THE ASTROPHYSICAL JOURNAL, 191:L37–L41, 1974 July 1

INFRARED PUMPING PROCESSES FOR SiO MASERS*

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Received 1974 April 5

ABSTRACT

The $J = 2 \rightarrow 1$ transition of the first excited vibrational state ($v = 1$) of $^{28}Si^{16}O$ has recently been shown to produce maser amplification near 86,245 MHz in Orion A and in several stars. Two possible pumping mechanisms are proposed for such masers. One involves the near coincidence between the frequencies of the 1–0 ($R0$) and 3–2 ($R18$) transitions in $^{28}Si^{16}O$. The other requires emission by SiO and reabsorption without the necessity for an accidental frequency coincidence. Each of these types of mechanisms may occur for other transitions of molecules in a medium illuminated by intense infrared radiation, or with strong temperature gradients.

Subject headings: infrared sources — masers — molecules

Snyder and Buhl (1974) have reported rather intense narrow lines near 86,245 MHz in Orion A, which Lovas and Johnson identified as the $J = 2 \rightarrow 1$, $v = 1$ transition of $^{28}Si^{16}O$ (Snyder and Buhl 1974). Subsequently Buhl, Snyder, and Kaifu (1974) detected the same line radiation from a number of late-type stars, including W Hya and NML Cyg; the localized nature of these sources strongly indicates that maser action is involved. Davis *et al.* (1974) and Thaddeus *et al.* (1974) found radiation of the $J = 3 \rightarrow 2$ and $J = 1 \rightarrow 0$, $v = 1$ transitions, respectively, of SiO from Orion A, confirming the molecular identification, but no detectable radiation from these transitions in NML Cyg. This pattern of phenomena appears to be explainable as the result of the near coincidence between two infrared transitions in $^{28}Si^{16}O$ involving quite different rotation-vibration states. An alternative mechanism involves infrared line radiation from hot SiO molecules in an optically thin cloud which is absorbed in a cooler region containing SiO.

The maser mechanism in this case cannot involve any microwave transitions between nearby levels if the source is isotropic and entirely within the antenna beam, because the total radiation of the $J = 3 \rightarrow 2$ rotational transition should then give antenna temperatures approximately as great as does the $J = 2 \rightarrow 1$ transition, which is not the case. The collision-radiation mechanism of Goldsmith (1972), for example, would be expected to give not only detectable radiation from the $J = 1 \rightarrow 0$ transition in the $v = 1$ state, but a still stronger maser in the $v = 0$ state.

Molecular collisions alone would not provide a pump mechanism since two different temperatures, not just the kinetic temperature, must be involved for a pump cycle to work. Hence, radiation quanta of some type are necessary, and one must examine which quanta that interact with SiO are adequately abundant. The number of quanta per second in a frequency range $\Delta\nu$ emerging from a small isotropic source is

$$N_\nu = \frac{4\pi R^2 F_\nu \Delta\nu}{h\nu} \quad (1)$$

where R is the distance to the source and F_ν is the power per unit area per unit frequency observed at the Earth. If such quanta are involved in the pump cycle, they are expected to be as least as numerous as the microwave quanta from the maser, or

$$\frac{4\pi R^2 F_\nu \Delta\nu}{h\nu} \geq 4\pi R^2 F_\mu \frac{\Delta\nu_\mu}{h\nu_\mu} . \quad (2)$$

Here $F_\mu = kT_A/\pi D^2/4$ is the microwave flux, where T_A is the antenna temperature and D its diameter. The quantity $2F_\mu$ should replace F_μ if the maser radiation is unpolarized. Since the frequency width to which molecules respond is very likely due to the Doppler effect, $\Delta\nu/\nu = \Delta\nu_\mu/\nu_\mu$, and formula (2) requires

$$F_\nu \geq \frac{kT_A}{\frac{1}{4}\pi D^2} . \quad (3)$$

For $T_A \approx 14°$ as observed by Snyder and Buhl at the Kitt Peak 36-foot (11-m) antenna, this gives $F_\nu \geq 2 \times 10^{-24}$ W m^{-2} Hz^{-1}. In the case of the Becklin-Neugebauer point source in Orion, heavy obscuration prevents precise knowledge of the available flux. However, the radiation observed from this object fulfills such a requirement for infrared wavelengths longer than about 8 μ. For the brighter infrared stars, the requirement is surpassed by about two orders of magnitude in much of the infrared region, but is not satisfied at microwave frequencies. Visible light from such stars is very marginal in providing enough quanta for pumping. Thus, there are enough infrared quanta to provide pumping, but generally not enough at other wavelengths.

The temperature of the radiation at the masing region near a star, of radius r and distance R from the Earth, must be approximately $T = \pi^{-1} (\lambda R/Dr)^2 \times T_A$, where λ is the wavelength. Values of λ, D, and T_A, and estimates $R = 10^{21}$ cm, $r = 10^{13}$ cm for a typical case give a temperature $T \approx 3 \times 10^9$ ° K. This implies an optical depth of ~15 if the maser amplifies thermal radiation of initial temperature ~1000° K. It can be deduced from the results of Wollman *et al.* (1973) that single rotation-vibration lines of the $\Delta v = 2$ bands of

* Work partially supported by NASA grant NGL 05-003-272 and NTR 05-003-452.

$^{28}Si^{16}O$ have optical depths as great as about unity in the atmospheres of some stars. This implies optical depths in the range 10–10^3 for rotational transitions for a radial path through a stellar atmosphere. Optical depths would be one or two orders of magnitude still greater than this for tangential paths through a stellar atmosphere or a circumstellar cloud. Hence, a modest fractional population inversion in material at some rather restricted range of radii about a star would be adequate to give maser action. Such amplification should occur, however, in a location and for states such that too much reabsorption of the radiation produced does not occur at still larger distances from the infrared source. This criterion is fulfilled especially easily for transitions within an excited vibrational state, which would have low population in the cooler regions around an infrared source.

Infrared radiation of importance in the pumping cycle can only be at one of the rotation-vibration transitions to one of the masing levels. Such transitions involving $\Delta v > 1$ are too weak by comparison with the more dominant $\Delta v = 1$ transitions to make them reasonable candidates. Hence, for the $J = 2 \rightarrow 1$, $v = 1$ maser, transitions in the 1–0 or 2–1 bands at about 8 μ wavelength which involve one of the two masing levels must be the important ones in the pumping cycle. Molecules in each of the levels $v = 1$, $J = 1$ and $v = 1$, $J = 2$ decay to the ground vibrational state at the same rate, except for a very small variation associated with small differences in frequencies, so that their spontaneous infrared emission cannot provide a significant selectivity in the populations of rotational states. Hence, one must look for some substantial difference in the radiation intensity of the 8-μ transitions which involve these two levels. Two possible mechanisms are suggested. The first involves an emission or absorption line of another atom or molecule which coincides in frequency with one of the SiO transitions involved, and thus disturbs the intensity of radiation at its frequency. The second requires emission of infrared radiation from a hot gas containing SiO which is not optically thick and hence produces radiation of different intensities to the $v = 1$, $J = 1$, 2, and 3 levels which is subsequently absorbed in molecules in ground vibrational states in a cooler region.

Because the maser is observed in a variety of objects, the first mechanism would most reasonably depend on a coincidence within the SiO spectrum, and hence coincidences of transitions in its spectrum were examined. For a coincidence to be important, the frequency difference between two transitions must not be much greater than half the stellar line width. Some late-type stars of high infrared luminosity are thought to have fractional Doppler half-widths of $\sim 1.5 \times 10^{-5}$ (Geballe, Wollman, and Rank 1972), or ~ 0.02 cm^{-1} at 1250 cm^{-1} (8 μ). Transitions to and from the $v = 1$, $J = 1$ and 2 masing levels are $R0$, $R1$, $P2$, and $P3$ in the 1–0 band, and $R1$, $R2$, $P1$, and $P2$ in the 2–1 band. Frequency coincidences with these transitions which differ by less than 0.1 cm^{-1} are listed in table 1, as are also those involving the adjacent rotational levels, $J = 0$ and $J = 3$. Frequencies have been derived from constants for the SiO molecule kindly supplied by Hall (1974). Transitions intensities relative to an arbitrary scale are given at 1500° and 2500° K.

The most striking coincidence in table 1 is that between the 1–0 ($R0$) and the intense 3–2 ($R18$) line. The eight other coincidences listed are probably not within the Doppler width, and most involve higher excited-state lines which are weaker than the 3–2 ($R18$) line. Figure 1 shows the effect of the coincidence. Equilibrium between the $v = 1$ and $v = 0$ states of SiO is established by 8-μ radiation if collisions can be neglected in comparison with radiative processes. When intensities at all transitions shown in figure 1 correspond to a blackbody distribution (i.e., are close to the same), the $v = 1$, $J = 1$ and 2 levels are populated approximately in a normal Boltzmann distribution. If radiation at the $R0$ frequency is substantially weaker than at the other transitions, the $v = 1$, $J = 1$ level will be underpopulated and there will be maser amplification in the transition $v = 1$, $J = 2 \rightarrow 1$. If the maser is saturated, this in turn can decrease the population of the $J = 2$ level enough that there may be maser amplification in the $v = 1$, $J = 3 \rightarrow 2$ transition, as is observed in Orion A. The relative intensities

TABLE 1

Transitions of $^{28}Si^{16}O$ Involving $v \leq 6$ Which Coincide in Frequency within 0.1 cm^{-1} with Those to the $v = 1$, $J = 0$, 1, 2, or 3 Levels

Transition	Frequency (cm^{-1})	Transition Intensities 1500° K	Transition Intensities 2500° K	Coinciding Transition	Coinciding Transition Intensities 1500° K	Coinciding Transition Intensities 2500° K	Frequency Difference (cm^{-1})
1–0 ($R0$).........	1231.054	0.034	0.011	3–2 ($R18$)	0.145	0.131	0.008
				5–4 ($R40$)	0.022	0.070	0.021
1–0 ($R2$).........	1233.900	0.101	0.033	4–3 ($R31$)	0.066	0.113	0.090
				5–4 ($R43$)	0.020	0.068	0.041
1–0 ($P1$).........	1228.167	0.034	0.011	5–4 ($R37$)	0.023	0.072	0.057
1–0 ($P4$).........	1223.762	0.132	0.043	4–3 ($R22$)	0.066	0.099	0.076
2–1 ($R0$).........	1219.148	0.021	0.011	4–3 ($R18$)	0.061	0.087	0.099
2–1 ($R2$).........	1221.974	0.062	0.032	5–4 ($R31$)	0.026	0.071	0.088
2–1 ($P1$).........	1216.281	0.021	0.011	1–0 ($P9$)	0.283	0.093	0.061

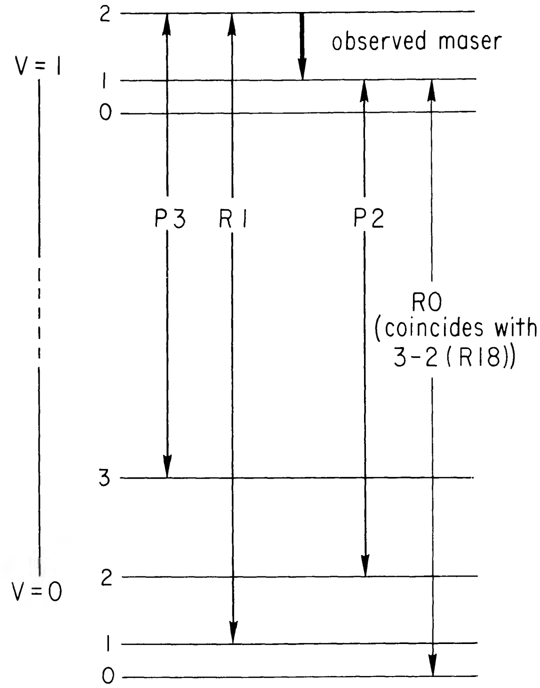

FIG. 1.—Energy levels and transitions involved in the $J = 2 \rightarrow 1$, $v = 1$ SiO maser.

of the two transitions which excite the $v = 1$, $J = 1$ level, the $R0$ and $P2$, is $\frac{1}{2}$. Hence, a decrease in the radiation intensity by a fraction ϵ at the $R0$ frequency due to absorption by the coinciding 3–2 ($R18$) line implies a fractional population inversion in the $J = 1$ and 2 levels of about $\frac{1}{3}\epsilon$. This uses the simplifying assumption that population of the $v = 2$ state is much smaller than that of the $v = 1$ state; when this is not true, as is likely for stellar atmospheres, the population inversion is somewhat reduced. Since the total optical depth in SiO is quite large, a fractional decrease as small as 10 percent in the radiation intensity at the $R0$ line appears to be adequate to provide the maser gain which occurs. If the $v = 1$, $J = 2 \rightarrow 1$ transition is completely saturated, then the $J = 2$ population is reduced, yielding a fractional population inversion for the $J = 3 \rightarrow 2$ transition of $\frac{1}{8}\epsilon$, again assuming that the $v = 2$ states can be neglected. This would make the $J = 3 \rightarrow 2$ maser amplification strong enough to give an antenna temperature about half that of the $J = 2 \rightarrow 1$ maser. However, such a value is an upper limit since the $J = 2 \rightarrow 1$ maser is unlikely to be completely saturated over its entire length. Furthermore, if the excitation temperature is high so that $v = 2$ states are abundantly populated, this inversion would tend to be suppressed. In a few cases, perhaps the $J = 4 \rightarrow 3$ transition would amplify, but still more weakly, as a result of saturation of the $J = 3 \rightarrow 2$ transition. If the 3–2 ($R18$) line were to produce excess radiation rather than a decrease in intensity, maser amplification would be expected in the $v = 1$, $J = 1 \rightarrow 0$ transition rather than at the $J = 2 \rightarrow 1$ and $J = 3 \rightarrow 2$ frequencies.

Consider now the typical situation which would reduce infrared intensity at the 1–0 ($R0$) frequency as a result of the 3–2 ($R18$) line. This can occur schematically as radiation from a star leaves a region where it can be represented by blackbody radiation, perhaps at 3000° K, and travels through an optically thin atmosphere of SiO at a lower temperature, perhaps between 1500° and 2500° K. Table 1 shows that at these temperatures the 3-2 ($R18$) line is much stronger than any of the lines involving the $v = 1$, $J = 1$ or 2 levels; hence it would cool the radiation temperature at the 1— 0($R0$) frequency substantially below that of the other transitions shown in figure 1. If the radiation traverses this absorbing layer to a still cooler, very attenuated layer of SiO, it will then excite some of the SiO molecules to the $v = 1$ rotation-vibration levels, providing an inverted population in the $v = 1$, $J = 2 \rightarrow 1$ transition as indicated above. This last absorbing region should not be optically very deep at 8 μ, and of density $\lesssim 10^{11}$ cm^{-3} so that collisions are not much faster than radiative processes there. The SiO relative abundance required appears to be reasonable; the total SiO needed would be a small fraction of that found in many stellar atmospheres. Of course, these three postulated layers are not in fact likely to be sharply separated. Rather, absorption cooling of radiation by the 3–2 ($R18$) line and excitation of the $v = 1$ level by the resulting modified radiation would likely take place simultaneously in the rarefied regions of a stellar atmosphere or circumstellar cloud. In the case of Orion A, where the $J = 1 \rightarrow 0$, $v = 1$ transition is observed, it is not unreasonable to suppose that in some parts of the source temperature distributions are such that the 3–2 ($R18$) line produces excess radiation, whereas in others it decreases the radiation intensity. This would allow observation of all three masers, $J = 1 \rightarrow 0$, $2 \rightarrow 1$, and $3 \rightarrow 2$, but perhaps at somewhat different Doppler velocities. In addition, relatively large line breadths or differences in Doppler velocities could produce effective coincidences for some of the other pairs of lines listed in table 1 and further modes for maser pumping. While the production of nonequilibrium radiation and of maser action would thus seem to be possible in a variety of temperature and density distributions like those which are thought to occur in stars or infrared sources, no models have yet been examined in detail.

It is possible that maser action could be produced by a coincidence between transitions of quite different molecular species. For example, an H_2O line at 1219.10 cm^{-1} corresponds fairly closely to the SiO 2–1 ($R0$) transition. However, important coincidences within a single molecular spectrum seem especially likely, and the maser mechanism discussed raises the question of how many other such cases can be expected. The fundamental bands of SiO and of CO hence have been examined to locate other coincidences where similar effects might occur, and these are in fact not very rare. Some coincidences, approximately within the Doppler width, are listed in tables 2 and 3. Not all of them appear to provide just the right relative intensities and other characteristics to easily produce maser action, and most of the masers which might result are

TABLE 2

$^{28}Si^{16}O$ COINCIDENCE CLOSER THAN 0.02 cm^{-1} WITH $v_{lower} < 5$ AND $J < 40$

Transition	Relative Intensity at 1500° K	Coinciding Transition	Relative Intensity at 1500° K	Frequency Difference (cm^{-1})
1–0 (*R*0).........	0.034	3–2 (*R*18)	0.145	0.008
1–0 (*R*16)........	0.478	2–1 (*R*26)	0.347	0.004
1–0 (*R*25)........	0.565	2–1 (*R*36)	0.310	0.005
1–0 (*P*21)........	0.505	3–2 (*P*6)	0.055	0.019
1–0 (*P*38)........	0.445	5–4 (*P*10)	0.015	0.003
2–1 (*P*9).........	0.173	3–2 (*P*1)	0.010	0.016
2–1 (*P*13)........	0.234	4–3 (*R*2)	0.012	0.015
2–1 (*P*27)........	0.324	3–2 (*P*20)	0.141	0.016
2–1 (*P*31)........	0.315	4–3 (*P*17)	0.054	0.008
3–2 (*R*14)........	0.125	5–4 (*R*35)	0.025	0.014
3–2 (*R*15)........	0.131	4–3 (*R*25)	0.067	0.012
3–2 (*R*24)........	0.160	4–3 (*R*35)	0.062	0.018
4–3 (*P*10)........	0.037	5–4 (*P*2)	0.003	0.016
4–3 (*P*28)........	0.063	5–4 (*P*21)	0.024	0.011

TABLE 3

COINCIDENCES IN THE CO FUNDAMENTAL ROTATION-VIBRATION BAND*

Transition	Relative Intensity at 1500° K	Coinciding Transition	Relative Intensity at 1500° K	Frequency Difference (cm^{-1})
$^{12}C^{16}O$ 1–0 (*R*1).........	0.282	$^{13}C^{16}O$ 2–1 (*R*24)	0.316	0.003
$^{12}C^{16}O$ 1–0 (*R*3).........	0.555	$^{12}C^{16}O$ 3–2 (*R*19)	0.072	0.029
$^{12}C^{16}O$ 1–0 (*R*9).........	1.204	$^{13}C^{16}O$ 1–0 (*R*25)	1.118	0.002
$^{12}C^{16}O$ 1–0 (*R*16)........	1.468	$^{12}C^{16}O$ 2–1 (*R*25)	0.290	0.027
$^{12}C^{16}O$ 1–0 (*P*4).........	0.544	$^{13}C^{16}O$ 1–0 (*R*8)	1.062	0.016
$^{12}C^{16}O$ 1–0 (*P*24).......	1.108	$^{13}C^{16}O$ 1–0 (*P*14)	1.279	0.028
$^{12}C^{16}O$ 2–1 (*R*1).........	0.072	$^{13}C^{16}O$ 1–0 (*R*7)	0.971	0.014
$^{12}C^{16}O$ 3–2 (*R*13)........	0.072	$^{13}C^{16}O$ 2–1 (*R*20)	0.363	0.015
$^{12}C^{16}O$ 3–2 (*P*26).......	0.051	$^{13}C^{16}O$ 1–0 (*P*28)	0.879	0.007
$^{12}C^{16}O$ 4–3 (*P*13).......	0.012	$^{13}C^{16}O$ 2–1 (*P*15)	0.348	0.016
$^{12}C^{17}O$ 1–0 (*R*1).........	0.273	$^{12}C^{16}O$ 1–0 (*P*5)	0.667	0.010
$^{12}C^{18}O$ 1–0 (*P*6)........	0.737	$^{13}C^{16}O$ 1–0 (*P*7)	0.842	0.004

* Coincidences closer than 0.03 cm^{-1} are listed through the 4–3 band of $^{12}C^{16}O$ and the 2–1 band of $^{13}C^{16}O$, with $J < 30$. Relative intensities given assume equal isotopic abundances. Frequencies were calculated using the constants of Rao and Mantz (1972).

at frequencies higher than the millimeter region, where in some cases spontaneous relaxation of the transitions may be rapid enough to quench the pumping action. Nevertheless, it would not be surprising for these coincidences to produce masers, including some at far-infrared wavelengths, in the vicinity of intense infrared sources.

The second radiation pumping mechanism depends on the fact that the two 8-μ $v = 1$–0 transitions from each of the rotational states $v = 1$, $J = 0$, 1, 2, and 3 have relative strengths which tend to increase with statistical weights of the levels, and thus with J. Transitions from a given level specified by $v = 1$, J, have relative intensities, when $kT \gg J(+ 1)B$, of $R(J-1) \propto J$ and $P(J+1) \propto J+1$, as is seen from table 1. A hot cloud of SiO which is optically thin at these transitions would therefore emit more radiation at rotation-vibration lines involving higher rotational states, the largest fractional differences occurring for low values of J. If such radiation is absorbed by a cooler, optically thin, cloud containing SiO which is mostly in the ground vibrational state, then the numbers of molecules n_J excited to the J, $v = 1$ state in the cool cloud is approximately proportional to $\frac{1}{2}(2J+1)^2$. This represents a population inversion whose magnitude increases with J, but a fractional population inversion which decreases with increasing J. More precisely, the fractional inversion defined by

$$\left(\frac{n_J}{2J+1} - \frac{n_{J-1}}{2J-1}\right) \Big/ \frac{1}{2}\left(\frac{n_J}{2J+1} + \frac{n_{J-1}}{2J-1}\right),$$

would be $(2J^2-1)/2J^3$. Hence, under these ideal assumptions, the fractional population inversion would be 0.500, 0.438, 0.315, and 0.242 for the $v = 1$, $J = 1 \rightarrow 0$, $J = 2 \rightarrow 1$, $J = 3 \rightarrow 2$, and $J = 4 \rightarrow 3$ masers, respectively. Clearly, maser action would tend to be suppressed by collisions, by the presence of a large continuum infrared radiation which would make the fractional variation in intensity smaller, or by optical depths which are not small in either the hot or cool clouds containing SiO. The latter two effects would suppress maser action for the larger J values most easily. Thus, it would be possible for the $v = 1$, $J = 2 \longrightarrow 1$ maser to be most prominent, as is often observed, although this result seems somewhat fortuitous.

The requirements on amounts of SiO and cloud densities for the above second mechanism to be operative are not very different from those for the first, and they are again not unreasonable for the environment of an infrared star. However, the second mechanism differs from the first in not producing a maser in a region around a star which decreases in temperature monotonically with the radius, and in not requiring as high temperatures, since the excited states $v = 2$ or 3 do not play a role. This second mechanism may also produce maser action in much the same way in the lower rotational states of other molecules which are suitably abundant. CO is certainly adequately abundant to similarly produce masers by this means in its $v = 1$ state. However, it may in fact be so abundant that in regions which are otherwise suitable its lines are optically thick and maser action is suppressed. Thus, the rarer molecules which are adequately stable at high temperatures could be better maser candidates.

We thank D. N. B. Hall and L. E. Snyder for providing important information on SiO before publication, and P. Thaddeus and J. Mather for both unpublished information and helpful discussion.

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