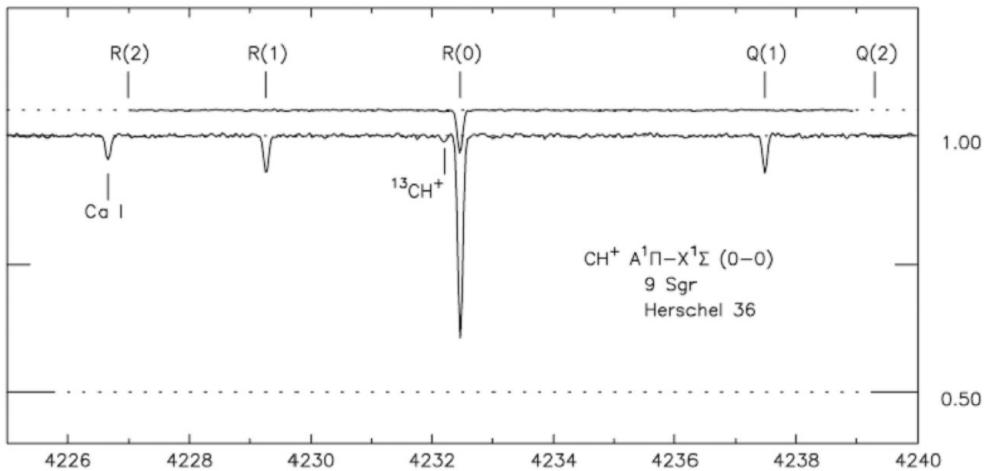


Figure 1. Comparison of ordinary CH^+ spectrum toward 9 Sgr (upper trace) and extraordinary spectrum toward Her 36 (lower trace). The two stars are less than 3 arcminutes away at similar distances from the sun of ~ 1.5 kpc.

2.1. Huge variation

This is not the first time that a variation of DIBs depending on sightlines is reported but the variations noted in the 3 DIBs of the left of Figure 2 are gigantic compared with previously reported (e.g. Cami *et al.* 2004). This is understandable if the variation of the radiative temperature is very large. The heavy molecules which produce the absorption have rotational constants orders of magnitude smaller and their rotational levels are much more closely spaced than those of CH^+ . While only the $J = 1$ population is affected in CH^+ , a great many J levels are radiatively excited for heavy molecules.

2.2. Sharp contrast

One immediately notes the sharp contrast between the three DIBs $\lambda 5780.5$, $\lambda 5797.1$, and $\lambda 6613.6$ on the left and the three DIBs $\lambda 5849.8$, $\lambda 6196.0$, and $\lambda 6379.3$ on the right. The former are greatly influenced by the high T_r while the latter are nearly insensitive. The molecules producing those two groups of DIBs must be qualitatively different. The most natural interpretation of this difference is that the carriers of the former three are polar molecules while those for the latter three are non-polar molecules.

2.3. The variation makes sense spectroscopically

The huge Extended Tail toward Red (ETR) is readily explained spectroscopically as due to reduction of the rotational constant upon excitation to the upper electronic state. For low rotational levels, the R branch lines ($J + 1 \leftarrow J$) and P branch lines ($J - 1 \leftarrow J$) are approximately equally spaced and symmetric but for high J levels the quadratic term $(B' - B)J(J + 1)$ takes over and makes the absorption asymmetric. The rotational constant in the excited electronic state, B' , is smaller than that in the ground state, B , because molecules are more loosely bound. This negative term causes the R -branch bandhead and the redward tail. The fractional variation of the rotational constant $\beta = (B' - B)/B$ is the most crucial molecular parameter since the width of the ETR is simply proportional to it. Some representative experimental values of β are - 5.7 %, - 1.8 %, and - 1.1 % for electronic transitions of C_4 (Linnartz *et al.* 2000), HC_6H^+ (Sinclair *et al.* 1999), and HC_8H^+ (Pfluger *et al.* 2000), respectively.

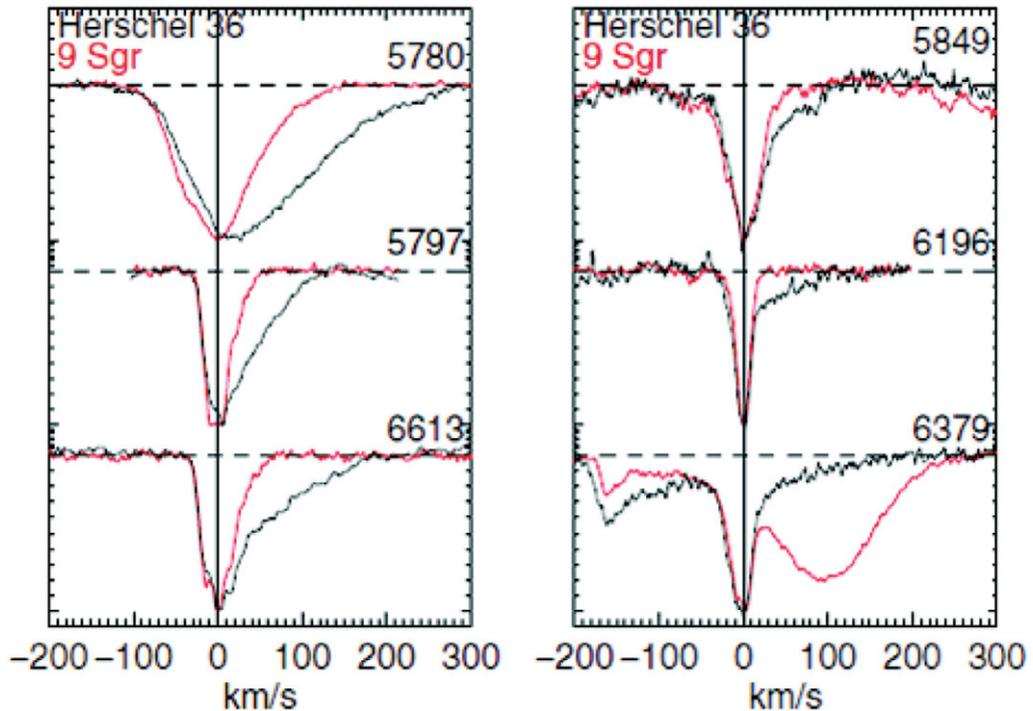


Figure 2. Comparison between the extraordinary DIBs toward Her 36 (in black) and ordinary DIBs toward 9 Sgr (red). The deep absorption near 100 km s⁻¹ for λ 6379 of 9 Sgr is stellar and should be ignored.

3. Model calculation

3.1. Rotational distribution

The distribution of molecules on rotational levels is determined by a subtle balance of radiative and collisional effects, which are governed by the radiative temperature T_r of Planck's law of radiation and the kinetic temperature T_k of Maxwell's velocity distribution, respectively. A general treatment of these effects for asymmetric top molecules with 3 rotational constants and 3 quantum numbers is beyond the scope of this work. We consider the simplest case of linear molecules with one rotational constant B , one quantum number J , and one component of dipole moment μ . The radiative effects can be calculated accurately from Einstein's formula of emission and absorption if Planck's law is assumed, but collisions are more difficult to treat. We have used Boltzmann's principle of detailed balancing as a guiding principle and a rough approximation for the J dependence of collision rates (Oka & Epp 2004). The equation of detailed balancing between J and $J - 1$ levels is written as

$$n(J)(A^J + B_{J-1}^{\downarrow} \rho + C_{J-1}^{\downarrow}) = n(J-1)(B_{J-1}^{\uparrow} \rho + C_{J-1}^{\uparrow}), \quad (3.1)$$

where A and B are Einstein's coefficients, ρ is Planck's distribution of radiation and C is the collision rate. The rate of spontaneous emission A^J is approximately proportional to J^3 and thus varies rapidly with J . For low J levels, it is nearly negligible and the thermalization process is collision dominated. As J increases, the two processes become competitive until the radiative effect dominates for high J levels. The rotational distribution $n(J)$ can be calculated numerically as a function of three molecular parameters,

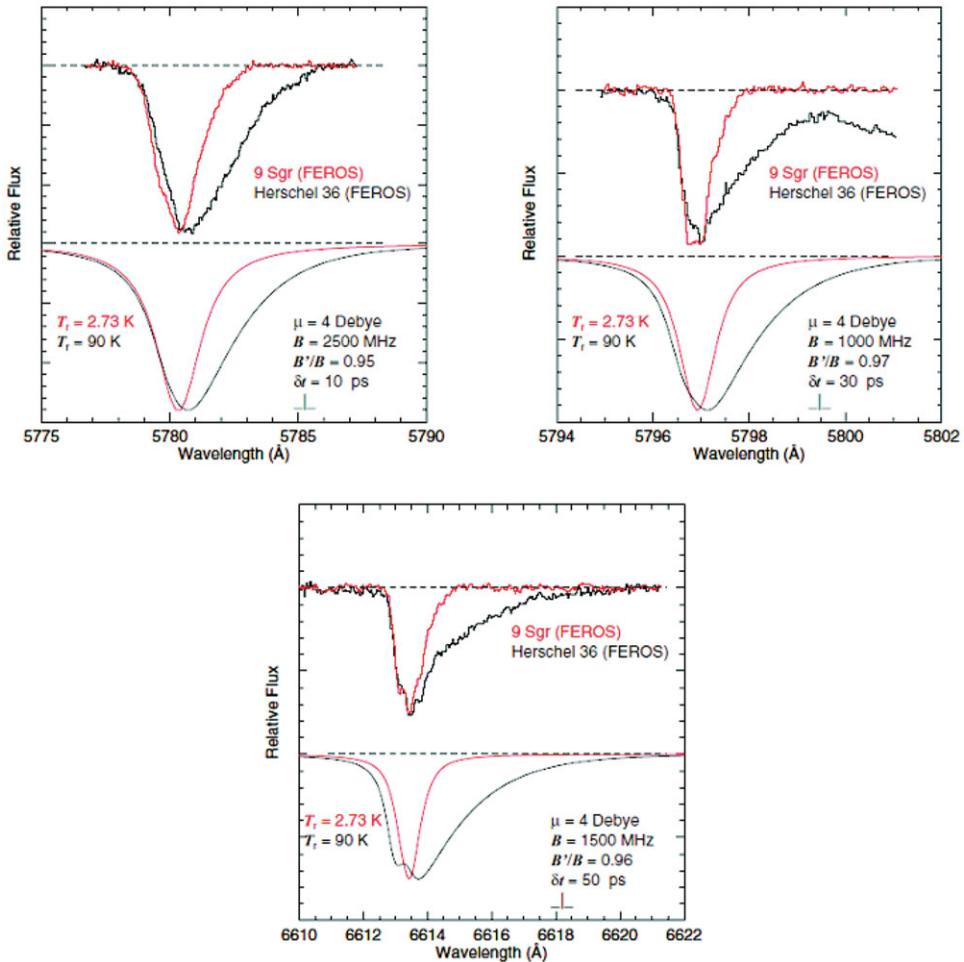


Figure 3. Comparison of observed DIBs, $\lambda 5780.5$, $\lambda 5797.1$, and $\lambda 6613.6$ (upper traces) and simulated DIBs (lower traces). From Oka *et al.* 2013.

B , β , and C and two temperatures T_r and T_k by an iterative procedure from this formula (See Oka *et al.* 2013 for details).

3.2. Spectral simulation

Once the rotational distribution is calculated, the simulation of the spectrum is straightforward by using the standard formula for the rotational energy $E_r = BJ(J + 1)$ and the Hönl-London intensity factor (Herzberg 1989). Two new molecular parameters enter – the rotational constant in the excited state (B' , which is expressed through β), and the intrinsic uncertainty linewidth $\Gamma = 1/2\delta t$ which is caused by the fast spontaneous emission and internal conversion of the carrier (Douglas 1977). The calculated spectra are shown in Figure 3 together with molecular parameters and T_r and T_k . A normalized collision parameter $C = 1 \times 10^{-7} \text{ s}^{-1}$ is used for all of them.

There are 7 parameters to simulate each DIB. One additional complication is that significant (but uncertain) contribution to the DIBs may arise in the foreground of the high T_r region – and should be subtracted from the observed profiles. It is thus a meaningless

exercise trying to determine the accurate values of the 5 molecular parameters and T_r and T_k . Nevertheless the two most crucial parameters, T_r (which is taken to be 90 K), and β (which is taken to be -5% , -3% , and -4%) for the 3 DIBs indicate that the ETRs can be explained by realistic molecular parameters if T_r is sufficiently high. Those two parameters are closely related. For molecules with lower β , higher T_r is needed. Although we studied only linear molecules, as long as we ascribe the ETRs to variation of rotational constants, this situation must be the same for general molecules with three rotational constants A , B , and C . The ETR requires carriers with large negative $A' - A$, $B' - B$, and $C' - C$.

4. Other possible interpretations

It is known that some molecules change their shape from non-linear in the ground electronic state to linear in the excited state (Herzberg 1989b). For such molecules the variation of A is 100 % and relatively low T_r may produce ETR. Such electronic transitions, however, tend to have many vibronic satellites with high Franck-Condon factors – which are not seen in the three DIBs considered above. Radiative excitation of vibrational states may cause spectral variation but not ETRs.

5. Conclusion, speculation, and headache

The carriers of $\lambda 5780.5$, $\lambda 5797.1$, and $\lambda 6613.6$ which show large ETR in the spectrum of Her 36 are polar molecules. If T_r is not much higher than 100 K, the molecules are not gigantic and should be detectable by radio observations. Since their distributions are subthermal, detection in absorption in the centimeter region is preferred. But then we are caught by a dilemma. When Maier *et al.* (2011) proposed H_2CCC as the carrier of DIBs $\lambda 4881$ and $\lambda 5450$, it was negated by radio observations by Araki *et al.* (2012) and Liszt *et al.* (2012) because the column density of that molecule determined from radio observations is orders of magnitude smaller than $5 \times 10^{14} \text{ cm}^{-2}$ inferred from DIBs. This dilemma applies to any molecules of medium size, but there must be a solution. The carriers of DIBs $\lambda 5849.8$, $\lambda 6196.0$, and $\lambda 6379.3$ that are not affected by high T_r are most likely non-polar molecules.

Acknowledgements

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