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Multi-transitional observations of methanol in Comet Hale-Bopp (1995 O1)

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Abstract. We have observed 9 rotational lines of methanol in comet Hale-Bopp (1995 O1) using the 45-m radio telescope at Nobeyama Radio Observatory in the frequency range 36–104 GHz. The observed transitions have upper state rotational energy levels of $E_{\rm u}$ = 7–159 K. Assuming the Haser model for density distribution, we estimated the excitation temperature and the production rate to be $T_{\rm ex} = 81 \pm 8$ K and $Q(\rm CH_3OH) = (1.2 \pm 0.1) \times 10^{29}$ molecule s^{-1}, respectively. We also observed the HCN $J = 1{-}0$ line at 88 GHz to derive the HCN production rate. We compared the production rate of CH_3OH with that of HCN and that of other molecules whose production rates have been determined previously. The abundance ratio $Q(\rm CH_3OH)/Q(X)$ is estimated to be in the range 3–121, where X denotes HCN, HNC, H_2CO, CS and CH_3CN. When we compare these abundance ratios with those in interstellar clouds: the bipolar flow L1157 B1/B2, the star-forming region SgrB2(M) and the dark cloud TMC-1, they are close to the values in L1157 B1/B2 or in SgrB2(M). We found that the abundance ratio $Q(\rm CH_3OH)/Q(H_2O)$ was similar to solid methanol ratio relative to water ice in interstellar medium. These results support the hypothesis that cometary nuclei are formed from dust grains outside of the primordial solar nebula so that the grain composition of the nebula remains in cometary nuclei.

Key words. comets: general – comets: individual: C/1995 O1(Hale-Bopp) – ISM: abundances

1. Introduction

Methanol is one of the most abundant interstellar molecules and was first detected in space more than 30 years ago (Ball et al. 1970). Not only gaseous methanol but also solid methanol has been detected in space. Several absorption features of methanol were found in W33A and other sources (Baas et al. 1988; Grim et al. 1991; Allamandola et al. 1992; Skinner et al. 1992; Sandford et al. 1993) by infrared observations. The distributions of methanol have also been observed toward from hot core, Orion-KL (Minh et al. 1993) to dark cloud, TMC-1 (Takakuwa et al. 1998; Takakuwa et al. 2000).

Methanol is expected to be present in comets if the cometary nucleus contains unmodified interstellar material, as is generally believed (Yamamoto 1985; Greenberg & Hage 1990). The first radio detection of methanol lines in comet was made in comet Austin(1990 V) by Bockelée-Morvan et al. (1990). Subsequently methanol was also detected in several other comets: in Levy(1990 XX) (Bockelée-Morvan et al. 1990), P/Swift-Tuttle(1992) (Bockelée-Morvan et al. 1994b), Hyakutake(C/1996 B2) (Womack et al. 1997), and Lee(C/1999 H1) (Biver et al. 2000). In comet Hale-Bopp(C/1995 O1), several methanol lines have been detected at 97, 145, 157, 242, 252, 304, and 307 GHz by Biver et al. (1999). They observed the comet in a range of heliocentric distance, $r_{\rm h}$, from 7 AU pre-perihelion to 4 AU post-perihelion and obtained a kinetic temperature of $T = (103 \pm 7) r_{\rm h}^{(-1.10 \pm 0.08)}$ K from average of pre and post-perihelion data of CH_3OH and CO.

In the present study, we have observed the 36, 44, 84, 95, 96 and 104 GHz lines of methanol using the Nobeyama 45-m radio telescope. This is the first detection of 36 and 44 GHz methanol lines in comet. From the multi-transitional observations of methanol, we have determined the excitation temperature and the production rate of methanol, and compare the abundance ratio of methanol in Hale-Bopp with observational results in interstellar medium.

2. Observations

Observations were made from the 9th to the 15th of February 1997, using the 45-m radio telescope at Nobeyama Radio

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Table 1. Characteristics of the NRO 45-m telescope.

Frequency (GHz)	beam width (″)	main beam efficiency
36.	47	0.87
44.	39	0.81
84.	18	0.48
95.	16	0.44
96.	16	0.44
104.	15	0.42

Observatory[1]. During the observation period, comet Hale-Bopp was approaching the perihelion, with a geocentric distance, Δ, and a heliocentric distance, r_h, in the ranges of 1.85–1.73 AU and 1.27–1.21 AU, respectively.

Three SIS receivers (100 GHz, 80 GHz and 40 GHz) were used at the frontend. The spectra of $\mathrm{CH_3OH}$ and HCN $J = 1-0$ line at 88 GHz, which was observed every day during the observation period in order to check the system, were simultaneously observed by using 100 GHz and 80 GHz receivers or 100 GHz and 40 GHz receivers, respectively. The system temperatures of the three receivers were 300–500 K, 280–550 K and 120–220 K, respectively, during the observations. The backend consists of two sets of acousto-optical spectrometers (AOSs). One is a bank of eight high-resolution AOSs with a frequency resolution of 37 kHz and a bandwidth of 40 MHz each. The other is a bank of eight wide-band AOSs with a frequency resolution of 250 kHz and a bandwidth of 250 MHz each. Pointing was checked every hour by observing nearest SiO maser emission from R-Aql. The estimated pointing accuracy was ∼5″ rms. The observations were made toward the cometary nucleus in position-switching mode, and the typical off position was 15′ west of the source position. The beam widths and main beam efficiencies are summarized in Table 1. The on-source integration time was 0.24–2.6 hours. The ephemeris and the radial velocity of comet Hale-Bopp were derived every hours. These values were calculated from the six orbital elements of the comet by taking into account perturbations from nine planets.

3. Results

Nine rotational transitions arising from methanol were detected. The corresponding line parameters are listed in Table 2. The observed line profiles of this molecule are shown in Fig. 1. Most of the lines have both blue and redshifted components, reflecting the expansion of $\mathrm{CH_3OH}$ from the comet nucleus. The redshifted component was generally stronger than the blueshifted component, indicating asymmetric expansion of methanol. This trend has been reported in other observations. According to Irvine et al. (1998), time variation in line shape of HCN and HNC was recognized in Hale-Bopp and asymmetric line shape of HCN whose redshifted component was stronger than blueshifted component at February 1997 was reported. They concluded that this result suggests asymmetric out-gassing from the nucleus. Since methanol and HCN are both thought to be parent molecule, asymmetric line shape of methanol may also indicate asymmetric out-gassing from the nucleus. We estimated the $\mathrm{CH_3OH}$ expansion velocity to be 0.86 ± 0.20 km s^{-1} from the difference between the blue and the redshifted components assuming Gaussian profiles for the two lines. This value is consistent, within the limits of error, with the value of 1.0 km s^{-1} at $r_\mathrm{h} = 1.24$ AU, determined from the expansion velocity $V_\mathrm{exp} = (1.12 \pm 0.014) r_\mathrm{h}^{(-0.41\pm0.01)}$ suggested by Biver et al. (1999). Observed antenna temperatures and integrated intensities are listed in Table 2. The antenna temperatures of double-peaked lines are peak temperatures of redshifted component and those of single-peaked lines are peak temperatures of the line. The fluxes, $S_\nu = 2k\nu^2 T_\mathrm{b}\Omega/c^2$ (Ω: solid angle of the 45-m telescope beam, $T_\mathrm{b} = T_\mathrm{a}^*/\eta_\mathrm{B}$: brightness temperature, η_B: beam efficiency), which are converted from the antenna temperatures, T_a^*, for each frequency observed with the 45-m telescope, are shown in the last column of Table 2.

In order to obtain the production rate of $\mathrm{CH_3OH}$, we analyzed the observed data using the method described by Schloerb et al. (1986). In this method it is assumed that the molecular distribution is described by the Haser model. That is, we assumed that the $\mathrm{CH_3OH}$ molecules flow spherically away from the nucleus at a constant expansion velocity.

Assuming a scale length of R_d for photodissociation and a constant expansion velocity V_exp, the number density of the parent molecule can be written as:

$$n(r) = \frac{Q}{4\pi r^2 V_\mathrm{exp}} \exp\left(-\frac{r}{R_\mathrm{d}}\right), \tag{1}$$

where r is the distance from the nucleus, and Q is the production rate of the parent molecule. For $\mathrm{CH_3OH}$, we adopted the photodissociation rate, $k_\mathrm{p} = 1.3 \times 10^{-5}$ s^{-1}, at the heliocentric distance of 1 AU for the quiet sun (Bockelée-Morvan et al. 1994a), and R_d ($= V_\mathrm{exp}/k_\mathrm{p} r_\mathrm{h}^2$) was calculated to be ∼101 700 km. Assuming that the temperature and the expansion velocity are constant on the line of sight, integration of $n(r)$ along the line of sight, z, gives the column density

$$N(a) = \int_{-\infty}^{\infty} n(r)\,\mathrm{d}z, \tag{2}$$

where N is the column density, a is the projected distance from the nucleus, and z is measured along the line of sight. Consider a point on the line of sight that has a distance a from the nucleus when ϕ is the angle between the point and the plane which passes through the nucleus, we obtain

$$N(a) = \frac{Q}{4\pi V_\mathrm{exp} a} \int_0^{\pi} \exp\left(-\frac{a}{R_\mathrm{d}\sin\phi}\right) \mathrm{d}\phi. \tag{3}$$

Assuming that the optical depth is small, the relation between the brightness temperature of the line and the column density averaged over the antenna beam, $\langle N \rangle$, is given as follows:

$$T_\mathrm{b} = [J(T_\mathrm{ex}) - J(T_\mathrm{bg})] \frac{8\pi^3}{3h} \frac{\mu^2 S \langle N \rangle}{\mathrm{d}v Z} \times \left[\exp\left(\frac{h\nu}{kT_\mathrm{ex}}\right) - 1\right] \exp\left(-\frac{E_\mathrm{u}}{kT_\mathrm{ex}}\right), \tag{4}$$

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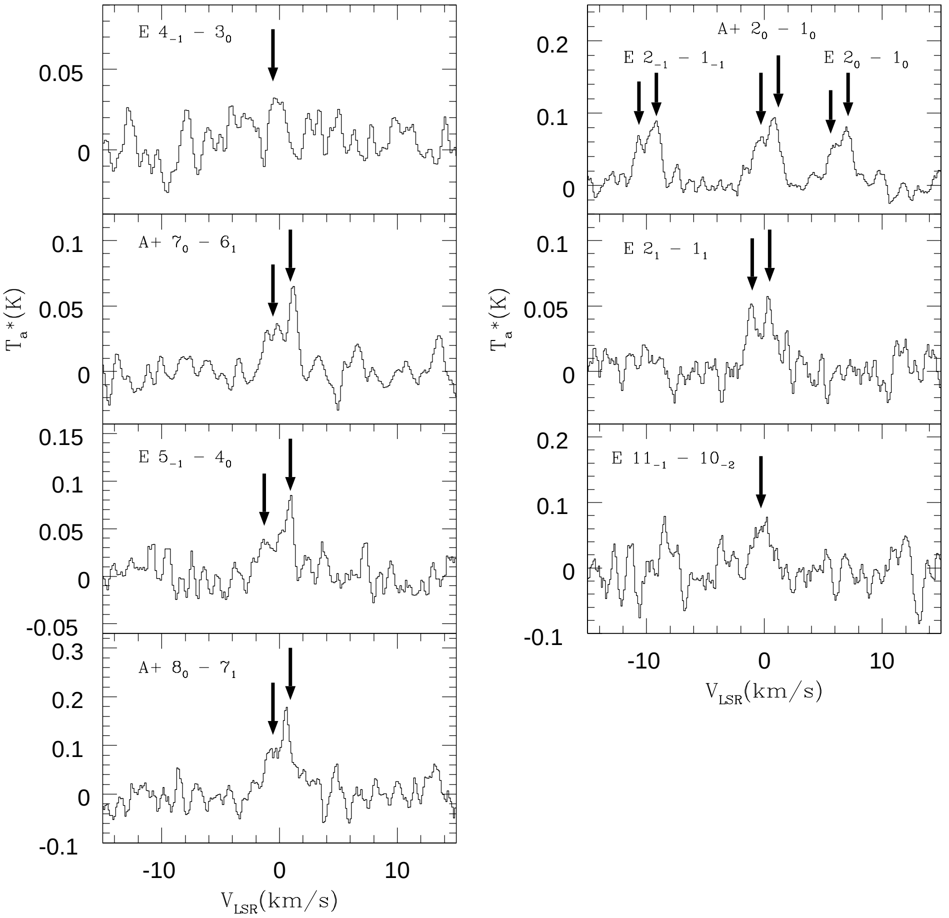

Fig. 1. Spectra of CH_3OH toward Comet Hale-Bopp (1995 O1) (heliocentric distance is about 1.24 AU). The transition is shown at the upper left, center or right of the frame. Arrows indicate blue and redshifted components.

where $J(T) = h\nu/k\,[\exp(h\nu/kT) - 1]^{-1}$, $T_{\rm ex}$ is the excitation temperature, $T_{\rm bg}$ is 2.7 K continuum background, μ is the permanent dipole moment, S is the line strength, and dυ is the line width. Since CH_3OH is a molecule with internal rotation, the partition function, Z, is given as follows:

$$Z = 2\left[\frac{\pi}{ABC}\left(\frac{kT_{\rm ex}}{h}\right)^3\right]^{0.5} = 1.2327 \times T_{\rm ex}^{1.5}, \tag{5}$$

where A, B, and C are the rotational constants of CH_3OH.

The antenna temperature produced by the brightness temperature distribution $T_{\rm b}(p)$ observed with a Gaussian beam of half-power beam width $\theta_{\rm B}$ and beam efficiency $\eta_{\rm B}$ is

$$T_{\rm a}^* = \eta_{\rm B}\,\frac{8\ln 2}{\theta_{\rm B}^2}\int_0^\infty T_{\rm b}(p)\exp\left[-4\ln 2\left(\frac{p}{\theta_{\rm B}}\right)^2\right] p\,{\rm d}p, \tag{6}$$

where p $(=a/\Delta$: Δ is geocentric distance) is the angular size of a and $T_{\rm b}(p)$ may be found by substituting $N(p)$ from Eq. (3) for $\langle N\rangle$ of Eq. (4). The integrated intensity of the line observed in the telescope's Gaussian beam is given as follows:

$$\int T_{\rm a}^*{\rm d}\upsilon = \eta_{\rm B}\,\frac{8\ln 2}{\theta_{\rm B}^2}[J(T_{\rm ex}) - J(T_{\rm bg})]\frac{8\pi^3}{3h}\frac{\mu^2 S}{Z} \times \frac{Q}{4\pi V_{\rm exp}}\left[\exp\left(\frac{h\nu}{kT_{\rm ex}}\right) - 1\right]\exp\left(-\frac{E_{\rm u}}{kT_{\rm ex}}\right)\frac{F(p)}{\Delta} \tag{7}$$

and $F(p)$ is

$$F(p) = \int_0^\infty {\rm d}p\int_0^\pi {\rm d}\phi\,\exp\left[-\frac{p\Delta}{R_{\rm d}\sin\phi}\right]\exp\left[-4\ln 2\left(\frac{p}{\theta_{\rm B}}\right)^2\right]\cdot \tag{8}$$

The excitation temperature, $T_{\rm ex}$, and the production rate, Q were derived from the observed lines by adjusting these two parameters of Eq. (7) by a least-squares fit, where the integration of $F(p)$ is calculated numerically by Simpson's rule. We obtained these parameters to be $T_{\rm ex} = 81 \pm 8$ K and $Q(CH_3OH) = (1.2\pm0.1)\times10^{29}$ molecule s^{-1}. Biver et al. (1999) observed evolution increase of production rates of several molecules with heliocentric distance (See Fig. 3 of their paper). We investigated the heliocentric distance dependence of $Q(CH_3OH)$ from their data and calculated $Q(CH_3OH)$ at $r_{\rm h} = 1.24$ AU to be 8.8×10^{28} molecule s^{-1}. This value is similar to our result. $T_{\rm ex}$ we obtained corresponds to the value of 81 K at $r_{\rm h} = 1.24$ AU, determined from the $T = (103 \pm 7)\ r_{\rm h}^{\ (-1.10\pm0.08)}$ suggested by Biver et al. (1999).

We also observed the HCN $J = 1{-}0$ line, with resolved hyperfine components, $F = 1{-}1,\ 2{-}1,\ 0{-}1$ at 88.63 GHz. Each line has blue and redshifted velocity components with an average interval of 1.44 km s^{-1}. We estimated the production rate of HCN from Feb. 10 data ($r_{\rm h} = 1.26$ AU), of which the quality is high, using Eq. (7). Assuming an HCN photodissociation rate of 1.3×10^{-5} s^{-1} ($r_{\rm h} = 1$ AU) for the quiet Sun and an excitation temperature equal to that for CH_3OH, the production rate of HCN is calculated to be

Table 2. Observed CH_3OH transitions with NRO 45-m telescope.

Transition		Rest freq.[a] [GHz]	E_u^b [K]	$\mu^2 S^c$ [D^2]	date (1997)	T_a^* (rms) [mK]	$\int T_a^* dv$ (rms) [K km s^{-1}]	S_ν (rms) [mJy]
4_{-1}–3_0	E	36.169290	28.789	2.518	Feb.11–13	32 (11)	0.049 (0.008)	87 (30)
7_0–6_1	A^+	44.069476	64.981	6.138	Feb.9–10	68 (16)	0.107 (0.013)	203 (48)
5_{-1}–4_0	E	84.521206	40.391	3.083	Feb.15	87 (22)	0.137 (0.019)	343 (87)
8_0–7_1	A^+	95.169516	83.539	7.221	Feb.13	179 (28)	0.303 (0.028)	771 (121)
2_{-1}–1_{-1}	E	96.739363	12.542	1.213	Feb.14	83 (16)	0.141 (0.014)	369 (71)
2_0–1_0	A^+	96.741377	6.965	1.617	Feb.14	97 (16)	0.169 (0.014)	431 (71)
2_0–1_0	E	96.744549	20.090	1.617	Feb.14	88 (16)	0.173 (0.014)	391 (71)
2_1–1_1	E	96.755507	28.011	1.244	Feb.14	59 (16)	0.112 (0.016)	263 (71)
11_{-1}–10_{-2}	E	104.300396	158.637	3.414	Feb.15	84 (28)	0.113 (0.022)	400 (133)

[a] Frequencies from Xu & Lovas (1997).

[b] Energy of the upper level of the transition.

[c] Square of dipole moment times line strength.

Q(HCN) = 7.6 × 10^{27} molecule s^{-1} from the integrated intensity in which the three hyperfine components were added. The integrated intensity, $\int T_a^* dv$, and $\mu^2 S$ which comprised the three hyperfine components are 1.645 K km s^{-1} and 8.9 D^2, respectively. The upper energy of each hyperfine component and the beam efficiency are 4.3 K and 0.48, respectively. The obtained production rate is lower than the value of $(1.7 \pm 0.3) \times 10^{28}$ molecule s^{-1} at r_h = 0.98 AU (Hirota et al. 1999), probably because of the larger heliocentric distance in the present observation. When we investigate the heliocentric distance dependence of Q(HCN) from the data of Biver et al. (1999), Q(HCN) at r_h = 1.26 AU was calculated to be 6.9 × 10^{27} molecule s^{-1}. This value is similar to our result.

4. Discussion and summary

The sublimation temperatures of HCN and CH_3OH are estimated to be 95 K and 99 K (Yamamoto 1985), respectively at a gas density of 10^{13} cm^{-3}. Both molecules are thought to be parent species and to be sublimated similarly. Therefore, the production rates of HCN and CH_3OH may reflect the original abundances in the comet nucleus. The abundance ratio [CH_3OH]/[HCN] was obtained from Q(CH_3OH) at r_h = 1.24 AU and Q(HCN) at r_h = 1.26 AU to be 16. This value agrees within a factor of 2 with the value of 9.6 at $r_h \sim$ 1 AU obtained by Bockelée-Morvan et al. (2000). When we compare our abundance ratios with those of previous comets, [CH_3OH]/[HCN] = 28 in Levy (Crovisier et al. 1993), 80 in Austin (Crovisier et al. 1993), and 40–70 in Swift-Tuttle (Despois et al. 1996) are larger than our result, but 20 in Hyakutake (Lis et al. 1997) is similar to our result.

Solid methanol has been identified toward W33A and several other protostellar objects (Baas et al. 1988; Grim et al. 1991; Allamandola et al. 1992; Skinner et al. 1992; Sandford et al. 1993), with an abundance of 7 to 40% relative to water ice. Dello Russo et al. (2000) obtained water production rate to be $Q(H_2O) = 8.35 \times 10^{30}\ r_h^{-1.88}$. We obtained $Q(H_2O)$ at r_h = 1.24 AU to be 5.6 × 10^{30} molecule s^{-1} from this equation. Therefore, [CH_3OH]/[H_2O] at r_h = 1.24 AU is 2%. This value agrees to within a factor of 4 with the smallest value in interstellar ice.

We compared the abundance ratios in Hale-Bopp with those in interstellar clouds. We obtained CH_3OH abundance ratio relative to other molecules, [CH_3OH]/[X], where X indicates HCN, HNC, H_2CO, CS and CH_3CN. There are no observational molecular data at $r_h \sim$ 1.24 AU except for CH_3OH and HCN, so that we investigated the heliocentric distance dependence of Q(X) from the data of Biver et al. (1999) and calculated Q(X) at r_h = 1.24 AU. The sublimation temperatures, production rates, and abundance ratios of molecules in Hale-Bopp are listed in Table 3 with the abundances in interstellar clouds for comparison. The abundance ratios in Hale-Bopp were obtained as ratios between the production rates and those in interstellar clouds were obtained as ratios between the column densities. The ratios [CH_3OH]/[X] in Hale-Bopp agree within a factor of 1–4 with those in the bipolar flow L1157 B1/B2 or the star-forming region SgrB2(M). On the other hand, the ratios [CH_3OH]/[X] in the dark cloud TMC-1 are 2–3 orders of magnitude smaller than those in Hale-Bopp.

In the bipolar flow L1157 B1/B2, methanol which is thought to be evaporated from dust grain is enhanced (Bachiller et al. 1997). In the star-forming region SgrB2, many organic molecules are enhanced and thought to be evaporated from dust grain (Miao et al. 1995). Methanol is thought to be one of such molecules . On the other hand, the kinetic temperature in dark cloud such as TMC-1 is low, molecules cannot be evaporated from dust grain. Therefore, methanol abundance ratios relative to other molecules in Hale-Bopp are similar to values in the molecular cloud in which methanol can evaporated from dust grain. This fact supports the hypothesis that when cometary nuclei are formed from dust grains outside of a primordial solar nebula, the nascent grain composition of the solar nebula may remain in the cometary nuclei.

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Table 3. Sublimation temperatures, production rates (Q) of molecules in Hale-Bopp, and abundance ratios [CH_3OH]/[X] in Hale-Bopp and interstellar clouds.

		Comet Hale-Bopp		interstellar space		
Molecule[a]	Subli. Temp.[b] [K]	Q (1.24 AU) [mol s^{-1}]	[CH_3OH]/[X]	[CH_3OH]/[X] L1157 B1/B2[c]	[CH_3OH]/[X] SgrB2(M)[d]	[CH_3OH]/[X] TMC-1[e]
CH_3OH	99	1.2×10^{29}	-	-	-	-
HCN	95	7.6×10^{27}[f]	16	3/41	1–6	0.11[h]
HNC	-	1.1×10^{27}	109	36/480	3–19	0.07[h]
(H_2CO)	64	3.8×10^{28}	3	3/60	2–13	0.05
(CS)	-	5.6×10^{27}	21	6/120	1–4	0.4
CH_3CN	91	9.9×10^{26}	121	-	70–470[g]	4

[a] Molecules in parentheses are thought to be “daughter” molecules.
[b] Yamamoto (1985).
[c] Observed molecular abundances in the bipolar flow by Bachiller et al. (1997).
[d] Observed molecular abundances in the star-forming region by Sutton et al. (1991).
[e] Observed molecular abundances in the dark cloud by Ohishi et al. (1998).
[f] Obtained from data at $r_h = 1.26$ AU.
[g] $N(CH_3CN)$ was adopted from Turner (1991).
[h] N(HCN) and N(HNC) were estimated from $H^{13}CN$ and $HN^{13}C$ data of Hirota et al. (1998) assuming $^{12}C/^{13}C = 60$.

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