Electronic Supplementary Information

$T_{v'}$ values of the 1 $^1\Pi$ state reported by Kasahara *et al.* for the overlapped energy region. We add the dissociation energy of the $X\,^1\Sigma^+$ state, 4217.822 ± 0.03 cm^{-1}, to the corresponding values reported from Physical Review A, 2007, **75**, 032511 in order to convert them to the $T_{v'}$ values. The discrepancies between our data and those of Kasahara et al. may come from the experimental resolution (~0.12 cm^{-1}), wavelength calibration errors (~0.2 cm^{-1}) in the MB experiment and probe laser linewidth (0.2 cm^{-1}) and the fitted uncertainty for the line positions is 0.3 cm^{-1} due to laser scan nonlinearity in the UM experiment.

(a) The 1 $^1\Pi$ state

	Our work		Kasahara *et al.*[13]	Okada *et al.*[12]
Vib. Num.	$T_{v'}$(cm^{-1}) MB	$T_{v'}$ (cm^{-1}) UM	$T_{v'}$ (cm^{-1})	$T_{v'}$ (cm^{-1})
$v' = 0$	15043.05			15043.019
1	15103.93			15103.964
2	15164.63			15164.427
3	15223.93			15224.303
4	15283.66			15283.691
5	15342.57			15342.496
6	15402.15			15400.747
7	15460.01	15459.55		15458.068
8	15512.29	15511.90		15514.803
9	15567.96			15569.756
10	15623.65	15623.59		15622.943
11	15677.20	15677.25		15675.841
12	15730.09	15730.13	15727.307	15725.984
13	15771.98	15771.96	15773.297	
14	15814.71	15814.73	15814.409	
15		15848.63	15849.356	
16		15880.09	15880.849	
17		15909.93	15910.403	
18		15938.65	15939.072	
19		15964.68	15966.599	
20		15993.45	15993.568	

(b) The 2 $^3\Sigma^+$ state

	Our work			Okada *et al.*[12]
Vib. Num.	$T_{v'}$(cm^{-1}) MB (Ω=1)	$T_{v'}$(cm^{-1}) UM (Ω=1)	$T_{v'}$(cm^{-1}) UM (Ω=0$^-$)	$T_{v'}$(cm^{-1}):
v_a	15116.18			
v_a +1	15154.19			
v_a +2	15190.37			
v_a +3	15226.49			
v_a +4	15256.46			
v_a +5	15291.52			15291.65
v_a +6	15324.97			
v_a +7	15359.08	15358.60	15359.44	15358.64
v_a+8	15390.24	15389.68	15390.65	
v_a +9	15423.23	15422.73	15424.81	
v_a +10	15453.41	15452.99	15457.43	
v_a +11	15486.57	15486.24	15488.88	
v_a+12	15520.40	15520.21	15520.96	15517.65
v_a +13	15548.40	15548.84	15550.06	
v_a +14	15581.57	15581.33	15582.15	
v_a +15		15612.46	15615.35	
v_a +16	15640.49	15640.27	15637.85	15640.88
v_a +17		15669.26	15668.10	
v_a +18	15695.89	15695.92		
v_a +19	15722.32	15722.30		
v_a +20	15755.35	15755.18	15753.47	
v_a +21	15785.79	15785.71	15782.62	
v_a +22	15814.41	15814.73		
v_a +23		15837.28	15835.54	
v_a +24		15860.91		
v_a +25		15890.66	15888.85	
v_a +26		15916.30	15914.60	
v_a +27		15942.73	15941.12	
v_a +28		15964.68		
v_a +29		15990.88	15990.85	
v_a +30		16016.16		
v_a +31		16037.76		
v_a +32		16062.86		
v_a +33		16087.40	16086.69	

*Vibrational number assignments were made by comparing the energies from theoretical calculations[15] with the experimental ones. Here we estimate v_a =34. Above 15850 cm^{-1} there are no MB spectra so that we do not know the Ω assignments;We assume here that the Ω=1 level remains above the Ω=0 level since this is the case in the region 15637- 15837 cm^{-1}.

(c) The *b* $^3\Pi$ state

	Our work				Okada *et al.*[12]
Vib. Num.	$T_{v'}$(cm^{-1}) MB (Ω=1)	$T_{v'}$ (cm^{-1}) UM (Ω=2)	$T_{v'}$ (cm^{-1}) UM (Ω=1)	$T_{v'}$ (cm^{-1}) UM (Ω=0$^{\pm}$)	$T_{v'}$ (cm^{-1}) (Ω=1)
v_a	15355.10				15357.25
v_a +1	15402.12				15401.41
v_a +2	15445.06				
v_a +3	~15492	~15493	15490.45		
v_a +4	~15532	~15535	15531.70	15526.69	
v_a +5	~15573	~15577	15574.61	15569.96	
v_a +6			15617.25	15612.46	
v_a +7	~15658		15657.67	15651.62	
v_a +8	~15701		15700.36	15695.92	
v_a +9	~15739	15744.21	15739.9	15734.32	
v_a +10	~15778	15782.62	15778.41	15775.05	
v_a +11			15819.95	15814.73	
v_a +12		15860.91	15856.61	15852.94	
v_a +13		15897.41	15893.13	15888.85	
v_a +14			15932.91		
v_a +15			15971.99	15966.69	
v_a +16			16005.80		
v_a +17			16041.89	16037.76	
v_a +18			16076.05		
v_a +19			16107.34		

*Vibrational number assignments are made by comparing the energies from theoretical calculation[15] with the experimental ones. According to the theoretical calculation, Ω=2 for same vibrational quantum number has the highest energy and Ω=1 is between the Ω=2 and the Ω=0. Here we estimate v_a =87.