Model for Cameron band emission in comets: A case for EPOXI mission target comet 103P/Hartley 2

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ABSTRACT

The CO_2 production rate has been derived in comets using the Cameron band ($a^3\Pi$ - $X^1\Sigma$) emission of CO molecule assuming that photodissociative excitation of CO_2 is the main production mechanism of CO in $a^3\Pi$ metastable state. We have devoloped a model for the production and loss of CO($a^3\Pi$) which has been applied to comet 103P/Hartley 2: the target of EPOXI mission. Our model calculations show that photoelectron impact excitation of CO and dissociative excitation of CO_2 can together contribute about 60-90% to the Cameron band emission. The modeled brightness of (0-0) Cameron band emission on comet Hartley 2 is consistent with Hubble Space Telescope observations for 3-5% CO_2 (depending on model input solar flux) and 0.5% CO relative to water, where photoelectron impact contribution is about 50-75%. We suggest that estimation of CO_2 abundances on comets using Cameron band emission may be reconsidered. We predict the height integrated column brightness of Cameron band of ~1300 R during EPOXI mission encounter period.

Key words: comets:general-comets:103P/Hartley 2–molecular processes-astrochemistry

1 INTRODUCTION

In the exploration of the solar system, comets have been targeted by various space missions. After successful encounter of comet 9P/Temple 1 on 4 July 2005, the NASA's Deep impact mission, also called EPOXI mission, under it's extended investigation program DIXI will encounter comet 103P/Hartley 2 on 4 November 2010, with closest approach around 700 km from the nucleus. This comet has been observed by several space telescopes in different spectral regions (Weaver et al. 1994; Crovisier et al. 1999; Colangeli et al. 1999; Groussin et al. 2004; Lisse et al. 2009; Snodgrass et al. 2008, 2010).

The first clear detection of the Cameron band ($a^3\Pi$ - $X^1\Sigma$) of CO was reported by Weaver et al. (1994) in HST/FOS spectrum of comet 103 P/Hartley 2. Since Cameron band emission is a forbidden transition, resonance fluorescence is not an effective excitation mechanism. The upper state of this emission ($a^3\Pi$) is a metastable state with lifetime of 3 ms (Gilijamse et al. 2007), which is quite small. Thus, Cameron band emissions are treated as "prompt emissions" and can be used to probe distribution of parent species if this emission is produced in dissociative excitation of a molecular species. Photodissociative excitation of CO_2 is considered as the major production mechanism of CO Cameron band and has been used to trace the distribution and abundance of CO_2 on comets (Feldman et al. 1997; Weaver et al. 1994).

Besides photodissociative excitation of CO_2, there are other

channels of excitation of CO molecule in the $a^3\Pi$ state. It has been shown that photoelectrons generated by solar EUV radiation also play an important role in excitation, dissociation, and ionization processes leading to emission and chemistry in cometary comae (e.g., Ip 1986; Boice et al. 1986; Körösmezey et al. 1987; Bhardwaj et al. 1990, 1996; Bhardwaj 1999, 2003; Weaver et al. 1994; Haider & Bhardwaj 2005; Capria et al. 2008). Recently, Campbell & Brunger (2009) demonstrated the importance of photoelectron impact excitation in comets, and showed that electron impact on CO gives 40% contribution to the total CO Fourth positive emission. The presence of photoelectron excitation in cometary coma is clearly publicised by detection of OI 1356 Å emission in comets (e.g., Sahnow et al. 1993; McPhate et al. 1999), since this emission being a spin-forbidden transition cannot be produced by solar fluorescence. There are other siginificant evidences for an important role of photoelectron excitation in cometary coma (e.g., Tozzi et al. 1998; Bhardwaj 1999; Feldman et al. 2009). In addition to photon and electron impact reactions, dissociative electron recombination reactions of CO^+-bearing ions can also produce CO in the $a^3\Pi$ excited state.

Our aim in this paper is to study various production and loss mechanisms of CO($a^3\Pi$) and to estimate the contribution of photoelectron impact excitation of CO and CO_2 in the production of Cameron band for different relative abundances of CO_2 on comet 103 P/Hartley 2: the target of EPOXI mission. Since model calculations depend on input solar flux, we have estimated its sensitivity on the calculated intensity of Cameron band emission. We show that photoelectron impact on CO and CO_2 are dominant processes (~60–90% contribution) in producing CO molecule in ($a^3\Pi$) state.

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Around the EPOXI encounter epoch predictions are made for the brightness of Cameron band on for comet 103P/Hartley 2, which will be observed by several space-based telescopes including HST.

2   MODEL

We have developed a model for the production of Cameron band emission on comets, which uses the basic coupled chemistry model described in detail in our earlier papers (Bhardwaj et al. 1996; Bhardwaj 1999; Haider & Bhardwaj 2005). Various sources of production and loss of $CO(a^3\Pi)$ are summarized in Table 1. The total water production rate is taken as 6.3×10^{28} s^{-1} for comet 103P/Hartley 2 (Weaver et al. 1994).

To evaluate the effect of solar EUV flux on model calculations, we have considered 2 solar flux models: EUVAC model of Richards et al. (1994) and SOLAR 2000 (S2K) model of Tobiska et al. (2000). The degradation of the solar UV-EUV radiation and solar EUV-generated photoelectrons in the coma is modeled using the method of Bhardwaj et al. (1990, 1996) and further developed by Bhardwaj (1999, 2003). The electron impact production rates are calculated using the Analytical Yield Spectrum (AYS) approach, which is based on the Monte Carlo method. Details of AYS approach are given in several of the previous papers (Bhardwaj et al. 1990, 1996; Bhardwaj 1999; Bhardwaj & Michael 1999a,b; Bhardwaj & Jain 2009). The current model takes into account the most recently published cross sections for the photon impact and electron impact dissociation, ionization, and excitation processes for the gases in the coma. The cross section for photodissociative excitation of CO_2 producing CO in $a^3\Pi$ state is calculated using absorption cross sections of CO_2 and yield of Cameron band measured by Lawrence (1972). The cross section for electron impact excitation of $CO(a^3\Pi)$ from CO is taken from Jackman et al. (1977) and for dissociative excitation of CO_2 is taken from Bhardwaj & Jain (2009). The electron temperature profile required for dissociative recombination reactions is taken from Körösmezey et al. (1987) and is assumed to be same as on comet Halley. Calculations are made for the comet 103P/Hartley 2 at heliocentric distance of 0.96 AU.

3   RESULTS AND DISCUSSION

The photodissociation of CO_2 producing CO in $a^3\Pi$ state is determined by solar flux mainly in the wavelength region 550 to 1050 Å. Table 2 presents the calculated photon production frequencies of $CO(a^3\Pi)$ for two different solar flux models. The $CO(a^3\Pi)$ production frequencies calculated for photoelectron impact on CO_2 and CO are also shown in the same table for the corresponding solar flux models. Our calculated photodissociation frequencies are about 50% to a factor of 2 lower than those reported by Huebner et al. (1992).

Using EUVAC solar flux, the calculated radial profile of volume production rate for the various sources of $CO(a^3\Pi)$ at the relative abundance of 4% CO_2 and 0.5% CO are shown in Figure 1. At 100 km cometocentric distance, the dominant source of production of $CO(a^3\Pi)$ is electron impact of CO_2 ($\sim$50%) followed by electron impact of CO ($\sim$25%), and photodissociation of CO_2 ($\sim$15%). The contributions from dissociative recombination reactions are quite small ($\leqslant$5%) at lower cometocentric distances, but the recombination of CO_2^+ is a significant ($<$30%) source at 1000

km and beyond. Figure 2 shows radial profile of various loss processes of $CO(a^3\Pi)$ for the same relative composition of CO_2 and CO. Since lifetime of CO in excited state ($a^3\Pi$) is very short ($\sim$3 ms; Gilijamse et al. 2007), the radiative decay is the dominant loss process. Collisional quenching of $CO(a^3\Pi)$ by cometary neutral species is negligible since 103P/Hartley 2 is a low production rate comet. But in the case of large production rate comets, like Hale-Bopp, quenching by water would be a dominant loss process in the innermost part of the coma.

Figure 3 shows the modeled limb brightness profiles of Cameron band emission for different production processes of $CO(a^3\Pi)$. The cometary coma is assumed to be spherically symmetric. The production rates are integrated up to 10^5 km along the line of sight at a given projected distances from the cometary nucleus, and converted into brightness. The brightness profiles are averaged over the projected area of slit (2870×954 km) corresponding to the HST observation (Weaver et al. 1994). The volume emission rate for 3 transitions (0-0, 1-0, 0-1) of Cameron band emission are calculated using the following formula

$$V_{\nu'\nu''}(r) = q_{o\nu'}(A_{\nu'\nu''} / \sum_{\nu''} A_{\nu'\nu''})\, V(r)\, exp(-\tau) \qquad (1)$$

where V(r) is total volume excitation rate of $CO(a^3\Pi)$ at cometocentric distance r, $q_{o\nu'}$ is the Franck-Condon factor for transition, $A_{\nu'\nu''}$ is Einstein transition probability from upper state ν' to lower state ν'', and τ is optical depth. Since resonance fluorescence is not an effective excitation mechanism for the Cameron band and the total gas production rate is only 6.3×10^{28} s^{-1}, the cometary coma can be safely assumed to be optically thin. The Franck-Condon factors are taken from Nicholls (1962) and branching ratios from Conway (1981). The relative contributions of (1-0), (0-0), (0-1) transitions to the total Cameron band are 13.9%, 10.4%, and 14.7%, respectively.

Table 3 presents the model calculated slit-averaged brightness of (1-0), (0-0), (0-1) transitions of Cameron band, as well as total Cameron band brightness and height-integrated column brightness for different relative abundances of CO and CO_2 corresponding to the HST observation of comet 103P/Hartley 2 on September 18-19, 1991. Due to the absence of CO Fourth positive emission in this comet (Weaver et al. 1994), the abundance of CO is constrained to 0.5%. However, we do consider a case of 1% of CO to evaluate it's implications on the results. This table also depicts fractional contribution of photodissociation of CO_2, photoelectron impact of CO and CO_2, and dissociative recombination of CO_2^+ to the total calculated brightness at 3 projected distances (10^2, 10^3, and 10^4 km) from the nucleus. Since the production rates of photodissociative excitation of CO_2, and photoelectron impact of CO and CO_2, are dependent on input solar flux model, results are presented for the EUVAC and S2K solar fluxes relevant to the date of comet observation which was in solar maximum condition.

The HST observation of 0-0 transition of Cameron band is 35 Rayleigh (Weaver et al. 1994), which is consistent with model calculated brightness for the relative abundance of 4 to 5% of CO_2 and 0.5% CO when EUVAC solar flux is used. In this case, at 100 km, the photoelectron impact of CO_2 (50%) and CO (25%) contribute around 75%, while photodissociative excitation of CO_2 is $<$15%. At 1000 km and beyond, the contribution due to electron impact of CO_2 and CO is about 60–70% while those of dissociative recombination of CO_2^+ is $\sim$15–30% and of photodissociative excitation of CO_2 $\sim$10% only. On an average, the photoelectron impact of CO_2 and CO contribute about 60-75% to the production of Cameron band emission, while photodissociative excitation of

CO_2 contribute about 10-15% only. In the case of S2K solar flux model, the CO_2 abundance of 3 to 4% is required to match HST-observed Cameron band 0-0 transition brightness. Here the contribution of photodissociative excitation of CO_2 is ~20%, while the electron impact of CO_2 and CO together contribute ~65%, to the total Cameron band emission. When the CO abundance is doubled to 1% of water the relative contribution due to electron impact on CO increases resulting in the reduction (by ~1%) in the requirement for CO_2 abundace to match the HST-observation brightness. However, there is no major change in the percentage contributions due to photodissociation and photoelectron impact excitation of CO and CO_2. Hence, we conclude that the photodissociative excitation of CO_2 is not the dominant source for the production of Cameron band in comets.

4 SUMMARY

The summery of Table 3 and the above results is that whatever be the relative abundances of CO_2 and CO, and the solar input flux, the photodissociation contribution is in the range of 5–20%, while photoelectron impact excitation contribution is about 50–80%. We conclude that photoelectron impact excitation of Cameron band in comets is much more important than was thought previously. Further, the contribution due to photoelectron impact excitation of CO is significant and vary between 20-50%. We have also shown that dissociative recombination of CO_2^+ ion is also a significant source of Cameron band at cometocentric distances $\geqslant 1000$ km with contribution of as high as 30%. Hence, the derivation of CO_2 abundances based on the assumption that photodissociation of CO_2 is major mechanism should be revisited. The results presented in this paper suggest that Cameron band emission may not be used to probe cometary CO_2 abundance uniquely.

5 PREDICTION

The EPOXI mission will encounter the comet 103P/Hartley 2 on 4 November 2010 when comet will be at heliocentric distance of 1.06 AU and geocentric distance 0.15 AU. In the current solar minimum period, using our model we have estimated the intensity of Cameron band around mission encounter date by taking solar flux on 1 sept. 2010 for both EUVAC and S2K solar flux models. The calculated Cameron band intensity is tabulated in table 3 for the relative abundance of 4% of CO_2 and 0.5% of CO. For EUVAC solar flux, the predicted height-integrated column intensity of Cameron band is 1365 R, in which 1-0, 0-0, and 0-1 band transitions contribute 189, 142, 200 R, respectively. Figure 3 presents the total Cameron band predicted brightness profile as a function of projected distances from the nucleus. For the same relative abundances of CO_2 and CO and the solar S2K flux, the predicted intensity is 1258 R. The results presented in the paper will help in understanding and interpretation of the extensive data to be obtained during EPOXI encounter period.

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Table 1. Reactions for the production and loss of $CO(a^3\Pi)$

Reaction	Rate(cm^{-3} s^{-1} or s^{-1})	Reference
$CO_2 + h\nu \rightarrow CO(a^3\Pi) + O(^3P)$	Model	Shunk & Nagy (2009); Lawrence (1972)
$CO + h\nu \rightarrow CO(a^3\Pi)$	1.69×10^{-9}	Weaver et al. (1994)
$CO_2 + e_{ph}^- \rightarrow CO(a^3\Pi) + O + e^-$	Model	*Present work*
$CO + e_{ph}^- \rightarrow CO(a^3\Pi) + e^-$	Model	*Present work*
$CO_2^+ + e^- \rightarrow CO(a^3\Pi) + O$	6.5×10^{-7} (300/Te)$^{0.8}$ $\times 0.87^\dagger \times 0.29^\ddagger$	Seiersen et al. (2003); Rosati et al. (2003),
$HCO^+ + e^- \rightarrow CO(a^3\Pi) + H$	$0.23^\S \times 2.4 \times 10^{-7}$ (300/Te)$^{0.7}$	Rosati et al. (2007); Schmidt et al. (1988)
$CO(a^3\Pi) + h\nu \rightarrow C + O$	7.2×10^{-5}	Huebner et al. (1992)
$CO(a^3\Pi) + h\nu \rightarrow CO^+ + e^-$	8.58×10^{-6}	Huebner et al. (1992)
$CO(a^3\Pi) + h\nu \rightarrow O + C^+ + e^-$	2.45×10^{-8}	Huebner et al. (1992)
$CO(a^3\Pi) + h\nu \rightarrow C + O^+ + e^-$	2.06×10^{-8}	Huebner et al. (1992)
$CO(a^3\Pi) + H_2O \rightarrow CO + H_2O$	3.3×10^{-10}	Wysong (2000)
$CO(a^3\Pi) + CO_2 \rightarrow CO + CO_2$	1.0×10^{-11}	Skrzypkowski et al. (1998)
$CO(a^3\Pi) + CO \rightarrow CO + CO$	5.7×10^{-11}	Wysong (2000)
$CO(a^3\Pi) + e_{ph}^- \rightarrow CO^+ + 2e^-$	Model	*Present work*
$CO(a^3\Pi) \longrightarrow CO + h\nu$	1.6×10^{-9}	Weaver et al. (1994)

†0.87 is yield of dissociative recombination of CO_2^+ producing CO; ‡0.29 is yield of $CO(a^3\Pi)$ produced from CO; §0.23 is yield of dissociative recombination of HCO^+ producing $CO(a^3\Pi)$; e_{ph}^- = photoelectron.

Table 2. Production frequency (s^{-1}) of $CO(a^3\Pi)$ for three different processes at 1 AU

Solar flux	Photodissociation of CO_2		Photoelectron impact of CO_2		Photoelectron impact of CO	
	Solar min (2010 Sep 1)	Solar max (1991 Sep 18)	Solar min (2010 Sep 1)	Solar max (1991 Sep 18)	Solar min (2010 Sep 1)	Solar max (1991 Sep 18)
S2K	1.1×10^{-7}	5.6×10^{-7}	3.4×10^{-7}	9.7×10^{-7}	1.5×10^{-6}	4.3×10^{-6}
EUVAC	1.7×10^{-7}	2.6×10^{-7}	3.5×10^{-7}	8.9×10^{-7}	1.5×10^{-6}	3.7×10^{-6}
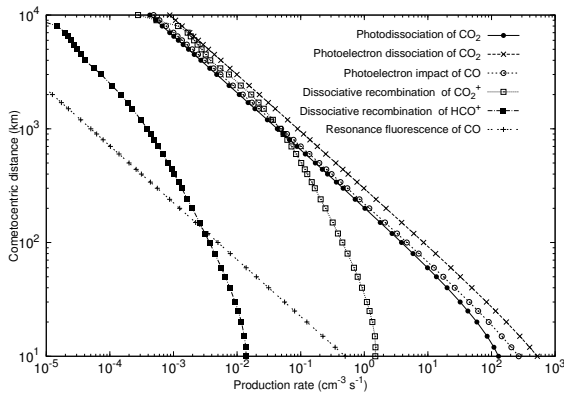
Figure 1. Radial profiles of the production processes of $CO(a^3\Pi)$ in comet 103P/Hartley 2 for 0.5% CO and 4% CO_2 using EUVAC solar flux on 18-19 sept 1991.
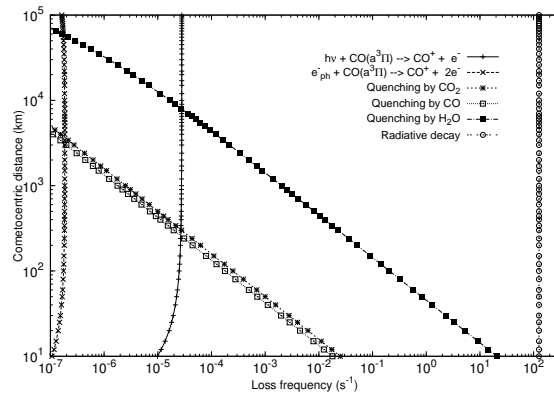

Figure 2. Radial profiles of the loss frequencies of $CO(a^3\Pi)$ in comet 103P/Hartley 2 for 0.5% CO and 4% CO_2 using EUVAC solar flux on 18-19 sept 1991.

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Table 3. Calculated brightness of Cameron band on comet 103P/Hartley 2 for different conditions

Relative abundance		HST-slit averaged brightness (R)			Percentage contribution to total Cameron band for different process at three different projected radial distances (km)												Total Cameron band brightness (R)	
					Photodissociation of CO_2			Photoelectron impact of CO_2			Photoelectron impact of CO			Recombination of CO_2^+				
CO_2 (%)	CO (%)	(1-0)	(0-0)	(0-1)	10^2	10^3	10^4	10^2	10^3	10^4	10^2	10^3	10^4	10^2	10^3	10^4	HST-Slit Avg.	Height integrated nadir view
EUVAC[*]																		
7	0.5	68	51	72	15	12	15	57	42	51	17	12	15	10	32	17	489	4769
5	0.5	51	39	54	14	11	14	53	40	48	22	17	21	9	30	16	369	3710
4	0.5	43	32	45	13	11	13	50	38	45	26	20	25	9	29	15	309	3172
3	0.5	34	26	36	12	10	12	46	36	42	32	26	30	8	26	13	250	2628
2	0.5	26	20	28	11	9	10	39	32	36	42	34	40	7	23	12	190	2078
4	1	51	38	54	11	9	11	40	32	36	41	33	38	7	24	12	311	3948
3	1	43	32	46	10	8	10	35	29	32	48	40	45	6	21	11	311	3420
S2K[*]																		
7	0.5	86	64	91	26	21	25	48	36	44	15	11	14	10	31	16	622	5928
5	0.5	65	48	68	25	20	24	45	35	42	20	15	19	9	29	15	467	4586
4	0.5	54	40	57	23	19	22	43	33	40	24	19	22	8	28	14	390	3903
3	0.5	43	32	46	22	18	21	40	31	37	30	23	28	8	26	13	313	3210
2	0.5	33	25	35	19	16	18	35	28	32	39	32	37	8	23	11	236	2508
3	1	53	40	56	17	15	17	31	25	29	45	37	42	6	21	10	384	4093
2	1	43	32	45	14	12	14	25	21	23	55	47	52	5	18	8	308	3411
Prediction EUVAC[†]																		
4	0.5	189[‡]	142[‡]	200[‡]	21	18	20	46	37	42	25	20	23	7	23	12	-	1365
S2K[†]																		
4	0.5	175[‡]	130[‡]	185[‡]	16	14	16	50	41	46	28	23	25	7	23	13	-	1258

[*] Solar flux for 18 sept. 1991; [†] Solar flux for 1 sept. 2010 [‡] Relative contribution of band in total nadir view intensity.
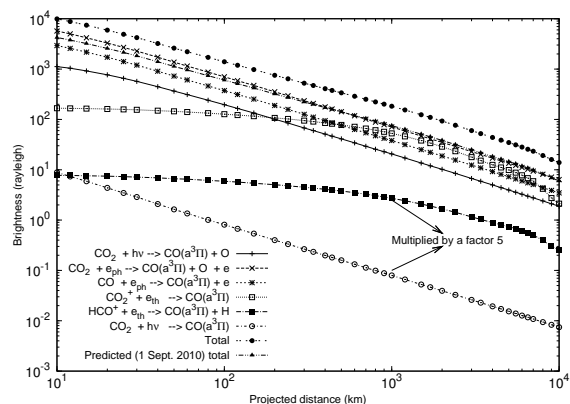
Figure 3. Brightness profile of Cameron band on comet 103P/Hartley 2 as a function of projected distance from nucleus for 4% CO_2 and 0.5% of CO using EUVAC solar flux on 18-19 sept 1991. Resonance fluorescence values and dissociative recombination profiles are plotted after multiplication by a factor 5. Total brightness predicted profile for EPOXI mission period is also shown