

Letter to the Editor

Carbon molecules in the inner wind of the oxygen-rich Mira IK Tauri

Debiprosad Duari¹, Isabelle Cherchneff¹, and Karen Willacy²

¹ Department of Physics, UMIST, P.O. Box 88, Manchester, M60 1QD, UK

² Jet Propulsion Laboratory, Pasadena, CA 91109, USA

Received 2 November 1998 / Accepted 17 November 1998

Abstract. The gas-phase non-equilibrium chemistry of the inner wind of the oxygen-rich Mira variable IK Tau (NML Tau) is investigated using a physio-chemical model describing the periodically shocked gas close to the stellar photosphere. We predict the formation in large amounts of a few carbon species in the inner envelope, in particular CO₂, which has been recently detected with ISO in the spectra of several oxygen-rich semi-regular and Mira stars. The theoretical abundances are also in excellent agreement with values derived from millimeter and sub-millimeter observations, pointing to the fact that some carbon species in oxygen stars do form from shock chemistry in the inner layers and travel the envelope as “parent” species.

Key words: stars: abundances – stars: AGB and post-AGB – stars: circumstellar matter – stars: late-type

1. Introduction

Carbon-bearing molecules have been identified in the outer envelopes of many oxygen-rich (O-rich), late-type stars at millimeter and microwave wavelengths (Deguchi & Goldsmith 1985, Lindqvist et al. 1988, Omont et al. 1993, Bujarrabal et al. 1994) and include HCN, CS, OCS, HNC and CN. Because HNC is typically formed in the outer envelopes of AGB stars from ion-molecule chemistry triggered by the penetration of cosmic rays and ultra-violet radiation, it was first thought that the observed carbon species could be produced in the outer wind of oxygen stars. Photo-chemical models of several oxygen Miras by Willacy & Millar (1997, hereafter WM97) tried to reproduce the observations and relied on the injection of methane, CH₄, ammonia, NH₃, silicon sulfide, SiS and hydrogen sulfide, H₂S, to generate a carbon-rich chemistry at large radii. These input molecular abundances are questionable since there exist no observational or theoretical evidences for the formation of these species in the inner and intermediate envelopes of O-rich Miras. The model succeeded in reproducing the observed values of certain species but failed to reproduce some molecular abundances, in particular that of hydrogen cyanide, HCN, which is known to be a “parent” molecule in carbon stars and forms

Table 1. IK Tau - stellar parameters: γ and α are defined as in Cherchneff et al. (1992) and $X(Y) \equiv X \times 10^Y$.

| | | | |
|--|---------------|-----------------------|---------------------------|
| T_* | 2100 K | L_* | $2.0 \times 10^3 L_\odot$ |
| R_* | 305 R_\odot | M_* | 1 M_\odot |
| P | 470 days | $n(r_{\text{shock}})$ | 3.7 (15) cm^{-3} |
| r_{shock} | 1.0 R_* | α | 0.6 |
| $\gamma = v_{\text{shock}}/v_{\text{esc}}$ | 0.89 | C/O ratio | 0.75 |

in the inner regions of the winds (Willacy & Cherchneff 1998, hereafter WC98).

The recent ISO detection of several infrared (IR) emission bands of CO₂ in various O-rich Miras and semi-regular stars by Justanont et al. (1998) suggests that this carbon species has to form in the deep layers of the stellar winds in order to excite the IR transitions observed. In this letter, we investigate the non-equilibrium chemistry of the inner regions close to the stellar photosphere of the oxygen Mira IK Tau (NML Tau) and raise the following questions: (a) Can some of these carbon molecules form in the inner parts of the wind and be ejected as “parent” species?; (b) Can methane and ammonia form in the inner wind of O-rich Mira stars?

2. A model for the inner wind

IK Tau is a variable O-rich Mira of spectral type M6. The stellar parameters considered in this study are listed in Table 1. Its distance was derived by Le Sidaner & Le Bertre (1994) to be 220 pc while its pulsation period is ~ 470 days (Hale et al. 1997). Le Sidaner & Le Bertre assumed a stellar temperature of 2000 K for their radiative transfer model of the IR excess, in good agreement with the value used in this study. In order to derive a radius for the star we assumed a luminosity close to the canonical value for typical Miras stars given by the Period-Luminosity relation derived by Feast (1996). The derived radius satisfies the standard pulsation equation for Miras of Fox & Wood (1982)

$$Q = P(M/M_\odot)^{0.5} (R/R_\odot)^{-1.5} \quad (1)$$

where we assume that the star is pulsating in its fundamental mode ($Q = 0.09$). This gives a stellar mass of 1 M_\odot , typical

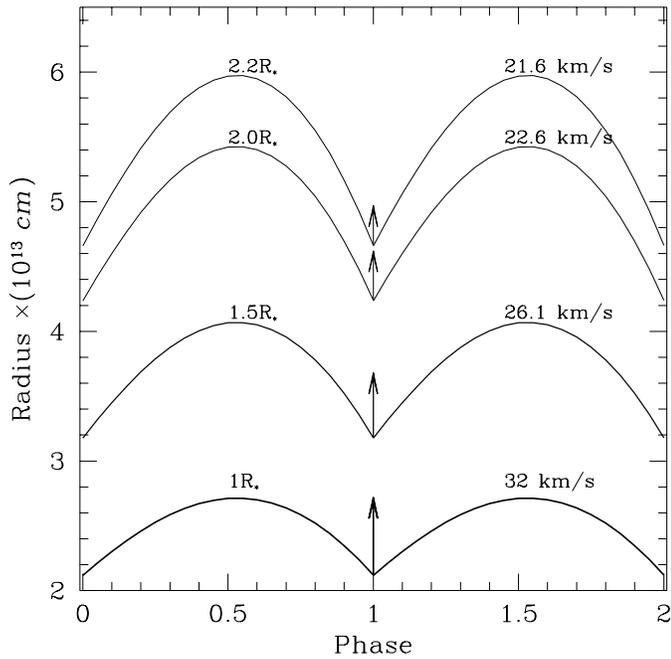


Fig. 1. Gas excursions induced by an initial shock of 32 km s^{-1} . The arrows show the shock position.

of O-rich Miras variables. There exists observational evidence for O-rich Miras to pulsate in their first overtone (Feast 1996) and we will study the impact of this result on our stellar and chemical model in a forthcoming paper.

We consider the inner wind as a narrow region above the photosphere which experiences the passage of strong, periodic shocks generated by stellar pulsation. The model describes both the immediate region (thermal cooling region) and the hydrodynamical cooling region of the post-shock structure as described by Fox & Wood (1985), Bertschinger & Chevalier (1985) and WC98. More details on the model for the inner winds of AGB stars are given in Cherchneff et al. (1998). In our model of IK Tau, we choose a shock speed $v_{\text{shock}} = 32 \text{ km s}^{-1}$ in agreement with shock velocities derived from the CO IR line analysis of Hinkle et al. (1997). The periodic shocks steepen at $r_{\text{shock}} = 1 R_*$ in our model and levitate the nearby gas layers to larger radii, these regions falling down to their initial position because of stellar gravity. This periodic motion generates a pattern of gas excursions as illustrated in Fig. 1. The physical parameters characterising the shocked, inner wind are listed in Table 2.

3. The chemistry

We consider 68 chemical species and 752 reactions and include all possible chemical routes at work in a dense gas, that is, termolecular and bimolecular neutral-neutral reactions. No photoprocesses (dissociation or ionisation) are considered as the UV stellar radiation field is low for the effective temperature quoted in Table 1. Also, we do not consider radiative processes in the post-shock gas on the ground of the theoretical models of post-shock structures by Fox & Wood (1985). Indeed, for a molecular, cool pre-shock gas, they find that the ionization level in the

thermal cooling region is low and we consider the collisional dissociation of molecular hydrogen to be the dominant coolant in the immediate post-shock region (WC 1998, Cherchneff et al. 1998).

The reaction rates are taken from the RATE95 UMIST database (Millar et al. 1997), Baulch et al. (1992), Cherchneff et al. (1992), Mick et al. (1994) and the NIST database (Mallard et al. 1994). Details about assumptions involved in the chemistry used in the model are given by WC98.

We assume thermal equilibrium (TE) for the stellar photosphere and derive molecular abundances for the effective temperature, gas number density and C/O ratio given in Table 1 for IK Tau. We then “shock” the photosphere and investigate the chemistry in the immediate cooling layer and the hydrodynamical cooling part (\equiv excursion) of the post-shock region. The model (the immediate post-shock region followed by excursion at one position in the envelope) is run over two pulsation cycles to check for periodicity. The output abundances for one model are then used as the input to that for the shock at the next distance and are rescaled according to the local gas number density.

4. Results and discussion

The molecular abundances relative to the total gas number density are listed in Table 3 for various shock strengths and positions in the wind. As we do not know precisely the position where the wind is chemically frozen due to the acceleration induced by grains, we have considered gas layers very close to the photosphere. Therefore, abundances at $2.2 R_*$ may not be the exact values frozen in the outflow but are indicative of trends on destruction/formation of species in the inner wind. The dominant molecules are, apart from molecular hydrogen, CO, H_2O , N_2 and SiO. This was known already from TE calculations applied to O-rich AGB stars and confirms the “parent” character of these molecules. However, and as for the case of carbon stars (see WC98), caution should be exerted in comparing observations with TE calculations. For some “parent” species, the non-equilibrium chemistry does not alter significantly the initial TE abundances. However, other species abundant in the TE photosphere according to Table 3 (e.g. OH, O, SiS and HS) are quickly destroyed in the outflow by the non-equilibrium chemistry generated by shocks.

This chemistry is also responsible for the formation of several carbon-bearing species close to the star, in particular CO_2 , HCN, and CS. The theoretical values derived for HCN and CS are in excellent agreement with the abundances derived from millimeter lines in the outer envelope. Chemically, these species are quite stable and in carbon stars, they travel the entire envelope unaltered until they reach the photo-dissociation regions of the outer wind. The same should occur in O-rich winds as these molecules do not participate to the formation of dust grains (e.g., silicate, corundum) in the inner envelope.

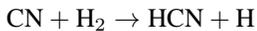
The chemical processes responsible for the formation of HCN and CS are linked in that both CS and HCN are produced from reactions involving cyanogen, CN. While HCN is formed by the reaction

Table 2. Pre-shock, shock front and excursion (\equiv post-shock) gas temperature and number density as a function of position in the envelope and shock strengths. M is the Mach number associated with each shock speed.

| Position (R_*) | Shock Vel. (km s^{-1}) | M | Pre-shock | | Shock Front | | Start of excursion | |
|-----------------------|--------------------------------------|------|-----------|----------------------------|-------------|--------------------------|--------------------|--------------------------|
| | | | T_0 (K) | n_0 (cm^{-3}) | T (K) | n (cm^{-3}) | T (K) | n (cm^{-3}) |
| 1.0 | 32.0 | 10.6 | 2100.0 | 3.62 (15) | 47861 | 2.08 (16) | 6271 | 1.32 (17) |
| 1.5 | 26.1 | 9.74 | 1646.5 | 1.49 (13) | 31924 | 8.49 (13) | 4711 | 4.80 (14) |
| 2.0 | 22.6 | 9.19 | 1385.5 | 5.02 (11) | 24059 | 2.84 (12) | 3838 | 1.49 (13) |
| 2.2 | 21.6 | 9.02 | 1308.5 | 1.78 (11) | 21934 | 1.01 (12) | 3572 | 5.13 (12) |

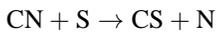
Table 3. Calculated fractional abundances (relative to the total gas number density) versus shock strength and radius. Data from millimeter observations are listed with the following references: 1 – Bujarrabal et al. (1994), 2 – Lindqvist et al. (1988), 3 – Omont et al. (1993), 4 – Justtanont et al. (1998); *in other O-rich miras. No observations for IK Tau*, 5 – Menten & Alcolea (1995).

| Species | T.E. | 32 km s^{-1} | 26.1 km s^{-1} | 22.6 km s^{-1} | 21.6 km s^{-1} | Observational values | |
|-------------------------------|-------------------|-----------------------|-------------------------|-------------------------|-------------------------|------------------------------|-----------------------|
| | 1. R_* | 1. R_* | 1.5 R_* | 2. R_* | 2.2 R_* | | |
| H | 6.65 (-2) | 1.08 (-3) | 6.82 (-3) | 1.85 (-1) | 3.19 (-1) | | |
| H ₂ | 6.52 (-1) | 7.08 (-1) | 7.03 (-1) | 5.51 (-1) | 4.36 (-1) | | |
| Si | 1.03 (-8) | 7.85 (-13) | 4.42 (-16) | 4.19 (-22) | 2.63 (-22) | | |
| S | 1.37 (-5) | 1.20 (-6) | 7.92 (-6) | 1.96 (-5) | 1.84 (-5) | | |
| C ₂ H ₂ | 8.56 (-17) | 5.99 (-12) | 6.05 (-15) | 4.59 (-17) | 6.52 (-12) | | |
| CS | 1.32 (-10) | 8.09 (-6) | 1.14 (-5) | 5.15 (-7) | 2.75 (-7) | 1.0 (-7) ¹ | 3.0 (-7) ² |
| SiS | 2.89 (-7) | 3.42 (-6) | 1.59 (-7) | 1.36 (-9) | 3.82 (-10) | 4.4 (-7) ¹ | 7.0 (-7) ² |
| CH₄ | 5.05 (-14) | 7.86 (-10) | 4.41 (-15) | 8.59 (-20) | 1.24 (-20) | | |
| HS | 6.49 (-6) | 5.96 (-6) | 1.06 (-6) | 1.63 (-8) | 3.70 (-9) | | |
| H ₂ S | 1.03 (-6) | 1.92 (-6) | 2.15 (-8) | 3.95 (-12) | 2.82 (-13) | | |
| NS | 4.36 (-11) | 5.75 (-12) | 3.68 (-11) | 1.91 (-12) | 7.45 (-13) | | |
| N ₂ | 8.05 (-5) | 2.76 (-6) | 5.07 (-5) | 7.30 (-5) | 6.90 (-5) | | |
| HCN | 4.37 (-11) | 1.61 (-4) | 6.47 (-5) | 5.24 (-6) | 2.12 (-6) | 9.8 (-7) ¹ | 6.0 (-7) ² |
| CN | 1.73 (-13) | 8.88 (-10) | 6.06 (-10) | 4.75 (-10) | 2.40 (-10) | | |
| NH₃ | 1.20 (-10) | 5.16 (-11) | 7.87 (-13) | 3.33 (-16) | 3.12 (-17) | ~ 1.0 (-6) ⁵ | |
| O | 1.63 (-7) | 9.41 (-12) | 7.45 (-11) | 2.89 (-9) | 1.11 (-9) | | |
| OH | 2.30 (-6) | 1.10 (-8) | 1.20 (-8) | 6.34 (-8) | 5.53 (-8) | | |
| H ₂ O | 1.86 (-4) | 3.68 (-4) | 2.70 (-4) | 1.49 (-4) | 1.02 (-4) | | |
| CO | 6.95 (-4) | 5.50 (-4) | 6.40 (-4) | 6.14 (-4) | 5.38 (-4) | | |
| CO₂ | 4.09 (-8) | 1.34 (-7) | 2.76 (-7) | 3.39 (-5) | 6.44 (-5) | ISO detection ⁴ | |
| O ₂ | 1.99 (-11) | 1.73 (-15) | 1.13 (-14) | 3.56 (-13) | 1.25 (-13) | | |
| SiO | 4.28 (-5) | 4.12 (-5) | 4.43 (-5) | 4.06 (-5) | 3.75 (-5) | 1.7 (-5) ¹ | 3.0 (-6) ³ |
| NO | 1.04 (-9) | 1.70 (-13) | 1.41 (-11) | 6.11 (-9) | 1.46 (-8) | | |
| SO | 2.18 (-8) | 4.87 (-9) | 3.13 (-8) | 8.27 (-8) | 7.79 (-8) | 2.6 (-6) ¹ | 1.8 (-6) ³ |
| OCS | 5.37 (-39) | 1.60 (-9) | 1.53 (-11) | 1.18 (-13) | 2.52 (-14) | | |



(2) where hydroxyl OH is formed from the collisional destruction of water, H₂O, with atomic hydrogen, and

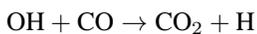
the formation of CS results from the reaction



(3)

CN acts as an intermediate in the formation of the two molecules and is quickly destroyed by atomic hydrogen. Furthermore, the destruction of HCN by atomic hydrogen possesses a high activation barrier while Reaction (2) is highly dependent on temperature and then quite fast in the gas excursions.

The chemical routes to the formation of CO₂ are



(4)



(5)

Reaction (4) represents the dominant formation pathway at small radii while Reaction (5) becomes important at larger radii, explaining the jump in the CO₂ abundance at 2 R_* . The rate for Reaction (4) has been determined experimentally but that of Reaction (5) was calculated from thermodynamical data. In view of the uncertainty of this rate, we also consider Reaction (5) to proceed with a typical three-body reaction rate of $k = 2 \times 10^{-32} \text{ cm}^6 \text{ s}^{-1}$ to test the variation of CO₂ abundance with radius. The abundance was lower than that quoted in Table 3 but

of the order of $\sim 10^{-6}$. Therefore, CO_2 is a direct result of shock chemistry involving the destruction of CO by OH radicals.

Other species appear to be absent from the inner regions of the wind but are observed in the outer envelopes of Miras stars. This is the case for SO which is produced in the photo-dissociation regions by ion-molecule reactions according to WM97. However, WM97 inject at large radii SiS when the molecule does not appear to be “parent” and has a very low abundance in the inner wind (see Table 3). This could explain the discrepancy found by WC97 between their theoretical value and the observed value for SiS which is much lower, implying that SiS is produced in the outer envelope of IK Tau. As for methane and ammonia, they are also absent from the inner wind of Mira stars, a result already derived for carbon stars (WC98). This points to the necessity of invoking formation processes different from pure gas-phase mechanisms and these species have to be produced in the intermediate regions of the wind from gas-grain interaction as first suggested by Nejad & Millar (1988). Whether they enter the outer envelope of IK Tau with the large abundances used by WM97 needs to be confirmed by theoretical models or observations. The same conclusion is drawn for hydrogen sulphide, H_2S , which has a very low abundance at small stellar radii. Omont et al. (1993) have proposed a formation route for H_2S from gas-grain chemistry in the intermediate wind of Miras involving atomic sulphur and atomic hydrogen. We notice from Table 3 that both S and H enter the intermediate part of the wind with quite large abundances. This result for sulphur could be tested observationally with the search of the [S I] fine structure lines at 25 and 56 microns.

We conclude that the inner envelopes of O-rich Miras are regions of efficient formation of molecules and dust. As for carbon stars, the non-equilibrium chemistry is triggered by the propagation of periodic shocks induced by stellar pulsation. Some of the carbon molecules so far observed in these stars,

in particular HCN, CS and CO_2 are formed in the inner wind and act as “parent” species throughout the envelope. This prediction awaits confirmation from new ISO data and sub-millimeter observations on O-rich Mira stars.

Acknowledgements. The authors wish to thank K. Justtanont for useful discussion and the referee, M. Lindqvist, for his helpful comments.

References

- Baulch, D. L. et al., 1992, *J. Phys. Chem. Ref. Data* 21, 411
 Bertschinger, E., Chevalier, R. A., 1985, *ApJ* 299, 167
 Bujarrabal, V., Fuente, A., Omont A., 1994, *A&A* 285, 247
 Cherchneff, I., Barker, J. R., Tielens, A. G. G. M., 1992, *ApJ* 401, 269
 Cherchneff, I., P. Cau, Tielens, A. G. G. M., 1998, *A&A*, submitted
 Deguchi, S., Goldsmith, P. F., 1985, *Nature* 317, 336
 Feast, M., 1996, *MNRAS* 278, 11
 Fox, M. W., Wood, P. R., 1982, *ApJ* 259, 198
 Fox, M. W., Wood, P. R., 1985, *ApJ* 297, 455
 Hale, D. S. et al., 1997, *ApJ* 490, 411
 Hinkle, K.H., Lebzelter, T., Scharlach, W. W. G., 1997, *Astron. J.* 114, 2686
 Justtanont, K. et al., 1998, *A&A* 330, L17
 Le Sidaner, P., Le Bertre, T., 1996, *A&A* 314, 896
 Lindqvist, M., Nyman, L. -A., Olofsson, H., Winnberg, A., 1988 *A&A* 205, L15
 Mallard, W.G. et al., 1994, *NIST Chemical Kinetics Database: Version 6.0*, N.I.S.T., Gaithersburg (MD).
 Menten, K.M., Alcolea, J., 1995, *ApJ* 448, 416
 Mick, H.R., Roth, P., Smirnov, V. N., Zaslanko, I.S., 1994, *Kinetics & Catalysts* 35, 485
 Millar, T.J., Farquhar, P. R. A., Willacy, K., 1997, *A&AS* 121, 139
 Nejad, L., Millar, T. J., 1988, *MNRAS* 230, 79
 Omont, A., Lucas, R., Morris, M., Guilloteau, S., 1993, *A&A* 267, 490
 Willacy, K. and Millar, T. J., 1997 (WM97), *A&A* 324, 237
 Willacy, K. and Cherchneff, I., 1998 (WC98), *A&A* 330, 676