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INVESTIGATION OF A FEW SIMPLE MOLECULAR GASES AS A POSSIBLE MOLECULAR LASER MATERIAL

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REPORT

by THE OHIO STATE UNIVERSITY RESEARCH FOUNDATION COLUMBUS, OHIO 43212

Sponsor	National Aeronautics and Space Administration Office of Grants and Research Contracts Washington, D.C. 20546
Grant Number	NsG - 74 - 60
Investigation of	Receiver Techniques and Detectors for Use at Millimeter and Submillimeter Wavelengths
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Submitted by	P.K-L Yin and S.H. Koozekanani Antenna Laboratory Department of Electrical Engineering
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ABSTRACT

Energy levels of a few simple molecular gases which have a resonant energy level with the N_2 metastable level have been investigated for possible molecular laser material.

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INVESTIGATION OF A FEW SIMPLE MOLECULAR GASES AS A POSSIBLE MOLECULAR LASER MATERIAL

I. INTRODUCTION

Coherent sources lying in the infrared or the far-infrared region of the spectrum would be best and more efficiently produced with molecular gas lasers rather than atomic gas lasers. The reason lies simply in the fact that in atomic gases, disregarding the hyperfine or magnetic splitting, the electronic transitions necessary to reproduce an infrared photon would, in general, be between states having high quantum numbers n where the energy states lie close to each other. This fact reduces the efficiency greatly; moreover the upper states of atomic levels tend to have long life-times, which in turn can be shown to cause these states to be saturated at very low current discharges or low pressures. Hence atomic lasers at these wavelengths suffer both from low efficiency and low output power. However, the above problems are alleviated to a great extent when one considers molecular systems where one need not work between the electronically excited levels. The vibrational levels are rich in energy states and are low-lying in the energy scale. This feature could greatly enhance the efficiency. The following discussions will concern a few possible mechanisms of inversion and will review only a few of the many promising molecules suitable for laser action in the infrared region, so that investigators equipped to handle these gases may experiment with them.

II. MECHANISMS OF INVERSION

Among the few possible methods of population inversion of some of the energy levels of a certain gas with respect to its other levels, the method of resonant transfer has one of the highest efficiencies. In this method a gas molecule which has been excited to a metastable level, upon collision with another molecule, relinquishes its energy to the colliding particle and relaxes from its metastable level to the ground state. The excitation cross section for this process has its greatest value when the energy levels of the colliding particles are in resonance, or differ by less than kT. Among the lasers which use this process for excitation are the $He-Ne^{1}$ laser in which the metastable levels of He are responsible for the inversion of the neon levels, and also the $CO_2-N_2^{2}$ laser in which the vibrationally excited metastable level of N_2 excites the vibrational (001) level of CO_2 . The energy levels in both the above processes are very close to each other. Yet another process which can aid greatly the inversion of some of the vibrational levels of the molecular gases is the addition of light gases in the discharge. When a particle collides with a vibrating molecule it can cause the vibrating level to relax to the ground state by transferring the vibrational energy to its kinetic energy. ³ Since the cross sections for this process for all of the vibrational levels are not equal, this can help to bring about a non-thermal distribution. An example of such a laser system is the He-CO₂ mixture.

III. REVIEW OF SOME SIMPLE MOLECULAR GASES

We shall now review some of the simple molecular gases which have energy levels close to the vibrationally excited metastable level (v = 1) of N₂. Most of these gases are extremely poisonous and a few may not be stable in a discharge; however, in the latter case, it is possible to excite the N₂ in another chamber and then mix it with the gas in question. The review is presented in a series of ten tables, which follow.

Energy level (cm ⁻¹)	Designation	Species
2215	00003 ¹	πu
1973. 8	01000	Σ_{g}^{+}
1956	0002°11	^π u
*1460	00002	Σ_{g}^{+} , Δ_{g}
1328. 1	0001111	Σ_{u}^{+}
*1224	00021	$\Sigma^+_{ extbf{g}}$, $\Delta_{ extbf{g}}$
729. 1	000011	πu
611.8	000110	πg

TABLE I C_2H_2 : Linear with center of symmetry $(D_{\infty}h)$

*Not observed Spectroscopically. Values are estimated without including the anharmonic correction.

Remark: $00003^1 - 0000^{\circ}0^{\circ}$ is weak. Hence, it is not very favorable for laser action.

C ₂ D ₂ : Linear	with center of sym	metry (D_{ω}^n)
Energy level	Designation	Species_
2311	01001	^π u
1762. 4	01000	σ_{g}^{+}
1610	00003	π
1044	01001	Σ_{u}

TABLE II C2D2: Linear with center of symmetry (D_oh)

Remark: 01001 -00000 is weak. Hence, it is not very favorable for laser action.

			ΓABLE	ΪÏ		
C_2N_2 :	Linear	with	center	of	symmetry ($D_{\infty}h$)

Energy level	Designation	Species
226	00001	π _u
506	00010	π _g
732	00011	Σ_{u}^{+}
848	01000	σ+ g
1026	00002	Σ_{g}^{+} , Δ_{g}
2149	00100	σ_{u}^{+}
2322	10000	σ_{g}^{+}

Remark: 10000 level is very close to that of $N_2(v = 1)$. However, since transition to the ground state is forbidden, collision cross section is small.

Energy level	Designation	Species
2329	02°1	Σ_{u}^{+}
2183.9	10°1	Σ_{u}^{+}
1523	00°1	Σ_{u}^{+}
796	02°0	Σ_{g}^{+}
656.5	10°0	Σ_{g}^{+}
396. 7	0110	π _u

TABLE IV CS₂: Linear with center of symmetry (C₂v)

Energy level	Designation	Species
2305	200	A1
1871	011	\mathbf{B}_1
1361	001	bı
1151.2	100	aı

TABLE V SO₂: Asymmetric top nonlinear (C_2v)

TABLE VI H_2O : Asymmetric top nonlinear (C_2v)

Energy level	Designation	Species
6874	021	B ₁
5332	011	B ₁
3755.8	001	B ₁
3651.4	100	A ₁
3151.4	020	A ₁
1595	010	A ₁

Remark: The lifetime of $N_2(v = 3)$ is short. Hence, a slim chance of laser action is expected with $N_2(v = 3)$.

	TAB	LE	VII	
H ₂ S:	Asymmetric	top	nonlinear	(C_2v)

Energy level	Designation	Species
2422	020	A ₁
1290	010	aı

Remark: It may not be very favorable for laser action because 020 level of H_2S lies above that of N_2 (v = 1).

Energy level	Designation	Species
2220	011	B _I
1621	001	bı
1320	100	al
1373	020	
648	010	aı

TABLE VIII N₂O: Asymmetric top nonlinear (C_2v)

Energy level	Designation	Species
2162	ν ₃	E
2115. 2	ν_1	A ₁
1812	2 v ₂	A1
999.4	V4	E
906	ν ₂	A ₁

TABLE IX A₃H₃: Symmetric top (C₃v)

	· · · · · · · · · · · · · · · · · · ·	
Energy level	Designation	Species
2290	ν ₃	σ_{u}^{+}
2200	<i>v</i> ₁	σ ⁺ g
2190		πu
1980	-	πu
1850	-	^π u
1760	-	π _u
1670	_	"u
1570	V ₄	$\sigma_{\mathbf{u}}^{+}$
1470	-	$\pi_u \text{ or } \sigma_u^+$
1387	_	πu
1225	_	Σ_{u}^+
1226	_	Σ_u^+ or π_u
1114		Σ_{g}^{+}
1024	_	π _u
909	-	πu
1176	_	Σ_{g}^{+}
843		σġ
586	v ₅	πg
557	V 7	π _u

TABLE $\ensuremath{\overset{\,\,}{x}}$ $C_3\,O_2\text{:}$ Linear with center of symmetry ($D_\infty h)$

Remark: v_3 is very strong. But when warm it decomposes.























Fig. 6. Vibrational energy level diagram of H_2O .













Fig. 10. Vibrational energy level diagram of $C_3 O_2$.

IV. SUMMARY

A few of the simple gases having resonant energy level with the v = l vibrational level of N₂ have been investigated. The vibrational level of N₂(v = l) is about 2330 cm⁻¹ above the ground level and is a metastable state. Because of its long lifetime it is a suitable gas for transferring its energy to other gases being in resonance with it.