

Interaction of a dinuclear fluorescent Cd(II) complex of calix[4]arene conjugate by phosphates and its applicability in cell imaging

V.V. Sreenivasu Mummidivarapu, Vijaya Kumar Hinge and Chebrolu Pulla Rao*

^aDepartment of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India

E-mail cprao@iitb.ac.in

Supporting Information

SI01. Synthesis and characterization of L	2
SI02. Synthesis and characterization of [Cd L] ₂	3
SI03. Preliminary crystallographic data for [Cd L] ₂	5
SI04. Fluorescence studies of [Cd L] ₂ in buffer	13
SI05. Fluorescence and absorption titration details	13
SI06. Fluorescence studies of [Cd L] ₂ with anions	14
SI07. Dilution experiment by maintaining the ratio of [Cd L] ₂ :H ₂ PO ₄ ¹⁻ as 1:2	15
SI08. Fluorescence studies of [Cd L] ₂ with Na ⁺ counter cation	16
SI09. Absorption titration studies of [Cd L] ₂ with anions	17
SI10. ¹ H NMR titration studies of [Cd L] ₂ with phosphates	18
SI11. ESI MS titration studies of [Cd L] ₂ with phosphates	20
SI12. Minimized structures and metric data of [Cd LX] ₂ complexes	22
SI13. Cartesian coordinates for MM minimized structure of [Cd LH PO ₄ ²⁻] ₂	26
SI14. Cartesian coordinates for MM minimized structure of [Cd LH ₂ PO ₄ ⁻] ₂	31
SI15. Cartesian coordinates for MM minimized structure of [Cd L PPi ⁴⁻] ₂	36
SI16. Cartesian coordinates for MM minimized structure of [Cd L AMP ²⁻] ₂	41
SI17. Cartesian coordinates for MM minimized structure of [Cd L ADP ²⁻] ₂	46
SI18. Cartesian coordinates for MM minimized structure of [Cd L ATP ²⁻] ₂	51
SI 19. Details of cell culture studies	57

SI01. Synthesis and characterization of L

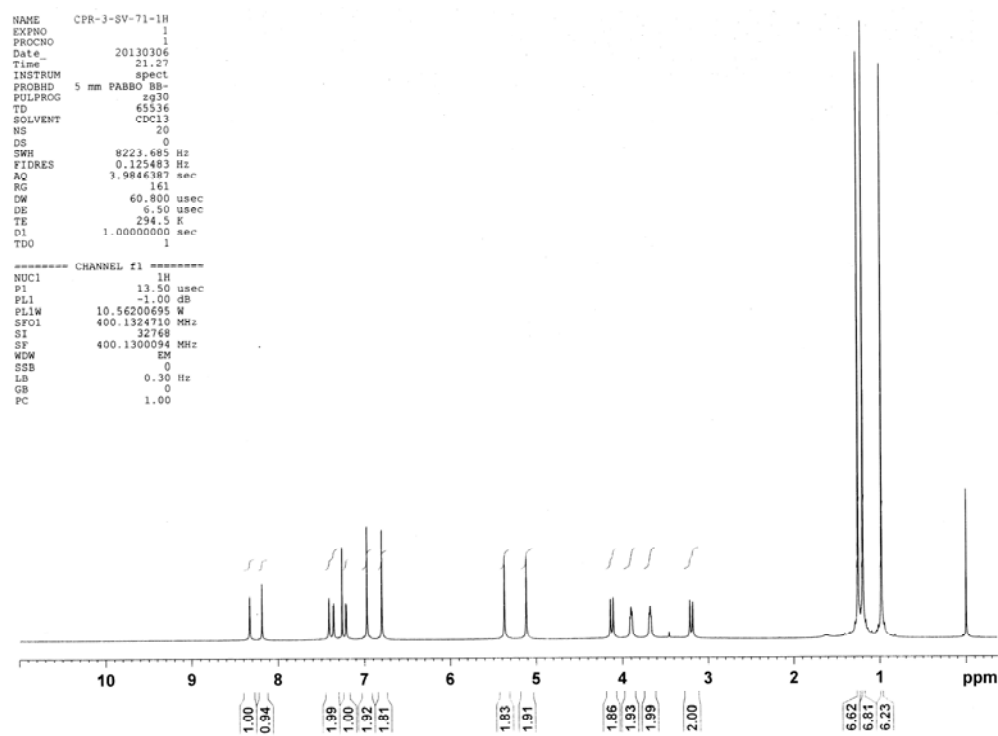


Figure S01 ^1H NMR spectrum (CDCl_3 , 400 MHz) of compound **L**.

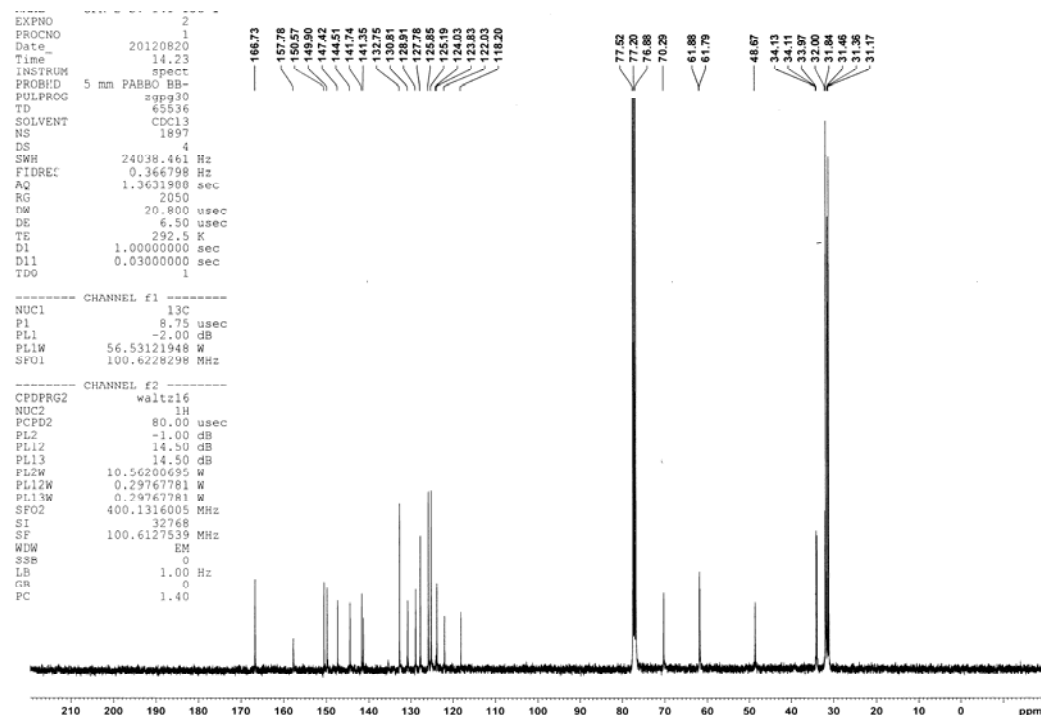


Figure S02 ^{13}C NMR spectrum (CDCl_3 , 100 MHz) of **L**

Single Mass Analysis (displaying only valid results)

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 200.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

66 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Waters(Micromass) : Q-ToF micro(YA-105)

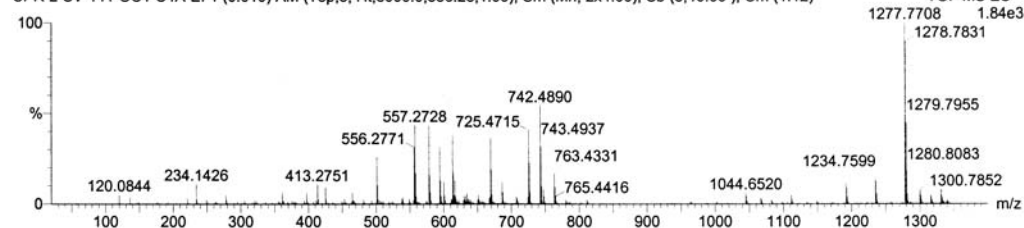
Dept. Of Chemistry - I.I.T.(B)

19-Aug-2012 17:04:32

C78H100N8O8

CPR-2-SV-141-OC1-C4A-EI 1 (0.010) AM (Top,5, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00); Cm (1:12)

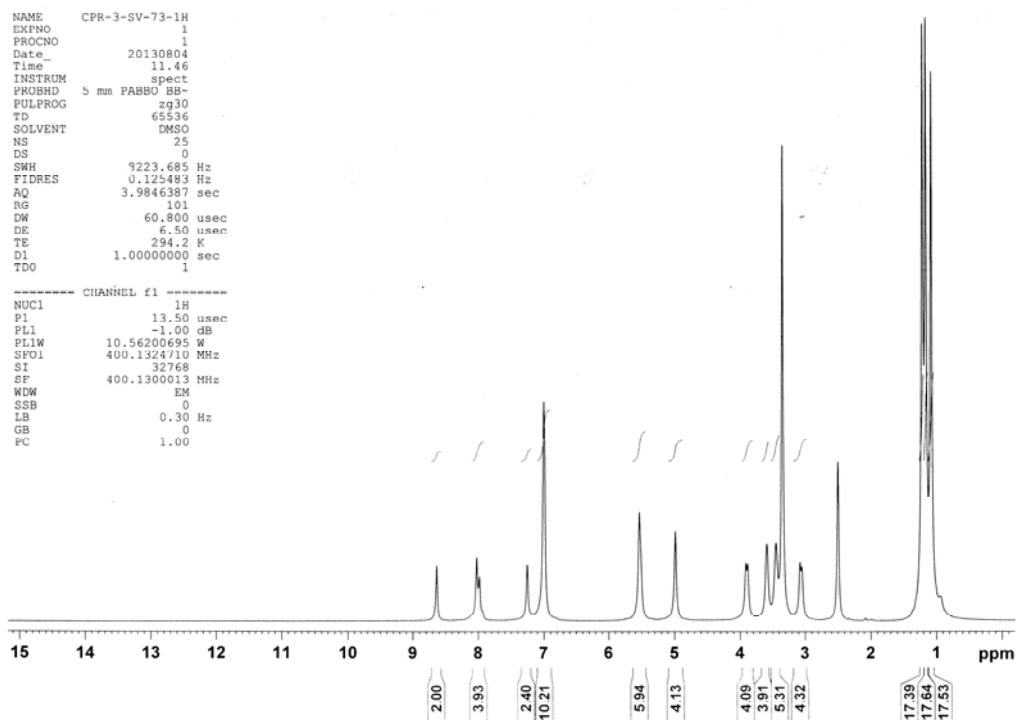
TOF MS ES+



Minimum: -1.5
Maximum: 200.0 20.0 200.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
1277.7708	1277.7742	-3.5	-2.7	32.5	1	C78 H101 N8 O8

Figure S03 HRMS Spectrum of L.

SI02. Synthesis and characterization of [CdL]₂Figure S04 ¹H NMR spectrum (DMSO-d₆, 400 MHz) of [CdL]₂

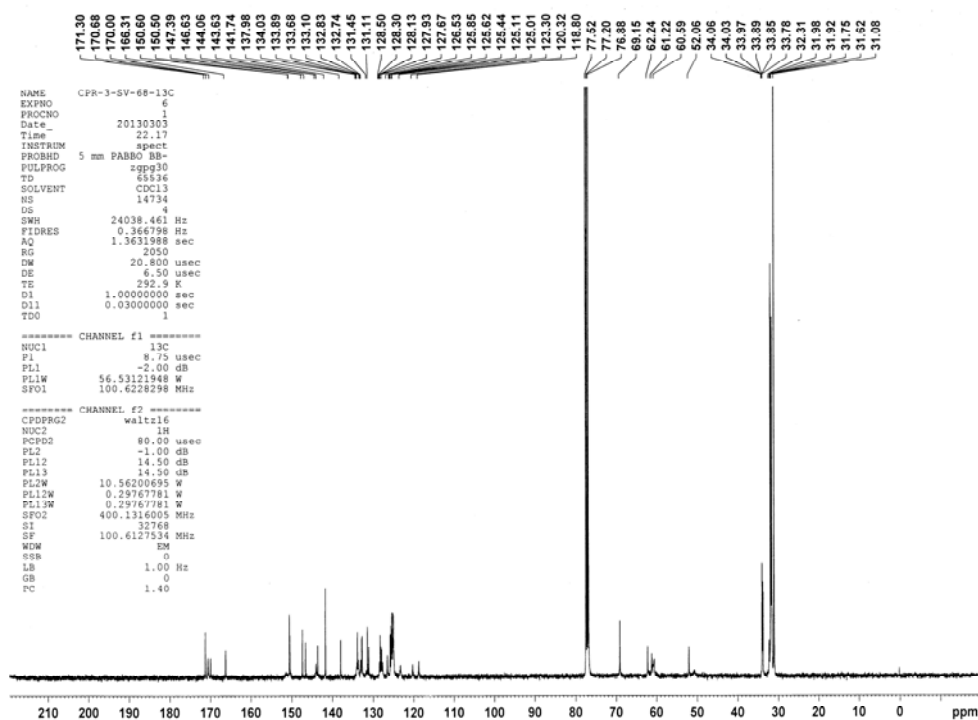


Figure S05 ^{13}C NMR spectrum (DMSO- d_6 , 100 MHz) of $[\text{CdL}]_2$.

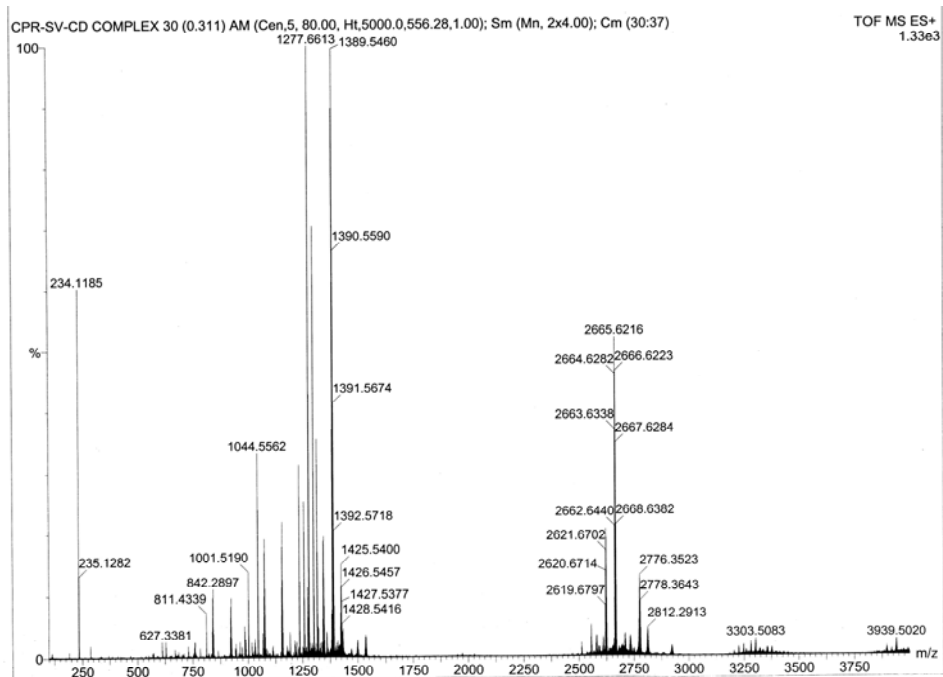


Figure S06 ESI MS of compound $[\text{CdL}]_2$.

SI03. Crystallographic data for [CdL]₂

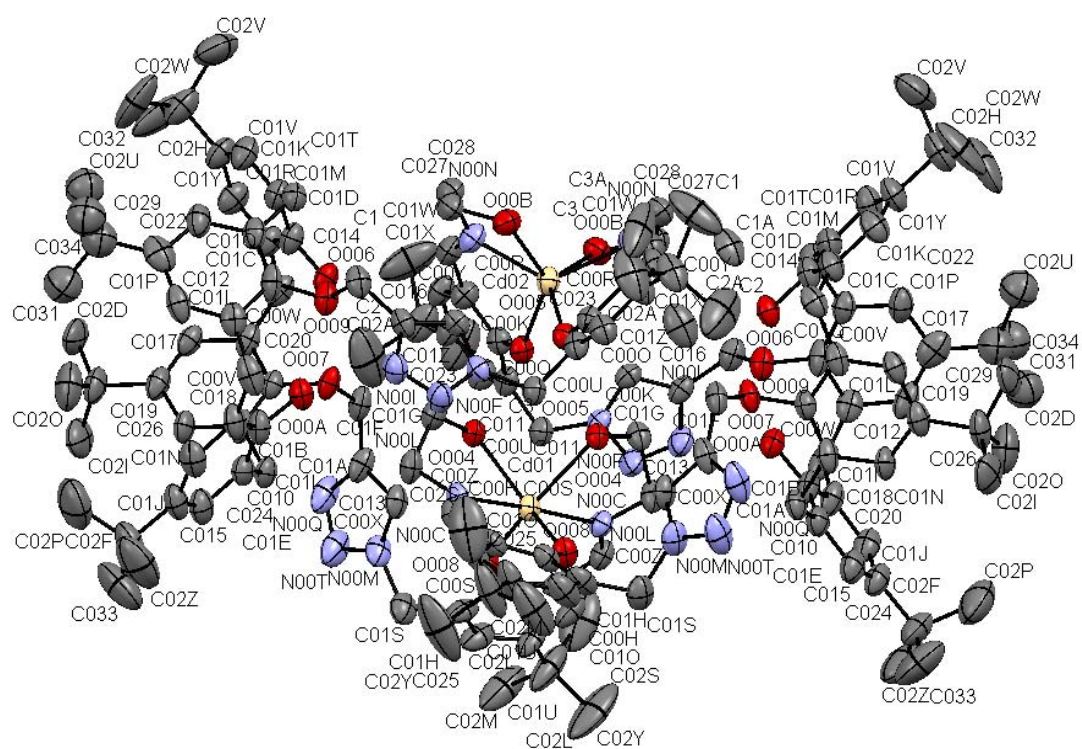


Figure S07. ORTEP diagram of [CdL]₂

Table S01. Bond length and bond angles of crystal structure [CdL]₂

Cd01	O004	2.405(5)	N00Q	N00T	1.330(9)
Cd01	O004	2.406(5)	N00Q	C01A	1.358(7)
Cd01	O008	2.236(4)	C00R	C00Y	1.410(7)
Cd01	O008	2.236(4)	C00R	C01W	1.467(8)
Cd01	N00C	2.266(7)	C00S	C01H	1.422(7)
Cd01	N00C	2.266(7)	C00U	C011	1.501(8)
Cd02	O005	2.253(4)	C00U	C023	1.400(7)
Cd02	O005	2.253(4)	C00V	C00W	1.411(7)
Cd02	O00B	2.506(7)	C00V	C014	1.501(9)
Cd02	O00B	2.506(7)	C00V	C017	1.424(7)
Cd02	N00N	2.271(5)	C00W	C018	1.357(8)
Cd02	N00N	2.271(5)	C00X	H00C	0.9900 .
O004	H004	0.874(9)	C00X	H00D	0.9900 .
O004	C01G	1.427(7)	C00X	C01G	1.536(8)
O005	C00O	1.295(6)	C00Y	H00Y	0.9500 .
O006	H006	0.8400 .	C00Y	C01Z	1.386(8)
O006	C01D	1.373(7)	C00Z	H00Z	0.9500 .
O007	C00W	1.395(6)	C010	C015	1.390(9)
O007	C01F	1.458(7)	C010	C01B	1.431(8)
O008	C00S	1.280(7)	C010	C01E	1.500(9)
O009	C01Q	1.389(6)	C011	H01A	0.9900 .
O009	C01X	1.450(6)	C011	H01B	0.9900 .
O00A	H00A	0.8400 .	C012	H012	0.9500 .
O00A	C01B	1.379(7)	C012	C01L	1.387(8)
O00B	H00B	0.879(10)	C012	C01P	1.425(11)
O00B	C028	1.482(7)	C013	H013	0.9500 .
N00C	C00X	1.476(7)	C013	C01A	1.386(8)
N00C	C00Z	1.281(7)	C014	H01C	0.9900 .
N00F	C00K	1.328(7)	C014	H01D	0.9900 .
N00F	N00L	1.367(6)	C014	C01R	1.521(8)
N00F	C011	1.451(7)	C015	H015	0.9500 .
C00H	C00S	1.443(8)	C015	C01J	1.407(10)
C00H	C00Z	1.421(8)	C016	C01X	1.493(8)
C00H	C01O	1.424(8)	C017	H017	0.9500 .
N00I	N00L	1.286(7)	C017	C019	1.379(9)
N00I	C016	1.350(8)	C018	C01E	1.516(8)
C00K	H00K	0.9500 .	C018	C01N	1.413(7)
C00K	C016	1.373(7)	C019	C01N	1.419(8)
N00M	N00T	1.336(6)	C019	C026	1.538(8)
N00M	C013	1.326(8)	C01A	C01F	1.481(9)
N00M	C01S	1.555(9)	C01B	C01I	1.388(8)
N00N	C01W	1.270(8)	C01C	C01M	1.502(8)
N00N	C027	1.453(8)	C01C	C01Q	1.388(9)
C00O	C00R	1.421(8)	C01C	C022	1.389(8)
C00O	C00U	1.434(7)	C01D	C01R	1.383(7)

C01D	C01T	1.414(9)	C026	C02D	1.517(10)
C01E	H01E	0.9900 .	C026	C02I	1.522(10)
C01E	H01F	0.9900 .	C026	C02O	1.485(12)
C01F	H01G	0.9900 .	C027	H02C	0.9900 .
C01F	H01H	0.9900 .	C027	H02D	0.9900 .
C01G	H01I	0.9900 .	C027	C028	1.493(9)
C01G	H01J	0.9900 .	C028	H02E	0.9900 .
C01H	C01S	1.495(9)	C028	H02F	0.9900 .
C01H	C025	1.382(9)	C029	C02U	1.628(13)
C01I	C020	1.494(9)	C029	C031	1.499(13)
C01I	C024	1.402(9)	C029	C034	1.463(13)
C01J	C024	1.399(10)	C02A	C1 1	.548(5) .
C01J	C02F	1.529(9)	C02A	C2 1	.548(4) .
C01K	H01K	0.9500 .	C02A	C3 1	.548(6) .
C01K	C01R	1.419(8)	C02A	C1A	1.548(5)
C01K	C01Y	1.381(9)	C02A	C2A	1.548(5)
C01L	C01Q	1.419(8)	C02A	C3A	1.548(5)
C01L	C020	1.499(10)	C02D	H02G	0.9800 .
C01M	H01L	0.9900 .	C02D	H02H	0.9800 .
C01M	H01M	0.9900 .	C02D	H02I	0.9800 .
C01M	C01T	1.524(8)	C02F	C02P	1.599(15)
C01N	H01N	0.9500 .	C02F	C02Z	1.463(13)
C01O	H01O	0.9500 .	C02F	C033	1.490(13)
C01O	C01U	1.386(8)	C02H	C02V	1.610(14)
C01P	C022	1.386(10)	C02H	C02W	1.490(12)
C01P	C029	1.509(11)	C02H	C032	1.502(14)
C01S	H01P	0.9900 .	C02I	H02J	0.9800 .
C01S	H01Q	0.9900 .	C02I	H02K	0.9800 .
C01T	C01V	1.374(9)	C02I	H02L	0.9800 .
C01U	C025	1.383(10)	C02L	C02M	1.462(12)
C01U	C02L	1.545(10)	C02L	C02S	1.669(18)
C01V	H01V	0.9500 .	C02L	C02Y	1.536(11)
C01V	C01Y	1.403(9)	C02M	H02M	0.9800 .
C01W	H01W	0.9500 .	C02M	H02N	0.9800 .
C01X	H01R	0.9900 .	C02M	H02O	0.9800 .
C01X	H01S	0.9900 .	C02O	H02P	0.9800 .
C01Y	C02H	1.529(9)	C02O	H02Q	0.9800 .
C01Z	C023	1.371(8)	C02O	H02R	0.9800 .
C01Z	C02A	1.548(4)	C02P	H02S	0.9800 .
C020	H02A	0.9900 .	C02P	H02T	0.9800 .
C020	H02B	0.9900 .	C02P	H02U	0.9800 .
C022	H022	0.9500 .	C02S	H02V	0.9800 .
C023	H023	0.9500 .	C02S	H02W	0.9800 .
C024	H024	0.9500 .	C02S	H02X	0.9800 .
C025	H025	0.9500 .	C02U	H02Y	0.9800 .
C02U	H02Z	0.9800 .			
C02U	H02{	0.9800 .			

C02V	H02	0.9800 .			
C02V	H02	0.9800 .			
C02V	H02}	0.9800 .			
C02W	H0AA	0.9800 .			
C02W	H1AA	0.9800 .			
C02W	H02~	0.9800 .			
C02Y	H2AA	0.9800 .			
C02Y	H3AA	0.9800 .			
C02Y	H4AA	0.9800 .			
C02Z	H5AA	0.9795 .			
C02Z	H6AA	0.9798 .			
C02Z	H7AA	0.9809 .			
C031	H03A	0.9800 .			
C031	H03B	0.9800 .			
C031	H03C	0.9800 .			
C032	H03D	0.9800 .			
C032	H03E	0.9800 .			
C032	H03F	0.9800 .			
C033	H03G	0.9800 .			
C033	H03H	0.9800 .			
C033	H03I	0.9800 .			
C034	H03J	0.9800 .			
C034	H03K	0.9800 .			
C034	H03L	0.9800 .			
C1 H	1A 0.	9800 . ?			
C1 H	1B 0.	9800 . ?			
C1 H	1C 0.	9800 . ?			
C2 H	2A 0.	9800 . ?			
C2 H	2B 0.	9800 . ?			
C2 H	2C 0.	9800 . ?			
C3 H	3A 0.	9800 . ?			
C3 H	3B 0.	9800 . ?			
C3 H	3C 0.	9800 . ?			
C1A	H1AB	0.9800 .			
C1A	H1AC	0.9800 .			
C1A	H1AD	0.9800 .			
C2A	H2AB	0.9802 .			
C2A	H2AC	0.9798 .			
C2A	H2AD	0.9800 .			
C3A	H3AB	0.9800 .			
C3A	H3AC	0.9800 .			
C3A	H3AD	0.9800 .			
C02U	H02Z	0.9800 .			

O004	Cd01	O004	84.5(2) 2	C01O	C00H	C00S	119.8(5) .
O008	Cd01	O004	87.34(17)	N00L	N00I	C016	109.2(5) .
O008	Cd01	O004	148.67(14)	N00F	C00K	H00K	127.5 . .
O008	Cd01	O004	148.68(14)	N00F	C00K	C016	104.9(4) .
O008	Cd01	O004	87.33(17)	C016	C00K	H00K	127.5 . .
O008	Cd01	O008	113.9(2) .	N00I	N00L	N00F	107.5(5) .
O008	Cd01	N00C	96.61(17)	N00T	N00M	C01S	119.9(5) .
O008	Cd01	N00C	81.74(17)	C013	N00M	N00T	112.7(5) .
O008	Cd01	N00C	81.74(17)	C013	N00M	C01S	127.3(5) .
O008	Cd01	N00C	96.60(17)	C01W	N00N	Cd02	123.8(4) .
N00C	Cd01	O004	109.60(13)	C01W	N00N	C027	119.0(5) .
N00C	Cd01	O004	72.74(14)	C027	N00N	Cd02	117.1(4) .
N00C	Cd01	O004	72.74(14)	O005	C00O	C00R	125.5(5) .
N00C	Cd01	O004	109.60(13)	O005	C00O	C00U	118.7(5) .
N00C	Cd01	N00C	177.0(2) 2	C00R	C00O	C00U	115.7(4) .
O005	Cd02	O005	95.7(2) .	N00T	N00Q	C01A	108.6(5) .
O005	Cd02	O00B	80.52(19)	C00O	C00R	C01W	124.8(5) .
O005	Cd02	O00B	137.92(13)	C00Y	C00R	C00O	120.3(5) .
O005	Cd02	O00B	137.92(13)	C00Y	C00R	C01W	114.9(5) .
O005	Cd02	O00B	80.52(19)	O008	C00S	C00H	125.4(5) .
O005	Cd02	N00N	83.15(18)	O008	C00S	C01H	119.5(5) .
O005	Cd02	N00N	134.05(18)	C01H	C00S	C00H	115.2(5) .
O005	Cd02	N00N	83.14(18)	N00Q	N00T	N00M	106.3(5) .
O005	Cd02	N00N	134.05(18)	C00O	C00U	C011	119.2(4) .
O00B	Cd02	O00B	129.0(2) 2	C023	C00U	C00O	121.1(5) .
N00N	Cd02	O00B	87.43(18)	C023	C00U	C011	119.7(5) .
N00N	Cd02	O00B	71.08(17)	C00W	C00V	C014	123.4(5) .
N00N	Cd02	O00B	87.43(18)	C00W	C00V	C017	117.4(5) .
N00N	Cd02	O00B	71.08(17)	C017	C00V	C014	119.0(5) .
N00N	Cd02	N00N	129.2(3) 2	O007	C00W	C00V	116.8(5) .
Cd01	O004	H004	136.5(18)	C018	C00W	O007	120.3(4) .
C01G	O004	Cd01	112.2(3) .	C018	C00W	C00V	122.9(5) .
C01G	O004	H004	108.0(16)	N00C	C00X	H00C	110.0 . .
C00O	O005	Cd02	123.0(3) .	N00C	C00X	H00D	110.0 . .
C01D	O006	H006	109.5 . .	N00C	C00X	C01G	108.6(4) .
C00W	O007	C01F	113.9(4) .	H00C	C00X	H00D	108.3 . .
C00S	O008	Cd01	131.0(3) .	C01G	C00X	H00C	110.0 . .
C01Q	O009	C01X	113.9(4) .	C01G	C00X	H00D	110.0 . .
C01B	O00A	H00A	109.5 . .	C00R	C00Y	H00Y	118.4 . .
Cd02	O00B	H00B	138(2) . .	C01Z	C00Y	C00R	123.2(5) .
C028	O00B	Cd02	108.5(3) .	C01Z	C00Y	H00Y	118.4 . .
C028	O00B	H00B	108.1(17)	N00C	C00Z	C00H	128.1(5) .
C00X	N00C	Cd01	112.6(3) .	N00C	C00Z	H00Z	116.0 . .
C00Z	N00C	Cd01	128.5(4) .	C00H	C00Z	H00Z	116.0 . .
C00Z	N00C	C00X	118.9(4) .	C015	C010	C01B	118.3(6) .
C00K	N00F	N00L	110.0(4) .	C015	C010	C01E	121.1(5) .
C00K	N00F	C011	129.4(4) .	C01B	C010	C01E	120.2(5) .
N00L	N00F	C011	120.6(4) .	N00F	C011	C00U	112.2(4) .
C00Z	C00H	C00S	124.6(4) .	N00F	C011	H01A	109.2 . .
C00Z	C00H	C01O	115.5(5) .	N00F	C011	H01B	109.2 . .
C00U	C011	H01A	109.2 . .	O007	C01F	H01H	109.1 . .
C00U	C011	H01B	109.2 . .	C01A	C01F	H01G	109.1 . .
H01A	C011	H01B	107.9 . .	C01A	C01F	H01H	109.1 . .

C01L	C012	H012	118.6 . .	H01G	C01F	H01H	107.8 . .
C01L	C012	C01P	122.7(6) .	O004	C01G	C00X	107.8(4) .
C01P	C012	H012	118.6 . .	O004	C01G	H01I	110.2 . .
N00M	C013	H013	128.0 . .	O004	C01G	H01J	110.2 . .
N00M	C013	C01A	104.1(5) .	C00X	C01G	H01I	110.2 . .
C01A	C013	H013	128.0 . .	C00X	C01G	H01J	110.2 . .
C00V	C014	H01C	109.7 . .	H01I	C01G	H01J	108.5 . .
C00V	C014	H01D	109.7 . .	C00S	C01H	C01S	117.8(5) .
C00V	C014	C01R	110.0(5) .	C025	C01H	C00S	122.2(6) .
H01C	C014	H01D	108.2 . .	C025	C01H	C01S	120.0(5) .
C01R	C014	H01C	109.7 . .	C01B	C01I	C020	121.0(5) .
C01R	C014	H01D	109.7 . .	C01B	C01I	C024	118.8(6) .
C010	C015	H015	119.2 . .	C024	C01I	C020	120.1(6) .
C010	C015	C01J	121.7(6) .	C015	C01J	C02F	120.9(6) .
C01J	C015	H015	119.2 . .	C024	C01J	C015	118.4(6) .
N00I	C016	C00K	108.3(5) .	C024	C01J	C02F	120.6(6) .
N00I	C016	C01X	122.2(5) .	C01R	C01K	H01K	118.7 . .
C00K	C016	C01X	129.4(5) .	C01Y	C01K	H01K	118.7 . .
C00V	C017	H017	119.4 . .	C01Y	C01K	C01R	122.6(6) .
C019	C017	C00V	121.1(5) .	C012	C01L	C01Q	117.0(6) .
C019	C017	H017	119.4 . .	C012	C01L	C020	120.3(5) .
C00W	C018	C01E	124.2(5) .	C01Q	C01L	C020	122.6(5) .
C00W	C018	C01N	119.0(5) .	C01C	C01M	H01L	109.7 . .
C01N	C018	C01E	116.8(5) .	C01C	C01M	H01M	109.7 . .
C017	C019	C01N	119.3(5) .	C01C	C01M	C01T	109.8(5) .
C017	C019	C026	122.4(5) .	H01L	C01M	H01M	108.2 . .
C01N	C019	C026	118.3(6) .	C01T	C01M	H01L	109.7 . .
N00Q	C01A	C013	108.2(6) .	C01T	C01M	H01M	109.7 . .
N00Q	C01A	C01F	122.7(5) .	C018	C01N	C019	120.3(6) .
C013	C01A	C01F	129.0(5) .	C018	C01N	H01N	119.9 . .
O00A	C01B	C010	114.4(5) .	C019	C01N	H01N	119.9 . .
O00A	C01B	C01I	124.5(5) .	C00H	C01O	H01O	118.6 . .
C01I	C01B	C010	121.1(5) .	C01U	C01O	C00H	122.9(6) .
C01Q	C01C	C01M	121.9(5) .	C01U	C01O	H01O	118.6 . .
C01Q	C01C	C022	117.7(5) .	C012	C01P	C029	119.5(6) .
C022	C01C	C01M	120.2(6) .	C022	C01P	C012	116.5(6) .
O006	C01D	C01R	123.3(5) .	C022	C01P	C029	124.0(7) .
O006	C01D	C01T	115.6(5) .	O009	C01Q	C01L	117.2(5) .
C01R	C01D	C01T	120.9(5) .	C01C	C01Q	O009	120.2(5) .
C010	C01E	C018	111.0(4) .	C01C	C01Q	C01L	122.4(5) .
C010	C01E	H01E	109.4 . .	C01D	C01R	C014	121.6(5) .
C010	C01E	H01F	109.4 . .	C01D	C01R	C01K	118.4(5) .
C018	C01E	H01E	109.4 . .	C01K	C01R	C014	119.9(5) .
C018	C01E	H01F	109.4 . .	N00M	C01S	H01P	109.7 . .
H01E	C01E	H01F	108.0 . .	N00M	C01S	H01Q	109.7 . .
O007	C01F	C01A	112.6(4) .	C01H	C01S	N00M	109.8(5) .
O007	C01F	H01G	109.1 . .	C01H	C01S	H01P	109.7 . .
C01H	C01S	H01Q	109.7 . .	N00N	C027	H02C	109.8 . .
H01P	C01S	H01Q	108.2 . .	N00N	C027	H02D	109.8 . .
C01D	C01T	C01M	120.8(5) .	N00N	C027	C028	109.2(5) .
C01V	C01T	C01D	117.5(6) .	H02C	C027	H02D	108.3 . .
C01V	C01T	C01M	121.3(5) .	C028	C027	H02C	109.8 . .
C01O	C01U	C02L	119.6(6) .	C028	C027	H02D	109.8 . .

C025	C01U	C01O	116.6(5) .	O00B	C028	C027	109.1(5) .
C025	C01U	C02L	123.6(6) .	O00B	C028	H02E	109.9 . .
C01T	C01V	H01V	117.8 . .	O00B	C028	H02F	109.9 . .
C01T	C01V	C01Y	124.4(6) .	C027	C028	H02E	109.9 . .
C01Y	C01V	H01V	117.8 . .	C027	C028	H02F	109.9 . .
N00N	C01W	C00R	128.3(5) .	H02E	C028	H02F	108.3 . .
N00N	C01W	H01W	115.9 . .	C01P	C029	C02U	110.4(7) .
C00R	C01W	H01W	115.9 . .	C031	C029	C01P	111.6(7) .
O009	C01X	C016	109.8(4) .	C031	C029	C02U	101.3(8) .
O009	C01X	H01R	109.7 . .	C034	C029	C01P	110.7(8) .
O009	C01X	H01S	109.7 . .	C034	C029	C02U	103.5(8) .
C016	C01X	H01R	109.7 . .	C034	C029	C031	118.5(8) .
C016	C01X	H01S	109.7 . .	C01Z	C02A	C1 1	09.45(10) .
H01R	C01X	H01S	108.2 . .	C01Z	C02A	C2 1	09.48(13) .
C01K	C01Y	C01V	116.0(5) .	C01Z	C02A	C1A	110.6(7) .
C01K	C01Y	C02H	123.3(6) .	C01Z	C02A	C2A	108.8(8) .
C01V	C01Y	C02H	120.7(6) .	C01Z	C02A	C3A	111.8(9) .
C00Y	C01Z	C02A	120.9(4) .	C2 C	02A C	1 109	.45(15) . .
C023	C01Z	C00Y	116.7(5) .	C3 C	02A C	01Z 1	09.52(13) .
C023	C01Z	C02A	122.2(4) .	C3 C	02A C	1 109	.44(9) . .
C01I	C020	C01L	112.8(5) .	C3 C	02A C	2 109	.48(13) . .
C01I	C020	H02A	109.0 . .	C1A	C02A	C2A 1	08.5(5) . .
C01I	C020	H02B	109.0 . .	C3A	C02A	C1A 1	08.5(5) . .
C01L	C020	H02A	109.0 . .	C3A	C02A	C2A 1	08.5(5) . .
C01L	C020	H02B	109.0 . .	C026	C02D	H02G	109.5 . .
H02A	C020	H02B	107.8 . .	C026	C02D	H02H	109.5 . .
C01C	C022	H022	118.2 . .	C026	C02D	H02I	109.5 . .
C01P	C022	C01C	123.6(7) .	H02G	C02D	H02H	109.5 . .
C01P	C022	H022	118.2 . .	H02G	C02D	H02I	109.5 . .
C00U	C023	H023	118.5 . .	H02H	C02D	H02I	109.5 . .
C01Z	C023	C00U	122.9(5) .	C01J	C02F	C02P	105.9(7) .
C01Z	C023	H023	118.5 . .	C02Z	C02F	C01J	111.4(6) .
C01I	C024	H024	119.1 . .	C02Z	C02F	C02P	108.0(9) .
C01J	C024	C01I	121.8(6) .	C02Z	C02F	C033	112.1(9) .
C01J	C024	H024	119.1 . .	C033	C02F	C01J	112.8(7) .
C01H	C025	C01U	123.1(6) .	C033	C02F	C02P	106.2(9) .
C01H	C025	H025	118.5 . .	C01Y	C02H	C02V	108.1(7) .
C01U	C025	H025	118.5 . .	C02W	C02H	C01Y	112.1(6) .
C02D	C026	C019	110.6(6) .	C02W	C02H	C02V	107.1(9) .
C02D	C026	C02I	107.7(6) .	C02W	C02H	C032	112.7(9) .
C02I	C026	C019	109.5(5) .	C032	C02H	C01Y	108.7(7) .
C02O	C026	C019	109.4(5) .	C032	C02H	C02V	107.9(9) .
C026	C02I	H02L	109.5 . .	H0AA	C02W	H02~	109.5 . .
H02J	C02I	H02K	109.5 . .	H1AA	C02W	H02~	109.5 . .
H02J	C02I	H02L	109.5 . .	C02L	C02Y	H2AA	109.5 . .
H02K	C02I	H02L	109.5 . .	C02L	C02Y	H3AA	109.5 . .
C01U	C02L	C02S	107.3(8) .	C02L	C02Y	H4AA	109.5 . .
C02M	C02L	C01U	114.0(8) .	H2AA	C02Y	H3AA	109.5 . .
C02M	C02L	C02S	105.7(9) .	H2AA	C02Y	H4AA	109.5 . .
C02M	C02L	C02Y	115.6(8) .	H3AA	C02Y	H4AA	109.5 . .
C02Y	C02L	C01U	107.6(7) .	C02F	C02Z	H5AA	110.6 . .
C02Y	C02L	C02S	106.1(10)	C02F	C02Z	H6AA	108.6 . .
C02L	C02M	H02M	109.5 . .	C02F	C02Z	H7AA	109.3 . .

C02L	C02M	H02N	109.5 ..	H5AA	C02Z	H6AA	109.5 ..
C02L	C02M	H02O	109.5 ..	H5AA	C02Z	H7AA	109.4 ..
H02M	C02M	H02N	109.5 ..	H6AA	C02Z	H7AA	109.4 ..
H02M	C02M	H02O	109.5 ..	C029	C031	H03A	109.5 ..
H02N	C02M	H02O	109.5 ..	C029	C031	H03B	109.5 ..
C026	C02O	H02P	109.5 ..	C029	C031	H03C	109.5 ..
C026	C02O	H02Q	109.5 ..	H03A	C031	H03B	109.5 ..
C026	C02O	H02R	109.5 ..	H03A	C031	H03C	109.5 ..
H02P	C02O	H02Q	109.5 ..	H03B	C031	H03C	109.5 ..
H02P	C02O	H02R	109.5 ..	C02H	C032	H03D	109.5 ..
H02Q	C02O	H02R	109.5 ..	C02H	C032	H03E	109.5 ..
C02F	C02P	H02S	109.5 ..	C02H	C032	H03F	109.5 ..
C02F	C02P	H02T	109.5 ..	H03D	C032	H03E	109.5 ..
C02F	C02P	H02U	109.5 ..	H03D	C032	H03F	109.5 ..
H02S	C02P	H02T	109.5 ..	H03E	C032	H03F	109.5 ..
H02S	C02P	H02U	109.5 ..	C02F	C033	H03G	109.5 ..
H02T	C02P	H02U	109.5 ..	C02F	C033	H03H	109.5 ..
C02L	C02S	H02V	109.5 ..	C02F	C033	H03I	109.5 ..
C02L	C02S	H02W	109.5 ..	H03G	C033	H03H	109.5 ..
C02L	C02S	H02X	109.5 ..	H03G	C033	H03I	109.5 ..
H02V	C02S	H02W	109.5 ..	H03H	C033	H03I	109.5 ..
H02V	C02S	H02X	109.5 ..	C029	C034	H03J	109.5 ..
H02W	C02S	H02X	109.5 ..	C029	C034	H03K	109.5 ..
C029	C02U	H02Y	109.5 ..	C029	C034	H03L	109.5 ..
C029	C02U	H02Z	109.5 ..	H03J	C034	H03K	109.5 ..
C029	C02U	H02{	109.5 ..	H03J	C034	H03L	109.5 ..
H02Y	C02U	H02Z	109.5 ..	H03K	C034	H03L	109.5 ..
H02Y	C02U	H02{	109.5 ..	C02A	C1 H	1A 10	9.5 ..
H02Z	C02U	H02{	109.5 ..	C02A	C1 H	1B 10	9.5
C02H	C02V	H02	109.5 ..	C02A	C1 H	1C 10	9.5
C02H	C02V	H02	109.5 ..	H1A	C1 H1	B 109	.5 ..
C02H	C02V	H02}	109.5 ..	H1A	C1 H1	C 109	.5
H02	C02V	H02	109.5 ..	H1B	C1 H1	C 109	.5
H02	C02V	H02}	109.5 ..	C02A	C2 H	2A 10	9.5
H02	C02V	H02}	109.5 ..	C02A	C2 H	2B 10	9.5
C02H	C02W	H0AA	109.5 ..	C02A	C2 H	2C 10	9.5
C02H	C02W	H1AA	109.5 ..	H2A	C2 H2	B 109	.5
C02H	C02W	H02~	109.5 ..	H2A	C2 H2	C 109	.5
H0AA	C02W	H1AA	109.5 ..	H2B	C2 H2	C 109	.5
C02A	C3 H	3A 10	9.5 ..				
C02A	C3 H	3B 10	9.5 ..				
C02A	C3 H	3C 10	9.5 ..				
H3A	C3 H3	B 109	.5 ..				
H3A	C3 H3	C 109	.5 ..				
H3B	C3 H3	C 109	.5 ..				
C02A	C1A	H1AB	109.5 ..				
C02A	C1A	H1AC	109.5 ..				
C02A	C1A	H1AD	109.5 ..				
H1AB	C1A	H1AC	109.5 ..				
H1AB	C1A	H1AD	109.5 ..				
H1AC	C1A	H1AD	109.5 ..				
C02A	C2A	H2AB	108.8				
C02A	C2A	H2AC	109.3				

C02A	C2A	H2AD	110.3
H2AB	C2A	H2AC	109.5
H2AB	C2A	H2AD	109.4
H2AC	C2A	H2AD	109.5
C02A	C3A	H3AB	109.5
C02A	C3A	H3AC	109.5
C02A	C3A	H3AD	109.5
H3AB	C3A	H3AC	109.5
H3AB	C3A	H3AD	109.5
H3AC	C3A	H3AD	109.5

SI04. Fluorescence studies of $[\text{CdL}]_2$ in buffer

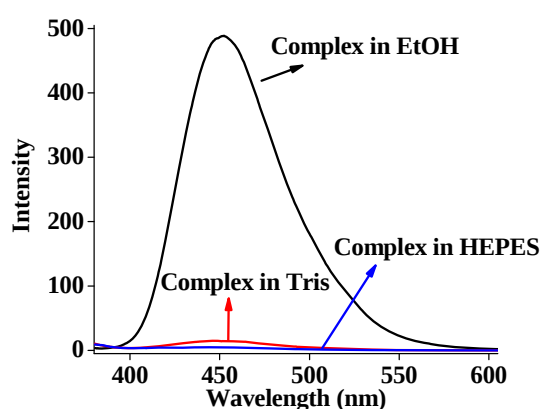
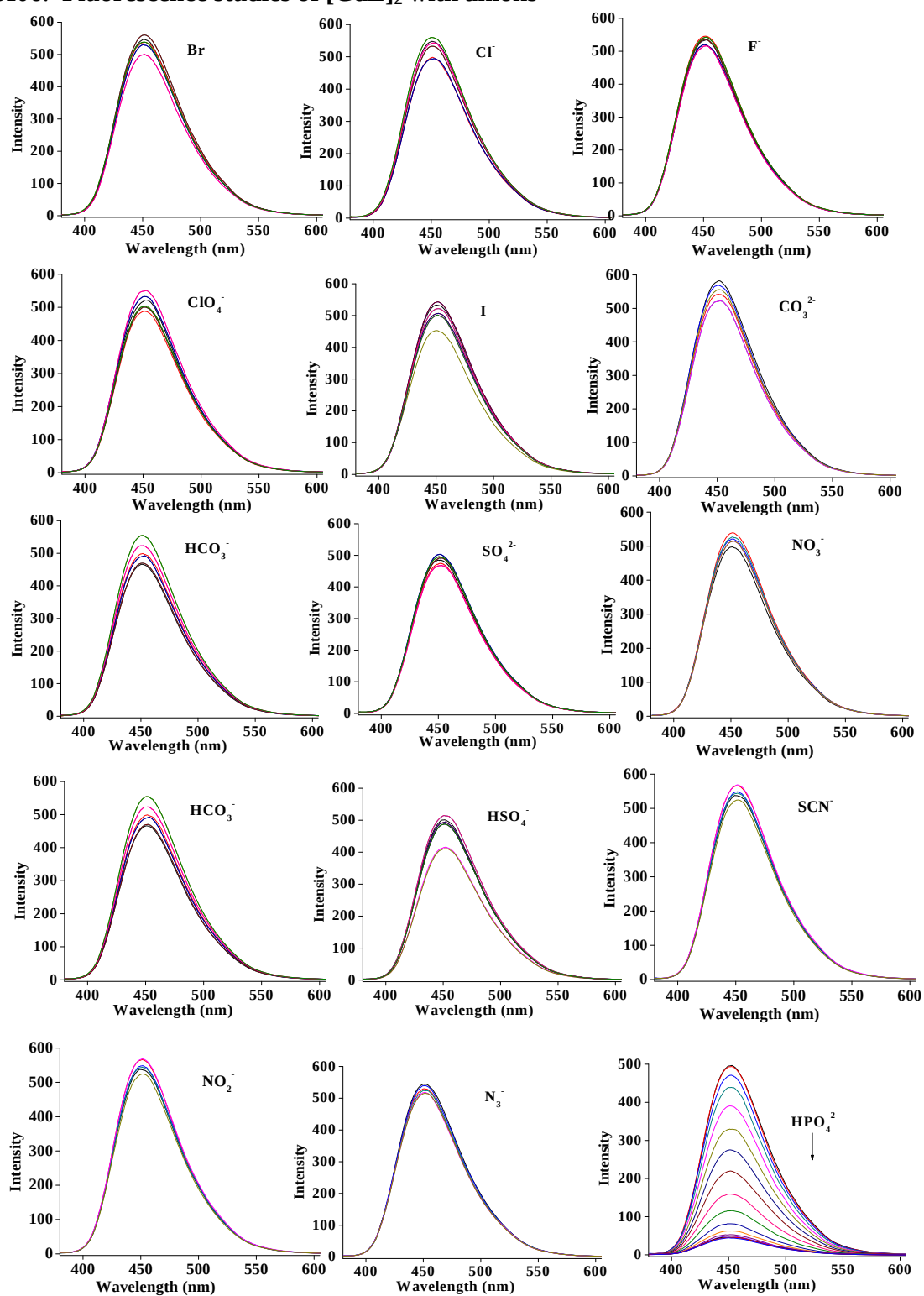


Figure S08 Fluorescence spectra obtained during the titration of $[\text{CdL}]_2$ in buffer.

SI05. Fluorescence and absorption details

Bulk solutions of $[\text{CdL}]_2$ was dissolved in DMSO and the anion salts were prepared in $\text{C}_2\text{H}_5\text{OH}$ by initially dissolving water. The concentration of the bulk solution of $[\text{CdL}]_2$ has been maintained as 6×10^{-4} M throughout the titration. All the fluorescence titrations were carried out by exciting $[\text{CdL}]_2$ at 370 nm of the solutions taken in 1 cm quartz cells by maintaining a final $[\text{CdL}]_2$ at 5 μM in a total volume of 3 mL achieved by diluting with $\text{C}_2\text{H}_5\text{OH}$. All the metal ions used for the fluorescence and absorption titrations were used as their tetrabutyl and sodium salts. Absorption studies were carried out in a similar manner as in fluorescence studies.

SI06. Fluorescence studies of [CdL]₂ with anions



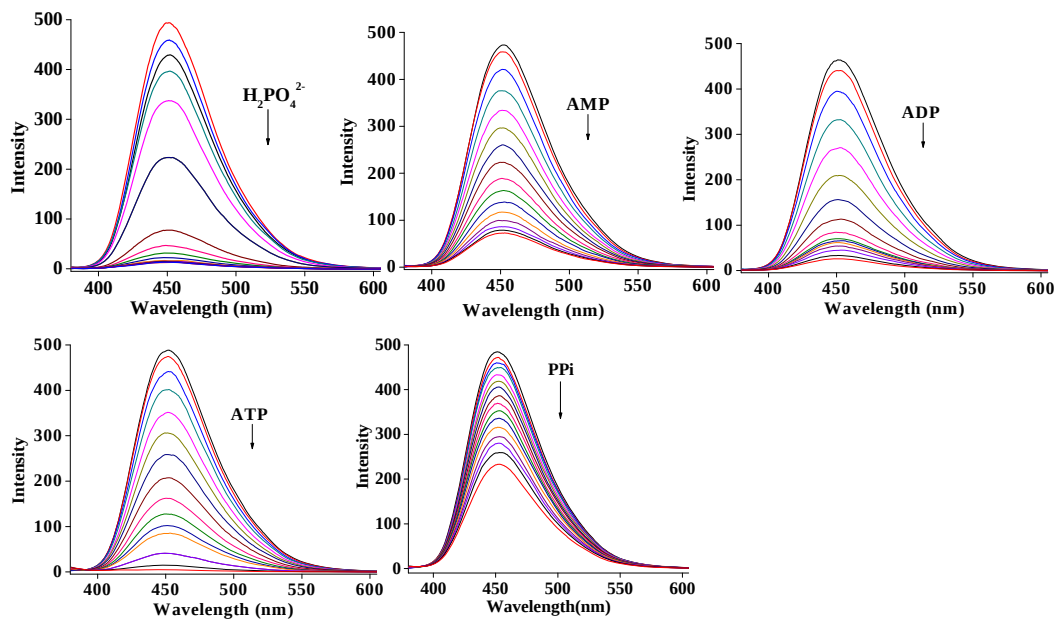


Figure S09 Fluorescence spectra obtained during the titration of $[\text{CdL}]_2$ with anions in ethanol.

SI07. Dilution experiment by maintaining the ratio of $[\text{CdL}]_2$:Phosphates as 1:2

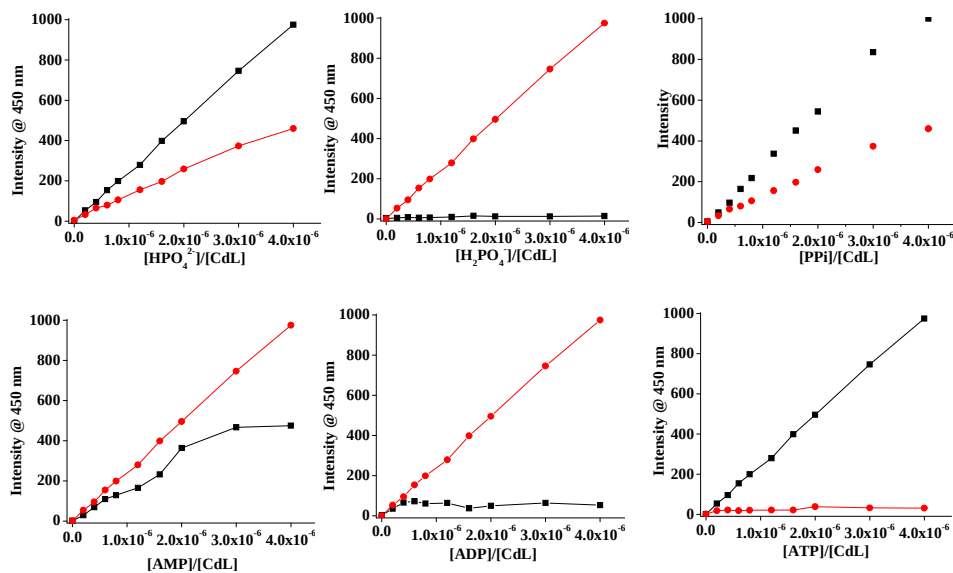


Figure S10 Determination of minimum concentration of phosphates that can be detected by $[\text{CdL}]_2$.

SI08. Fluorescence studies of $[\text{CdL}]_2$ with Na^+ counter cation

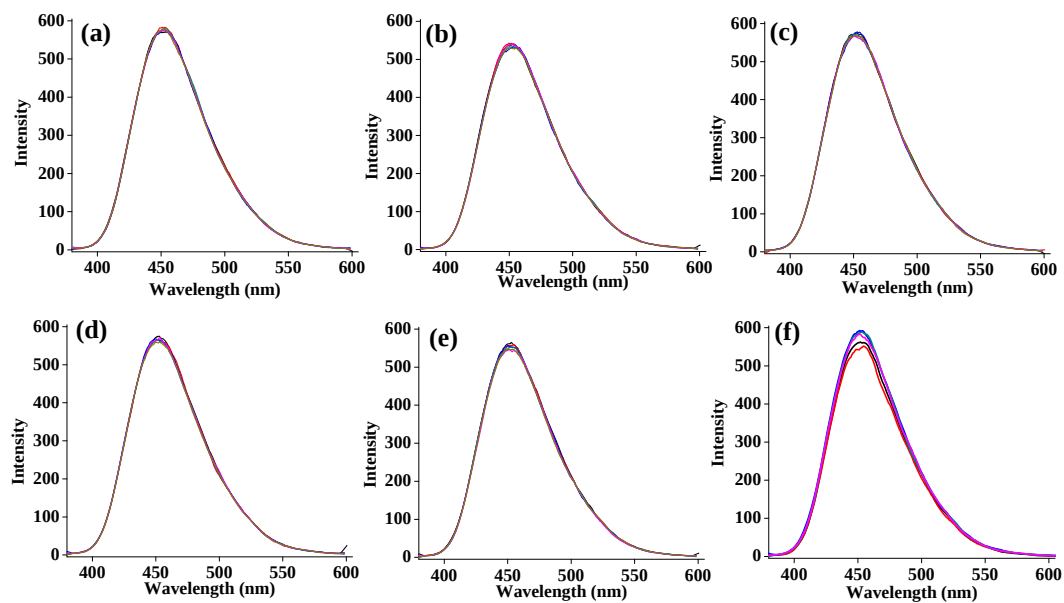


Figure S11 Fluorescence titration of $[\text{CdL}]_2$ with anions (a) NaF; (b) NaCl; (c) NaBr; (d) NaI; (e) NaHSO₄; (f) NaClO₄.

SI09. Absorption titration studies of $[\text{CdL}]_2$ with anions

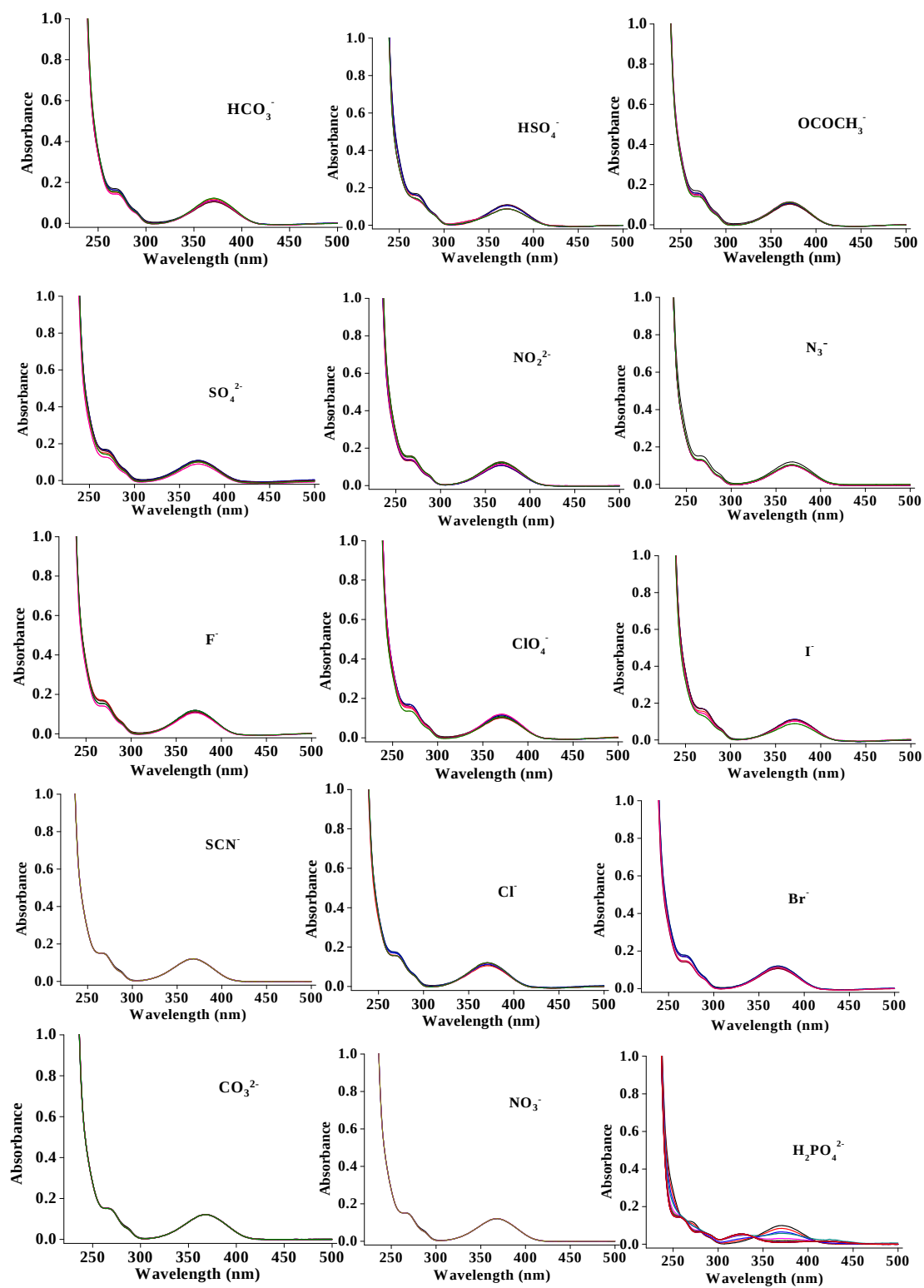


Figure S12 Absorbance spectra obtained during the titration of $[\text{CdL}]_2$ with anions.

SI10. ^1H NMR titration studies of $[\text{CdL}]_2$ with phosphates

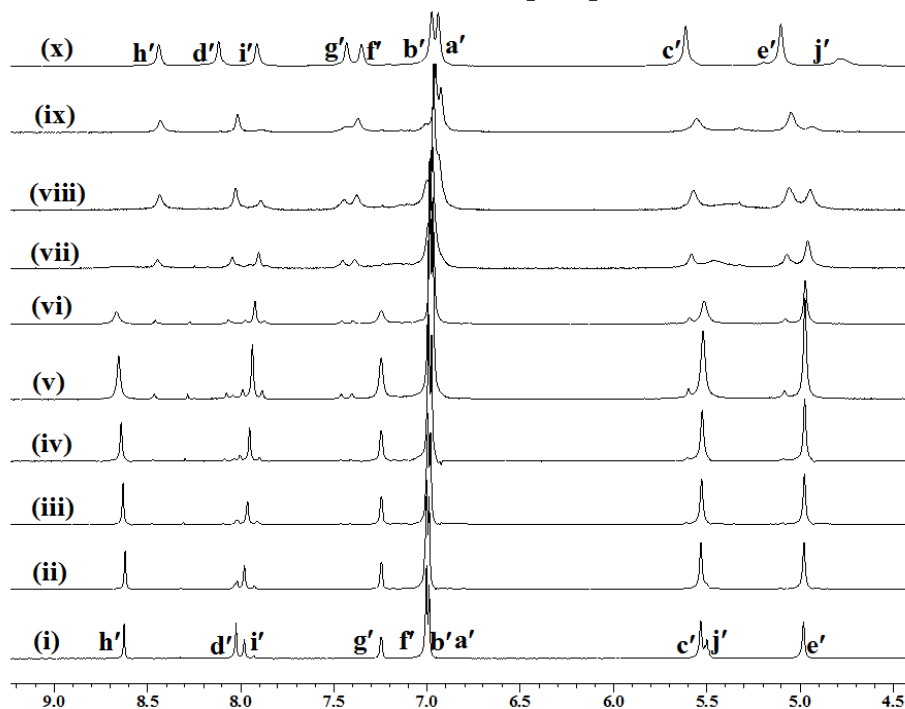


Figure S13 ^1H NMR spectral titration of $[\text{CdL}]_2$ with Na_2HPO_4 in DMOS-d_6 : (i) $[\text{CdL}]_2$. $[\text{CdL}]_2$ followed by n equivalents of Na_2HPO_4 , where, (ii) $n = 0.5$; (ii) $n = 1$; (iii) 1.5; (iv) 2; (v) 2.5; (vi) 3.0; (vii) 3.5; (viii) 4; (ix) 5 and (x) **L**

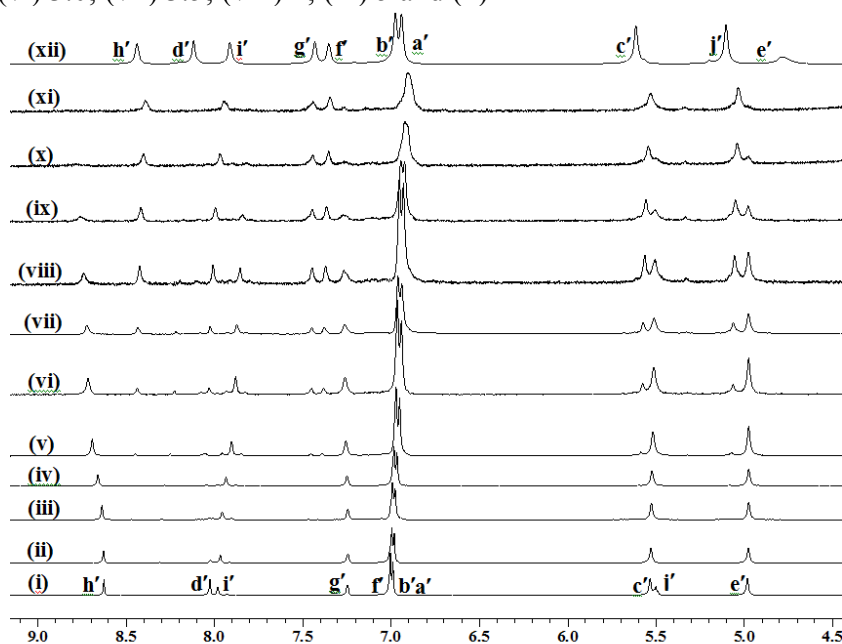


Figure S14 ^1H NMR spectral titration of $[\text{CdL}]_2$ with $\text{Na}_2\text{P}_2\text{O}_7$ in DMOS-d_6 : (i) $[\text{CdL}]_2$. $[\text{CdL}]_2$ followed by n equivalents of $\text{Na}_2\text{P}_2\text{O}_7$, where, (ii) $n = 1$; (ii) $n = 2$; (iii) 3; (iv) 4; (v) 5; (vi) 6; (vii) 7; (viii) 8; (ix) 9; (x) 10; (xi) 11; (xii) **L**.

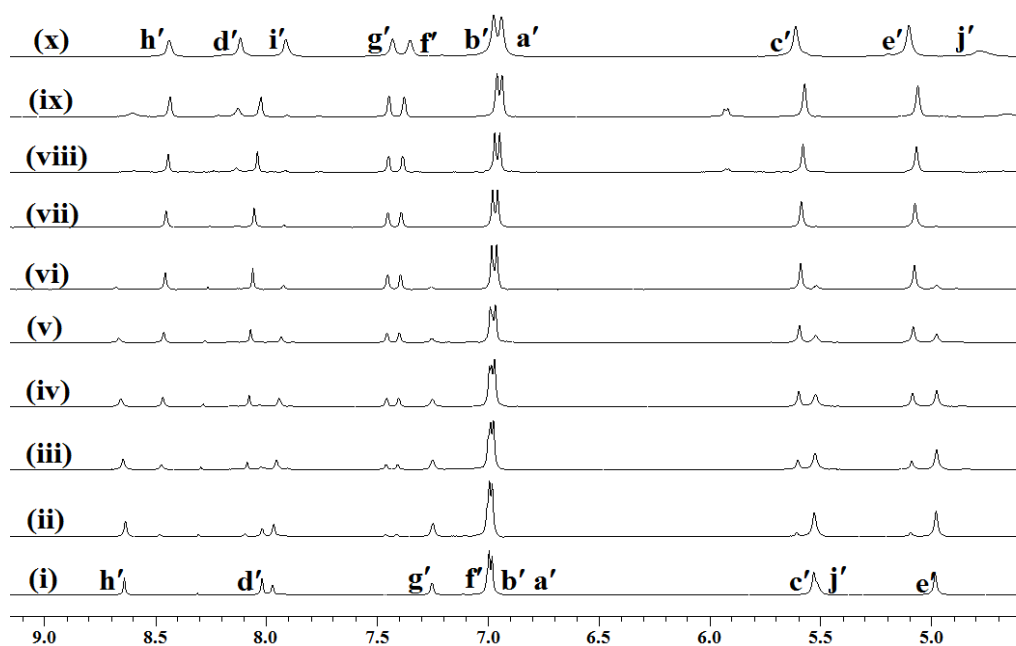


Figure S15 ^1H NMR spectral titration of $[\text{CdL}]_2$ with Na_2ATP in DMOS-d_6 : (i) $[\text{CdL}]_2$. $[\text{CdL}]_2$ followed by n equivalents of Na_2ATP , where, (ii) $n = 0.3$; (ii) $n = 0.6$; (iii) 0.9 ; (iv) 1.2 ; (v) 1.5 ; (vi) 1.8 ; (vii) 2.1 ; (viii) 2.4 ; (ix) 3 and (x) **L**

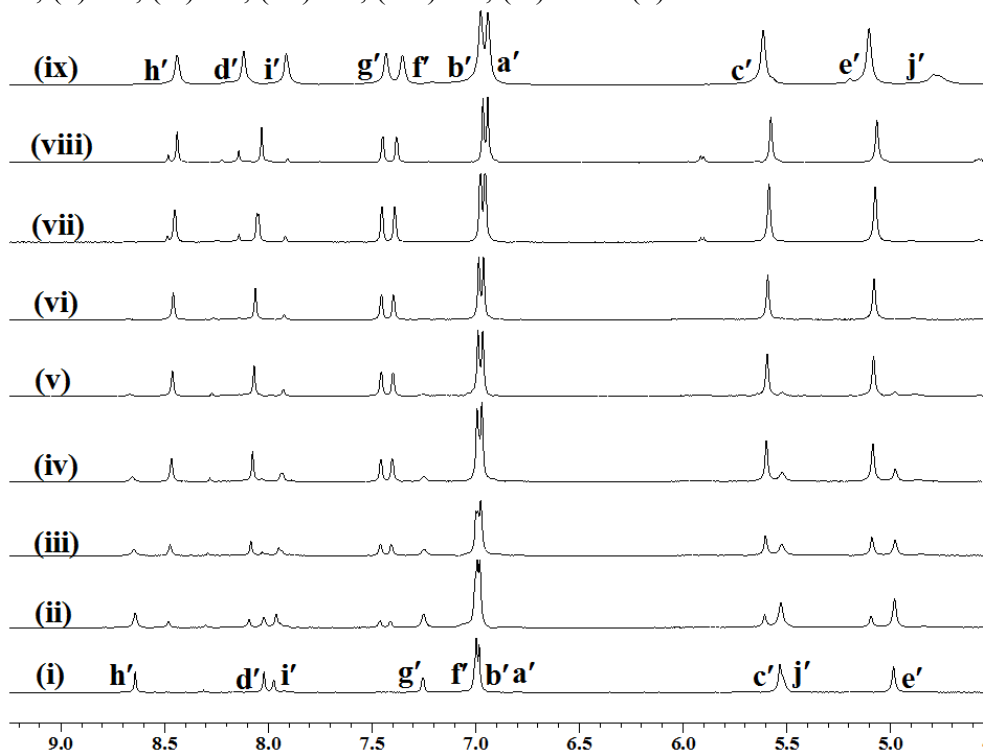
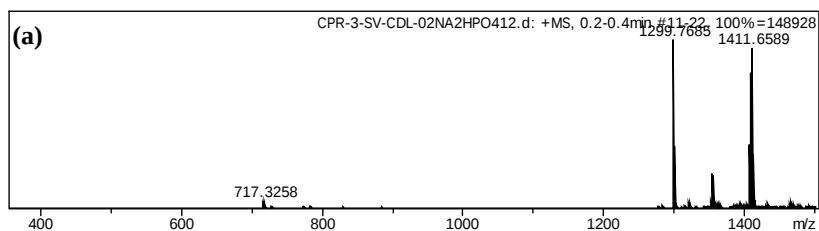


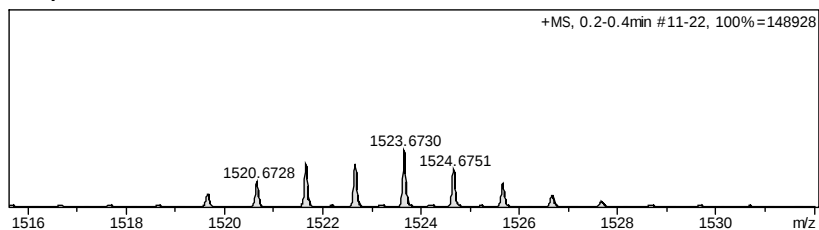
Figure S16 ^1H NMR spectral titration of $[\text{CdL}]_2$ with Na_2ADP in DMOS-d_6 : (i) $[\text{CdL}]_2$. $[\text{CdL}]_2$ followed by n equivalents of Na_2ADP , where, (ii) $n = 0.4$; (ii) $n = 0.8$; (iii) 1.2 ; (iv) 1.6 ; (v) 2.0 ; (vi) 2.5 ; (vii) 3.0 ; (viii) 3.5 and (ix) **L**.

SI11. ESI MS titration studies of $[\text{CdL}]_2$ with phosphates

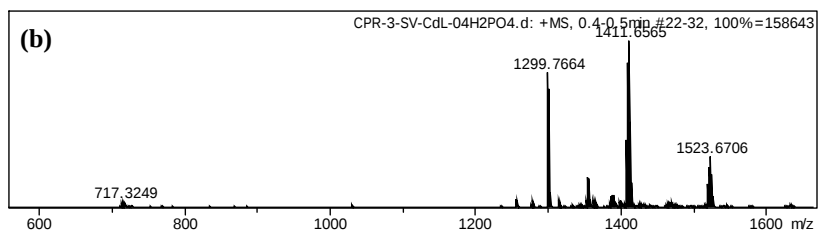
Spectrum View



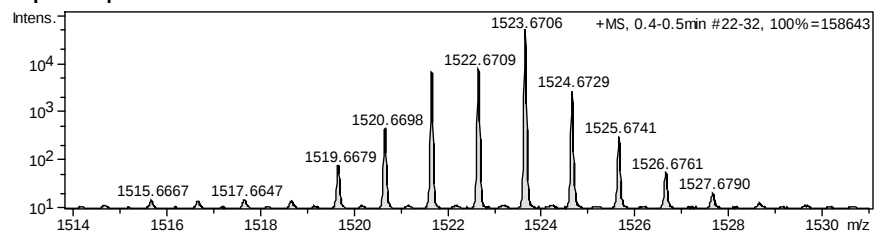
Compound Spectra



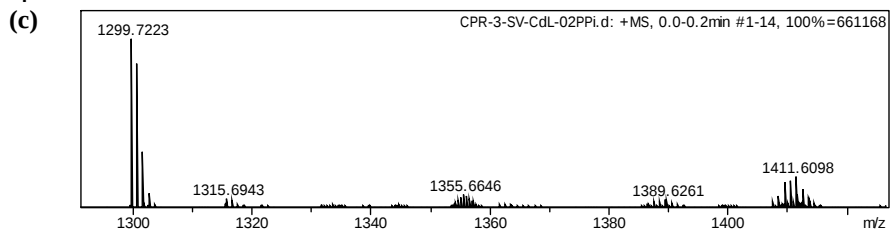
Spectrum View



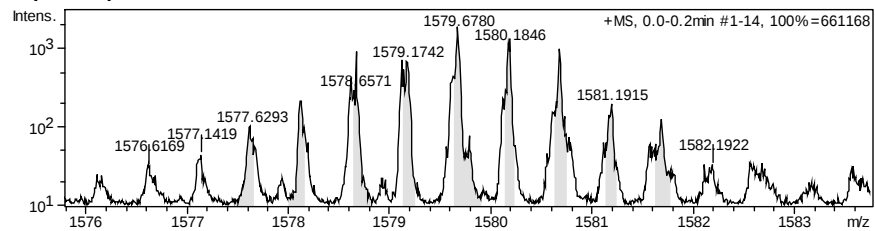
Compound Spectra



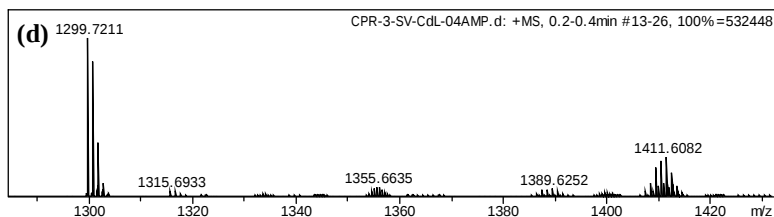
Spectrum View



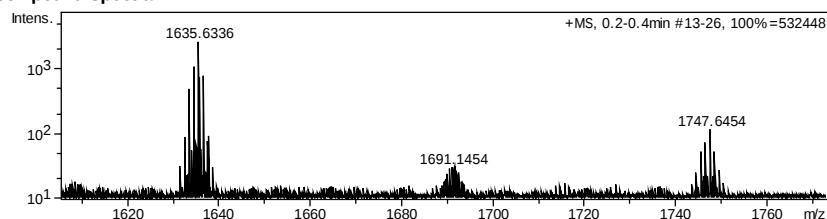
Compound Spectra



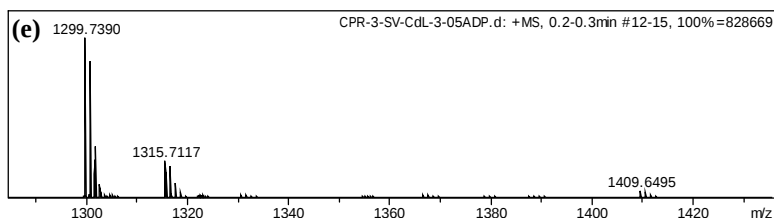
Spectrum View



Compound Spectra



Spectrum View



Compound Spectra

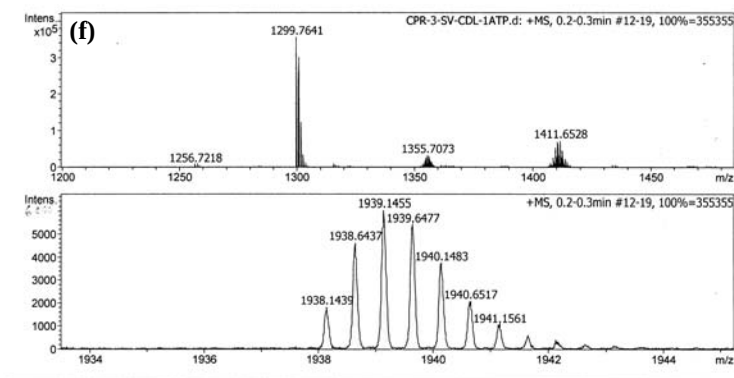
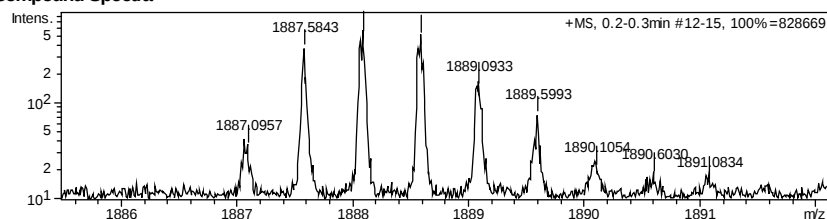


Figure S17 Ternary complexes of phosphates: (a) HPO_4^{2-} , (b) H_2PO_4^- , (c) $\text{P}_2\text{O}_7^{4-}$, (d) AMP^{2-} , (e) ADP^{2-} and (f) ATP^{2-}

SI12. Minimized structures and metric data of $[\text{CdLX}]_2$ complexes

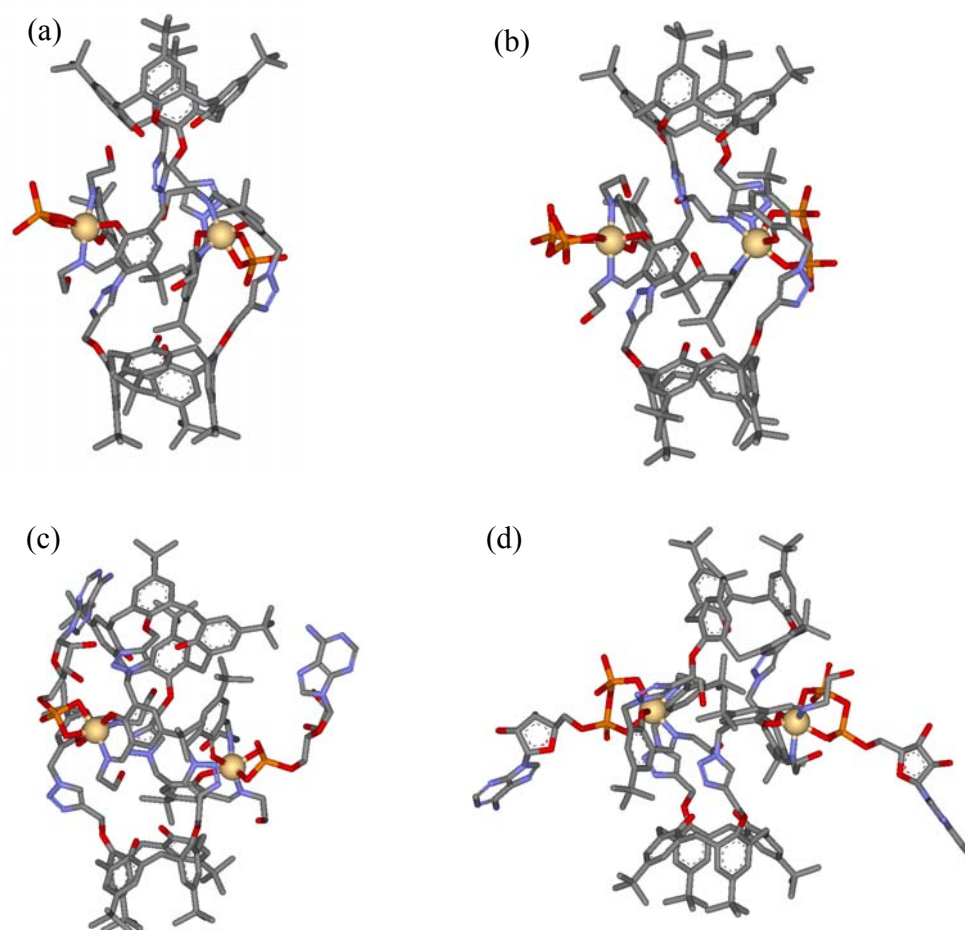


Figure S18. The MM minimized structures of ternary complexes (a) $[\text{CdLHPO}_4^{2-}]_2$, (b) $[\text{CdLPPi}^{4-}]_2$, (c) $[\text{CdLAMP}^{2-}]_2$ & (d) $[\text{CdLADP}^{2-}]_2$

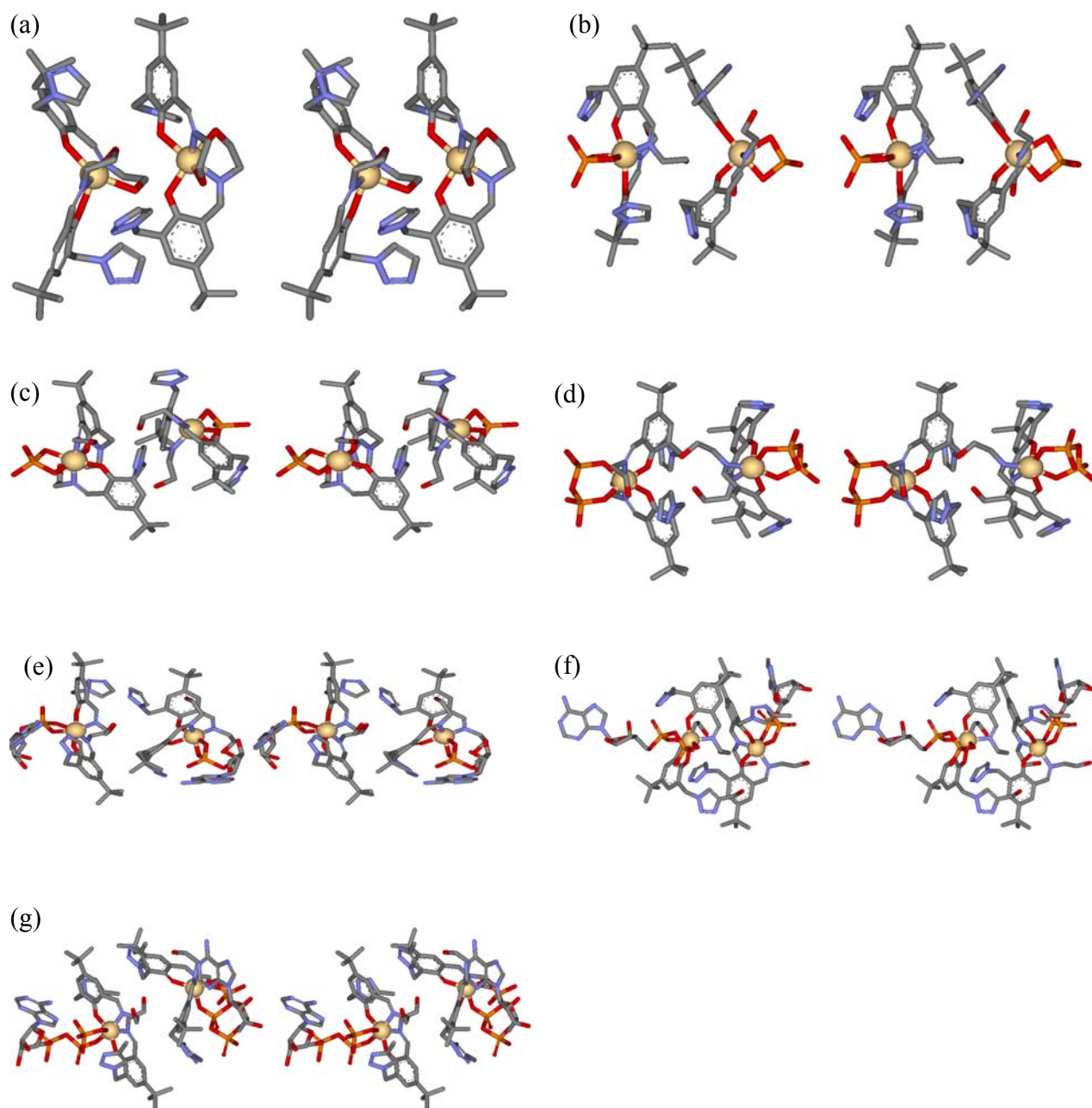


Figure S19. Stereo view of the binding cores of crystal and MM minimized structures (a to g) (a) crystal structure of $[\text{CdL}]_2$ (b) $[\text{CdLH}_2\text{PO}_4]_2$, (c) $[\text{CdLHPO}_4^{2-}]_2$, (d) $[\text{CdLPPi}^{4-}]_2$, (e) $[\text{CdLAMP}^{2-}]_2$, (f) $[\text{CdLADP}^{2-}]_2$ & (g) $[\text{CdLATP}^{2-}]_2$.

Table S02. The calculated metric data {bond distances (Å)} of Cd1 coordination sphere of MM minimized structures of [CdLX]₂ complexes.

Bond distances	Crystal	HPO ₄ ²⁻	H ₂ PO ₄ ⁻	P ₂ O ₇ ⁴⁻	AMP ²⁻	ADP ²⁻	ATP ²⁻
O1-Cd1	2.25	2.07	2.07	2.05	2.03	2.06	2.05
O2-Cd1	2.25	2.04	2.04	2.10	2.06	2.04	2.05
N1-Cd1	2.27	2.11	2.11	2.05	2.08	2.15	2.13
N2-Cd1	2.27	2.09	2.09	2.11	2.12	2.14	2.09
O3-Cd1	2.51	3.97	4.94	4.87	4.08	3.35	5.27
O4-Cd1	2.51	4.99	5.15	4.07	3.90	5.12	5.08
OP1-Cd1		2.19	2.16	2.12	2.12	2.16	2.09
OP2-Cd1		2.12	2.16		2.14		
OP3-Cd1							
OP4-Cd1				2.11		2.15	2.08

Table S03. The calculated metric data {bond distances (Å)} of Cd2 coordination sphere of MM minimized structures of [CdLX]₂ complexes.

Bond distances	Crystal	HPO ₄ ²⁻	H ₂ PO ₄ ⁻	P ₂ O ₇ ⁴⁻	AMP ²⁻	ADP ²⁻	ATP ²⁻
O1-Cd2	2.24	2.05	2.05	2.05	2.08	2.06	2.06
O2-Cd2	2.24	2.05	2.04	2.12	2.07	2.05	2.04
N1-Cd2	2.27	2.12	2.10	2.10	2.13	2.14	2.13
N2-Cd2	2.27	2.10	2.10	2.03	2.12	2.11	2.09
O3-Cd2	2.41	5.22	3.79	5.24	4.97	4.86	5.12
O4-Cd2	2.41	3.59	4.93	3.68	3.62	3.84	4.05
OP1-Cd2		2.13	2.13	2.13	2.15	2.16	2.10
OP2-Cd2		2.13	2.13		2.14		
OP3-Cd2							
OP4-Cd2				2.13		2.13	2.10

Table S04. The calculated metric data {bond angles (deg)} of Cd1 coordination sphere of MM minimized structures of [CdLX]₂ complexes.

Bond angles	Crystal	HPO ₄ ²⁻	H ₂ PO ₄ ⁻	P ₂ O ₇ ⁴⁻	AMP ²⁻	ADP ²⁻	ATP ²⁻
O1-Cd1-O2	113.9	160.0	159.9	156.4	174.3	162.7	154.9
O1-Cd1-N1	81.7	92.5	87.4	91.2	85.1	88.6	88.0
O1-Cd1-N2	96.5	93.3	107.3	102.0	96.8	104.3	112.7
O1-Cd1-O3/OP1	148.7	97.5	87.2	100.1	93.2	82.9	84.0
O1-Cd1-O4/OP4	113.9	73.5	82.4	72.0	80.5	81.6	78.5
O2-Cd1-N1	96.6	107.1	93.5	109.8	93.7	96.2	98.5
O2-Cd1-N2	81.7	87.1	92.4	89.1	88.7	92.1	91.6
O2-Cd1-O3/OP1	87.3	82.9	73.0	73.9	81.3	80.2	70.8
O2-Cd1-O4/OP4	148.7	87.0	97.3	86.63	99.1	98.7	103.4
N1-Cd1-N2	176.9	96.9	96.6	88.7	103.4	90.4	88.9
N1-Cd1-O3/OP1	72.8	82.0	104.9	80.9	95.6	94.8	104.2
N1-Cd1-O4/OP4	109.6	154.5	169.0	163.3	161.0	158.1	153.2
N2-Cd1-O3/OP1	109.6	169.1	154.5	155.6	159.0	171.1	159.2
N2-Cd1-O4/OP4	72.7	105.0	82.3	94.54	90.7	73.1	75.3
O3/OP1-Cd1-O4/OP4	84.5	78.8	78.9	101.6	72.8	103.3	97.4

Table S05. The calculated metric data {bond angles (deg)} of Cd2 coordination sphere of MM minimized structures of [CdLX]₂ complexes.

Bond angles	Crystal	HPO ₄ ²⁻	H ₂ PO ₄ ⁻	P ₂ O ₇ ⁴⁻	AMP	ADP	ATP
O1-Cd2-O2	95.7	95.4	94.7	80.0	68.0	78.8	77.5
O1-Cd2-N1	83.2	90.3	91.1	89.3	94.1	85.6	86.3
O1-Cd2-N2	134.1	80.4	83.7	77.5	146.9	83.8	85.1
O1-Cd2-O3/OP1	137.9	101.0	94.8	102.8	105.1	115.1	119.3
O1-Cd2-O4/OP4	80.5	168.1	166.9	157.9	78.2	145.0	150.0
O2-Cd2-N1	134.0	90.5	83.3	95.4	93.8	139.9	144.7
O2-Cd2-N2	83.2	91.9	93.0	90.1	87.5	92.1	92.8
O2-Cd2-O3/OP1	80.5	163.4	164.0	169.0	163.7	67.6	72.2
O2-Cd2-O4/OP4	137.9	86.7	94.7	79.4	117.8	119.6	115.1
N1-Cd2-N2	129.2	170.6	173.5	164.5	110.0	122.7	116.9
N1-Cd2-O3/OP1	71.1	87.5	83.7	79.3	71.4	86.7	89.5
N1-Cd2-O4/OP4	87.4	101.2	98.9	98.9	140.6	93.7	94.3
N2-Cd2-O3/OP1	87.4	92.7	100.6	95.4	103.7	147.2	146.0
N2-Cd2-O4/OP4	71.0	87.9	86.7	96.2	95.1	67.2	67.8
O3/OP1-Cd2-O4/OP4	129.0	77.5	78.0	98.8	73.4	99.6	90.6

SI13. Cartesian coordinates for MM minimized structure of $[\text{CdLHPO}_4^{2-}]_2$

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
6	-7.533	10.496	1.012	6	-8.057	8.684	9.036
6	3.67	10.208	6.282	6	-7.328	7.946	7.922
48	-3.468	16.832	7.605	8	-7.146	8.966	10.11
48	-4.437	8.927	7.751	6	-6.253	12.602	0.636
8	1.543	15.619	9.802	6	-8.3	12.654	2.058
8	-3.566	16.867	9.669	6	-1.717	10.373	14.474
7	-1.807	11.555	3.723	-6	11.668	10.449	7.322
8	1.982	14.38	5.778	8	-9.682	16.66	5.176
8	2.225	12.029	7.996	8	-3.821	17.334	5.661
7	-5.048	15.43	7.661	7	-6.987	12.091	11.25
8	2.342	10.894	3.811	-8	10.316	14.599	8.994
6	-5.871	16.241	9.825	-8	10.364	12.885	6.202
6	2.725	15.311	9.439	7	-1.959	15.49	7.082
6	-4.578	16.684	10.396	-8	10.806	10.729	10.084
7	-0.855	10.296	2.364	6	-2.058	16.01	4.657
6	-0.502	11.854	3.822	-6	10.852	16.197	5.39
6	3.337	16.082	8.335	6	-3.192	16.977	4.628
6	-5.968	15.446	8.579	7	-8.258	11.33	12.71
6	3.615	14.35	10.151	6	-8.116	11.769	10.596
7	-2.049	10.6	2.839	-6	11.589	16.659	6.584
6	1.567	10.941	2.613	6	-1.498	15.347	5.872
6	4.728	16.286	8.372	-6	11.628	15.361	4.431
6	-2.841	12.235	4.499	7	-7.064	11.871	12.551
6	2.562	15.351	5.207	-6	10.267	10.588	11.399
6	0.111	11.024	2.943	-6	12.979	16.841	6.452
6	-4.949	11.956	3.168	6	-5.813	12.687	10.624
6	2.474	16.856	7.36	-6	11.152	15.326	9.609
6	3.28	11.531	8.491	6	-8.938	11.265	11.555
6	-6.195	10.288	5.153	6	-3.846	12.145	12.104
6	-4.204	11.619	4.305	-6	10.845	17.175	7.798
6	-0.26	16.175	11.231	-6	11.25	12.302	5.507
6	5.561	15.634	9.32	6	-2.728	10.289	10.219
6	4.994	14.63	10.15	6	-4.571	11.887	10.93
6	3.149	13.003	10.667	6	-7.764	17.508	4.029
7	-2.025	17.198	11.876	-6	13.695	16.385	5.312
6	-6.873	10.701	3.986	-6	13.015	15.576	4.362
6	4.148	11.25	5.297	-6	11.035	14.168	3.716
6	2.716	13.948	3.02	7	-5.845	18.416	3.779
7	-0.165	17.491	10.988	6	-2.085	10.591	11.433
6	2.948	15.235	3.783	-6	12.401	11.227	8.395
6	0.809	15.17	10.934	-6	11.674	13.479	11.414
6	-4.766	10.666	5.292	7	-7.525	18.395	5.008
6	3.706	12.891	3.451	-6	11.836	14.881	10.858

6	3.648	16.29	3.179	6	-8.901	16.537	3.991
6	-7.01	16.282	10.645	6	-4.1	10.827	10.009
6	2.887	16.618	5.922	-6	12.445	12.485	10.577
6	5.07	13.2	3.439	-6	12.746	15.756	11.472
6	-1.466	15.976	11.825	6	-1.479	15.646	3.426
6	-6.265	11.477	2.967	-6	11.465	16.677	9.086
6	5.226	10.001	8.258	-6	13.822	12.683	10.402
6	-6.961	16.646	12.013	6	-6.673	17.518	3.221
6	-4.508	16.958	11.859	6	-2.63	11.476	12.398
6	3.776	11.89	9.851	-6	12.897	10.478	5.123
7	-1.245	18.142	11.377	6	-1.938	16.129	2.176
6	-3.277	17.513	12.555	6	-3.585	17.565	3.324
6	4.957	11.285	10.32	-6	11.656	12.881	4.206
6	5.493	11.655	5.274	7	-6.358	18.994	4.852
6	7.066	15.994	9.377	6	-4.523	18.754	3.264
6	-7.069	11.807	1.685	-6	12.666	12.255	3.459
6	5.701	10.357	9.544	-6	13.778	11.503	8.264
6	3.597	17.617	5.234	-6	15.202	16.71	5.185
6	7.841	15.211	10.466	6	-1.854	11.713	13.718
6	-5.705	16.947	12.597	-6	13.305	11.066	3.899
6	3.986	17.478	3.874	-6	12.383	17.482	9.778
6	5.984	12.583	4.321	-6	15.828	16.193	3.866
6	7.468	13.01	4.271	6	-2.967	17.103	2.152
6	-8.087	17.114	14.298	-6	13.037	17.046	10.96
6	-8.267	16.619	12.843	-6	14.514	12.187	9.269
6	7.217	17.498	9.691	-6	16.036	12.445	9.151
6	6.165	18	2.718	6	-1.944	16.119	-0.409
6	8.057	12.632	2.896	-6	14.469	10.416	3.113
6	4.792	18.572	3.131	6	-1.244	15.633	0.883
6	-9.328	17.527	12.181	-6	15.401	18.242	5.222
6	8.173	10.231	9.067	-6	15.452	17.187	11.677
6	7.442	10.229	11.453	-6	16.764	11.621	10.231
6	7.728	15.685	8.02	-6	14.09	17.916	11.688
6	-8.792	15.17	12.905	6	0.209	16.149	0.859
6	7.575	14.54	4.47	-6	15.742	10.422	3.989
6	8.337	12.331	5.358	-6	14.807	11.155	1.795
6	5.051	19.833	3.99	-6	15.972	16.067	6.354
8	-4.015	10.206	6.197	6	-1.241	14.086	0.847
8	-7.473	14.26	6.101	-6	16.338	13.948	9.366
7	-6.468	8.85	7.153	-6	16.615	12.042	7.772
6	-6.214	14.734	5.594	-6	14.299	19.303	11.031
6	-5.093	14.441	6.583	8	-4.872	10.403	9.103
6	3.289	11.665	4.173	8	-2.898	12.944	8.138
6	4.061	10.551	7.703	7	-2.372	9.167	8.048
6	-6.973	9.486	6.134	6	-1.504	13.283	8.138
6	-1.33	14.8	8.204	1	1.469	15.082	11.828
-6	11.772	11.477	9.711	1	0.321	14.197	10.706

-6	11.911	11.044	5.95	1	3.958	16.165	2.144
6	-1.901	9.637	9.167	1	-7.954	15.951	10.215
6	-0.476	9.589	6.513	1	5.4	14.012	2.801
6	-1.48	8.573	7.052	1	-1.906	15.052	12.194
8	0.231	9.018	5.4	1	5.796	9.304	7.648
6	-2.556	12.714	14.668	1	-3.224	17.118	13.597
6	-0.446	12.271	13.41	1	5.307	11.587	11.302
6	7.051	9.774	10.026	1	6.156	11.219	6.007
6	6.979	8.23	10.035	1	3.839	18.518	5.788
-6	13.644	18.157	13.147	1	7.399	15.388	11.474
6	4.019	19.021	1.87	1	8.906	15.537	10.505
-6	14.101	8.961	2.748	1	7.841	14.117	10.248
15	-4.056	6.199	8.362	1	-5.635	17.214	13.647
8	-4.438	7.58	9.405	1	-9.062	17.113	14.84
8	-5.29	4.921	8.509	1	-7.397	16.448	14.866
8	-4.184	7.033	6.803	1	-7.693	18.157	14.315
8	-2.385	5.646	8.646	1	6.77	18.131	8.892
15	-2.858	19.545	7.879	1	6.715	17.746	10.654
8	-1.812	18.113	7.925	1	8.293	17.779	9.774
8	-4.414	18.725	7.638	1	6.724	17.65	3.616
8	-2.831	20.399	9.443	1	6.779	18.776	2.204
8	-2.464	20.565	6.47	1	6.059	17.141	2.017
1	-6.655	9.847	0.785	1	9.132	12.921	2.834
1	2.563	10.116	6.236	1	7.977	11.532	2.73
1	4.085	9.216	5.988	1	7.52	13.148	2.068
1	1.698	14.394	6.745	-1	10.273	17.529	12.771
1	1.64	12.698	8.473	1	-8.953	18.575	12.114
1	-0.06	12.594	4.485	1	-9.582	17.187	11.156
1	-6.816	14.766	8.494	1	9.166	9.861	9.414
1	1.746	9.993	2.057	1	8.211	11.345	9.019
1	1.855	11.759	1.922	1	8.016	9.845	8.035
1	5.161	16.989	7.664	1	6.669	9.92	12.194
1	-2.572	12.214	5.576	1	7.577	11.335	11.496
1	-2.876	13.304	4.195	1	8.826	15.871	8.063
1	-4.474	12.616	2.449	1	7.316	16.329	7.211
1	2.535	17.939	7.619	1	7.563	14.618	7.748
1	1.402	16.581	7.467	1	-9.755	15.118	13.465
1	5.626	14	10.766	1	-8.052	14.511	13.413
1	3.432	12.913	11.741	1	-8.965	14.765	11.886
1	2.052	12.882	10.636	1	6.97	14.856	5.348
1	-7.91	10.393	3.862	1	8.632	14.854	4.634
1	2.811	14.113	1.921	1	7.206	15.099	3.581
1	8.332	11.223	5.239	-1	13.394	9.577	5.475
1	7.975	12.593	6.379	1	-4.082	19.581	3.868
1	9.398	12.666	5.284	-1	12.952	12.729	2.526
1	5.658	19.586	4.891	-1	14.27	11.16	7.363
1	5.62	20.597	3.41	-1	12.589	18.462	9.359

1	4.09	20.302	4.306	-1	16.894	16.507	3.784
1	-6.267	15.827	5.421	-1	15.812	15.079	3.825
1	-6.006	14.229	4.624	-1	15.285	16.604	2.983
1	-4.133	14.472	6.031	1	-3.289	17.548	1.216
1	-5.207	13.412	6.998	1	-1.882	17.227	-0.509
1	-8.041	9.375	5.93	1	-1.454	15.688	-1.313
1	-8.882	8.045	9.427	1	-3.014	15.806	-0.42
1	-8.496	9.629	8.65	-1	16.475	18.506	5.086
1	-6.723	7.135	8.368	-1	15.076	18.676	6.194
1	-8.071	7.446	7.254	-1	14.814	18.728	4.408
1	-5.958	13.602	1.032	-1	16.241	17.815	12.153
1	-5.339	12.039	0.335	-1	15.409	16.226	12.237
1	-7.976	13.588	2.57	-1	15.764	16.966	10.63
1	-2.723	9.94	14.679	-1	16.561	10.534	10.094
-1	12.008	9.388	7.358	-1	16.426	11.91	11.253
-1	10.574	10.425	7.523	-1	17.865	11.785	10.176
-1	10.048	13.677	9.297	1	0.785	15.779	1.736
-1	10.039	12.549	7.095	1	0.736	15.807	-0.062
1	-8.291	11.863	9.526	1	0.227	17.263	0.881
1	-0.659	14.672	5.716	-1	15.613	9.806	4.907
-1	10.979	10.932	12.184	-1	16.61	10.005	3.428
-1	10.105	9.502	11.58	-1	15.992	11.463	4.301
-1	13.509	17.36	7.245	-1	15.642	10.647	1.26
1	-5.692	13.725	11.003	-1	15.132	12.202	1.998
1	-5.951	12.748	9.52	-1	13.928	11.165	1.109
1	-4.253	12.891	12.78	-1	15.655	16.494	7.332
1	-9.78	16.847	7.765	-1	15.793	14.968	6.369
-1	10.836	18.289	7.769	-1	17.068	16.243	6.253
-1	13.561	15.048	3.587	1	-0.579	13.656	1.628
1	-9.955	14.079	3.915	1	-0.862	13.709	-0.131
-1	11.165	14.289	2.616	1	-2.273	13.691	0.999
1	-1.109	10.147	11.615	-1	17.378	14.202	9.055
-1	10.599	13.237	11.439	-1	16.247	14.241	10.436
1	-8.448	15.53	3.931	-1	15.629	14.57	8.778
1	-9.522	16.741	3.087	-1	17.702	12.281	7.712
-1	13.26	15.408	12.365	-1	16.515	10.945	7.599
1	-0.644	14.95	3.443	-1	16.101	12.592	6.95
-1	14.34	13.31	11.123	-1	15.055	19.898	11.595
1	-6.46	16.891	2.356	-1	13.35	19.888	11.028
-1	14.674	19.197	9.987	1	7.923	7.792	10.435
1	-1.024	12.818	9.028	1	6.135	7.887	10.678
1	-1.014	12.869	7.23	1	6.833	7.815	9.014
1	-1.785	15.163	9.147	-1	12.64	18.64	13.17
1	-0.248	15.038	8.219	-1	14.365	18.823	13.676
1	-0.826	9.586	9.348	-1	13.589	17.208	13.725
1	-1.009	10.503	6.182	1	4.551	19.854	1.355
1	0.259	9.87	7.299	1	3.913	18.195	1.132

1	-0.935	7.709	7.498	1	2.999	19.375	2.148
1	-2.087	8.198	6.199	1	1.673	13.625	3.215
1	-1.975	12.838	15.612	-1	12.033	13.422	12.467
1	-2.64	13.72	14.197	1	-4.629	19.136	2.222
1	-0.522	13.204	12.811	1	-3.393	18.619	12.626
1	-8.88	12.936	1.148	-1	13.156	8.937	2.158
1	-8.988	12.099	2.734	-1	13.964	8.329	3.654
1	-8.234	9.923	1.659	-1	14.907	8.49	2.138
1	-8.067	10.708	0.057	1	-2.181	5.018	7.851
1	-6.857	12.779	-0.284	1	-3.314	21.132	6.315
1	-1.13	9.63	13.888	1	0.102	12.506	14.352
1	-1.192	10.519	15.447	1	0.176	11.544	12.842
1	-3.572	12.351	14.948	1	8.408	9.768	11.765

SI14. Cartesian coordinates for MM minimized structure of $[\text{CdLH}_2\text{PO}_4]_2$

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
6	-7.61	10.485	1.442	7	-6.158	8.436	7.508
6	3.838	10.27	6.41	6	-6.232	14.716	5.668
48	-3.474	16.673	7.736	6	-5.133	14.336	6.653
48	-4.101	8.571	7.914	6	3.327	11.584	4.236
8	1.497	15.711	9.846	6	4.253	10.693	7.801
8	-3.597	16.722	9.798	6	-6.736	9.067	6.525
7	-1.768	11.303	3.918	6	-7.79	8.178	9.348
8	1.918	14.211	5.731	6	-6.934	7.478	8.3
8	2.344	12.076	8.102	8	-6.956	8.665	10.412
7	-5.064	15.281	7.77	6	-6.692	12.81	1.396
8	2.408	10.748	3.951	6	-8.613	12.283	2.889
6	-5.884	16.028	9.964	6	-1.866	10.421	14.764
6	2.671	15.439	9.435	-6	11.583	10.777	6.779
6	-4.603	16.516	10.528	8	-9.745	16.728	5.12
7	-0.828	10.035	2.559	8	-3.789	17.178	5.789
6	-0.461	11.6	4.006	7	-7	11.8	11.05
6	3.185	16.132	8.226	-8	10.264	14.622	8.788
6	-5.974	15.261	8.699	-8	10.519	13.355	5.709
6	3.651	14.559	10.144	7	-1.972	15.311	7.233
7	-2.019	10.345	3.04	-8	10.813	10.702	9.581
6	1.599	10.682	2.776	6	-2.07	15.788	4.798
6	4.576	16.341	8.15	-6	10.977	16.429	5.275
6	-2.793	11.995	4.694	6	-3.17	16.794	4.761
6	2.408	15.205	5.12	7	-8.435	11.105	12.387
6	0.146	10.76	3.131	6	-8.071	11.504	10.292
6	-5.014	11.754	3.545	-6	11.644	16.874	6.521
6	2.239	16.764	7.227	6	-1.521	15.134	6.023
6	3.442	11.658	8.578	-6	11.858	15.804	4.237
6	-6.045	9.941	5.533	7	-7.213	11.605	12.34
6	-4.152	11.349	4.571	-6	10.326	10.408	10.892
6	-0.257	16.232	11.344	-6	13.016	17.18	6.455
6	5.401	16.107	9.313	6	-5.769	12.388	10.539
6	5.011	14.906	10.01	-6	11.093	15.312	9.454
6	3.29	13.198	10.707	6	-9.002	11.051	11.172
7	-2.066	17.17	11.995	6	-3.916	11.953	12.195
6	-6.833	10.41	4.461	-6	10.826	17.256	7.739
6	4.232	11.287	5.363	-6	11.396	12.738	5.035
6	2.611	13.758	2.967	6	-2.596	10.1	10.447
7	-0.216	17.553	11.119	6	-4.558	11.611	10.995
6	2.773	15.077	3.691	6	-7.735	17.466	4.066
6	0.854	15.278	11.039	-6	13.804	16.891	5.311
6	-4.609	10.342	5.558	-6	13.226	16.127	4.263

6	3.664	12.778	3.425	-6	11.42	14.688	3.312
6	3.395	16.158	3.047	7	-5.779	18.305	3.87
6	-7.016	16.016	10.795	6	-2.037	10.479	11.681
6	2.649	16.512	5.79	-6	12.337	11.443	7.912
6	5.006	13.166	3.369	-6	11.621	13.355	11.135
6	-1.455	15.974	11.932	7	-7.49	18.339	5.056
6	-6.351	11.295	3.464	-6	11.758	14.797	10.687
6	5.457	10.219	8.343	6	-8.932	16.577	3.962
6	-6.97	16.376	12.164	6	-3.984	10.539	10.153
6	-4.536	16.802	11.99	-6	12.407	12.448	10.219
6	3.956	12.092	9.909	-6	12.643	15.644	11.375
7	-1.324	18.153	11.513	6	-1.516	15.385	3.566
6	-3.33	17.421	12.676	-6	11.413	16.69	9.014
6	5.173	11.555	10.37	-6	13.775	12.698	10.041
6	5.549	11.771	5.29	6	-6.626	17.442	3.284
6	6.947	16.313	9.127	6	-2.68	11.369	12.578
6	-7.296	11.718	2.313	-6	12.885	10.787	4.624
6	5.942	10.639	9.605	6	-1.983	15.852	2.311
6	3.28	17.538	5.063	6	-3.543	17.383	3.454
6	7.647	16.311	10.508	-6	11.933	13.351	3.796
6	-5.725	16.736	12.737	7	-6.295	18.889	4.939
6	3.666	17.383	3.705	6	-4.437	18.604	3.385
6	5.967	12.673	4.279	-6	12.92	12.67	3.065
6	7.424	13.176	4.17	-6	13.706	11.766	7.785
6	-8.094	16.786	14.462	-6	15.28	17.358	5.271
6	-8.269	16.298	13.003	6	-1.987	11.708	13.921
6	7.241	17.686	8.473	-6	13.409	11.396	3.457
6	5.778	18.001	2.471	-6	12.298	17.465	9.781
6	8.033	12.659	2.851	-6	15.984	17.038	3.929
6	4.389	18.505	2.921	6	-2.964	16.874	2.283
6	-9.361	17.177	12.356	-6	12.927	16.966	10.951
6	8.407	10.587	9.07	-6	14.449	12.356	8.843
6	7.734	10.661	11.471	-6	15.951	12.701	8.708
6	7.548	15.196	8.251	6	-2.114	15.704	-0.265
6	-8.747	14.832	13.057	-6	14.535	10.672	2.68
6	7.453	14.725	4.17	6	-1.33	15.315	1.013
6	8.327	12.689	5.33	-6	15.34	18.889	5.47
6	4.608	19.792	3.752	-6	15.326	17.096	11.72
8	-3.77	9.865	6.371	-6	16.755	11.826	9.69
8	-7.52	14.322	6.169	-6	13.954	17.803	11.753
6	0.094	15.891	0.897	1	6.677	18.495	8.993
-6	15.767	10.514	3.599	1	8.328	17.929	8.526
-6	14.993	11.432	1.412	1	6.38	17.689	3.356
-6	16.074	16.666	6.395	1	6.335	18.803	1.934
6	-1.259	13.768	1.047	1	5.699	17.132	1.78
-6	16.179	14.194	9.05	1	9.088	13.002	2.741
-6	16.508	12.456	7.284	1	8.021	11.545	2.828

-6	14.153	19.233	11.192	1	7.46	13.031	1.97
8	-4.684	10.029	9.234	-1	10.302	17.143	12.953
8	-2.982	12.829	8.305	1	-9.021	18.237	12.295
7	-2.079	8.94	8.336	1	-9.612	16.837	11.33
6	-1.578	13.123	8.349	1	9.421	10.274	9.409
6	-1.352	14.632	8.368	1	8.397	11.697	8.969
-6	11.742	11.52	9.264	1	8.244	10.146	8.061
-6	11.919	11.403	5.438	1	6.997	10.347	12.247
6	-1.684	9.474	9.455	1	7.818	11.773	11.465
6	-0.234	9.471	6.788	1	8.63	15.383	8.062
6	-1.109	8.382	7.396	1	7.023	15.152	7.273
8	0.542	8.914	5.714	1	7.45	14.201	8.74
6	-2.763	12.75	14.763	1	-9.703	14.746	13.625
6	-0.573	12.279	13.659	1	-7.982	14.192	13.554
6	7.326	10.129	10.076	1	-8.919	14.427	12.038
6	7.314	8.586	10.153	1	6.816	15.129	4.988
-6	13.481	17.943	13.217	1	8.49	15.11	4.306
6	3.553	18.889	1.679	1	7.082	15.146	3.209
-6	14.045	9.277	2.231	1	8.417	11.577	5.328
15	-3.629	5.81	8.162	1	7.925	13.021	6.314
8	-3.894	7.058	9.396	1	9.359	13.099	5.231
8	-4.872	4.536	8.263	1	5.246	19.587	4.643
8	-3.876	6.821	6.727	1	5.127	20.571	3.146
8	-1.953	5.208	8.227	1	3.634	20.222	4.082
15	-2.852	19.382	7.999	1	-6.214	15.812	5.509
8	-1.816	17.943	8.082	1	-6.057	14.21	4.692
8	-4.409	18.57	7.736	1	-4.168	14.349	6.112
8	-2.854	20.258	9.552	1	-5.29	13.296	7.025
8	-2.424	20.381	6.588	1	-7.808	8.915	6.376
1	-6.67	10.056	1.024	1	-8.52	7.452	9.773
1	2.736	10.126	6.405	1	-8.357	9.02	8.892
1	4.29	9.286	6.146	1	-6.258	6.774	8.819
1	1.656	14.233	6.704	1	-7.582	6.862	7.632
1	1.735	12.725	8.577	1	-6.436	13.723	1.983
1	-0.012	12.347	4.657	1	-5.78	12.436	0.874
1	-6.816	14.574	8.601	1	-8.394	13.092	3.622
1	1.785	9.696	2.294	1	-2.874	9.983	14.949
1	1.855	11.447	2.013	-1	11.835	9.691	6.779
1	4.986	16.792	7.253	-1	10.484	10.835	6.951
1	-2.496	12.017	5.763	1	-9.986	13.685	9.035
1	-2.851	13.053	4.354	-1	10.11	12.998	6.558
1	-4.62	12.464	2.823	1	-8.139	11.583	9.208
1	2.193	17.857	7.437	1	-0.703	14.432	5.877
1	1.202	16.389	7.371	-1	11.066	10.676	11.681
1	5.762	14.23	10.407	-1	10.182	9.307	10.96
1	3.614	13.16	11.773	-1	13.476	17.672	7.306
1	2.201	13.015	10.719	1	-5.696	13.436	10.904

1	-7.861	10.061	4.397	1	-5.789	12.425	9.425
1	2.69	13.893	1.863	1	-4.395	12.708	12.812
1	1.567	15.276	11.896	1	-9.778	16.89	7.637
1	0.419	14.266	10.888	-1	10.765	18.368	7.796
1	3.692	16.026	2.01	-1	13.843	15.727	3.464
1	-7.95	15.653	10.372	-1	10.33	14.599	3.224
1	5.277	13.95	2.67	-1	11.786	14.91	2.283
1	-1.856	15.028	12.287	1	-1.049	10.096	11.928
1	6.044	9.528	7.744	-1	10.55	13.094	11.139
1	-3.252	17.034	13.72	1	-8.554	15.534	3.905
1	5.528	11.903	11.334	1	-9.498	16.853	3.042
1	6.25	11.418	6.032	-1	13.145	15.245	12.253
1	3.465	18.469	5.589	1	-0.697	14.671	3.589
1	7.175	17.062	11.182	-1	14.291	13.264	10.812
1	8.728	16.563	10.405	1	-6.42	16.825	2.411
1	7.599	15.316	11.002	-1	13.28	9.827	4.947
1	-5.66	17.01	13.785	1	-3.982	19.411	4.006
1	-9.062	16.741	15.012	-1	13.301	13.162	2.176
1	-7.371	16.143	15.016	-1	14.187	11.543	6.841
1	-7.742	17.844	14.485	-1	12.499	18.472	9.428
1	6.975	17.7	7.393	-1	17.019	17.453	3.917
-1	17.844	12.053	9.62	-1	16.073	15.938	3.775
1	0.707	15.611	1.781	-1	15.429	17.489	3.074
1	0.605	15.505	-0.015	1	-3.274	17.319	1.344
1	0.062	17.004	0.842	1	-2.07	16.802	-0.45
-1	15.542	9.877	4.484	1	-1.674	15.215	-1.166
-1	16.611	10.036	3.051	1	-3.179	15.383	-0.185
-1	16.106	11.51	3.967	-1	16.389	19.259	5.39
-1	15.791	10.866	0.877	-1	14.962	19.192	6.472
-1	15.417	12.429	1.675	-1	14.727	19.404	4.694
-1	14.145	11.566	0.701	-1	16.095	17.699	12.256
-1	15.686	16.948	7.4	-1	15.287	16.097	12.209
-1	16.011	15.56	6.283	-1	15.663	16.956	10.667
-1	17.149	16.96	6.359	-1	16.605	10.746	9.46
1	-0.522	13.403	1.793	-1	16.435	12.003	10.743
1	-0.932	13.359	0.064	1	-7.418	13.11	0.605
1	-2.258	13.337	1.291	1	-1.242	9.655	14.251
-1	17.195	14.532	8.74	1	-1.391	10.637	15.749
-1	16.101	14.386	10.143	1	-3.781	12.375	15.02
-1	15.421	14.825	8.535	1	-0.104	12.629	14.608
-1	17.583	12.747	7.222	1	0.11	11.518	13.222
-1	16.448	11.377	7.01	1	8.729	10.257	11.773
-1	15.95	13.059	6.531	1	8.287	8.201	10.54
-1	14.887	19.801	11.809	1	6.504	8.239	10.835
-1	13.194	19.801	11.205	1	7.153	8.123	9.153
-1	14.552	19.201	10.151	-1	12.476	18.423	13.254
1	-1.146	12.675	9.273	-1	14.19	18.573	13.803

1	-1.066	12.662	7.476	-1	13.417	16.957	13.729
1	-1.782	15.038	9.305	1	4.027	19.735	1.13
1	-0.262	14.829	8.366	1	3.462	18.042	0.964
1	-0.616	9.504	9.677	1	2.527	19.2	1.986
1	-0.873	10.288	6.394	1	1.59	13.383	3.181
1	0.455	9.892	7.554	-1	11.985	13.222	12.18
1	-0.471	7.624	7.908	1	-4.509	18.999	2.344
1	-1.653	7.874	6.572	1	-3.502	18.521	12.745
1	-2.234	12.957	15.723	-1	13.121	9.373	1.615
1	-2.852	13.717	14.217	-1	13.82	8.618	3.099
1	-0.625	13.141	12.958	-1	14.822	8.762	1.62
1	-9.254	12.7	2.078	1	-1.829	4.692	7.34
1	-9.218	11.501	3.399	1	-3.235	21.009	6.459
1	-8.121	9.691	2.033	1	-4.731	3.968	7.411
1	-8.279	10.76	0.593	1	-3.416	19.665	10.185

SI15. Cartesian coordinates for MM minimized structure of $[\text{CdLPPi}^{4-}]_2$

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
6	-6.686	11.387	0.897	7	-6.607	8.225	6.671
6	3.865	10.51	7.03	6	-6.425	15.1	5.664
48	-3.673	16.978	7.561	6	-5.248	14.606	6.497
48	-4.655	8.035	7.464	6	3.42	11.563	4.71
8	1.246	16.328	9.769	6	4.193	11.108	8.382
8	-3.863	17.295	9.581	6	-6.973	9.047	5.726
7	-1.542	11.295	4.249	6	-8.491	7.949	8.241
8	1.816	14.2	5.95	6	-7.583	7.28	7.214
8	2.211	12.42	8.447	8	-7.754	8.205	9.446
7	-5.088	15.418	7.705	6	-5.696	13.607	1.479
8	2.575	10.646	4.449	6	-7.922	12.974	2.409
6	-5.836	15.983	9.993	6	-1.323	10.231	13.76
6	2.402	15.977	9.367	-6	11.973	10.634	6.832
6	-4.73	16.883	10.396	8	-9.478	16.851	4.957
7	-0.616	10.302	2.669	8	-3.758	17.451	5.568
6	-0.226	11.382	4.503	7	-6.982	11.4	10.634
6	2.886	16.471	8.058	8	-9.998	14.236	8.854
6	-5.902	15.245	8.705	-8	10.49	13.02	5.838
6	3.388	15.2	10.171	7	-2.19	15.539	7.204
7	-1.806	10.643	3.127	-8	10.949	10.471	9.538
6	1.824	10.456	3.251	6	-2.137	15.853	4.746
6	4.277	16.644	7.91	-6	10.636	16.395	5.236
6	-2.564	11.782	5.171	6	-3.139	16.944	4.594
6	2.254	15.241	5.107	7	-8.292	10.708	12.096
6	0.368	10.722	3.476	6	-8.124	11.128	9.98
6	-4.577	12.063	3.693	-6	11.215	16.633	6.579
6	1.906	16.956	7.01	6	-1.651	15.3	6.042
6	3.306	12.118	9.008	-6	11.546	15.722	4.263
6	-6.074	10.008	5.037	7	-7.069	11.181	11.935
6	-3.956	11.381	4.745	-6	10.352	10.116	10.786
6	-0.462	17.061	11.232	-6	12.621	16.756	6.647
6	5.152	16.56	9.061	6	-5.813	12.014	10.021
6	4.745	15.522	9.98	-6	10.748	15.012	9.518
6	3.027	13.922	10.905	6	-8.974	10.682	10.941
7	-2.293	18.032	11.752	6	-3.755	11.629	11.408
6	-6.606	10.727	3.947	-6	10.314	16.895	7.771
6	4.286	11.412	5.891	-6	11.454	12.579	5.147
6	2.656	13.555	3.185	6	-2.784	9.543	9.691
7	-0.467	18.329	10.797	6	-4.563	11.237	10.339
6	2.7	14.959	3.733	6	-7.613	17.705	3.742
6	0.657	16.09	11.04	-6	13.406	16.867	5.436
6	-4.664	10.265	5.411	-6	12.922	15.98	4.406

6	3.731	12.705	3.817	-6	11.101	14.521	3.46
6	3.229	16.004	2.97	7	-5.634	18.481	3.501
6	-6.836	15.697	10.941	6	-2.051	10.003	10.798
6	2.338	16.622	5.605	-6	12.568	11.339	8.033
6	5.063	13.127	3.756	-6	11.459	13.135	11.22
6	-1.639	16.864	11.878	7	-7.404	18.741	4.568
6	-5.884	11.736	3.256	-6	11.474	14.573	10.745
6	5.377	10.74	9.036	6	-8.861	16.885	3.672
6	-6.782	16.148	12.283	6	-4.16	10.086	9.509
6	-4.664	17.329	11.813	-6	12.369	12.295	10.354
6	3.745	12.732	10.295	-6	12.282	15.505	11.417
7	-1.592	18.948	11.106	6	-1.587	15.299	3.573
6	-3.615	18.312	12.3	-6	10.911	16.415	9.078
6	4.947	12.288	10.877	-6	13.733	12.619	10.307
6	5.601	11.9	5.793	6	-6.469	17.54	3.028
6	6.696	16.597	8.763	6	-2.514	11.01	11.674
6	-6.531	12.423	2.029	-6	13.323	10.999	4.747
6	5.777	11.31	10.269	6	-1.967	15.708	2.268
6	2.867	17.613	4.769	6	-3.418	17.456	3.233
6	7.466	16.911	10.069	-6	11.828	13.268	3.895
6	-5.698	16.964	12.689	7	-6.189	19.241	4.43
6	3.318	17.329	3.456	6	-4.269	18.693	3.03
6	6.028	12.694	4.694	-6	12.931	12.81	3.166
6	7.503	13.109	4.49	-6	13.926	11.727	8.041
6	-7.655	16.171	14.721	-6	14.967	16.86	5.629
6	-7.937	15.782	13.249	6	-1.613	11.448	12.853
6	7.051	17.717	7.752	-6	13.702	11.7	3.58
6	5.377	18.042	2.188	-6	11.712	17.283	9.838
6	8.024	12.461	3.19	-6	15.655	17.309	4.318
6	3.92	18.417	2.539	6	-2.845	16.812	2.128
6	-9.211	16.523	12.801	-6	12.415	16.851	10.993
6	8.274	11.203	9.901	-6	14.542	12.307	9.186
6	7.45	11.586	12.224	-6	16.057	12.623	9.246
6	7.175	15.242	8.201	6	-2.09	15.304	-0.277
6	-8.189	14.255	13.225	-6	14.972	11.25	2.822
6	7.62	14.648	4.367	6	-1.303	15.047	1.033
6	8.429	12.65	5.643	-6	15.396	17.864	6.73
6	3.944	19.822	3.188	-6	14.797	17.224	11.738
8	-4.044	9.574	6.262	-6	16.706	11.732	10.325
8	-7.657	14.552	6.162	-6	13.361	17.791	11.779
6	-2.039	8.674	8.731	6	0.115	15.623	0.871
6	-0.892	8.271	5.935	-6	16.193	11.351	3.764
6	-1.698	7.302	6.796	-6	15.278	12.111	1.572
8	-0.021	7.534	5.06	-6	15.465	15.45	6.01
6	-2.252	12.545	13.74	6	-1.212	13.511	1.209
6	-0.281	12.01	12.307	-6	16.285	14.109	9.616
6	7.129	10.875	10.886	-6	16.788	12.35	7.909

6	7.107	9.356	11.16	-6	13.412	19.229	11.207
-6	12.887	17.892	13.246	8	-4.999	9.602	8.702
6	3.085	18.519	1.243	8	-3.207	13.057	8.239
-6	14.805	9.789	2.35	7	-2.568	8.021	7.734
15	-4.012	5.799	9.641	6	-1.828	13.404	8.43
15	-4.384	4.931	6.948	6	-1.654	14.922	8.418
8	-3.166	5.086	8.242	-6	11.848	11.353	9.326
8	-2.955	6.399	10.678	-6	12.24	11.385	5.547
8	-4.785	4.655	10.447	1	6.769	17.441	6.711
8	-4.698	6.378	6.126	1	6.543	18.67	8.028
8	-5.757	4.31	7.482	1	8.15	17.903	7.73
8	-5.131	7.009	9.27	1	5.98	17.92	3.117
8	-3.848	3.892	5.859	1	5.85	18.836	1.564
15	-1.597	19.277	6.982	1	5.431	17.092	1.611
15	-4.34	19.985	7.457	1	9.093	12.726	3.017
8	-2.987	20.177	6.306	1	7.942	11.351	3.249
8	-1.973	18.102	8.139	1	7.441	12.805	2.305
8	-0.577	20.303	7.66	-1	10.08	16.238	13.438
8	-3.877	20.192	8.974	1	-9.067	17.626	12.871
8	-5.119	18.493	7.313	1	-9.458	16.282	11.746
8	-0.765	18.579	5.81	1	9.264	10.94	10.342
8	-5.435	21.116	7.181	1	8.278	12.291	9.659
1	-5.691	10.972	0.613	1	8.176	10.636	8.948
1	2.768	10.32	6.986	1	6.669	11.366	12.988
1	4.363	9.521	6.907	1	7.53	12.688	12.079
1	2.678	13.876	6.42	1	8.215	15.322	7.807
1	1.556	13.095	8.811	1	6.502	14.905	7.382
1	0.233	11.843	5.377	1	7.171	14.45	8.983
1	-6.677	14.481	8.619	1	-8.961	13.967	13.976
1	1.927	9.388	2.955	1	-7.249	13.705	13.46
1	2.209	11.053	2.396	1	-8.564	13.907	12.239
1	4.649	16.985	6.951	1	7.089	15.153	5.202
1	-2.35	11.39	6.191	1	8.687	14.969	4.385
1	-2.508	12.889	5.224	1	7.189	15.023	3.412
1	-4.006	12.854	3.217	1	8.443	11.539	5.727
1	1.774	18.056	7.134	1	8.102	13.083	6.614
1	0.907	16.497	7.182	1	9.479	12.98	5.464
1	5.489	14.931	10.503	1	4.574	19.826	4.108
1	3.303	14.04	11.978	1	4.377	20.574	2.487
1	1.941	13.722	10.89	1	2.913	20.16	3.443
1	-7.615	10.485	3.623	1	-6.472	16.21	5.702
1	2.786	13.551	2.078	1	-6.288	14.784	4.608
1	1.401	16.237	11.857	1	-4.332	14.685	5.883
1	0.236	15.063	11.075	1	-5.375	13.527	6.753
1	3.581	15.772	1.97	1	-8.013	9.026	5.392
1	-7.675	15.084	10.62	1	-9.341	7.271	8.481
1	5.33	13.853	2.997	1	-8.904	8.904	7.843

1	-2.005	15.966	12.373	1	-7.051	6.443	7.708
1	6.012	10	8.555	1	-8.196	6.838	6.392
1	-3.543	18.287	13.413	1	-5.526	14.374	2.269
1	5.244	12.762	11.807	1	-4.713	13.255	1.09
1	6.293	11.627	6.577	1	-7.844	13.579	3.338
1	2.929	18.614	5.174	1	-2.278	9.783	14.121
1	7.106	17.869	10.509	-1	12.4	9.605	6.782
1	8.559	17.004	9.871	-1	10.875	10.496	6.956
1	7.346	16.11	10.831	1	-9.832	13.273	9.097
1	-5.648	17.352	13.701	-1	10.182	12.602	6.702
1	-8.483	15.831	15.386	1	-8.3	11.237	8.91
1	-6.712	15.697	15.08	1	-0.82	14.596	5.992
1	-7.583	17.277	14.84	-1	10.994	10.402	11.651
1	-3.162	15.024	-0.152	-1	10.26	9.007	10.814
-1	16.497	18.039	6.705	-1	13.093	16.85	7.616
-1	15.171	17.485	7.752	1	-5.719	13.055	10.4
-1	14.885	18.844	6.586	1	-5.939	12.076	8.914
-1	15.509	17.911	12.25	1	-4.111	12.45	12.017
-1	14.865	16.237	12.248	1	-9.33	16.395	7.615
-1	15.132	17.095	10.682	-1	10.106	17.988	7.824
-1	16.55	10.654	10.084	-1	13.617	15.422	3.785
-1	16.267	11.93	11.329	-1	10.026	14.331	3.612
-1	17.803	11.923	10.388	-1	11.258	14.722	2.375
1	0.72	15.423	1.781	1	-1.064	9.583	10.962
1	0.634	15.162	-0.001	-1	10.417	12.774	11.205
1	0.075	16.726	0.719	1	-8.572	15.867	3.347
-1	16.102	10.664	4.635	1	-9.551	17.34	2.924
-1	17.132	11.081	3.227	-1	12.833	15.163	12.29
-1	16.299	12.391	4.152	1	-0.832	14.526	3.687
-1	16.199	11.749	1.058	-1	14.148	13.191	11.134
-1	15.453	13.175	1.855	1	-6.244	16.801	2.262
-1	14.443	12.055	0.836	-1	13.908	10.144	5.068
-1	14.863	15.042	6.852	1	-3.803	19.539	3.586
-1	15.372	14.74	5.157	-1	13.19	13.364	2.273
-1	16.537	15.477	6.313	-1	14.502	11.544	7.143
1	-0.465	13.222	1.979	-1	11.809	18.301	9.475
1	-0.881	13.017	0.266	-1	16.759	17.383	4.455
1	-2.204	13.091	1.491	-1	15.485	16.591	3.486
-1	17.357	14.39	9.498	-1	15.273	18.307	4.002
-1	16.016	14.319	10.675	1	-3.082	17.207	1.146
-1	15.675	14.776	8.969	1	-2.022	16.37	-0.594
-1	17.869	12.61	7.987	1	-1.672	14.706	-1.119
-1	16.729	11.271	7.634	1	-2.305	6.682	6.11
-1	16.353	12.96	7.086	1	-1.581	12.807	14.591
-1	14.095	19.871	11.811	1	-2.422	13.481	13.157
-1	12.403	19.702	11.231	1	-0.479	12.858	11.616
-1	13.798	19.228	10.161	1	-8.337	13.618	1.599

1	-1.489	13.002	9.409	1	-8.662	12.162	2.586
1	-1.21	12.933	7.635	1	-7.339	10.541	1.21
1	-2.174	15.349	9.302	1	-7.143	11.855	-0.005
1	-0.573	15.157	8.507	1	-6.221	14.105	0.631
1	-0.959	8.603	8.878	1	-0.747	9.444	13.224
1	-1.591	8.874	5.32	1	-0.72	10.533	14.648
1	-0.277	8.951	6.566	1	-3.219	12.195	14.17
1	-1.011	6.623	7.354	1	0.364	12.38	13.137
1	3.468	19.336	0.588	1	0.3	11.238	11.755
1	3.123	17.578	0.65	1	8.426	11.234	12.634
1	2.019	18.735	1.486	1	8.054	9.028	11.648
1	1.647	13.149	3.4	1	6.258	9.098	11.836
-1	11.795	13.062	12.28	1	6.998	8.768	10.222
1	-4.302	18.99	1.956	-1	11.837	18.263	13.288
1	-3.936	19.34	12.01	-1	13.53	18.598	13.821
-1	13.897	9.69	1.711	-1	12.932	16.908	13.763
-1	14.707	9.086	3.208	-1	15.689	9.461	1.755

SI16. Cartesian coordinates for MM minimized structure of $[\text{CdLAMP}^{2-}]_2$

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
6	-7.359	10.884	1.252	6	-1.407	15.932	0.3
6	2.043	11.167	6.886	-6	11.89	7.63	5.005
48	-4.063	19.252	6.759	-6	12.38	8.722	2.817
48	-2.586	9.612	6.096	-6	15.999	14.228	8.506
8	1.631	16.158	11.228	6	-3.757	15.132	0.062
8	-3.496	19.439	8.753	-6	13.714	12.829	10.92
7	-1.926	13.677	3.516	-6	13.587	10.685	9.65
8	2.602	15.815	7.395	-6	14.164	18.364	12.309
8	1.356	13.175	8.825	8	-2.113	11.144	7.384
7	-4.843	17.362	7.345	8	-1.671	16.767	7.862
8	1.933	12.865	4.562	7	-1.255	8.389	7.206
6	-5.356	18.173	9.576	6	-0.55	17.551	7.422
6	2.702	15.47	11.119	6	-1.025	18.919	6.93
6	-4.157	19.023	9.743	6	-8.681	12.555	9.768
7	-0.539	12.533	2.465	6	-9.792	11.265	6.347
6	-0.733	14.209	3.819	6	-0.926	8.602	8.448
6	3.882	16.125	10.506	6	0.651	7.167	6.21
6	-5.427	17.179	8.491	6	-0.839	7.152	6.55
6	2.921	14.09	11.669	8	0.919	8.152	5.2
7	-1.839	12.675	2.655	6	-1.577	12.09	13.719
6	1.641	13.472	3.306	6	-0.212	10.016	13.498
6	5.164	15.66	10.845	6	3.452	8.253	10.787
6	-3.164	14.096	4.166	6	2.461	7.125	10.423
6	3.725	16.375	7.235	-6	12.258	18.067	13.887
6	0.163	13.467	3.125	6	7.708	19.07	5.362
6	-5.308	13.144	3.223	-6	10.028	8.108	3.37
6	3.735	17.369	9.658	7	-6.798	6.047	0.538
6	1.84	12.103	9.296	6	-5.799	5.157	1.134
6	-5.284	10.929	5.048	6	-7.959	5.691	-0.034
6	-4.227	13.029	4.105	6	-8.683	6.81	-0.301
6	-0.349	17.081	12.159	7	-7.997	7.898	0.094
6	5.365	14.503	11.637	6	-6.272	4.596	2.488
6	4.241	13.71	11.981	6	-6.839	7.404	0.607
6	1.857	13.016	11.754	8	-4.539	5.864	1.326
7	-1.541	18.847	11.99	15	-2.714	8.601	3.51
6	-6.337	11.119	4.134	8	-3.61	9.66	2.548
6	3.195	11.985	6.35	6	-4.346	5.938	2.758
6	3.83	15.412	4.828	6	-5.049	4.736	3.363
7	-0.257	17.823	13.272	6	-9.97	6.701	-0.816
6	4.43	16.234	5.946	7	-8.443	4.442	-0.24
6	0.415	15.828	11.885	-7	10.455	5.439	-1.038
6	-4.08	11.783	4.877	6	-2.85	5.962	3.124
6	4.08	13.934	5.038	6	-9.703	4.322	-0.762

6	5.694	16.813	5.795	8	-2.157	7.138	2.62
6	-6.207	18.034	10.685	8	-1.488	9.474	4.264
6	4.374	17.178	8.301	8	-3.632	8.234	4.865
6	5.378	13.499	5.329	8	-7.362	5.376	3.039
6	-1.171	17.748	11.313	-7	10.782	7.873	-1.05
6	-6.324	12.156	3.158	8	-5.389	4.977	4.747
6	2.636	9.782	8.913	-7	10.258	21.982	4.803
6	-6.07	18.905	11.828	6	-9.249	23.001	4.497
6	-3.758	19.382	11.126	-6	11.429	21.783	4.18
6	2.113	11.916	10.748	-6	12.074	20.741	4.762
7	-1	18.914	13.195	-7	11.335	20.267	5.779
6	-2.379	19.906	11.442	6	-8.716	22.885	3.06
6	2.648	10.69	11.182	-6	10.224	21.049	5.791
6	4.522	11.648	6.662	8	-8.124	22.905	5.419
6	6.809	14.089	12.014	15	-5.077	21.763	7.385
6	-7.422	12.189	2.07	8	-3.566	21.338	6.788
6	2.891	9.609	10.296	6	-6.953	22.65	4.604
6	5.645	17.718	8.058	6	-7.252	23.221	3.227
6	6.866	12.862	12.957	-6	13.306	20.315	4.276
6	-4.685	19.148	12.155	-7	11.939	22.464	3.112
6	6.321	17.546	6.826	-7	13.832	20.996	3.199
6	5.625	12.357	6.125	6	-5.685	23.241	5.235
6	7.087	11.965	6.436	-6	13.163	22.06	2.622
6	-6.864	19.677	14.145	8	-5.798	23.249	6.676
6	-7.034	18.613	13.032	8	-5.895	20.335	7.052
6	7.513	15.259	12.739	8	-4.943	21.889	9.062
6	8.716	16.957	6.301	8	-8.87	21.535	2.558
6	7.777	11.53	5.127	-7	13.969	19.273	4.821
6	7.737	18.118	6.579	8	-6.422	22.626	2.206
6	-8.502	18.7	12.554	1	-6.358	10.773	0.775
6	4.814	7.984	10.11	1	1.071	11.663	6.659
6	3.672	8.198	12.319	1	2.033	10.183	6.368
6	7.592	13.737	10.734	1	2.065	15.87	8.246
6	-6.766	17.214	13.627	1	1.113	13.973	9.389
6	7.841	13.177	7.032	1	-0.543	14.995	4.549
6	7.206	10.797	7.446	1	-5.919	16.229	8.704
6	8.296	18.919	7.78	1	2.124	12.883	2.493
8	-2.933	11.433	5.269	1	1.989	14.515	3.218
8	-6.935	15.206	6.488	1	6.022	16.22	10.483
7	-4.524	9.407	6.83	1	-2.956	14.304	5.24
6	-6.082	16.034	5.681	1	-3.521	15.041	3.701
6	-4.748	16.269	6.385	1	-5.338	14.021	2.586
6	2.976	12.975	5.281	1	4.201	18.225	10.199
6	2.147	10.984	8.382	1	2.666	17.649	9.52
6	-5.499	9.994	6.192	1	4.374	12.743	12.455
6	-5.356	9.076	9.139	1	1.852	12.614	12.793
6	-4.776	8.425	7.883	1	0.837	13.376	11.579

8	-4.389	9.949	9.743	1	-7.182	10.435	4.183
6	-7.275	13.37	1.079	1	4.244	15.721	3.84
6	-8.804	12.306	2.733	1	0.615	15.318	12.856
6	-2.717	9.911	13.293	1	-0.214	15.195	11.221
6	-8.85	11.242	7.534	1	6.204	16.671	4.848
-8	10.805	16.438	5.332	1	-6.96	17.249	10.665
8	-4.817	19.119	4.832	1	6.205	14.126	5.015
7	-3.438	14.007	9.338	1	-1.467	17.484	10.303
8	-9.458	15.899	8.579	1	2.857	8.974	8.22
8	-9.96	13.663	6.236	1	-2.464	20.741	12.176
7	-2.139	18.777	5.99	1	2.871	10.598	12.239
8	-7.412	12.414	9.749	1	4.675	10.808	7.326
6	-2.916	18.1	3.742	1	6.103	18.274	8.865
-6	11.845	15.854	5.788	1	6.278	13.049	13.885
6	-4.305	18.62	3.789	1	7.917	12.644	13.259
7	-4.743	14.588	10.851	1	6.479	11.948	12.45
6	-4.523	13.226	9.188	1	-4.353	19.253	13.183
-6	12.437	16.427	7.026	1	-7.68	19.595	14.901
6	-1.891	18.339	4.788	1	-5.91	19.549	14.703
-6	12.57	14.684	5.164	1	-6.893	20.703	13.711
7	-3.59	14.909	10.292	1	7.634	16.146	12.077
6	-6.471	12.774	10.759	1	6.926	15.568	13.635
-6	13.741	16.066	7.394	1	8.533	14.962	13.074
6	-2.118	13.646	8.825	1	8.726	16.247	7.16
-6	10.262	16.195	9.512	1	9.753	17.34	6.152
6	-5.366	13.602	10.185	1	8.436	16.394	5.383
6	-1.564	12.178	10.793	1	8.837	11.239	5.317
-6	11.72	17.51	7.811	1	7.247	10.656	4.681
-6	10.366	12.536	5.83	1	7.78	12.354	4.378
6	-1.319	9.807	9.209	1	-9.204	18.538	13.403
6	-1.691	12.311	9.401	1	-8.709	19.702	12.112
6	-9.033	17.286	3.997	1	-8.737	17.934	11.789
-6	14.495	15.108	6.679	1	5.264	7.037	10.488
-6	13.867	14.388	5.632	1	5.522	8.818	10.321
-6	11.991	13.71	4.146	1	4.713	7.885	9.006
7	-7.462	18.56	3.308	1	2.714	8.367	12.864
6	-1.204	9.77	10.609	1	4.422	8.958	12.64
6	-9.493	11.808	8.782	1	8.625	13.399	10.981
6	-9.021	14.691	11.273	1	7.68	14.617	10.057
7	-8.896	18.348	4.802	1	7.078	12.916	10.184
-6	10.079	15.713	10.909	1	-7.437	17.024	14.497
-6	10.061	16.212	4.146	1	-5.711	17.132	13.975
6	-1.702	11.084	8.573	1	-6.947	16.414	12.875
6	-9.436	13.309	10.807	1	7.238	13.646	7.84
-6	10.996	16.131	11.89	1	8.827	12.873	7.455
6	-2.501	17.399	2.591	1	8.05	13.951	6.262
-6	11.428	17.059	9.222	1	6.736	9.87	7.044

-6	10.717	12.845	11.144	1	6.728	11.064	8.418
6	-8.103	17.416	3.016	1	8.275	10.558	7.652
6	-1.378	10.919	11.422	1	8.391	18.272	8.683
-6	10.158	10.06	5.727	1	9.312	19.318	7.552
6	-3.348	17.183	1.472	1	7.642	19.791	8.016
6	-5.132	18.49	2.565	1	-6.583	17.006	5.493
-6	11.42	12.459	4.788	1	-5.913	15.53	4.704
7	-7.931	19.151	4.393	1	-3.984	16.535	5.631
6	-6.462	19.186	2.453	1	-4.4	15.336	6.888
-6	11.729	11.201	4.237	1	-6.527	9.749	6.454
-6	10.807	11.448	9.141	1	-5.626	8.283	9.872
-6	15.965	14.844	7.094	1	-6.275	9.656	8.898
6	-1.463	10.746	12.959	1	-3.821	7.917	8.142
-6	11.09	10.003	4.66	1	-5.481	7.646	7.508
-6	12.289	17.425	10.269	1	-7.376	14.347	1.606
-6	16.706	13.877	6.138	1	-6.291	13.328	0.557
6	-4.652	17.732	1.489	1	-8.824	13.185	3.412
-6	12.088	16.989	11.604	1	-3.632	10.408	12.894
-6	11.425	11.927	10.328	1	-8.52	10.203	7.763
-6	12.872	11.546	10.719	1	-7.937	11.824	7.268
6	-3.021	17.277	-1.038	1	-8.639	15.323	8.705
-6	11.35	8.64	3.97	1	-9.231	13.779	6.922
6	-2.883	16.393	0.223	1	-4.587	12.338	8.562
-6	16.751	16.176	7.096	1	-0.859	18.099	4.523
-6	13.741	16.114	13.299	1	-6.922	13.273	11.639
-6	12.842	10.743	12.035	1	-6.021	11.836	11.156
-6	13.052	17.382	12.752	-1	14.183	16.564	8.253
-1	12.14	6.659	4.517	1	-1.373	14.417	9.125
-1	12.813	8.027	5.488	1	-2.142	13.628	7.711
-1	12.533	7.721	2.351	1	-1.674	13.083	11.382
-1	13.37	9.071	3.191	-1	10.762	17.806	7.326
-1	12.023	9.408	2.013	-1	12.351	18.429	7.819
-1	15.538	14.907	9.258	-1	14.385	13.561	5.157
-1	15.449	13.26	8.514	-1	11.24	14.136	3.47
-1	17.049	14.033	8.826	-1	12.812	13.432	3.443
1	-3.645	14.47	0.951	1	-1.005	8.808	11.074
1	-3.453	14.552	-0.84	1	-8.057	15.007	10.819
1	-4.833	15.392	-0.05	1	-9.519	15.247	4.216
-1	14.798	12.59	11.014	-1	10.732	16.261	3.258
-1	13.428	13.37	11.849	-1	10.861	15.757	12.902
-1	13.573	13.521	10.059	1	-1.485	17.016	2.586
-1	14.632	10.453	9.961	-1	11.211	13.299	11.998
-1	13.065	9.71	9.507	1	-7.926	16.776	2.154
-1	13.638	11.226	8.676	1	-9.693	9.144	6.081
-1	14.814	18.64	13.171	1	-6.315	20.239	2.758
-1	13.724	19.305	11.905	-1	12.452	11.181	3.429
-1	14.822	17.901	11.537	-1	11.339	10.78	8.471

1	0.163	17.682	8.267	-1	13.131	18.059	10.012
1	-0.028	17.007	6.602	-1	17.777	13.772	6.432
1	-1.334	19.535	7.797	-1	16.261	12.856	6.173
1	-0.177	19.461	6.447	-1	16.678	14.258	5.091
1	-0.332	7.853	8.976	1	-5.305	17.594	0.63
1	1.26	7.388	7.114	1	-2.457	18.229	-0.906
1	0.949	6.166	5.822	1	-2.617	16.753	-1.936
1	-1.072	6.275	7.201	1	-4.082	17.525	-1.258
1	-1.411	7.03	5.614	-1	17.831	16	7.312
1	-1.605	11.921	14.821	-1	16.378	16.879	7.873
1	-0.702	12.745	13.502	-1	16.67	16.674	6.102
1	0.705	10.586	13.244	-1	14.453	16.372	14.116
1	-9.609	12.423	1.971	-1	13.003	15.391	13.713
1	-9.038	11.397	3.324	-1	14.312	15.606	12.488
1	-7.537	9.997	1.899	-1	12.235	9.816	11.909
1	-8.135	10.879	0.452	-1	12.395	11.341	12.862
1	-8.069	13.332	0.298	-1	13.873	10.451	12.343
1	-2.654	8.892	12.848	1	-1.25	15.241	1.157
1	-2.834	9.793	14.395	1	-1.116	15.38	-0.623
1	-2.516	12.626	13.448	1	-0.722	16.806	0.398
1	-0.259	9.92	14.608	-1	11.144	7.415	5.801
1	-0.113	8.987	13.09	1	6.963	19.883	5.525
1	4.06	7.2	12.627	1	2.742	15.638	4.828
1	2.818	6.143	10.812	1	-8.861	14.665	12.376
1	1.459	7.334	10.863	1	-6.83	19.206	1.4
1	2.345	7.019	9.322	1	-1.895	20.322	10.529
-1	11.719	18.96	13.496	1	-9.615	8.84	2.639
-1	12.941	18.401	14.702	1	-9.26	7.929	4.155
-1	11.513	17.38	14.346	-1	10.193	7.142	2.839
1	8.707	19.537	5.201	1	-6.563	3.52	2.401
1	7.442	18.534	4.424	1	-6.063	8.023	1.054
1	-9.71	24.008	4.63	1	-4.852	6.861	3.125
1	-9.408	20.928	6.501	1	-2.361	5.066	2.679
1	-6.817	21.548	4.546	1	-2.727	5.872	4.226
1	-5.56	24.301	4.916	-1	10.118	3.334	-0.945
1	-4.781	22.696	4.874	1	-8.239	4.912	2.743
-1	13.601	22.577	1.776	-1	11.241	7.647	-1.984
1	-8.835	21.599	1.525	-1	11.611	7.695	-0.406
-1	13.578	18.745	5.638	1	-5.718	4.07	5.123
-1	14.895	18.971	4.429	1	-4.411	3.822	3.269
1	-6.605	23.162	1.339	1	-5.61	4.308	0.436
1	-7.129	24.332	3.227	1	-9.226	23.616	2.385

SI17. Cartesian coordinates for MM minimized structure of [CdLADP²⁻]₂

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
6	-6.623	10.98	-0.552	6	0.323	18.71	2.652
6	1.594	10.6	6.951	-6	14.201	8.226	3.821
48	-4.673	18.83	8.1	-6	12.593	8.447	1.928
48	-5.649	9.195	6.853	-6	15.095	12.786	4.973
8	1.539	16.715	9.458	6	-0.787	16.625	1.778
8	-4.067	19.204	10.018	-6	16.495	12.851	8.797
7	-3.482	13.371	4.12	-6	16.392	10.52	7.902
8	1.099	15.079	5.715	-6	15.373	18.681	8.808
8	1.125	13.053	8.387	8	-5.613	10.717	8.213
7	-6.221	17.561	8.754	8	-3.171	14.219	7.769
8	0.299	11.339	4.458	7	-3.518	9.2	6.67
6	-5.541	17.631	11.137	6	-2.432	14.985	8.736
6	2.617	16.135	9.098	6	-3.102	16.346	8.982
6	-4.45	18.648	11.086	-6	11.629	11.299	9.961
7	-1.971	13.458	2.693	-6	11.232	9.779	6.62
6	-2.613	12.407	4.47	6	-2.779	9.726	7.61
6	3.273	16.613	7.86	6	-3.736	8.16	4.397
6	-6.419	17.234	9.999	6	-2.815	8.575	5.538
6	3.36	15.105	9.894	8	-4.417	6.934	4.708
7	-3.092	14.053	3.057	6	-2.142	12.62	13.235
6	-0.526	11.492	3.304	6	-0.34	12.186	11.567
6	4.667	16.466	7.747	6	5.109	9.528	10.436
6	-4.845	13.45	4.627	6	4.477	8.166	10.799
6	1.934	15.689	4.982	-6	14.79	18.249	11.194
6	-1.626	12.479	3.543	6	4.29	18.064	1.022
6	-6.124	12.731	2.582	-6	12.208	6.688	3.652
6	2.513	17.444	6.847	7	-0.976	1.281	10.373
6	2.017	12.296	8.873	6	-1.775	2.296	11.058
6	-6.869	10.202	3.717	15	-7.166	8.379	9.583
6	-5.714	12.455	3.895	6	0.063	0.594	10.872
6	-0.011	17.807	10.889	6	0.479	-0.313	9.949
6	5.433	15.743	8.696	7	-0.292	-0.226	8.849
6	4.753	15.022	9.712	6	-2.864	1.669	11.93
6	2.695	14.028	10.726	6	-1.183	0.761	9.135
7	-1.439	19.24	11.582	8	-2.399	3.187	10.094
6	-7.256	10.574	2.414	15	-4.919	6.787	8.886
6	2.273	11.27	5.774	8	-6.176	9.327	10.725
6	1.536	13.932	3.107	8	-6.641	6.701	9.331
7	-0.063	18.864	10.065	6	-3.806	3.261	10.444
6	2.196	15.197	3.609	6	-3.976	2.687	11.845
6	0.808	16.577	10.67	6	1.54	-1.164	10.239
6	-6.023	11.134	4.486	7	0.637	0.711	12.095
6	2.192	12.711	3.709	7	2.127	-1.043	11.472

6	3.144	15.858	2.815	8	-8.661	8.312	10.201
6	-5.788	16.994	12.369	6	-4.3	4.705	10.349
6	2.679	16.891	5.447	8	-7.35	9.159	8.168
6	3.582	12.561	3.587	6	1.685	-0.12	12.39
6	-0.9	18.046	11.886	8	-4.145	5.173	8.989
6	-6.878	11.805	1.817	8	-4.762	7.296	7.355
6	3.23	10.128	8.816	8	-4.089	7.812	9.826
6	-5.077	17.291	13.558	8	-3.295	0.4	11.381
6	-3.738	18.972	12.344	7	2	-2.139	9.278
6	2.833	12.675	10.061	8	-5.28	2.086	12.005
7	-0.926	19.77	10.485	7	0.101	26.842	8.309
6	-2.527	19.876	12.319	6	-0.97	26.42	7.381
6	3.795	11.768	10.539	15	-6.131	21.559	7.977
6	3.673	11.205	5.617	6	1.043	27.789	8.113
6	6.973	15.696	8.543	6	1.797	27.923	9.23
6	-7.254	12.074	0.337	7	1.375	27.072	10.2
6	4.01	10.498	9.94	6	-2.225	27.273	7.534
6	3.612	17.487	4.578	6	0.326	26.425	9.595
6	7.677	14.931	9.69	8	-1.326	25.038	7.641
6	-4.061	18.278	13.519	15	-3.347	21.792	8.314
6	3.866	16.989	3.273	8	-5.733	21.957	6.282
6	4.342	11.809	4.517	8	-4.89	21.954	9.182
6	5.875	11.715	4.33	6	-2.636	25.04	8.272
6	-4.627	16.994	16.088	6	-3.082	26.487	8.499
6	-5.383	16.476	14.84	6	2.829	28.861	9.262
6	7.536	17.136	8.536	7	1.24	28.538	7.004
6	6.03	16.557	2.051	7	3.032	29.615	8.139
6	6.172	10.866	3.078	8	-7.508	22.308	8.386
6	4.94	17.611	2.348	6	-3.63	24.271	7.386
6	-6.894	16.538	15.162	8	-6.463	19.987	8.095
6	6.155	9.328	9.316	6	2.251	29.46	7.021
6	5.859	10.04	11.69	8	-3.099	22.98	6.987
6	7.339	14.999	7.219	8	-2.144	21.997	9.376
6	-4.966	15.007	14.613	8	-3.134	20.292	7.719
6	6.473	13.131	4.139	8	-1.931	28.605	8.014
6	6.597	11.062	5.535	7	3.605	29.033	10.357
6	5.642	18.845	2.965	8	-2.801	26.872	9.866
8	-5.538	10.837	5.609	1	-5.519	10.947	-0.401
8	-5.851	15.324	7.052	1	0.523	10.903	7.001
7	-6.943	8.354	5.358	1	1.611	9.496	6.8
6	-7.183	15.716	7.417	1	0.874	15.354	6.659
6	-7.217	17.204	7.74	1	0.894	13.96	8.76
6	1.477	11.799	4.646	1	-2.762	11.66	5.246
6	2.263	10.976	8.254	1	-7.284	16.612	10.241
6	-7.297	8.875	4.214	1	-0.998	10.508	3.085
6	-8.967	7.087	6.008	1	0.066	11.76	2.399
6	-7.469	7.033	5.716	1	5.164	16.941	6.905

8	-9.436	5.781	6.385	1	-4.852	13.256	5.724
6	-6.751	13.444	-0.183	1	-5.24	14.481	4.474
6	-8.788	12.05	0.161	1	-5.828	13.69	2.168
6	-1.461	10.269	12.755	1	2.882	18.495	6.903
-6	11.287	9.507	8.106	1	1.428	17.495	7.09
8	-9.501	15.505	4.363	1	5.293	14.333	10.356
8	-4.94	18.955	6.066	1	3.159	14.022	11.739
7	-6.987	12.908	10.641	1	1.625	14.203	10.899
-8	10.448	14.471	8.373	1	-7.85	9.868	1.837
8	-9.797	11.717	6.786	1	1.579	13.87	1.995
7	-3.399	17.14	7.778	1	1.496	16.463	11.539
-8	10.605	10.845	10.574	1	0.107	15.716	10.59
6	-2.873	17.883	5.481	1	3.341	15.458	1.823
-6	10.563	14.856	4.637	1	-6.554	16.223	12.396
6	-4.138	18.581	5.169	1	4.085	13.119	2.802
7	-8.261	13.057	12.28	1	-1.178	17.402	12.72
6	-7.953	12.005	10.415	1	3.41	9.173	8.328
-6	11.603	15.487	5.481	1	-2.179	20.119	13.35
6	-2.66	17.07	6.703	1	4.387	12.083	11.392
-6	10.924	13.522	4.073	1	4.235	10.668	6.371
7	-7.161	13.578	11.766	1	4.154	18.348	4.956
-6	10.001	11.299	11.782	1	7.42	15.375	10.679
-6	12.941	15.123	5.23	1	8.785	14.978	9.576
6	-5.911	13.202	9.706	1	7.396	13.852	9.684
-6	11.45	15.163	8.723	1	-3.474	18.505	14.403
6	-8.785	12.117	11.479	1	-4.917	16.415	16.996
6	-3.864	12.34	10.893	1	-3.525	16.876	15.969
-6	11.243	16.527	6.516	1	-4.869	18.065	16.279
-6	10.46	10.919	6.058	1	7.239	17.672	9.467
6	-3.294	10.456	8.799	1	8.649	17.126	8.476
6	-4.788	12.21	9.849	1	7.168	17.72	7.663
6	-7.726	16.318	3.011	1	6.484	16.194	3.002
-6	13.272	14.339	4.061	1	6.84	16.991	1.42
-6	12.295	13.303	3.82	1	5.616	15.68	1.505
6	-9.926	12.382	3.982	1	7.271	10.781	2.911
7	-6.603	18.136	2.925	1	5.753	9.84	3.197
6	-2.406	10.664	9.872	1	5.721	11.321	2.167
-6	12.157	10.516	8.821	1	-7.114	16.036	16.133
-6	11.857	13.764	10.917	1	-7.231	17.598	15.233
7	-7.924	16.945	1.841	1	-7.51	16.022	14.392
-6	12.19	14.922	9.995	1	6.983	8.666	9.661
6	-8.461	15.105	3.479	1	6.592	10.309	9.016
6	-4.62	11.108	8.881	1	5.705	8.858	8.413
-6	12.447	12.471	10.389	1	5.152	10.196	12.538
-6	13.298	15.734	10.292	1	6.397	10.992	11.473
6	-1.904	17.791	4.464	1	8.444	14.911	7.109
-6	11.919	16.258	7.843	1	6.961	15.57	6.341

-6	13.829	12.416	10.132	1	6.902	13.975	7.193
6	-6.876	17.092	3.726	1	-5.158	14.395	15.524
6	-2.695	11.537	10.955	1	-3.879	14.948	14.374
-6	11.925	8.933	5.738	1	-5.53	14.549	13.771
6	-2.125	18.261	3.144	1	6.061	13.828	4.902
6	-4.433	18.886	3.752	1	7.584	13.119	4.232
-6	10.472	11.111	4.593	1	6.244	13.546	3.133
7	-7.217	18.059	1.757	1	6.281	10.001	5.665
6	-5.82	19.302	3.325	1	6.39	11.626	6.473
-6	11.141	10.177	3.784	1	7.701	11.053	5.379
-6	13.535	10.581	8.546	1	6.182	18.57	3.901
-6	14.771	13.882	3.937	1	6.397	19.265	2.26
6	-1.679	11.658	12.115	1	4.905	19.652	3.185
-6	11.889	9.102	4.33	1	-7.524	15.129	8.297
-6	13.045	17.009	8.221	1	-7.869	15.499	6.569
-6	15.038	13.336	2.514	1	-8.238	17.49	8.088
6	-3.418	18.732	2.796	1	-7.018	17.778	6.814
-6	13.747	16.767	9.43	1	-7.951	8.3	3.555
-6	14.399	11.472	9.24	1	-9.527	7.422	5.109
-6	15.937	11.432	9.068	1	-9.166	7.793	6.842
6	-1.301	18.856	0.77	1	-6.962	6.664	6.628
-6	12.706	8.134	3.44	1	-7.264	6.303	4.898
6	-0.994	18.118	2.096	1	-7.196	14.28	0.405
-6	15.733	15.079	4.148	1	-5.639	13.506	-0.132
-6	16.218	16.611	9.915	1	-9.259	12.877	0.739
-6	16.561	10.887	10.368	1	-2.43	9.855	13.12
-6	15.011	17.57	9.824	-1	11.68	8.485	8.314
-1	16.363	16.08	8.946	-1	10.248	9.519	8.5
-1	16.18	9.862	10.583	-1	10.071	13.713	8.92
-1	16.31	11.539	11.236	1	-9.739	11.639	7.788
-1	17.672	10.84	10.284	1	-8.039	11.355	9.549
1	0.71	18.131	3.519	1	-1.842	16.356	6.65
1	1.123	18.691	1.877	-1	10.719	11.845	12.433
1	0.17	19.766	2.972	1	-9.665	10.405	12.354
-1	14.381	7.892	4.867	-1	13.715	15.511	5.885
-1	14.819	7.58	3.156	1	-5.522	14.23	9.893
-1	14.561	9.277	3.723	1	-6.302	13.184	8.664
-1	13.188	7.72	1.328	1	-4.061	13.11	11.633
-1	12.988	9.465	1.701	-1	10.142	16.544	6.678
-1	11.534	8.375	1.585	-1	11.521	17.532	6.123
-1	14.812	13.125	5.994	-1	12.614	12.329	3.469
-1	14.536	11.847	4.76	1	-8.986	12.639	4.515
-1	16.184	12.546	4.966	1	-9.666	12.212	2.917
1	-0.528	16.057	2.698	1	-1.451	10.142	9.85
1	0.04	16.487	1.043	-1	10.76	13.719	11.021
1	-1.718	16.186	1.351	1	-7.752	14.447	4.022
-1	17.565	12.81	8.487	1	-8.871	14.579	2.587

-1	16.457	13.492	9.705	-1	13.843	15.532	11.211
-1	15.918	13.355	7.991	1	-0.969	17.286	4.698
-1	17.499	10.557	7.776	-1	14.46	13.167	10.598
-1	16.126	9.455	8.097	1	-6.512	16.938	4.736
-1	15.928	10.844	6.944	-1	12.5	8.115	6.164
-1	16.277	19.242	9.141	1	-6.345	19.825	4.157
-1	14.541	19.416	8.711	-1	11.119	10.354	2.714
-1	15.604	18.246	7.808	-1	13.92	9.895	7.798
1	-2.398	14.421	9.693	-1	13.371	17.783	7.534
1	-1.378	15.109	8.399	-1	16.12	13.106	2.373
1	-4.049	16.14	9.512	-1	14.488	12.391	2.313
1	-2.457	16.946	9.659	-1	14.738	14.088	1.748
1	-1.692	9.64	7.534	1	-3.664	18.985	1.769
1	-4.464	8.958	4.169	1	-1.534	19.929	0.962
1	-3.124	7.993	3.482	1	-0.426	18.813	0.08
1	-2.076	9.3	5.121	1	-2.154	18.383	0.231
1	-2.246	7.684	5.894	-1	16.774	14.812	3.851
1	-1.408	12.634	14.074	-1	15.789	15.388	5.215
1	-2.222	13.665	12.855	-1	15.41	15.952	3.535
1	-0.503	13.145	11.024	-1	17.152	17.172	10.151
1	-9.061	12.189	-0.911	-1	16.078	15.849	10.714
1	-9.231	11.086	0.494	-1	12.773	5.977	3.007
1	-7.039	9.974	-0.322	1	-2.505	1.542	12.981
1	-6.821	11.181	-1.631	1	-1.976	1.077	8.458
1	-7.044	13.594	-1.248	1	-4.377	2.636	9.715
1	-1.022	9.545	12.033	1	-3.704	5.347	11.04
1	-0.761	10.338	13.62	1	-5.374	4.728	10.652
1	-3.125	12.3	13.653	1	2.171	-0.05	13.36
1	0.387	12.364	12.394	1	-3.711	-0.134	12.165
1	0.128	11.46	10.866	1	3.043	-1.932	9.236
1	6.623	9.299	12.024	1	2.028	-3.029	9.862
1	5.243	7.471	11.215	1	-5.376	1.871	13.014
1	3.676	8.303	11.563	1	-3.814	3.479	12.619
1	4.031	7.666	9.911	1	-1.106	2.914	11.704
-1	13.885	18.9	11.161	1	-6.235	8.807	11.616
-1	15.666	18.881	11.469	1	-2.743	27.331	6.544
-1	14.656	17.503	12.009	1	-0.266	25.664	10.095
1	5.045	18.538	0.353	1	-2.562	24.521	9.255
1	3.846	17.21	0.464	1	-3.807	24.858	6.456
1	3.486	18.809	1.221	1	-4.617	24.18	7.896
1	0.474	13.988	3.4	1	2.435	30.075	6.144
-1	12.258	13.95	11.94	1	-2.803	29.152	7.899
1	-5.756	20.027	2.48	1	4.372	29.749	10.354
1	-2.806	20.84	11.833	1	3.458	28.462	11.225
-1	11.127	6.609	3.392	1	-3.404	27.689	10.073
-1	12.339	6.355	4.706	1	-4.169	26.635	8.279
1	-6.604	21.768	5.758	1	-0.594	26.498	6.334

SI18. Cartesian coordinates for MM minimized structure of [CdLATP²⁻]₂

Z	Coordinates			Z	Coordinates		
	x	y	z		x	y	z
6	-7.54	7.543	3.391	6	-5.798	-0.502	8.844
6	2.482	9.723	6.868	7	-7.152	1.55	7.504
48	-3.782	17.998	6.157	7	-7.092	-0.164	9.179
48	-2.803	8.913	8.634	8	-1.326	8.65	7.17
8	1.297	16.034	9.88	6	-4.12	5.23	3.153
8	-3.487	18.706	8.056	8	0.002	7.792	5.202
7	-2.663	11.779	4.066	6	-7.766	0.849	8.519
8	1.517	14.309	5.913	8	-2.802	5.608	3.612
8	1.338	12.037	8.115	8	-4.413	6.518	6.198
7	-5.048	16.485	6.852	8	-3.773	4.31	7.694
8	1.351	10.535	4.328	8	-3.817	7.949	2.129
6	-5.339	17.542	9.069	8	-3.343	6.889	8.488
6	2.32	15.349	9.545	8	-0.98	7.586	2.509
6	-4.173	18.46	9.084	8	-5.614	0.958	3.693
7	-1.483	11.799	2.351	7	-5.157	-1.495	9.496
6	-1.486	11.251	4.444	8	-5.772	2.765	1.662
6	3.137	15.785	8.387	-7	11.396	23.109	7.351
6	-5.578	16.486	8.046	-6	10.269	23.963	7.775
6	2.863	14.191	10.315	15	-3.561	21.262	6.258
7	-2.676	12.15	2.798	-6	12.669	23.152	7.795
6	0.633	10.673	3.103	-6	13.439	22.31	7.063
6	4.507	15.459	8.4	-7	12.695	21.69	6.11
6	-3.764	12.084	4.972	-6	10.34	25.349	7.136
6	2.366	15.031	5.315	-6	11.442	22.213	6.316
6	-0.717	11.282	3.323	8	-8.999	23.352	7.422
6	-5.637	10.519	4.354	15	-6.199	20.135	6.015
6	2.565	16.697	7.324	15	-4.542	23.185	8.15
6	2.127	11.366	8.839	8	-5.069	21.324	5.297
6	-5.552	9.205	6.895	8	-3.744	21.591	8.007
6	-4.618	10.873	5.242	6	-8.155	24.412	6.895
6	-0.261	17.121	11.327	6	-8.885	25.746	7.086
6	5.133	14.936	9.596	-6	14.801	22.197	7.332
6	4.263	14.04	10.322	-7	13.169	23.918	8.809
6	1.994	13.06	10.838	-7	15.315	22.958	8.36
7	-1.571	18.849	11.103	8	-2.826	19.851	6.056
6	-6.548	8.918	5.95	6	-6.798	24.402	7.599
6	3.174	10.595	5.846	8	-2.533	22.324	5.649
6	2.349	13.369	3.325	-6	14.512	23.81	9.093
7	-0.683	17.503	12.562	8	-6.137	23.146	7.332
6	2.814	14.656	3.962	8	-6.23	20.244	7.609
6	0.506	15.87	11.053	8	-7.864	20.306	5.404
6	-4.429	10.063	6.457	8	-4.772	23.542	9.882

6	3.104	12.193	3.904	8	-5.694	18.657	5.688
6	3.765	15.451	3.317	8	-3.513	24.451	7.428
6	-6.223	17.595	10.163	-8	10.892	25.276	5.799
6	2.939	16.255	5.927	-7	15.604	21.384	6.615
6	4.509	12.206	3.905	8	-8.594	26.711	6.044
6	-0.831	17.962	10.398	1	-6.55	7.315	2.936
6	-6.571	9.5	4.659	1	1.378	9.755	6.723
6	3.662	9.438	9.075	1	2.792	8.664	6.708
6	-5.994	18.407	11.305	1	1.163	14.517	6.833
6	-3.855	19.167	10.344	1	0.857	12.861	8.434
6	2.425	11.732	10.247	1	-1.225	10.894	5.438
7	-1.476	18.551	12.389	1	-6.262	15.695	8.339
6	-2.513	19.828	10.546	1	0.479	9.657	2.685
6	3.284	10.904	10.985	1	1.199	11.231	2.326
6	4.579	10.703	5.832	1	5.105	15.772	7.552
6	6.607	14.408	9.427	1	-3.366	12.491	5.926
6	-7.664	9.059	3.656	1	-4.401	12.877	4.519
6	3.925	9.775	10.421	1	-5.699	11.078	3.428
6	3.882	16.994	5.199	1	2.925	17.733	7.526
6	7.268	14.266	10.819	1	1.459	16.744	7.397
6	-4.78	19.133	11.396	1	4.68	13.191	10.853
6	4.303	16.618	3.9	1	2.074	13.038	11.948
6	5.267	11.433	4.821	1	0.922	13.214	10.608
6	6.81	11.436	4.698	1	-7.333	8.226	6.236
6	-6.668	19.351	13.618	1	2.5	13.395	2.221
6	-7.06	18.445	12.426	1	1.16	15.662	11.931
6	7.476	15.405	8.618	1	-0.228	15.048	10.913
6	6.598	16.542	2.861	1	4.102	15.137	2.334
6	7.204	10.855	3.323	1	-7.112	16.97	10.127
6	5.356	17.426	3.108	1	5.013	12.883	3.22
6	-8.382	18.99	11.848	1	-0.757	17.919	9.319
6	6.306	8.943	10.527	1	4.144	8.572	8.634
6	5.132	9.4	12.678	1	-2.606	20.696	11.24
6	6.619	13.039	8.714	1	3.488	11.2	12.006
6	-7.289	17.023	12.98	1	5.124	10.176	6.609
6	7.353	12.88	4.809	1	4.292	17.873	5.677
6	7.507	10.579	5.782	1	7.224	15.234	11.369
6	5.831	18.703	3.843	1	8.338	13.968	10.721
8	-3.307	10.063	7.026	1	6.779	13.486	11.443
8	-6.049	13.549	7.097	1	-4.524	19.685	12.295
7	-4.801	8.589	9.162	1	-7.476	19.366	14.386
6	-6.441	14.493	6.086	1	-5.744	18.974	14.117
6	-5.305	15.487	5.804	1	-6.507	20.402	13.284
6	2.43	11.119	4.68	1	7.246	15.367	7.53
6	2.779	10.17	8.277	1	7.327	16.445	8.989
6	-5.759	8.722	8.288	1	8.559	15.156	8.708
6	-5.873	8.983	11.368	1	7.021	16.188	3.83

6	-5.059	8.031	10.492	1	7.389	17.114	2.321
8	-5.063	10.093	11.784	1	6.352	15.65	2.242
6	-7.566	9.777	2.288	1	8.312	10.818	3.211
6	-9.057	9.362	4.241	1	6.804	9.82	3.21
6	-1.825	12.28	15.45	1	6.803	11.475	2.489
-6	10.66	10.979	8.023	1	-9.177	19.004	12.629
8	-8.795	16.662	4.387	1	-8.243	20.028	11.465
8	-3.694	18.079	4.107	1	-8.747	18.363	11.007
7	-5.442	13.337	10.733	1	7.056	8.36	11.109
8	-9.038	15.395	8.708	1	6.672	9.992	10.439
8	-9.453	13.154	6.405	1	6.264	8.502	9.506
7	-2.192	16.586	6.097	1	4.173	9.372	13.246
8	-9.438	11.851	10.49	1	5.545	10.435	12.697
6	-1.744	16.741	3.668	1	7.661	12.741	8.456
6	-9.912	16.24	4.832	1	6.012	13.081	7.782
6	-2.886	17.593	3.271	1	6.188	12.239	9.357
7	-6.905	13.667	12.308	1	-8.009	17.038	13.831
6	-6.482	12.511	10.46	1	-6.328	16.587	13.339
-6	10.532	16.906	6.002	1	-7.715	16.348	12.207
6	-1.476	16.283	5.051	1	6.979	13.374	5.73
-6	10.748	15.189	4.177	1	8.468	12.884	4.839
7	-5.717	14.013	11.836	1	7.051	13.504	3.938
6	-8.684	11.996	11.691	1	7.183	9.515	5.716
-6	11.943	16.947	6.032	1	7.283	10.965	6.801
6	-4.146	13.387	10.042	1	8.614	10.599	5.652
6	-9.846	16.233	9.203	1	6.33	18.448	4.806
6	-7.408	12.737	11.454	1	6.573	19.261	3.226
6	-2.648	13.279	12.052	1	4.974	19.39	4.038
6	-9.686	17.638	7.024	1	-7.367	15.028	6.395
-6	10.354	12.442	5.876	1	-6.671	13.928	5.155
6	-1.675	10.663	11.428	1	-5.557	16.033	4.87
6	-3.095	12.685	10.868	1	-4.366	14.934	5.597
6	-7.215	17.341	2.753	1	-6.772	8.424	8.566
-6	12.704	16.534	4.873	1	-6.219	8.439	12.276
-6	12.144	15.351	4.267	1	-6.77	9.359	10.826
-6	10.174	13.866	3.719	1	-4.085	7.821	10.991
7	-5.492	18.416	1.966	1	-5.602	7.062	10.391
6	-1.299	11.331	12.602	1	-7.736	10.874	2.4
-6	11.265	11.977	8.986	1	-6.57	9.602	1.818
-6	10.232	14.815	11.376	1	-9.123	10.441	4.495
7	-7.46	18.674	2.861	1	-2.923	12.094	15.39
-6	10.458	16.057	10.545	-1	11.029	9.961	8.289
6	-8.159	16.269	3.176	1	-9.552	10.938	8.126
6	-2.625	11.327	10.521	1	-8.741	14.553	9.177
-6	11.061	13.665	10.85	1	-9.111	13.016	7.343
-6	11.346	17.035	11.009	1	-6.528	11.788	9.65
6	-0.884	16.268	2.658	1	-0.622	15.62	5.178

-6	10.195	17.442	8.434	1	-9.283	12.472	12.501
-6	12.456	13.821	10.812	1	-8.418	10.979	12.056
6	-5.988	17.168	2.158	-1	12.44	17.365	6.898
6	-1.783	12.612	12.948	1	-3.856	14.453	9.894
-6	12.026	10.613	5.947	1	-4.238	12.924	9.034
6	-1.066	16.562	1.284	1	-3.023	14.27	12.275
6	-3.084	17.877	1.827	1	-8.63	17.287	6.967
-6	10.778	12.717	4.49	1	-9.674	18.721	6.764
7	-6.394	19.294	2.376	-1	12.787	14.549	3.918
6	-4.204	18.782	1.355	1	-9.077	13.826	3.878
-6	11.804	11.952	3.923	-1	10.352	13.751	2.625
-6	12.651	12.229	8.971	1	-0.611	10.83	13.275
-6	14.265	16.536	5.035	1	-9.156	14.594	11.364
6	-1.377	13.222	14.31	1	-7.584	15.331	3.333
-6	12.45	10.913	4.633	1	-8.907	16.128	2.361
-6	11.079	18.374	8.991	-1	11.802	16.884	11.981
-6	14.94	16.322	3.658	1	-0.05	15.636	2.954
6	-2.166	17.368	0.895	-1	12.896	14.575	11.459
-6	11.677	18.185	10.259	1	-5.49	16.236	1.909
-6	13.273	13.108	9.899	-1	12.518	9.819	6.497
-6	14.809	13.304	9.949	1	-3.947	19.831	1.629
6	-0.376	16.39	-1.205	-1	12.103	12.205	2.915
-6	13.63	10.116	4.031	-1	13.241	11.705	8.226
6	-0.066	15.979	0.255	-1	11.318	19.24	8.387
-6	14.751	17.907	5.567	-1	16.046	16.439	3.736
-6	14.045	18.45	11.094	-1	14.758	15.303	3.254
-6	15.348	12.619	11.22	-1	14.562	17.067	2.921
-6	12.707	19.181	10.839	1	-2.329	17.618	-0.148
6	1.36	16.475	0.582	1	-0.335	17.498	-1.324
-6	14.887	10.328	4.905	1	0.373	15.953	-1.906
-6	13.989	10.545	2.587	1	-1.379	16.02	-1.519
-6	14.718	15.424	6.002	-1	15.86	17.994	5.495
6	-0.103	14.436	0.32	-1	14.498	18.056	6.64
-6	15.167	14.811	9.997	-1	14.297	18.732	4.972
-6	15.536	12.691	8.726	-1	14.824	19.162	11.453
-6	13.005	20.371	9.898	-1	13.943	17.657	11.868
8	-3.063	10.773	9.482	-1	14.411	17.976	10.154
8	-1.417	14.023	8.678	-1	15.111	11.53	11.206
7	-1.338	8.58	10.147	-1	14.893	13.062	12.135
6	-1.983	14.519	7.456	-1	16.455	12.738	11.293
6	-1.811	16.035	7.399	1	1.693	16.13	1.583
-6	10.474	12.502	10.122	1	2.095	16.09	-0.163
-6	11.007	11.321	6.594	1	1.396	17.589	0.568
6	-1.062	9.344	11.168	-1	14.746	9.928	5.934
6	0.84	7.541	9.617	-1	15.768	9.807	4.463
6	-0.618	7.311	10.006	-1	15.124	11.415	4.983
8	1.507	6.278	9.462	-1	14.839	9.94	2.194

6	-2.019	14.605	14.578	-1	14.302	11.615	2.556
6	0.155	13.4	14.367	-1	13.125	10.391	1.9
6	4.927	8.912	11.223	-1	14.194	15.524	6.977
6	4.418	7.456	11.29	-1	14.488	14.415	5.591
-6	12.177	19.763	12.168	-1	15.816	15.481	6.183
6	4.759	17.867	1.752	1	0.207	14.058	1.318
-6	13.276	8.613	3.993	1	0.588	13.99	-0.432
7	-5.084	1.74	6.241	1	-1.134	14.065	0.114
6	-5.429	2.803	5.299	-1	16.254	14.975	9.817
15	-1.435	7.688	5.893	-1	14.945	15.261	10.99
6	-5.87	1.207	7.185	-1	14.596	15.374	9.227
6	-5.194	0.216	7.818	-1	16.628	12.91	8.761
7	-3.967	0.093	7.282	-1	15.433	11.581	8.71
6	-6.129	2.262	4.054	-1	15.133	13.111	7.777
6	-3.922	1.041	6.309	-1	13.753	21.061	10.354
8	-4.235	3.518	4.884	-1	12.081	20.965	9.705
15	-3.299	5.953	7.192	-1	13.427	20.012	8.931
15	-2.575	7.355	3.266	1	-1.474	14.017	6.604
8	-1.681	6.005	6.434	1	-3.064	14.269	7.431
8	-2.677	8.321	4.769	1	-2.442	16.479	8.194
6	-4.357	3.751	3.457	1	-0.753	16.294	7.618
6	-5.749	3.289	3.013	1	-0.314	9.005	11.887
1	-8.784	1.092	8.803	1	0.883	8.092	8.654
1	-6.196	0.263	4.195	1	1.364	8.132	10.4
1	-4.171	-1.762	9.25	1	-0.677	6.727	10.955
1	-5.638	-2.02	10.267	1	-1.082	6.701	9.208
1	-5.005	2.076	1.562	1	-1.703	15.004	15.57
1	-1.02	7.024	1.643	1	-1.702	15.344	13.808
1	-2.959	3.954	8.223	1	0.494	14.066	13.544
1	-6.477	4.134	3.076	1	-9.86	9.126	3.504
1	-6.103	3.536	5.804	1	-9.264	8.77	5.16
-1	10.925	26.061	7.767	1	-7.646	6.948	4.325
-1	10.586	21.959	5.701	1	-8.332	7.2	2.685
1	-7.996	24.211	5.81	1	-8.341	9.395	1.584
1	-6.957	24.527	8.697	1	-1.302	11.298	15.405
1	-6.184	25.249	7.21	1	-1.6	12.727	16.446
-1	14.942	24.399	9.896	1	-3.131	14.533	14.585
-1	11.915	25.407	5.895	1	0.464	13.858	15.334
-1	15.232	20.818	5.815	1	0.689	12.428	14.273
-1	16.627	21.316	6.841	1	5.856	8.745	13.217
1	-8.71	26.249	5.124	1	5.107	6.823	11.896
1	-2.623	24.389	7.949	1	3.408	7.42	11.761
1	-8.087	21.306	5.54	1	4.35	6.995	10.279
1	-8.614	26.198	8.071	-1	11.213	20.296	11.998
-1	10.298	24.073	8.886	-1	12.904	20.491	12.597
-1	13.118	8.198	5.013	-1	12.011	18.97	12.93
-1	14.099	8.025	3.523	1	5.48	18.507	1.192

1	-7.238	2.226	4.191	1	4.52	16.996	1.101
1	-3.062	1.207	5.663	1	3.823	18.45	1.913
1	-3.567	3.151	2.947	1	1.258	13.272	3.512
1	-4.892	5.836	3.679	-1	10.498	14.996	12.444
1	-4.202	5.382	2.051	1	-4.317	18.739	0.247
-1	12.347	8.448	3.4	1	-2.116	20.222	9.583

SI 19. Details of cell culture studies

Cellular studies: Human cervical carcinoma (HeLa) cells were cultured in Dulbecco's Eagle's Minimal Essential Medium (DMEM) supplemented with 10% fetal bovine serum and 1% antibiotic-antimycotic solution containing streptomycin, amphotericin B and penicillin. Cells were maintained in humidified atmosphere of 5% CO₂ and 95% air in a 37 °C incubator. Stock solution (2 mM) of the **L** was prepared in DMSO. HeLa cells were seeded on a poly-lysine-coated glass bottom cell culture dishes at a density of 5×10^4 cells/ml. After 24 h of seeding, media was removed and dishes were washed twice, carefully with PBS. Cells were incubated in the presence of 20 μ M of **L** for 20 min. Then, the PBS containing some traces of ligand was removed and the dishes were washed three times with PBS thoroughly. After that the cells were imaged for the intrinsic fluorescence of the conjugates using Zeiss Axio Observer.Z1 microscope at 40 $\times$ magnification. The cells were further incubated with 20 μ M Cd(ClO₄)₂/pyrithione diluted in PBS buffer for 20 min. After this incubation, the PBS containing Cd²⁺ was removed and the cells were washed three times with PBS. Subsequently, the dishes already incubated with **L** and Cd²⁺ were treated with 80 μ M of H₂PO₄⁻ separately for 20 min. After the incubation, the dishes were washed three times with PBS and the cells were imaged using Zeiss Axio Observer.Z1 microscope at 40 $\times$ magnification. The exposure time was kept same for all the cases. The images were processed using Image-Pro Plus software (Media Cybernetics, Silver Spring, MD).

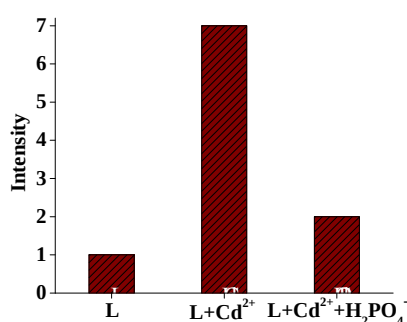


Figure S20. Histogram showing the fluorescence changes of **L** in the HeLa cells incubated with Cd²⁺ and followed by H₂PO₄⁻ as measured by selecting the area of the cells.