Supporting Information

A fluorescence-enhanced chemosensor based on mutifarene[2,2] and its recognition for metal cations

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School of Materials and Metallurgical Engineering, Guizhou Institute of Technology, Guiyang 550001, China.

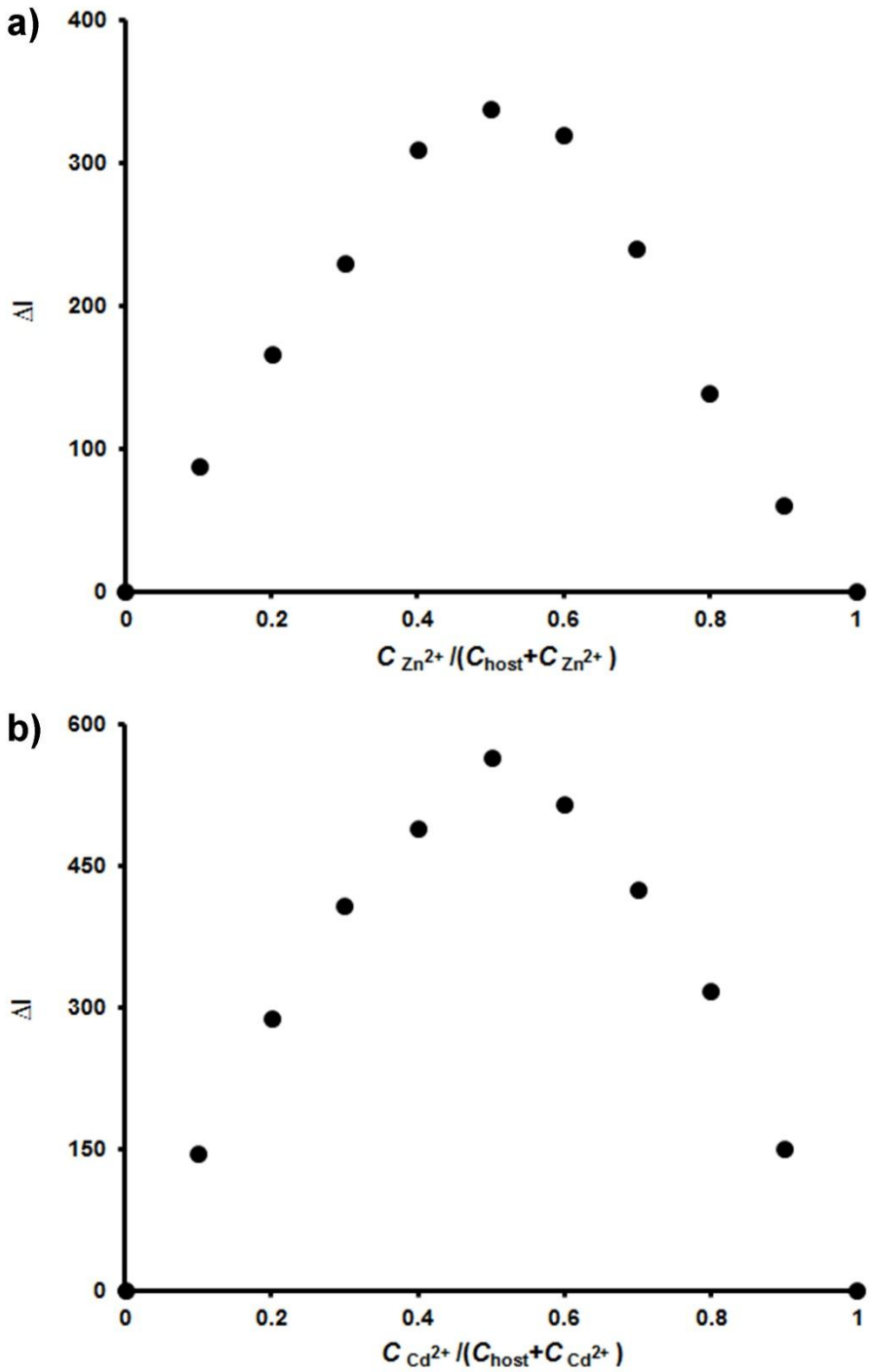

Figure S1. Job's plots of the interaction between **5** and a) Zn^{2+}; b) Cd^{2+}. The total concentration of the reactants was 2.0×10^{-5} mol·L^{-1}. (λ_{em} = 416 nm, λ_{ex} = 366 nm)

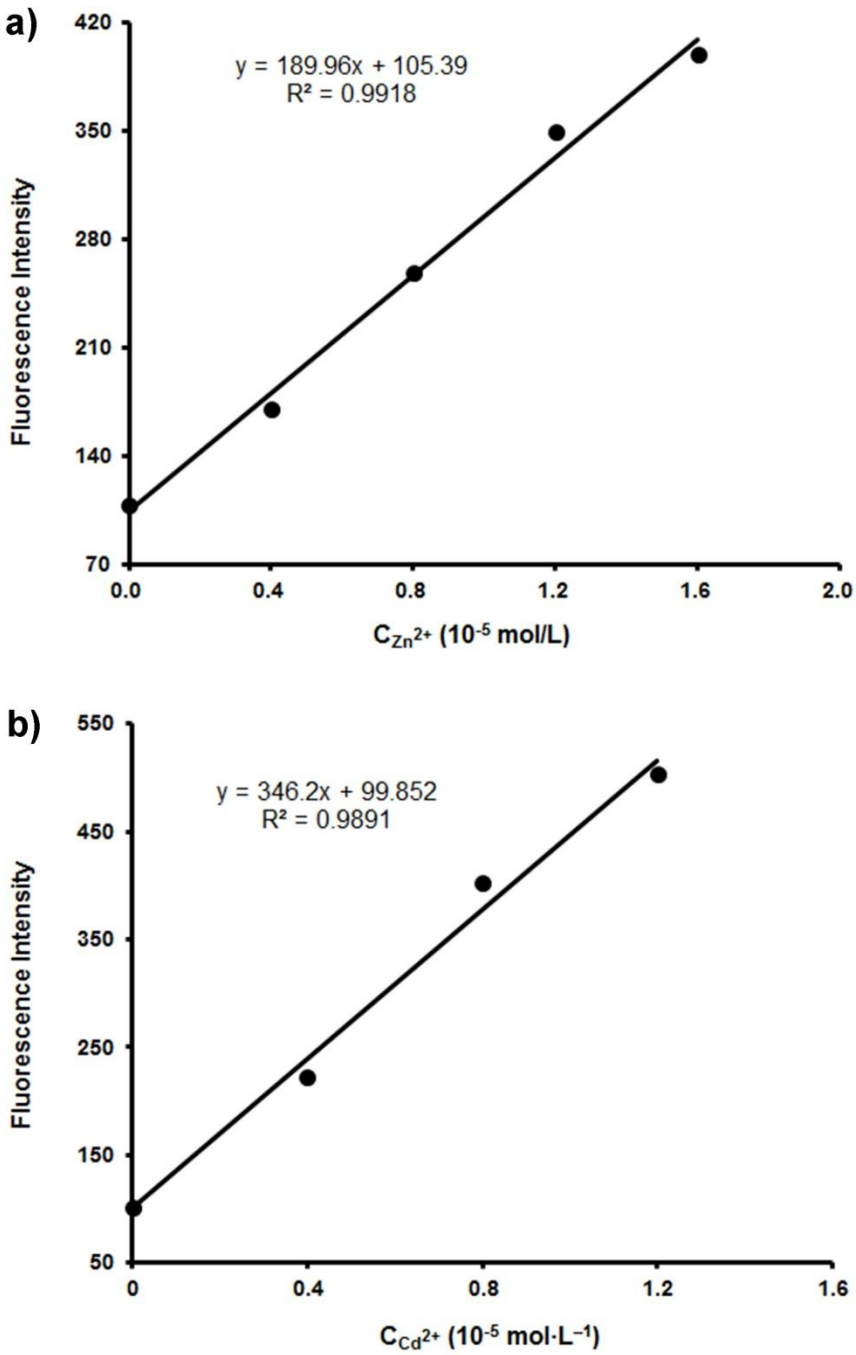

Figure S2. Linear dynamic response of **5** to a) Zn^{2+}; b) Cd^{2+}.

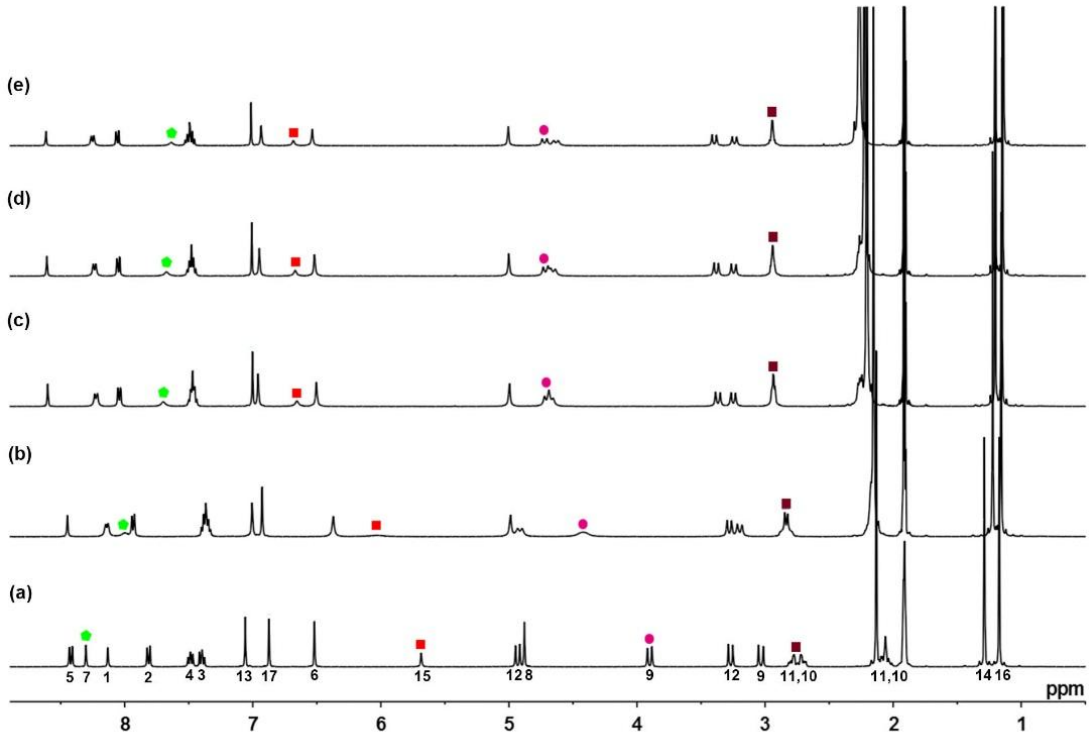

Figure S3. ^{1}H NMR titration spectra (400 MHz, CD_3CN) of **5** (5.0×10^{-3} mol·L^{-1}) in the presence of increasing amounts of Cd^{2+}. (a) Free **5**, (b c d and e) in the presence of 0.5, 1.0, 1.5, and 2.0 equiv. of Cd^{2+}, respectively.

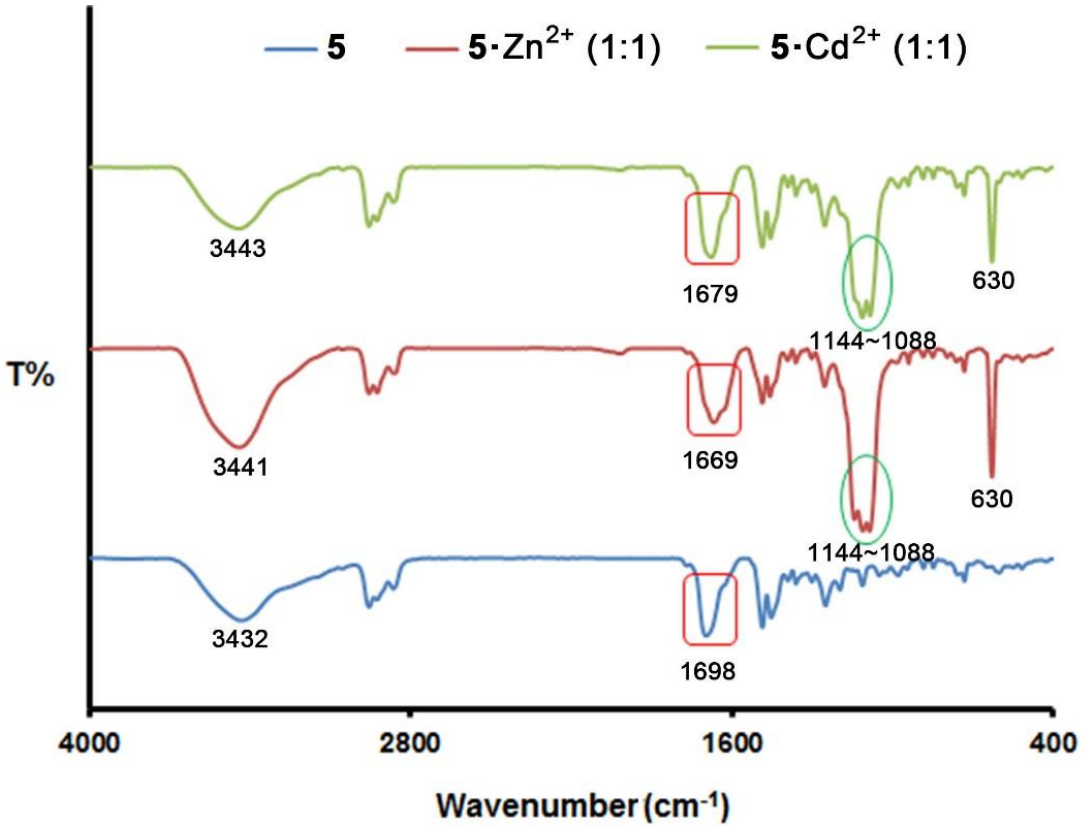

Figure S4. IR spectra of **5** and its coordination complexes with Zn^{2+} or Cd^{2+}.

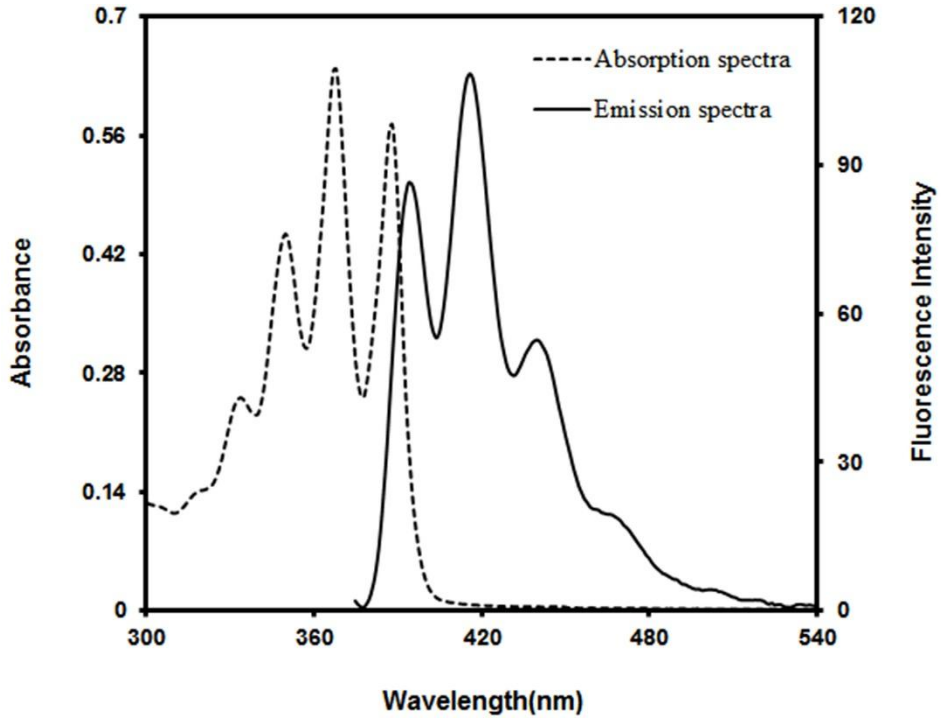

Figure S5. UV-Vis absorption (dash, 1.0×10^{-4} mol·L^{-1}) and fluorescence emission (solid, 2.0×10^{-5} mol·L^{-1}) spectra of **5** in CH_3CN.

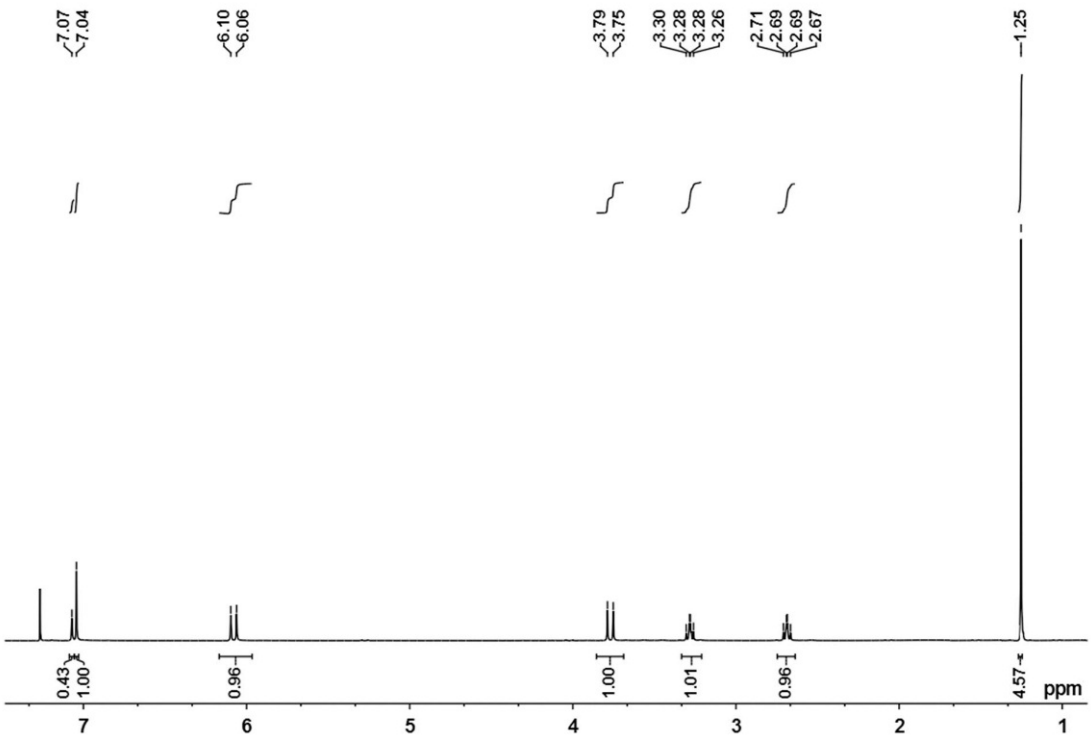

Figure S6. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of compound **1**.

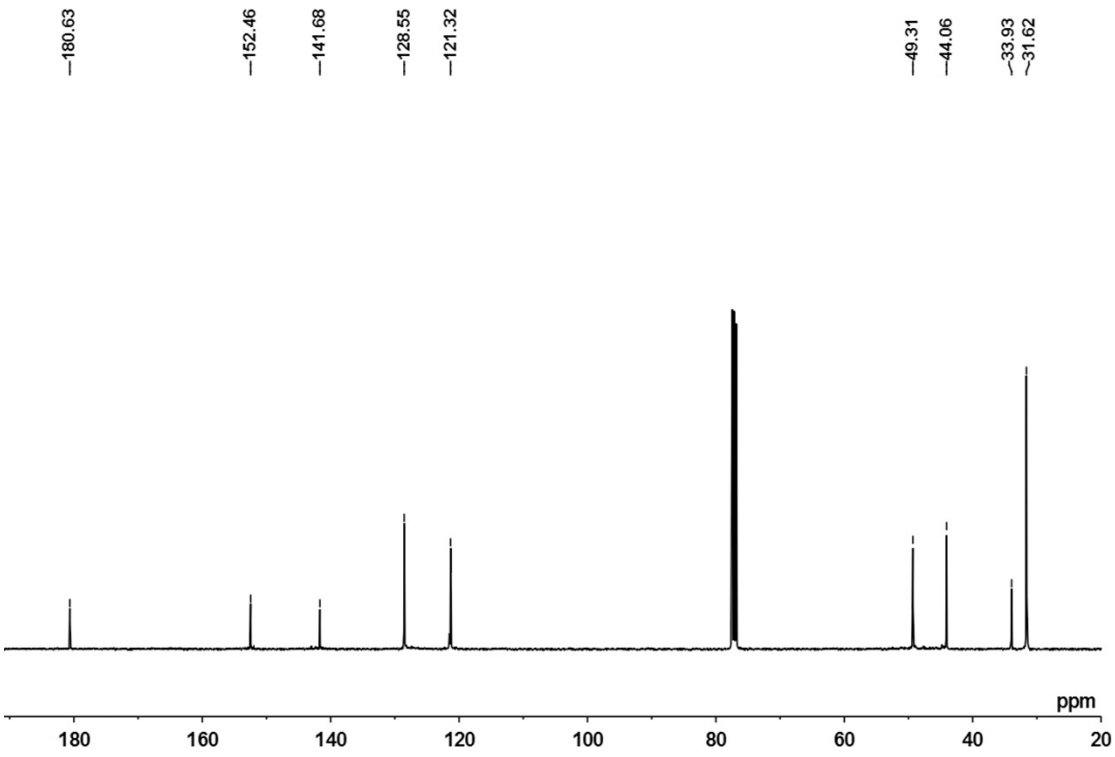

Figure S7. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of compound **1**.

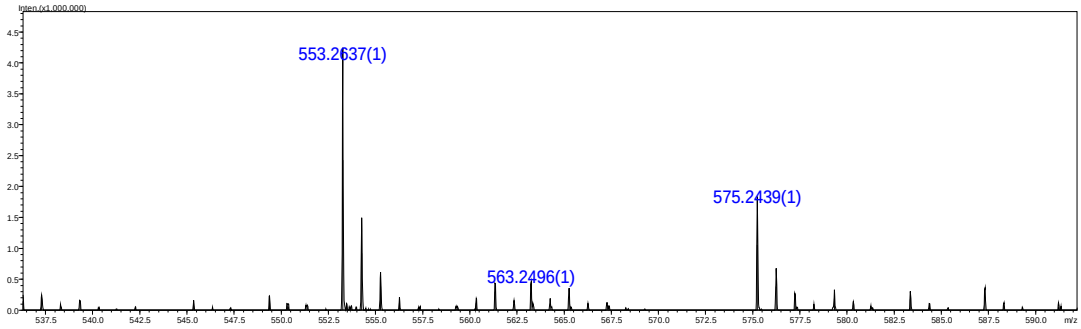

Figure S8. HRMS spectra of compound **1**.

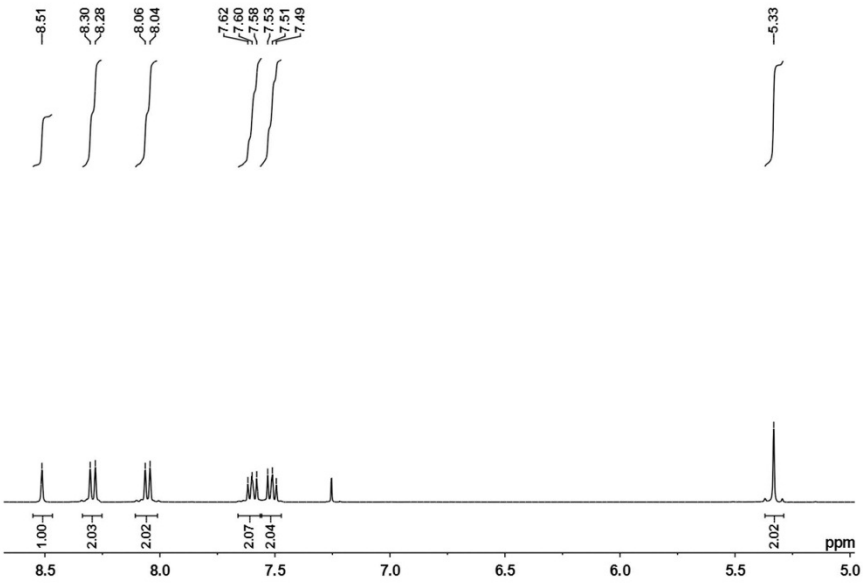

Figure S9. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of 9-azidomethylanthracene.

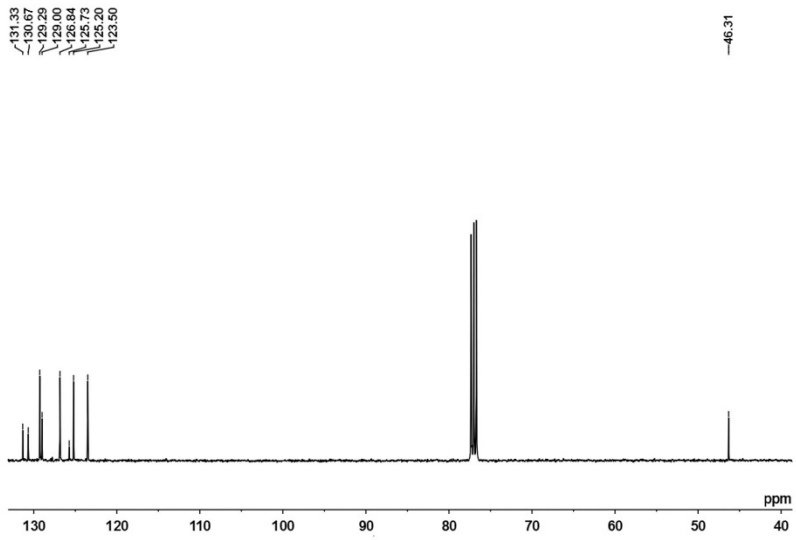

Figure S10. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of 9-azidomethylanthracene.

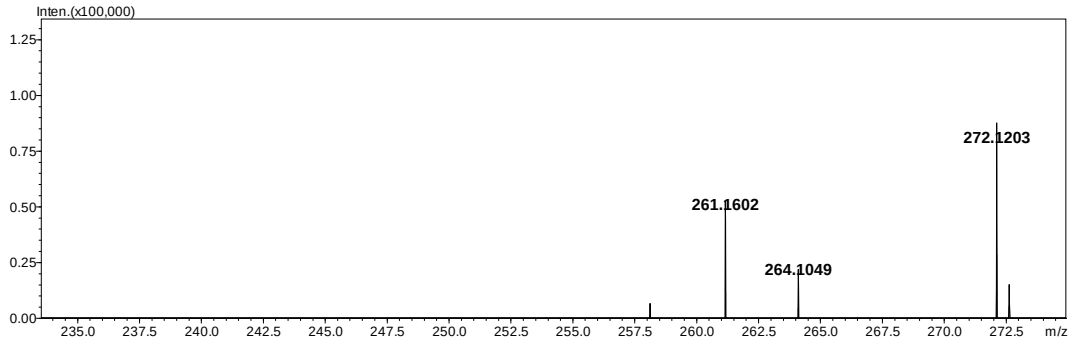

Figure S11. HRMS spectra of 9-azidomethylanthracene.

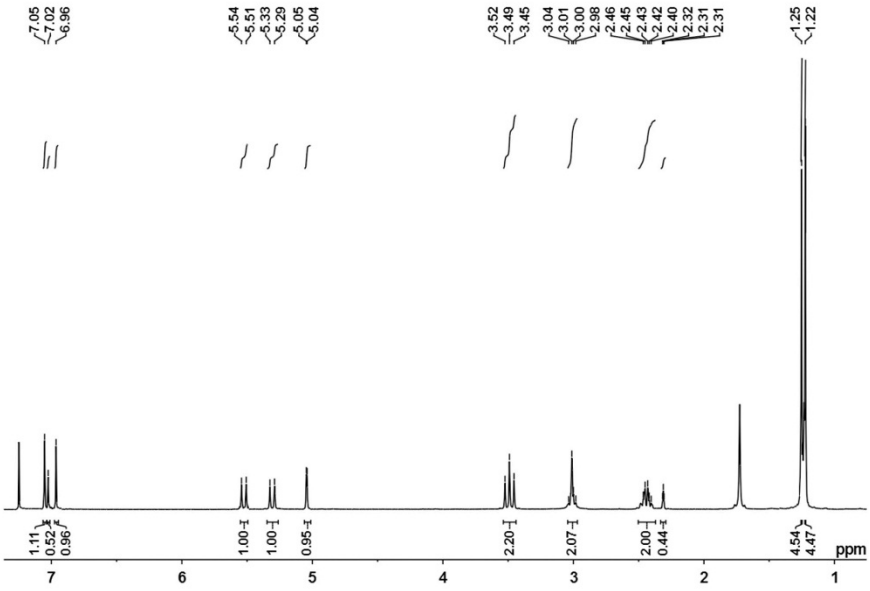

Figure S12. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of compound **2**.

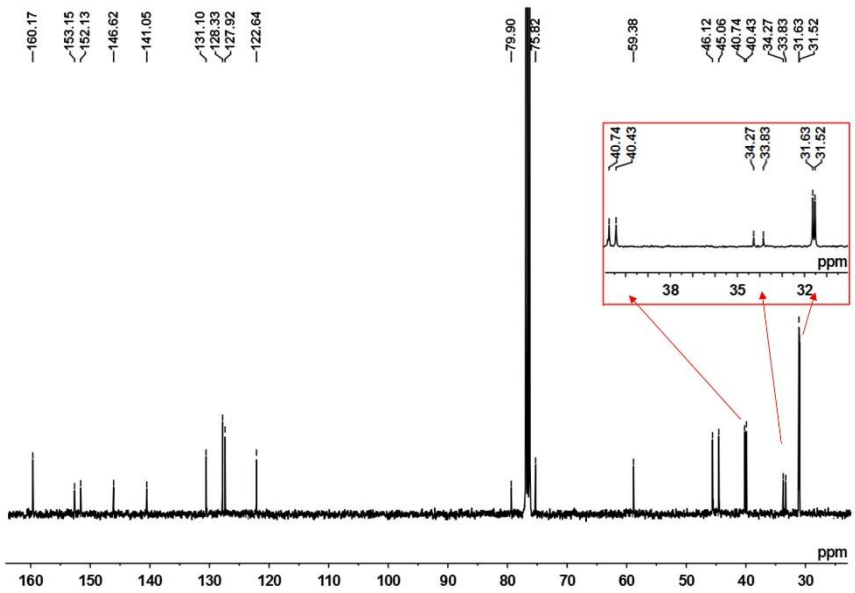

Figure S13. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of compound **2**.

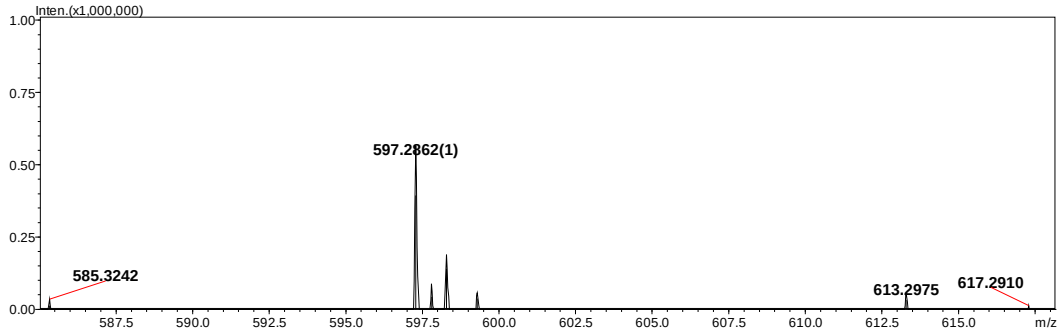

Figure S14. HRMS spectra of compound **2**.

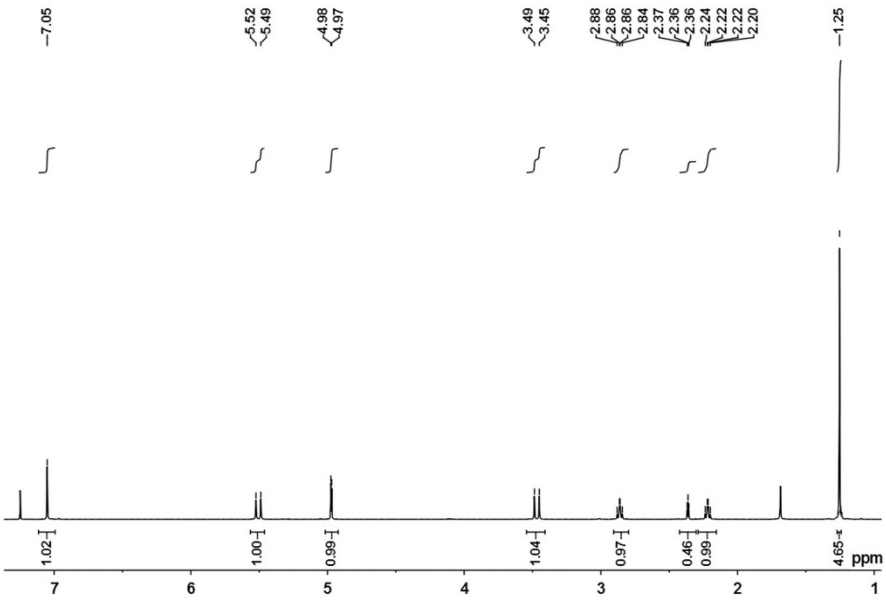

Figure S15. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of compound **3**.

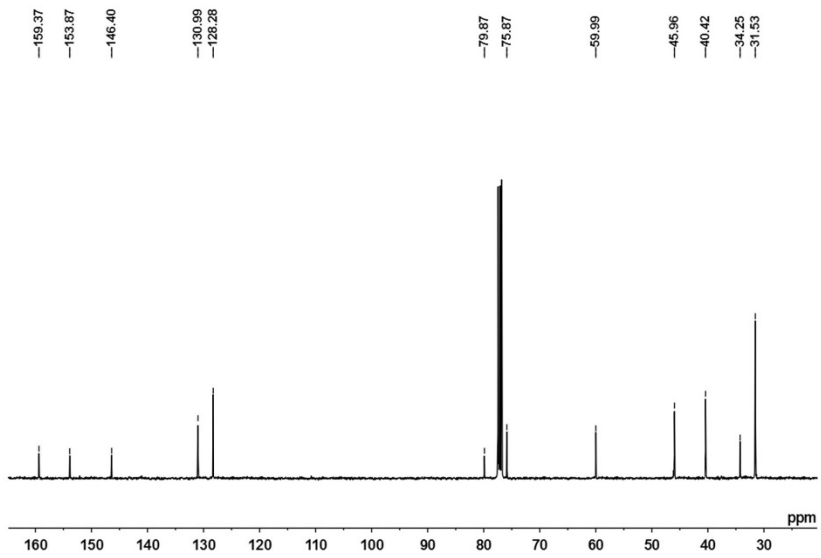

Figure S16. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of compound **3**.

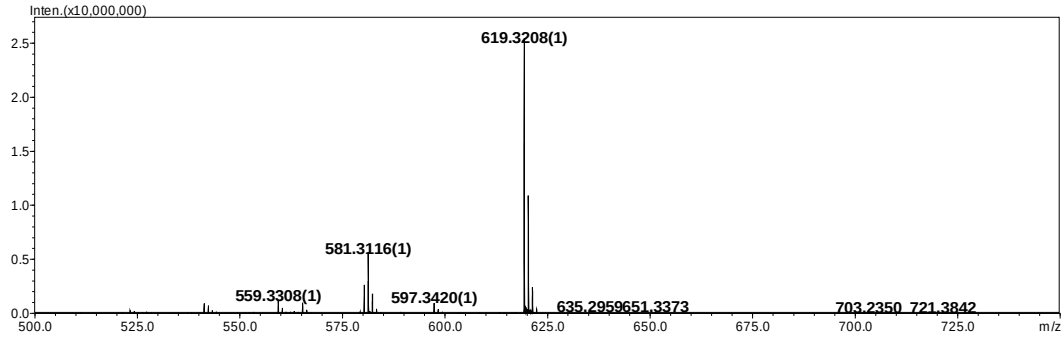

Figure S17. HRMS spectra of compound **3**.

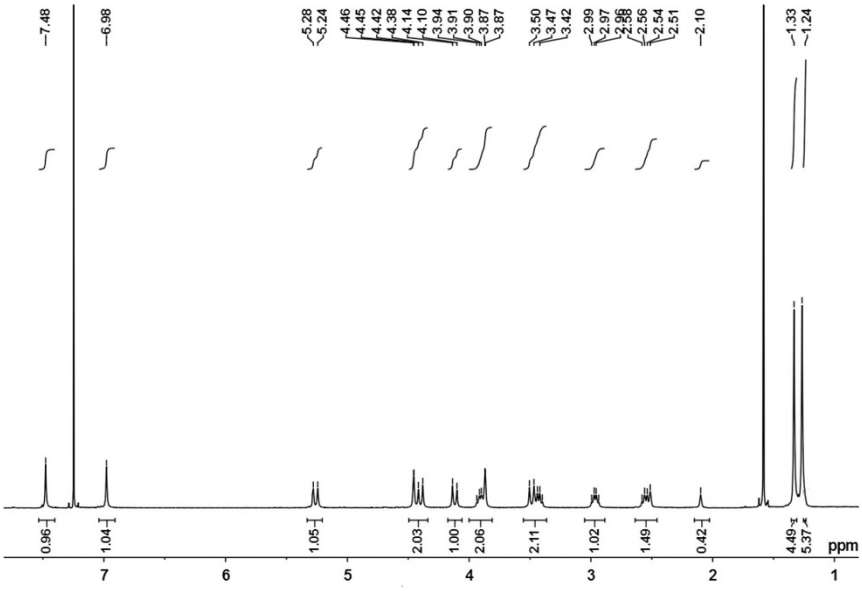

Figure S18. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of compound **4**.

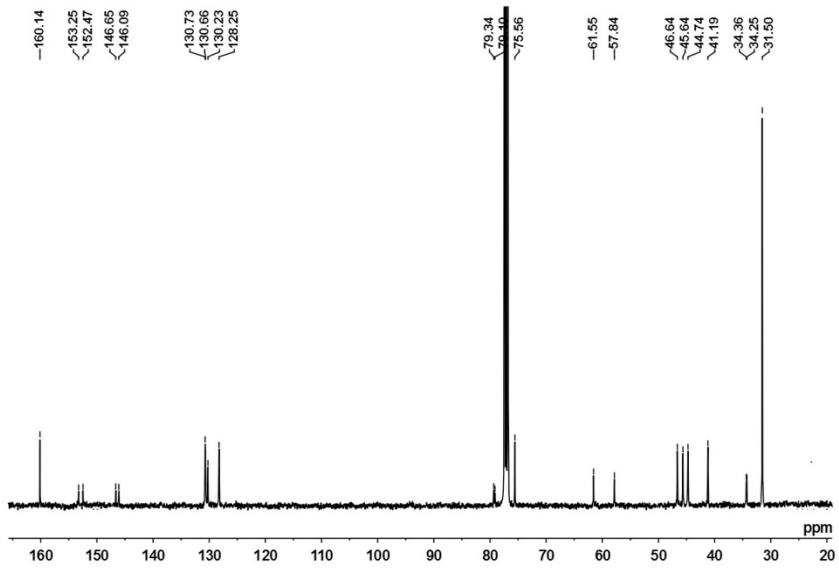

Figure S19. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of compound **4**.

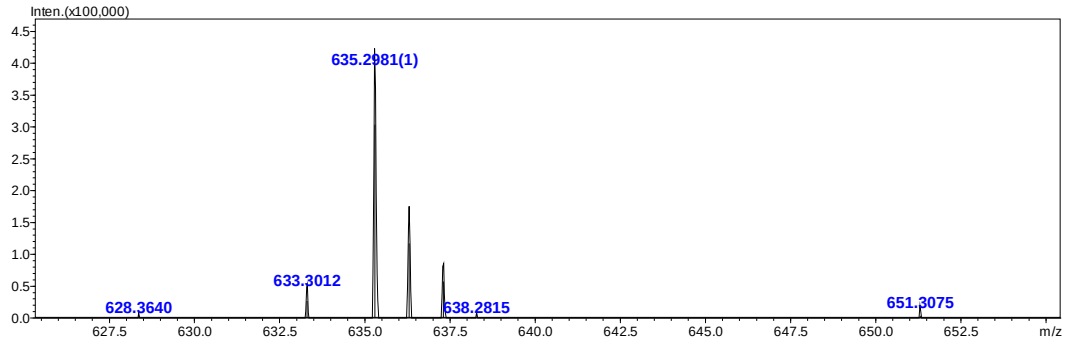

Figure S20. HRMS spectra of compound **4**.

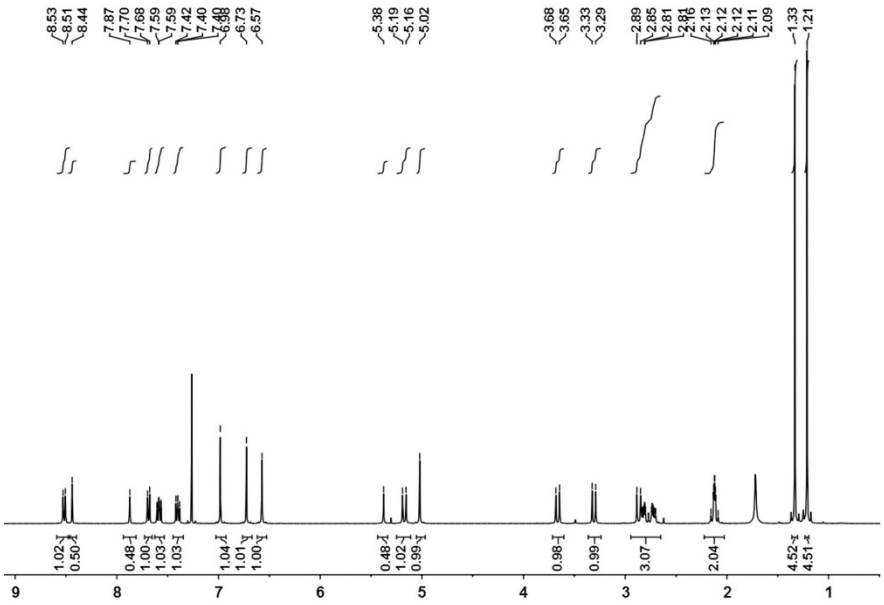

Figure S21. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of compound **5**.

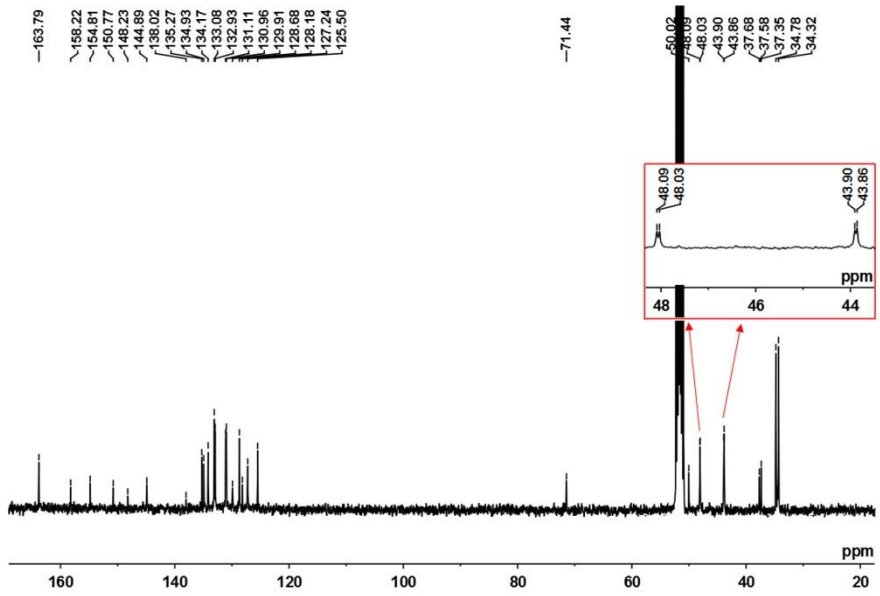

Figure S22. ^{13}C NMR spectra (400 MHz, CD_3OD) of compound **5**.

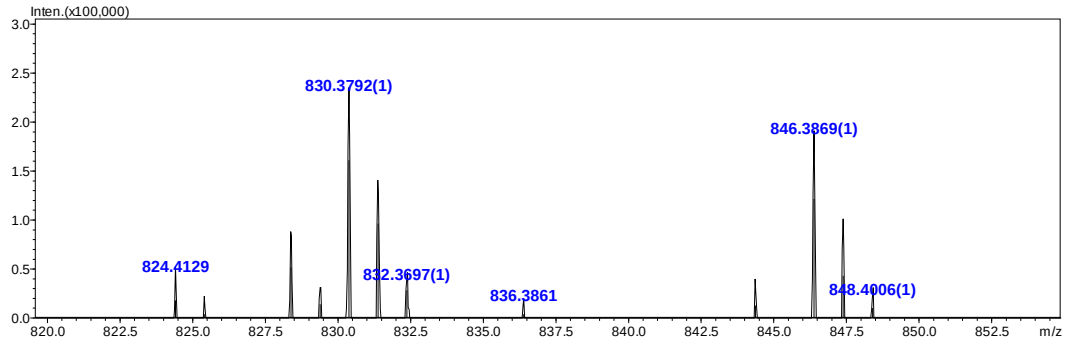

Figure S23. HRMS spectra of compound **5**.

Coordinates of the optimized structures

1.Compound **5**

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
S	0.64471500	-0.30930200	-3.14527100
S	-0.76598500	0.45021800	3.68949900
O	-0.67396500	-1.57877300	0.23316100
O	-1.53568700	1.19868700	0.24428300
N	-1.77176800	0.82798200	-2.63375700
N	-1.78602600	-1.38862300	-2.56195800
N	-2.78233600	-0.96414600	2.53969300
N	-3.12336000	1.22618100	2.56093600
C	-0.99182400	-0.28358800	-2.74638200
C	-3.18741400	0.48453500	-2.57223900
H	-3.66517800	0.65198100	-3.54896700
H	-3.70848000	1.09078700	-1.82877400
C	-3.15135600	-1.00436900	-2.20004600
H	-3.32357200	-1.15156600	-1.12792700
H	-3.88867200	-1.59453100	-2.75413300
C	-1.26248700	-2.72322900	-2.27096300
H	-0.17366900	-2.62422800	-2.27258000
H	-1.53438200	-3.41086900	-3.08230200
C	-1.78876000	-3.29227700	-0.96162500
C	-1.51446700	-2.66464400	0.26608700
C	-2.18087000	-3.08104700	1.43807200
C	-2.98954900	-4.21961900	1.36843100
H	-3.48570600	-4.53735700	2.28214400
C	-3.20497200	-4.93656600	0.18224600
C	-2.62031500	-4.41880000	-0.97797500
H	-2.80544300	-4.89037300	-1.93720700
C	-4.08689300	-6.19878200	0.19050000
C	-3.47148500	-7.24498300	1.14989000
H	-3.39613600	-6.86406400	2.17264200
H	-2.46544300	-7.52962700	0.82521000
H	-4.08914300	-8.14972400	1.17574400
C	-4.20280700	-6.83830400	-1.20592400
H	-4.67379800	-6.16266400	-1.92748700
H	-4.82155300	-7.73942700	-1.14832100
H	-3.22531200	-7.13349400	-1.60081700
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H	-5.50567400	-5.42023300	1.68576600
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H	-5.97539300	-5.10069300	0.01064000
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H	-2.71120400	-2.83115700	3.49848900
H	-1.16634200	-2.07813000	3.11816800
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C	-4.17341400	-0.81719200	2.12683300
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H	-4.13613800	0.87676500	0.74251200
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H	-1.74747700	2.70952400	2.86588700
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H	-5.82944200	7.22076100	-0.77510000
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H	-2.60815900	6.86623500	-2.62797100
H	-4.13124200	7.75122000	-2.49779900
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H	1.01540100	-2.67364000	0.80098000
C	1.50298000	-0.63954600	0.37658800
C	2.80005800	-0.75387000	-0.07128300

N	1.14015200	0.66797800	0.25381600
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H	4.30546800	2.07157700	-1.05411300
C	5.63999500	0.49585300	-0.40325600
C	6.38029500	-0.57668600	-0.95608800
C	6.07772100	1.13856900	0.78026500
C	5.96851800	-1.31397100	-2.11655800
C	7.62108600	-0.97732100	-0.32674800
C	7.31879300	0.72809200	1.39509700
C	6.72197400	-2.34402300	-2.61626100
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H	9.31099100	-2.33002300	-0.39966300
H	8.99376800	-0.61225000	1.28302400
H	8.53268300	-3.53517700	-2.41464100
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C	7.03569900	2.39745300	3.14514300
H	7.38467900	2.89201300	4.04647300
C	5.80290900	2.79409900	2.55559900
H	5.21760700	3.58156800	3.02058700
C	5.33921700	2.18948400	1.41579600
H	8.70827000	1.07048900	3.02196000
H	4.38137400	2.49736800	1.01281700
H	3.47404900	-1.59077300	-0.15532400

Total energy: -3191.7530147 a.u.

2. **5**·Zn^{2+}

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
S	0.09152800	-1.71570000	1.57886200
S	-0.55306700	-0.45892800	-3.00030300
O	0.41726400	1.18950400	-0.22644300
O	-1.92062900	-2.34468200	-0.63718500
N	-2.47073000	-1.54510000	2.49317700
N	-1.33904200	0.33049500	2.65562300
N	-2.14872900	1.69745000	-2.54347500
N	-3.24148300	-0.19757100	-2.75252300
C	-1.30583600	-0.94044600	2.24280200
C	-3.45338400	-0.59897800	3.02895800
C	-2.60182000	0.63727800	3.33292500
C	-0.28562300	1.33635700	2.54047900
C	-0.70215900	2.38214200	1.52703200
C	-0.46188500	2.19825800	0.17159200
C	-1.06686600	3.00273100	-0.79254800
C	-1.81971000	4.08511700	-0.35513100
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C	-4.12196100	-2.10645300	-1.52412800
C	-3.29201400	-2.38999300	-0.44337000
C	-3.81774700	-2.71044900	0.80314100
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C	-6.07188800	-2.58250100	-0.12545200
C	-5.49524100	-2.21189100	-1.34333500
C	-7.59316600	-2.70381600	-0.00235000
C	-8.09781400	-3.75324200	-1.00948600
C	-8.23391200	-1.33818600	-0.31097900
C	-8.02336900	-3.13511200	1.40459800
C	-2.92118500	-2.85161200	2.01786000
C	1.78098700	1.64391100	-0.35598100
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C	3.99466200	0.33357400	-0.83101100
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C	5.94038300	-3.19342200	2.55149600
C	7.90083800	-1.84733600	2.90784900
C	8.63875500	-0.31688100	1.13466600
C	7.02537100	-2.77816200	3.36960500
C	9.40866800	1.26266400	-0.57804900
C	9.26563500	1.83698900	-1.80052400
C	8.19820300	1.43387400	-2.64771500
C	7.31764400	0.47125600	-2.25826500
Zn	0.01750200	-0.90846000	-0.72740200
H	-1.50214900	-2.95404800	-0.01767500
H	-3.92974900	-1.01383600	3.91786600
H	-4.22262100	-0.40591900	2.27564000
H	-3.03802000	1.55341100	2.93401100
H	-2.41714800	0.76895900	4.40264200
H	0.63356100	0.82167500	2.26541900
H	-0.14133600	1.79009100	3.52404200
H	-2.27218900	4.72603600	-1.10499900
H	-1.62133700	3.64065500	2.98000800
H	-2.09761500	6.84380700	-0.24116500
H	-1.15942100	6.98037800	1.25312300
H	-2.74898300	7.74385700	1.12733800
H	-3.46196000	4.87644700	3.38512300
H	-3.53830800	6.62088700	3.17206000
H	-1.97376500	5.85149400	3.40354000
H	-4.25298100	5.42123200	-0.26877300
H	-4.86794400	6.31482000	1.11794600
H	-4.75105700	4.55266500	1.19541400
H	-1.20072400	3.51640300	-2.87942200
H	-0.13407100	2.14174700	-2.57143900
H	-3.80870700	2.91231900	-3.00919600
H	-3.70157300	2.41105900	-1.31035200
H	-5.03024200	0.52383600	-1.89850700
H	-4.82956400	0.85153500	-3.63236900

H	-2.61892800	-2.14477500	-3.08521600
H	-4.25696600	-1.77795100	-3.64535400
H	-5.59944700	-3.08463200	1.90753300
H	-6.13654400	-2.01087000	-2.19598800
H	-7.63985100	-4.72786400	-0.82280700
H	-7.88152600	-3.47059000	-2.04287200
H	-9.18090400	-3.86532200	-0.91959500
H	-7.88345800	-0.57292200	0.38820300
H	-9.32046900	-1.40604000	-0.21808400
H	-8.01340600	-1.00275000	-1.32805500
H	-7.61230000	-4.11184000	1.67440800
H	-9.11115300	-3.22020300	1.44215400
H	-7.72973900	-2.40560400	2.16563700
H	-2.03803800	-3.47117800	1.85234500
H	-3.47526500	-3.32335000	2.83142100
H	1.82644500	2.40435400	-1.14108000
H	2.09295800	2.10011300	0.58773800
H	4.82015100	1.01899000	-0.73220400
H	5.24216700	-2.72184500	-1.28031000
H	5.67244500	-1.51656600	-2.47580400
H	4.92274100	-3.02469100	0.71528500
H	5.24454600	-3.93364600	2.92948900
H	8.73348600	-1.51937100	3.52032500
H	9.45818500	0.00124500	1.77165200
H	7.14971700	-3.20955600	4.35526500
H	10.21770100	1.55850900	0.08068100
H	9.96059200	2.59625400	-2.13719900
H	8.09114000	1.89660600	-3.62196400
H	6.52449000	0.19462400	-2.94285600

Total energy: -3256.9546298 a.u.

3. **5**·Cd^{2+}

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
S	0.26663400	-1.89323200	1.24320800
S	-1.01812700	-0.27257400	-3.42009900
O	0.50085600	1.21147500	-0.63129800
O	-2.09870100	-2.35976900	-0.76280400
N	-2.16512300	-1.55015700	2.42124300
N	-0.91560400	0.25786900	2.42639300
N	-2.41304800	1.87274200	-2.48621400
N	-3.58180900	0.01185100	-2.56839600
C	-0.99813100	-1.01903400	2.03398900
C	-3.02545200	-0.53748900	3.03823300
C	-2.05966500	0.62545700	3.26515300
C	0.17600900	1.20620900	2.20150200
C	-0.32348000	2.32911800	1.31445300
C	-0.28819000	2.21208100	-0.06981200
C	-1.01132700	3.07554900	-0.89194300
C	-1.64298900	4.16029500	-0.29580500
C	-1.60780200	4.39181800	1.08231600
C	-0.96726400	3.43632400	1.86759000
C	-2.29453500	5.62868100	1.66601800
C	-1.66838500	6.88900000	1.04121100
C	-2.13841500	5.71051000	3.18886300
C	-3.79649800	5.57436600	1.32989300
C	-1.25981700	2.76353900	-2.35571800
C	-2.38398000	0.56157700	-2.76896900
C	-3.72659500	2.26398600	-1.96425200
C	-4.58563200	1.03125100	-2.25834500
C	-3.94824900	-1.39930000	-2.67997600
C	-4.37491300	-1.91956800	-1.32642100
C	-3.42920400	-2.29956500	-0.37899000
C	-3.79669300	-2.61143200	0.92510500
C	-5.15405900	-2.62658900	1.24704700
C	-6.14319800	-2.31969900	0.31728700
C	-5.71443500	-1.94677600	-0.95966700
C	-7.63935600	-2.36566600	0.63921800
C	-8.31320000	-3.39299000	-0.28901600
C	-8.25346900	-0.97323100	0.40672000
C	-7.90324600	-2.77580900	2.09266500
C	-2.75153900	-2.82299800	2.00488700
C	1.81151900	1.67550300	-1.02269400
C	2.69718600	0.49109400	-1.23319500

C	4.06141600	0.36641700	-1.19330700
N	2.19676000	-0.73053900	-1.53465400
N	3.16486100	-1.59281300	-1.67366200
N	4.28559900	-0.93410700	-1.48045600
C	5.58824800	-1.62815500	-1.54893100
C	6.48439700	-1.20416900	-0.41815300
C	6.29364200	-1.78340900	0.85128800
C	7.47578500	-0.22691400	-0.62841400
C	5.26427300	-2.73794200	1.13302300
C	7.15870100	-1.40750100	1.92835600
C	8.33158800	0.14012900	0.46338200
C	5.12765200	-3.28020900	2.37480100
C	6.98533300	-2.00522500	3.21386500
C	8.15783500	-0.46444300	1.70377700
C	6.00109600	-2.91566900	3.43443700
C	9.34826700	1.12441500	0.26367600
C	9.50834100	1.73199800	-0.94014100
C	8.65522700	1.38605100	-2.02297600
C	7.68097200	0.44632500	-1.87723500
Cd	-0.05377900	-1.03316400	-1.19879000
H	-1.64157400	-2.97944100	-0.18147100
H	-3.45704100	-0.91944200	3.96385800
H	-3.83748100	-0.27999900	2.35150000
H	-2.47716300	1.58194700	2.95166900
H	-1.73322800	0.70468200	4.30641200
H	1.00824800	0.66069900	1.76031500
H	0.49683200	1.59384500	3.17190600
H	-2.18694000	4.84738300	-0.93615800
H	-0.95341700	3.54702300	2.94557500
H	-1.80314500	6.92065000	-0.04289900
H	-0.59734000	6.94247300	1.25224200
H	-2.13946000	7.78294900	1.45649900
H	-2.60698400	4.86190600	3.69704900
H	-2.62803700	6.61456600	3.55573200
H	-1.08828500	5.76572200	3.48918300
H	-3.97637000	5.57953700	0.25155300
H	-4.30407400	6.44618200	1.74899000
H	-4.26217000	4.67882300	1.75262400
H	-1.47585900	3.68227700	-2.90512900
H	-0.41655100	2.27169800	-2.83707000
H	-4.08596400	3.16073300	-2.47041000
H	-3.65406300	2.47197500	-0.89298300
H	-5.19446500	0.72753600	-1.40636400
H	-5.23677900	1.17094800	-3.12598500

H	-3.08754800	-1.93658900	-3.07499800
H	-4.76599300	-1.48856600	-3.39932500
H	-5.43056000	-2.89018100	2.26123000
H	-6.45052500	-1.67627200	-1.71015700
H	-7.88448900	-4.38820500	-0.14673200
H	-8.20528300	-3.12656700	-1.34349600
H	-9.38243000	-3.45009400	-0.07126800
H	-7.78640400	-0.22464300	1.05393900
H	-9.32209800	-0.99367500	0.63313600
H	-8.14757200	-0.64548800	-0.63098900
H	-7.51062600	-3.77241900	2.31277500
H	-8.97985600	-2.80623200	2.27135200
H	-7.47659700	-2.06260700	2.80489100
H	-1.93652600	-3.48996300	1.71737400
H	-3.21756900	-3.27438000	2.88261900
H	1.71579800	2.26428400	-1.94035000
H	2.21078200	2.31999800	-0.23589000
H	4.86186600	1.05680800	-0.98389900
H	5.35465900	-2.69049700	-1.51894200
H	6.02012600	-1.42290300	-2.52577900
H	4.57458600	-3.04632100	0.35668900
H	4.34746000	-4.01005600	2.55863000
H	7.66332500	-1.71840900	4.01019000
H	8.81712900	-0.18821700	2.52078300
H	5.88098700	-3.37118200	4.40978100
H	9.99217700	1.37599000	1.09921600
H	10.28246200	2.47562400	-1.08376000
H	8.79138800	1.87308800	-2.98158200
H	7.06263500	0.21273500	-2.73564400

Total energy: -3239.4129483 a.u.