Electronic Supporting Information (ESI)

Facile Preparation, Mechanochromic Luminescence and Excitation Wavelength-Dependent Emission of Tetra(1H-benzo[d]imidazol-2-yl)ethene Zn (II) Complexes and Their Applications

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Section 1. Experimental Section

1.1 Materials and physical measurements

All chemicals and reagents in this work were purchased from commercial sources and used without further purification. C, H, and N elemental analyses were collected with a Vario EL elemental analyzer. The fluorescence spectra were recorded on an FLS980 fluorescence spectrophotometer. Fourier transform infrared (FTIR) spectra were measured in the range of 500–4000 cm^{-1} using an Avatar 360 FT-IR spectrometer with KBr pellets. The X-ray powder diffraction (PXRD) patterns were performed on SHIMADZU XRD-7000 diffractometer Cu-Kα radiation (λ = 1.5418 Å) and 2θ ranging from 5° to 50° at room temperature. Solid-state UV–Vis absorption spectra were recorded on a TU-1901 spectrophotometer in the range of 250–800 nm. Thermogravimetric data (TGA) were performed using a NETASCH STA449 F5 at a heating rate of 10 $℃ \cdot min^{-1}$ in the range of 25–500 ℃ under nitrogen flow. Single crystals X-ray diffraction data were collected on the XtaLAB Synergy-DW diffractometer with Cu-Kα radiation (λ = 1.54184 Å, powered at 4 kW) and Mo Kα radiation (λ = 0.71073 Å, powered at 4 kW).

Section 2. Supplementary Tables, Structural Figures and Scheme

2.1 Figure S1-S10

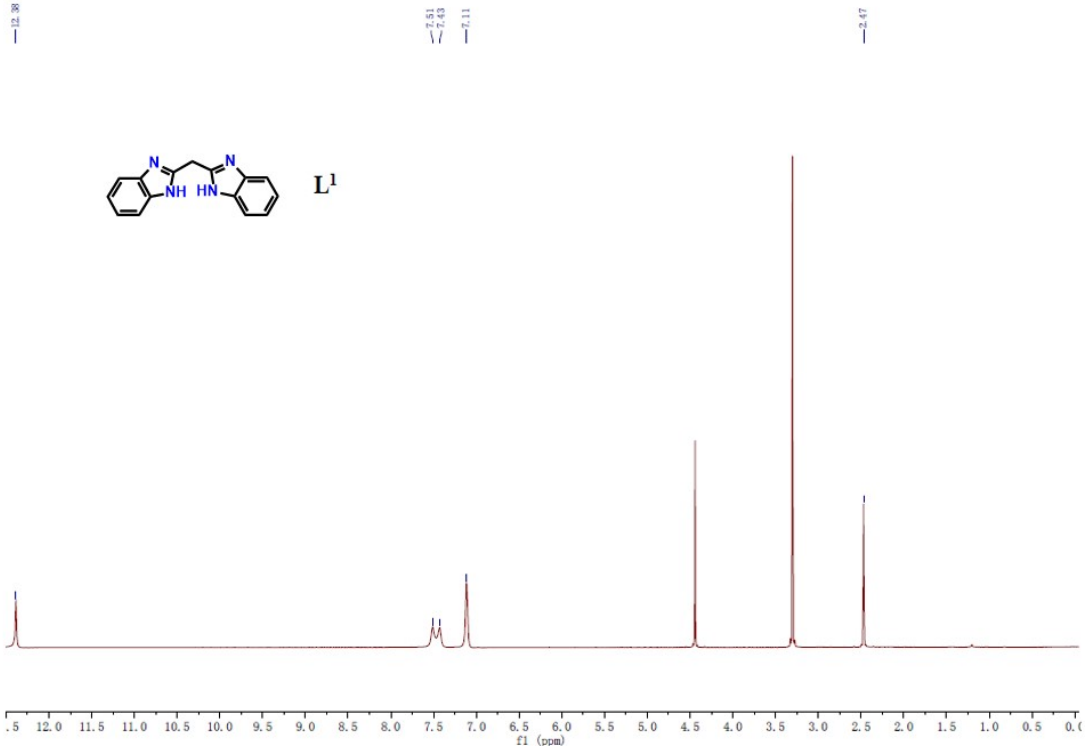

Figure S1 ^{1}H NMR spectra of L^{1}

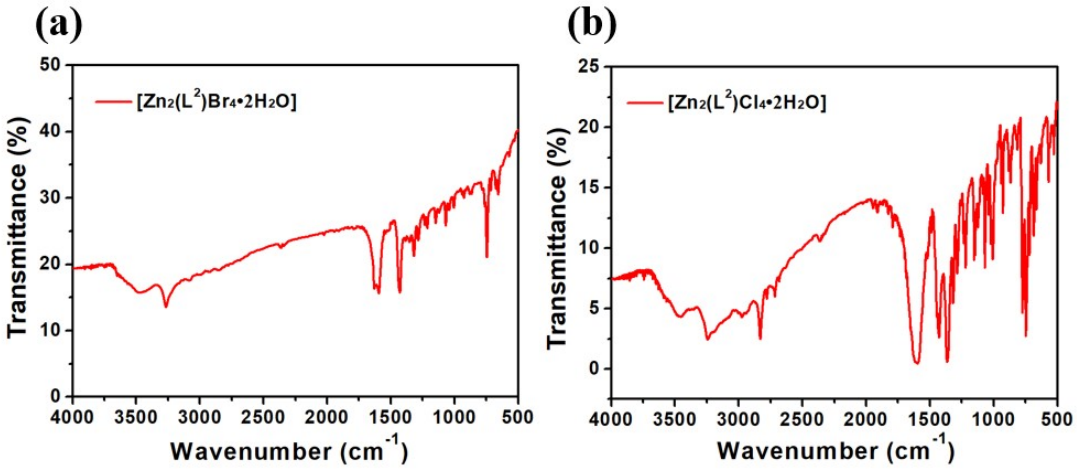

Figure S2 IR spectra of complex **1**(a) and complex **2** (b)

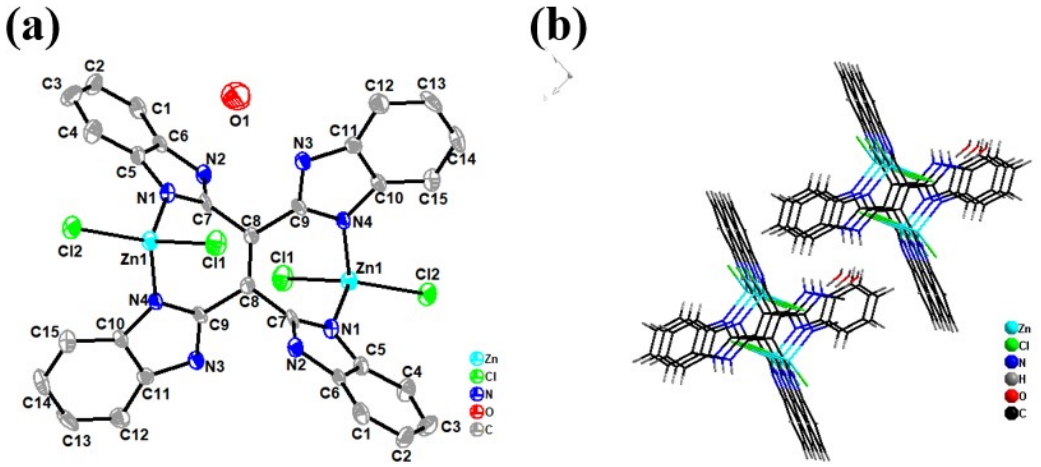

Figure S3 (a) Molecular structure of complex **2** (b) The stacking form of complex **2.**

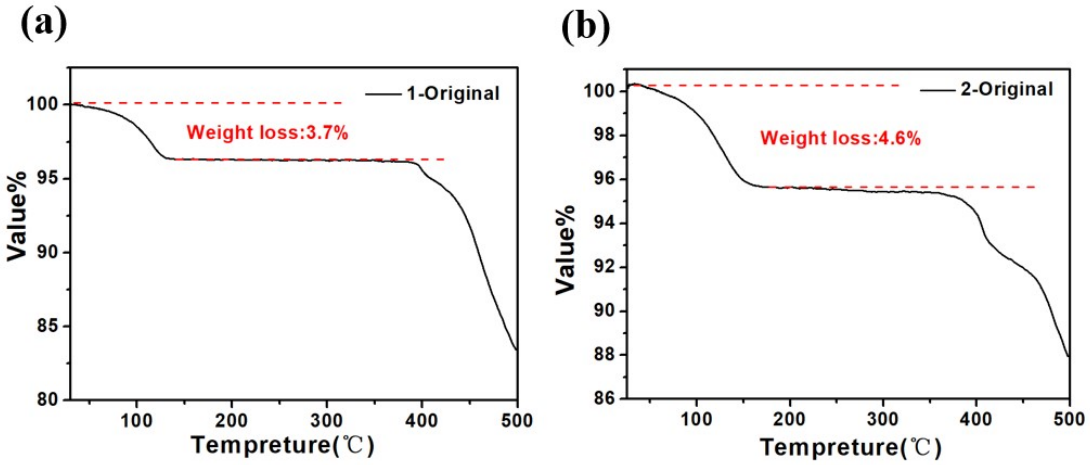

Figure S4 TGA curves of complex **1** (a) and complex **2** (b)

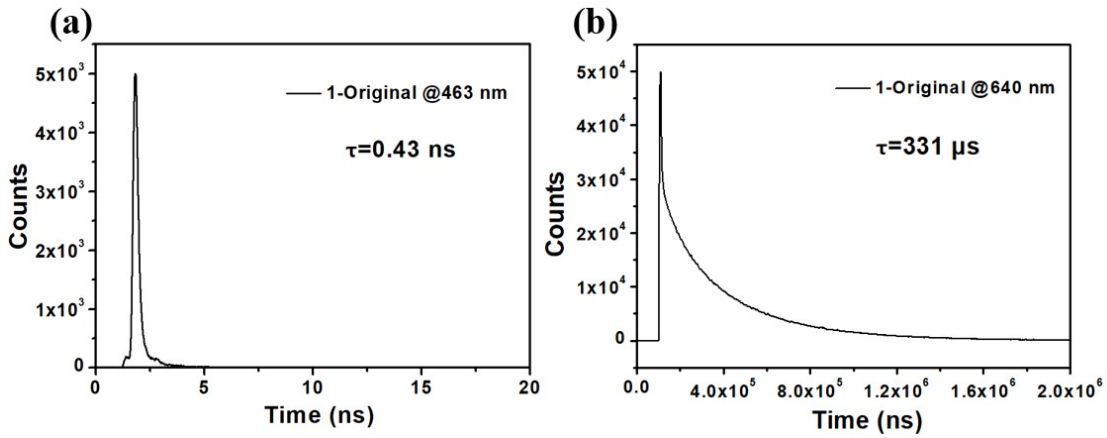

Figure S5 (a) Luminescence decay curves and fit results of complex **1** at 463 nm (b) Luminescence decay curves and fit results of complex **1** at 640 nm

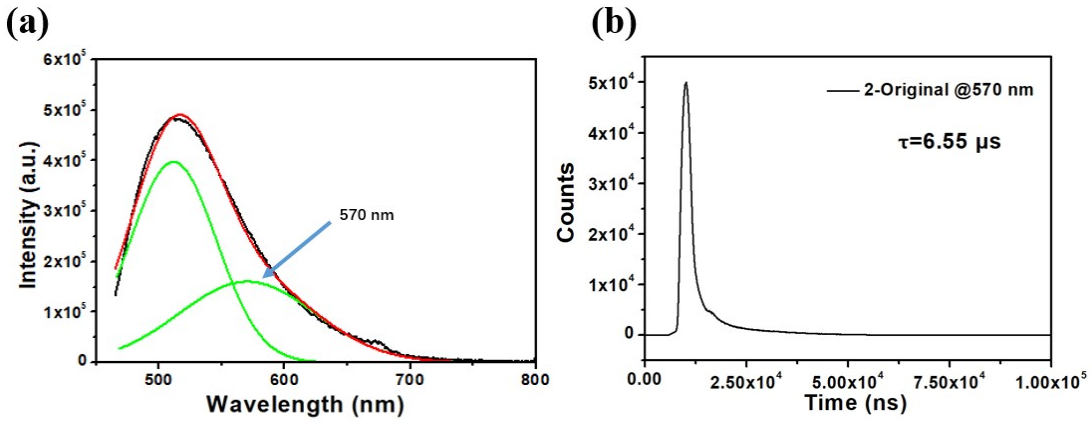

Figure S6 (a) The peak-splitting result of complex **2** luminescence emission (b) Luminescence decay curves and fit results of complex **2** at 570 nm

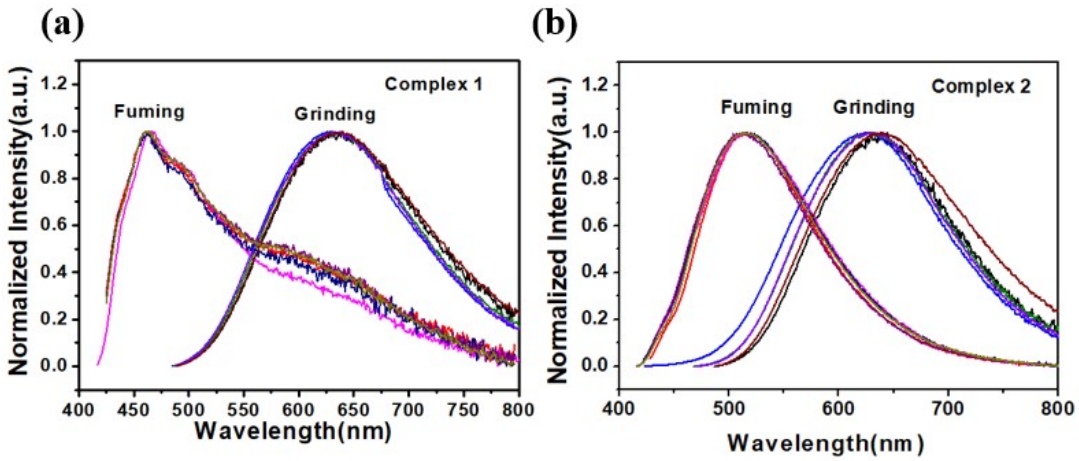

Figure S7 Luminescence emission spectra of complex **1** (a) and complex **2** (b) upon repeating the grinding-fuming processes

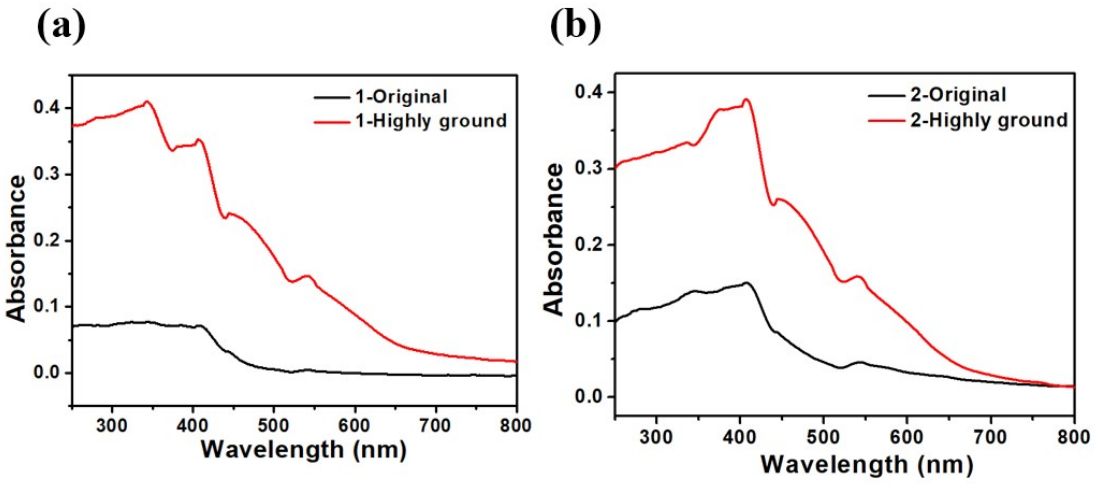

Figure S8 UV-Vis spectra of complex **1** (a) and complex **2** (b) upon repeating the grinding-fuming processes

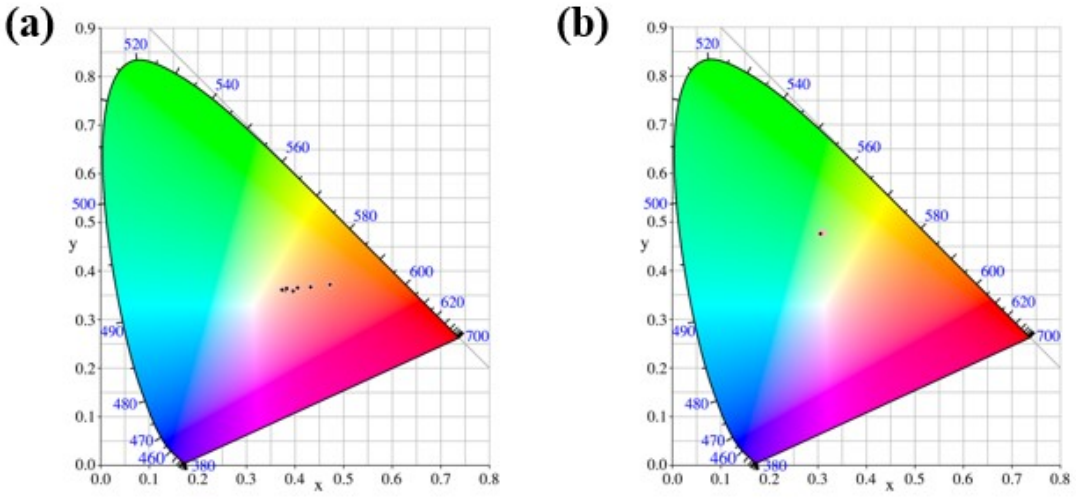

Figure S9 (a) The CIE chromaticity diagram reveals the dynamic luminescence color change of complex **1** in crystal state excited by different wavelengths of light (b) The CIE chromaticity diagram reveals the dynamic luminescence color change of complex **2** in crystal state excited by different wavelengths of light

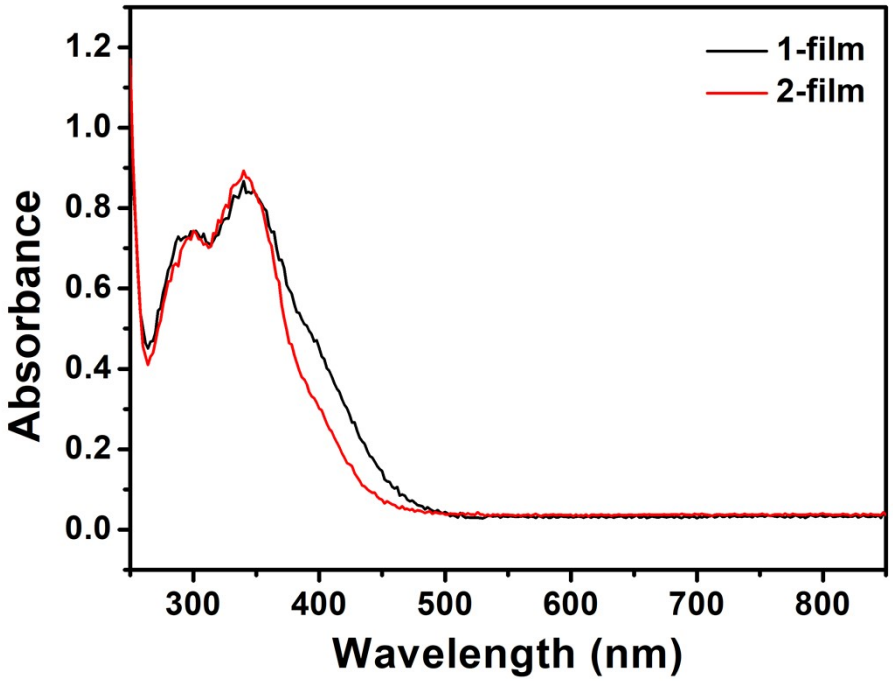

Figure S10 UV–Vis absorption spectra of complexes **1** and **2** in PMMA films.

Section 2. Supplementary Tables, Structural Figures and Scheme

2.2 Table S1-S3

Table S1 Crystal data and structure refinement parameters of complexes **1** and **2**

Table S2 Selected bond distances (Å) and angles (°) for complexes **1** and **2**

Table S3 Types of intramolecular and intermolecular interactions, corresponding bond distances and angles in complexes **1** and **2**.

Table S1 Crystal data and structure refinement parameters of complexes **1** and **2**

Empirical formula	$C_{15}H_{12}N_4OZnBr_2$(**1**)	$C_{15}H_{12}N_4OZnCl_2$(**2**)
Formula weight	489.48	400.56
Temperature/K	293(2)	99.99(10)
Crystal system	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a/Å	9.1124(5)	8.8194(5)
b/Å	9.9522(4)	9.7128(7)
c/Å	9.9964(6)	9.8023(5)
α/°	88.322(4)	91.156(5)
β/°	70.428(5)	95.778(4)
γ/°	83.041(4)	107.223(6)
Volume/Å^3	847.82(8)	796.85(9)
Z	2	2
ρ_{calc}g/cm^3	1.917	1.669
μ/mm^{-1}	6.169	1.884
F(000)	476.0	404.0
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2θ range for data collection/°	7 to 57.482	6.716 to 59.822
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 12, -13 ≤ l ≤ 12	-11 ≤ h ≤ 11, -7 ≤ k ≤ 13, -12 ≤ l ≤ 13
Reflections collected	6061	6772
Independent reflections	3547[R_{int} = 0.0201, R_{sigma} = 0.0408]	3744[R_{int} = 0.0612, R_{sigma} = 0.0955]
Data/restraints/parameters	3457/3/211	3744/4/214
Goodness-of-fit on F^2	1.038	1.025
Final R indexes [I>=2σ (I)]	R_1= 0.0340, wR_2 = 0.0672	R_1= 0.0488, wR_2 = 0.0968
Final R indexes [all data]	R_1= 0.0482, wR_2 = 0.0732	R_1= 0.0639, wR_2 = 0.1110
Largest diff. peak/hole / e Å^{-3}	0.62/-0.48	1.06/-0.67
CCDC number	2373214	2373223

Table S2 Selected bond distances (Å) and angles (°) for complexes **1** and **2**

1	Br2	Zn1	2.3340(5)		Zn1	N1	2.039(3)	
	Br1	Zn1	2.3611(5)		Zn1	N4[1]	2.049(2)	
	C8	C8[1]	1.347(6)		C8	C7	1.470(4)	
	C9	C8	1.476(4)					
	Br2	Zn1	Br1	116.08(2)	N1	Zn1	N4[1]	89.42(10)
	N1	Zn1	Br2	116.25(8)	N4[1]	Zn1	Br2	113.99(7)
	N1	Zn1	Br1	108.63(7)	N4[1]	Zn1	Br1	109.33(8)
	C7	C8	C8[1]	123.1(3)	C9	C8	C8[1]	124.0(4)
	C7	C8	C9	112.7(3)				
2	Cl2	Zn1	2.2136(8)		Zn1	N1	2.029(3)	
	Cl1	Zn1	2.2367(9)		Zn1	N4[1]	2.040(3)	
	C8	C8[1]	1.353(6)		C8	C7	1.456(4)	
	C9	C8	1.497(4)					
	Cl2	Zn1	Cl1	118.90(4)	N1	Zn1	N4[1]	89.82(11)
	N1	Zn1	Cl2	114.57(8)	N4[1]	Zn1	Cl2	112.99(7)
	N1	Zn1	Cl1	107.90(7)	N4[1]	Zn1	Cl1	108.80(8)
	C7	C8	C8[1]	124.5(3)	C9	C8	C8[1]	122.9(4)
	C7	C8	C9	112.5(3)				

[1]1-x, 1-y, 1-z

Table S3 Types of intramolecular and intermolecular interactions, corresponding bond distances and angles in complexes **1** and **2**.

Compound	Interactions	Distances (Å)	Angles (°)
1	N3-H3···Br2	2.67	143
	O1-H1···Br1	2.53	139
	N2-H2···O1	1.94	172
	C13-H13···πCg1	2.73	158
	πCg3···πCg3	3.945	180
2	N3-H3···Cl2	2.46	145
	O1-H1··· Cl1	2.38	168
	N2-H2···O1	1.94	166
	C13-H13···πCg1	2.61	158
	πCg3···πCg3	3.855	180