

Supporting Information

Ferrocene \cap Europium Assembly Showing Phototriggered Anticancer Activity and Fluorescent Modality Imaging

Jian Qu,^{a,b} Qing Xia,^b Wei Ji,^b Su Jing,^{*,b} Dunru Zhu,^{*,c} Lin Li,^a Ling Huang,^a Zhongfu An,^a Chenqi Xin,^a Yun Ni,^a Mengxue Li,^a Jidong Jia,^d Yinglin Song,^d and Wei Huang^{*,a}

^a*Institute of Advanced Materials, Nanjing Tech University, Nanjing 210009, P.R. China. E-mail, iamwhuang@njtech.edu.cn*

^b*School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, P.R. China. E-mail, sjing@njtech.edu.cn; Tel, 86-25-58139150*

^c*College of Chemical Engineering, Nanjing Tech University, Nanjing 210009, P.R. China. E-mail, zhudr@njtech.edu.cn*

^d*College of Physics, Optoelectronics and Energy, Soochow University, Suzhou 215006, P.R. China.*

Table of contents

Fig. S1 (a) View of the structure of (Et₂ChromenH)ClO ₄ . (b) $\pi\cdots\pi$ interactions involving intermolecular coumarin rings.....	3
Fig. S2 The FT-IR spectra of (a) fc1 ∩Eu and (b) fc2 ∩Eu.....	4
Fig. S3 TGA curves of the assemblies (a) fc1 ∩Eu and (b) fc2 ∩Eu.....	5
Fig. S4 Emission spectra of fc1 , fc2 and protonation of fc1 , fc2 under a 356 nm excitation light.....	6
Fig. S5 Emission spectra of fc1 , fc1 ∩Eu and fc2 , fc2 ∩Eu under a 381 nm excitation light.....	7
Table S1. Selected bond lengths (Å) and bond angles (°) for fc1 , fc2 , fc1 ⁺ ClO ₄ CH ₃ CN and (Et₂ChromenH)ClO ₄	8

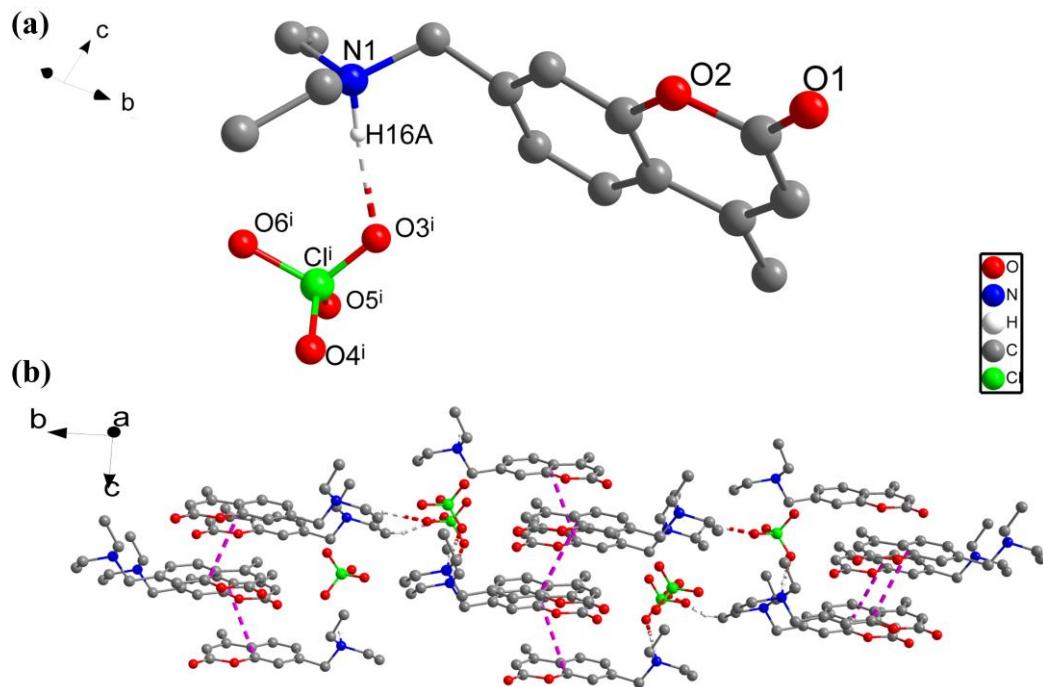


Fig. S1 (a)View of the structure of **(Et₂ChromenH)ClO₄**. (b) $\pi\cdots\pi$ interactions involving intermolecular coumarin rings. Part hydrogen atoms are omitted for clarity. Symmetry code: i) x, y, z+1.

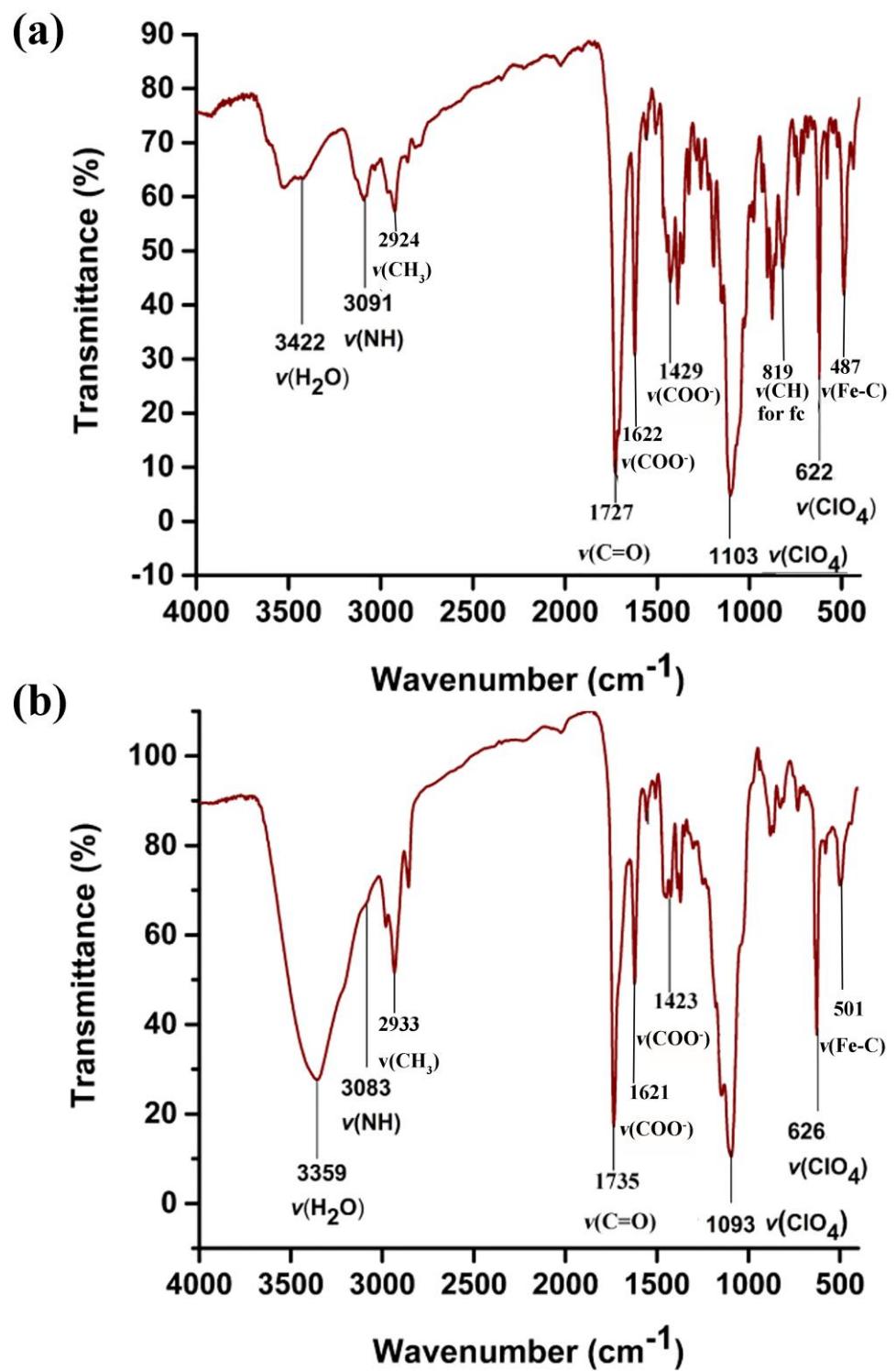


Fig. S2 The FT-IR spectra of (a) **fc1∩Eu** and (b) **fc2∩Eu**.

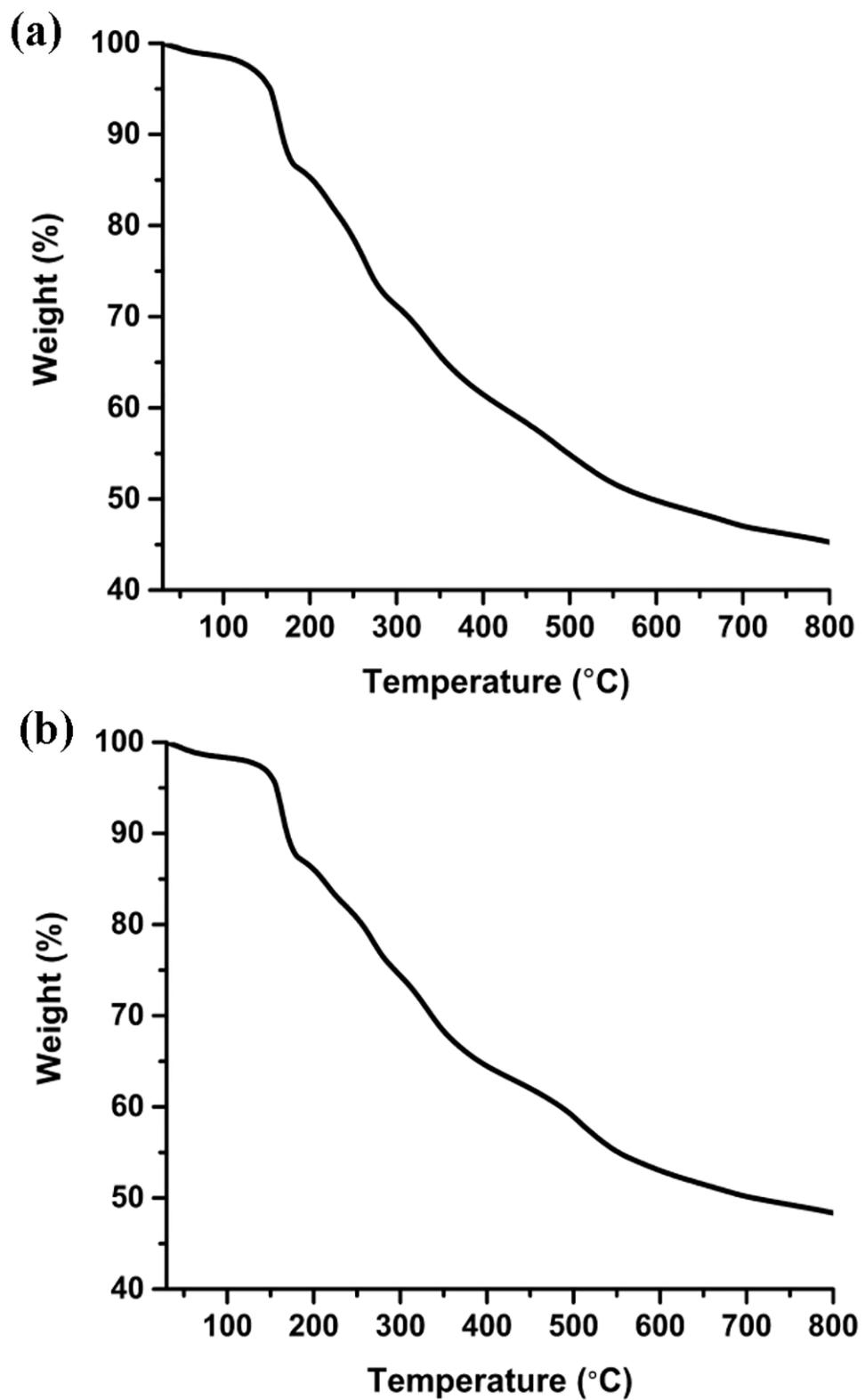


Fig. S3 TGA curves of the assemblies (a) $\text{fc1} \cap \text{Eu}$ and (b) $\text{fc2} \cap \text{Eu}$.

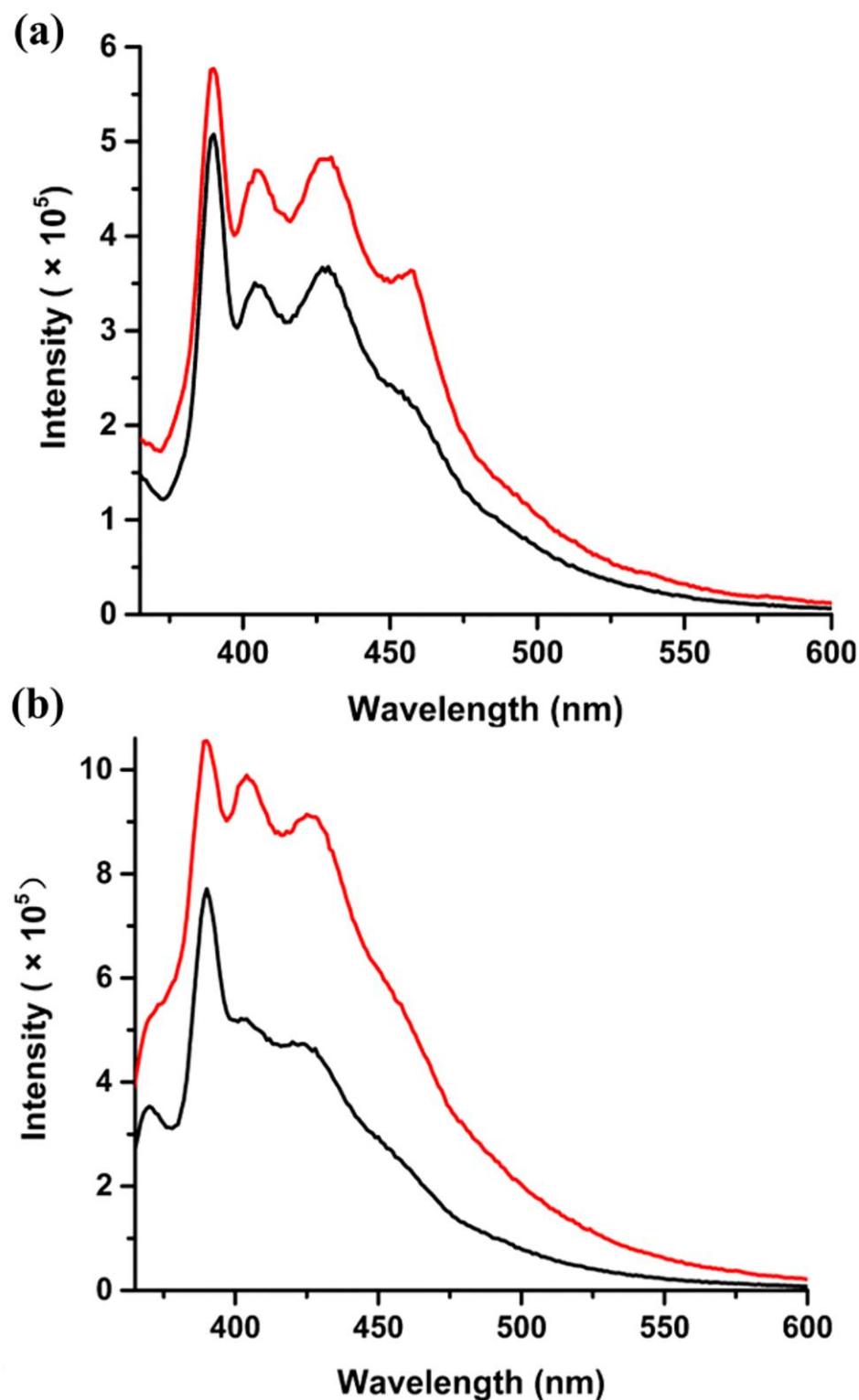


Fig. S4 (a) Emission spectra of **fc1** (black line) and protonation of **fc1** (red line) under a 365 nm excitation light. (b) Emission spectra of **fc2** (black line) and protonation of **fc2** (red line) under the same excitation light.

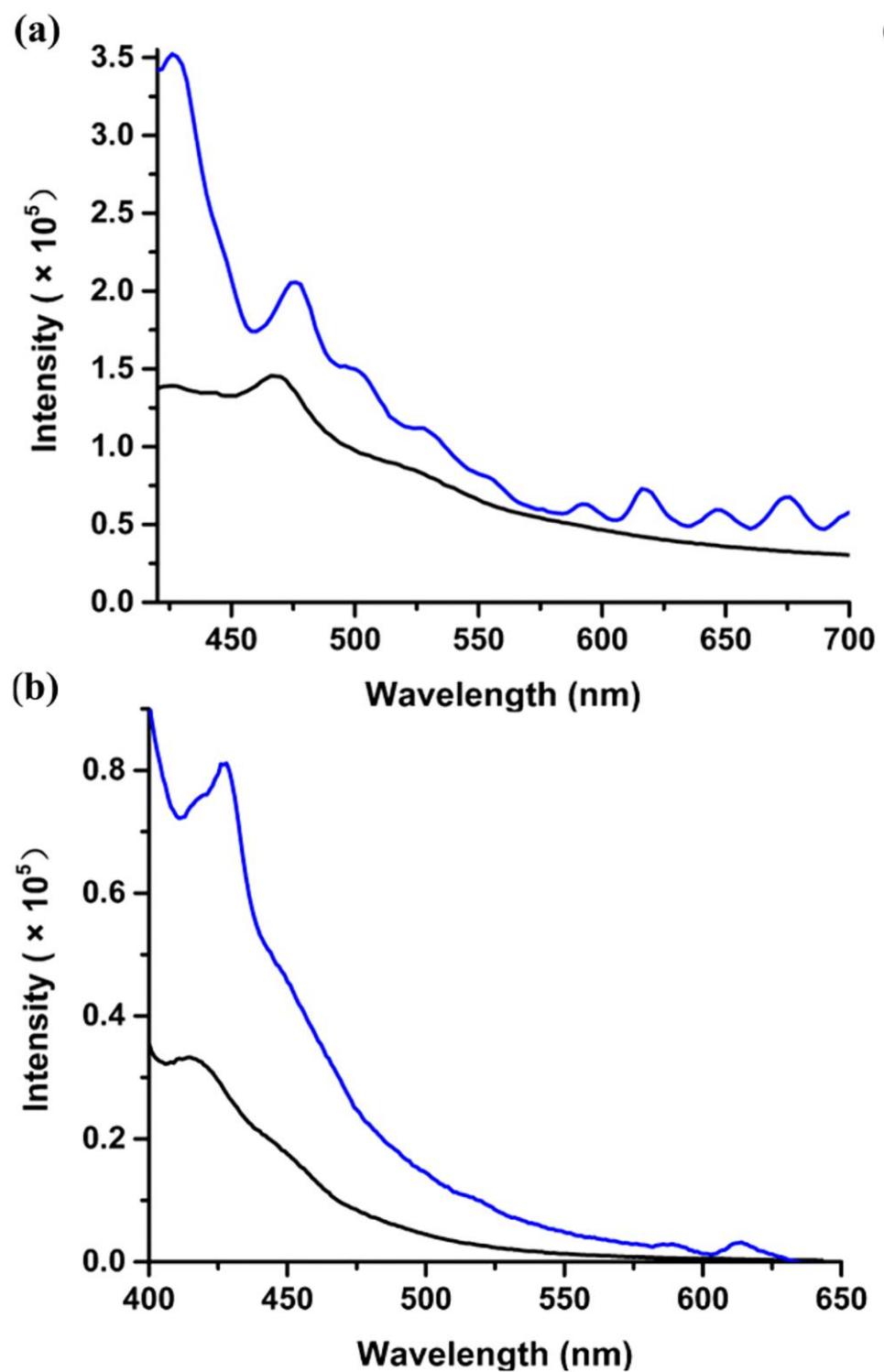


Fig. S5 (a)Emission spectra of **fc1** (black line) and **fc1** \cap **Eu**(blue line) under a 381 nm excitation light. (b) Emission spectra of **fc2** (black line) and **fc2** \cap **Eu** (blue line) under a 381 nm excitation light.

Table S1. Selected bond lengths (Å) and bond angles (°) for **fc1**, **fc2**, **fc1⁺ClO₄** CH₃CN and (**Et₂ChromenH**)ClO₄.

	fc1	fc2	fc1⁺ClO₄	CH ₃ CN(Et₂ChromenH)ClO ₄			
C1-Se1	1.891(6)	C1-Se1	1.904(3)	C1-Se1	1.898(9)	N1-H16A	0.9800
C11-Se1	1.944(6)	C11-Se1	1.962(3)	C14-Se1	1.963(8)	N1-C5	1.503(8)
Fe1-C1	2.056(6)	Fe1-C1	2.038(3)	Fe1-C1	2.114(6)	N1-C4	1.493(9)
Fe1-C6	2.065(6)	Fe1-C6	2.063(3)	Fe1-C6	2.106(6)	N1-C3	1.516(8)
C6-Se2	1.896(7)	C6-Se2	1.909(3)	C6-Se2	1.878(9)	O3 ⁱ -H16A	1.9514(3)
C14-Se2	1.963(7)	C13-Se2	1.955(3)	C11-Se2	1.945(8)	O3-Cl1	1.371(8)
N1-C12	1.456(8)	N1-C14	1.456(3)	N1-C12	1.498(9)	O4-Cl1	1.390(9)
N1-C13	1.424(8)	N1-C12	1.477(3)	N1-C13	1.493(10)	O5-Cl1	1.377(8)
N1-C15	1.460(8)	N1-C15	1.464(4)	N1-C15	1.498(10)	O6-Cl1	1.473(9)
C1-Se1-C11	103.2(3)	C1-Se1-C11	98.34(13)	C1-Se1-C14	101.9(4)	O1-C11	1.192(7)
C6-Se2-C14	101.6(3)	C6-Se2-C13	98.78(12)	C6-Se2-C11	99.1(4)	O2-C11	1.379(7)
C12-N1-C13	116.0(5)	C12-N1-C14	112.4(2)	C12-N1-C13	111.4(6)	O2-C15	1.380(6)
N1-C15-C16	112.9(5)	N1-C15-C16	113.1(2)	N1-C15-C16	108.7(6)	N1-H16A-O3 ⁱ	175.79(10)
		C18-O1-C19	121.6(3)	C18-O1-C19	120.9(7)	O3-Cl1-O4	106.6(9)
		O1-C19-O2	117.2(4)	O1-C19-O2	114.9(8)	O3-Cl1-O6	110.0(6)

Symmetry code: i) x, y, z+1.

