

## Long term puzzles of the CH and CD energetics and related phenomena revisited; Solutions sought through REMPI-photofragmentations of bromomethanes

Arnar Hafliðason, Huasheng Wang, and Ágúst Kvaran\*  
*Science Institute, University of Iceland, Dunhagi 3, 107 Reykjavík, Iceland.*

### Supporting information

<b>Content:</b>	<b>page:</b>
Table S1, CHBr <sub>3</sub> : REMPI spectral lines for C/C* atoms.....	2
Table S2, CHBr <sub>3</sub> : REMPI spectral lines for Br/Br* atoms.....	3

**Table S1.** CHBr<sub>3</sub>: Excitation wavenumbers of REMPI spectral lines for C/C\* atoms. The accuracy of atomic lines is about  $\pm 2.0 \text{ cm}^{-1}$  on the two-photon scale.

Configurations / Term symbols	C(2s <sup>2</sup> 2p <sup>2</sup> ; <sup>3</sup> P <sub>0</sub> ) <sup>a</sup>		C(2s <sup>2</sup> 2p <sup>2</sup> ; <sup>3</sup> P <sub>1</sub> ) <sup>a</sup>		C(2s <sup>2</sup> 2p <sup>2</sup> ; <sup>3</sup> P <sub>2</sub> ) <sup>a</sup>		C(2s <sup>2</sup> 2p <sup>2</sup> ; <sup>1</sup> D <sub>2</sub> ) <sup>a</sup>		C(2s <sup>2</sup> 2p <sup>2</sup> ; <sup>1</sup> S <sub>0</sub> ) <sup>b</sup>	
	This work <sup>c</sup> (intensity)	NIST <sup>1</sup>	This work <sup>c</sup> (intensity)	NIST <sup>1</sup>	This work <sup>c</sup> (intensity)	NIST <sup>1</sup>	This work <sup>c</sup> (intensity)	NIST <sup>1</sup>	This work <sup>c</sup> (intensity)	NIST <sup>1</sup>
2s <sup>2</sup> 2p3s / <sup>3</sup> P <sub>1</sub> <sup>o</sup>									38706.0 (m)	38704.6
2s <sup>2</sup> 2p4p / <sup>3</sup> D <sub>3</sub>					80793.6 (vw)	80791.2				
2s <sup>2</sup> 2p4p / <sup>3</sup> P <sub>0</sub>					81268.1 (vw)	81267.6				
2s <sup>2</sup> 2p4p / <sup>3</sup> P <sub>1</sub>					81281.8 (vw)	81282.4				
2s <sup>2</sup> 2p4p / <sup>3</sup> P <sub>2</sub>					81299.4 (m)	81300.6				
2s <sup>2</sup> 2p4p / <sup>3</sup> P <sub>0</sub>	81310.8 (vw)	81311.0								
2s <sup>2</sup> 2p4p / <sup>3</sup> P <sub>1</sub>			81308.4 (w)	81309.4						
2s <sup>2</sup> 2p4p / <sup>3</sup> P <sub>2</sub>			81326.7 (vw)	81327.6						
2s <sup>2</sup> 2p4p / <sup>3</sup> P <sub>2</sub>	81342.1 (vw)	81344.0								
2s <sup>2</sup> 2p6p / <sup>1</sup> D <sub>2</sub>							77024.4 (vw)	77025.6		
2s <sup>2</sup> 2p8p / <sup>1</sup> D <sub>2</sub>							78719.3 (vw)	78720.9		
2s <sup>2</sup> 2p9p / <sup>1</sup> D <sub>2</sub>							79157.1 (vw)	79157.5		

a. (2<sub>r</sub> + 1<sub>i</sub>)REMPI atomic lines

b. (1<sub>r</sub> + 1<sub>i</sub>)REMPI atomic lines

vw: very weak, w: weak, m: medium, s: strong, vs: very strong

**Table S2.** CHBr<sub>3</sub>: Excitation wavenumbers of REMPI spectral lines for Br/Br\* atoms. The accuracy of atomic lines is about  $\pm 2.0 \text{ cm}^{-1}$  on the two-photon scale.

Configurations / Term symbols	Br( $4s^2 4p^5; ^2P_{3/2}$ ) <sup>a</sup>		Br( $4s^2 4p^5; ^2P_{1/2}$ ) <sup>a</sup>	
	This work <sup>b</sup> (intensity)	NIST <sup>1</sup>	This work <sup>b</sup> (intensity)	NIST <sup>1</sup>
$4s^2 4p 4(^3P_2) 5p / ^4D^{\circ}_{3/2}$	76742.2 (m)	76743.1		
$4s^2 4p 4(^3P_1) 5p / ^2S^{\circ}_{1/2}$	78079.2 (vw)	78076.0		
$4s^2 4p 4(^3P_1) 5p / ^2D^{\circ}_{5/2}$	78509.8 (s)	78511.6		
$4s^2 4p 4(^3P_1) 5p / ^2D^{\circ}_{3/2}$	78674.6 (s)	78676.7		
$4s^2 4p 4(^3P_1) 5p / ^4S^{\circ}_{3/2}$	79177.2 (m)	79178.3		
$4s^2 4p 4(^3P_0) 5p / ^2P^{\circ}_{3/2}$	79697.0 (vs)	79695.9		
$4s^2 4p 4(^3P_0) 5p / ^2P^{\circ}_{1/2}$	79866.6 (m)	79868.0		
$4s^2 4p 4(^3P_0) 5p / ^2P^{\circ}_{3/2}$			76014.4 (vw)	76010.7
$4s^2 4p 4(^3P_0) 5p / ^2P^{\circ}_{1/2}$			76186.8 (w)	76182.8
$4s^2 4p 4(^3P_0) 6p / ^4P^{\circ}_{3/2}$			81903.0 (vw)	81901.1
$4s^2 4p 4(^3P_0) 6p / ^4P^{\circ}_{1/2}$			82117.0 (w)	82114.0
$4s^2 4p 4(^3P_2) 6p / ^4D^{\circ}_{5/2}$			82136.6 (w)	82135.3
$4s^2 4p 4(^3P_2) 6p / ^4D^{\circ}_{3/2}$			82258.8 (vw)	82258.6
$4s^2 4p 4(^1D) 5p / ^2F^{\circ}_{5/2}$			83375.4 (m)	83376.0
$4s^2 4p 4(^1D) 5p / ^2P^{\circ}_{1/2}$			83812.8 (m)	83813.8

a.  $(2_r + 1_i)$  REMPI

b. vw: very weak, w: weak, m: medium, s: strong, vs: very strong

## REFERENCE

1. NIST Chemistry WebBook - NIST Atomic Spectra Database Levels Data, <http://webbook.nist.gov/>, Accessed August 2015.