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Supporting information for article:

A new lanthanum coordination polymer built from a semi-rigid tripodal carboxylic acid ligand: synthesis, crystal structure and properties

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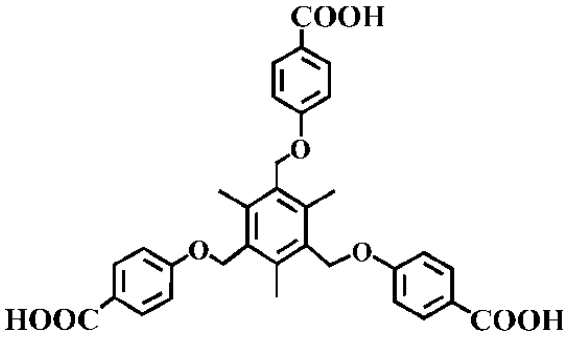

Scheme S1 Schematic structure of H_3L.

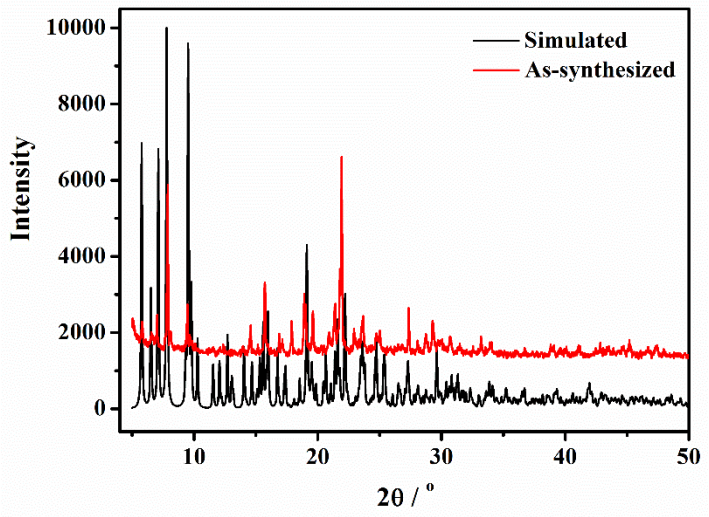

Figure S1 X-ray powder diffraction pattern of compound **1**.

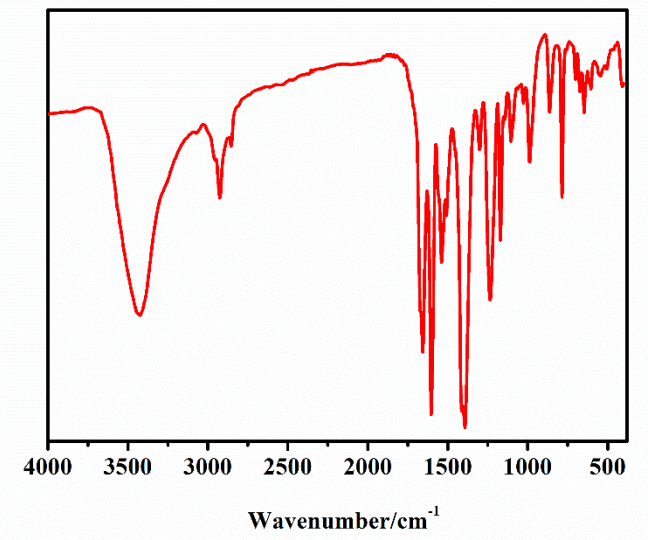

Figure S2 IR spectra of compound **1**.

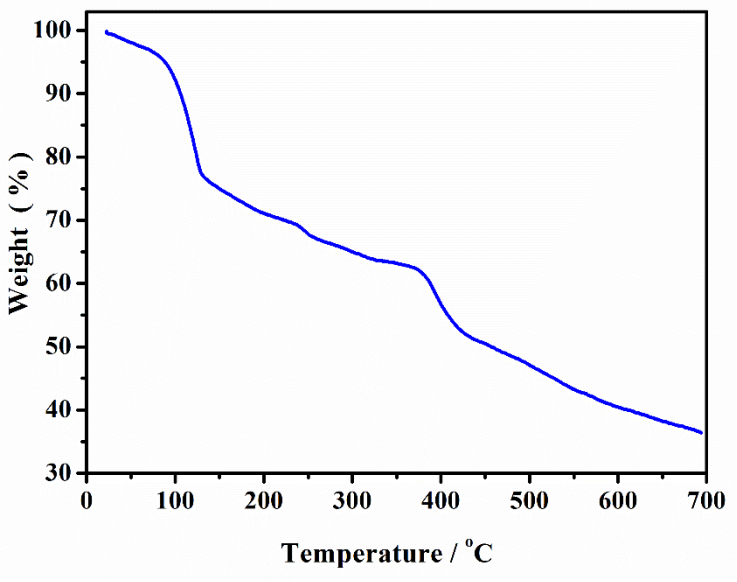

Figure S3 TGA curve of compound **1**.

Table S1 Selected hydrogen-bond parameters for **1**.

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
C23—H23···O14^{i}	0.93	2.31	3.063 (7)	137.8
C41—H41A···O12^{ii}	0.96	2.43	3.274 (8)	147.0
C47—H47B···O14^{iii}	0.96	2.41	3.284 (8)	151.5

Symmetry code(s): (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+2, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*+1.

Table S2 Selected geometric parameters (Å, º)

C1—C2	1.417 (7)	C34—O10	1.236 (6)
C1—C6	1.418 (6)	C35—H35A	0.9600
C1—C10	1.524 (7)	C35—H35B	0.9600

C2—C3	1.356 (7)	C35—H35C	0.9600
C2—C7	1.530 (5)	C35—N1	1.484 (6)
C3—C4	1.417 (6)	C36—H36A	0.9600
C3—C18^{i}	1.523 (7)	C36—H36B	0.9600
C4—C5	1.409 (7)	C36—H36C	0.9600
C4—C8	1.495 (7)	C36—N1	1.491 (6)
C5—C6	1.369 (7)	C37—H37	0.9300
C5—C26^{ii}	1.544 (5)	C37—N2	1.369 (7)
C6—C9	1.545 (7)	C37—O11	1.241 (6)
C7—H7A	0.9600	C38—H38A	0.9600
C7—H7B	0.9600	C38—H38B	0.9600
C7—H7C	0.9600	C38—H38C	0.9600
C8—H8A	0.9648	C38—N2	1.512 (7)
C8—H8B	0.9587	C39—H39A	0.9600
C8—H8C	0.9565	C39—H39B	0.9600
C9—H9A	0.9600	C39—H39C	0.9600
C9—H9B	0.9600	C39—N2	1.499 (6)
C9—H9C	0.9600	C40—H40	0.9300
C10—H10A	0.9700	C40—N3	1.377 (7)
C10—H10B	0.9700	C40—O12	1.258 (7)
C10—O1	1.442 (6)	C41—H41A	0.9600
C11—C12	1.396 (7)	C41—H41B	0.9600
C11—C16	1.371 (7)	C41—H41C	0.9600
C11—O1	1.361 (5)	C41—N3	1.485 (7)
C12—H12	0.9300	C42—H42A	0.9600
C12—C13	1.388 (7)	C42—H42B	0.9600
C13—H13	0.9300	C42—H42C	0.9600
C13—C14	1.382 (7)	C42—N3	1.481 (8)
C14—C15	1.408 (7)	C43—H43	0.9300
C14—C17	1.482 (6)	C43—N4	1.399 (7)
C15—H15	0.9300	C43—O13	1.259 (6)

C15—C16	1.382 (7)	C44—H44A	0.9600
C16—H16	0.9300	C44—H44B	0.9600
C17—La1	3.064 (5)	C44—H44C	0.9600
C17—O2	1.260 (6)	C44—N4	1.486 (7)
C17—O3	1.267 (5)	C45—H45A	0.9600
C18—H18A	0.9700	C45—H45B	0.9600
C18—H18B	0.9700	C45—H45C	0.9600
C18—O4	1.437 (6)	C45—N4	1.514 (7)
C19—C20	1.349 (7)	C46—H46	0.9300
C19—C24	1.367 (7)	C46—N5	1.355 (7)
C19—O4	1.414 (6)	C46—O14	1.248 (7)
C20—H20	0.9300	C47—H47A	0.9600
C20—C21	1.432 (6)	C47—H47B	0.9600
C21—H21	0.9300	C47—H47C	0.9600
C21—C22	1.389 (6)	C47—N5	1.481 (7)
C22—C23	1.399 (7)	C48—H48A	0.9600
C22—C25	1.488 (6)	C48—H48B	0.9600
C23—H23	0.9300	C48—H48C	0.9600
C23—C24	1.426 (7)	C48—N5	1.513 (7)
C24—H24	0.9300	C49—H49	0.9300
C25—O5	1.270 (6)	C49—N6	1.388 (7)
C25—O6	1.270 (5)	C49—O15	1.273 (6)
C26—H26A	0.9700	C50—H50A	0.9600
C26—H26B	0.9700	C50—H50B	0.9600
C26—O7	1.430 (6)	C50—H50C	0.9600
C27—C28	1.368 (7)	C50—N6	1.458 (6)
C27—C32	1.408 (7)	C51—H51A	0.9600
C27—O7	1.363 (5)	C51—H51B	0.9600
C28—H28	0.9300	C51—H51C	0.9600
C28—C29	1.422 (6)	C51—N6	1.472 (7)
C29—H29	0.9300	La1—La1^{iii}	4.1587 (8)

C29—C30	1.382 (7)	La1—O2	2.522 (3)
C30—C31	1.347 (7)	La1—O3^{iii}	2.448 (3)
C30—C33	1.460 (6)	La1—O3	2.827 (3)
C31—H31	0.9300	La1—O5	2.453 (4)
C31—C32	1.404 (6)	La1—O6^{iii}	2.459 (2)
C32—H32	0.9300	La1—O8	2.580 (3)
C33—La1	2.936 (4)	La1—O9	2.564 (3)
C33—O8	1.251 (6)	La1—O10	2.529 (3)
C33—O9	1.264 (6)	La1—O11	2.562 (3)
C34—H34	0.9300	O1W—H1WA	0.8500
C34—N1	1.368 (7)	O1W—H1WB	0.8500
C2—C1—C6	119.3 (5)	H41A—C41—H41B	109.5
C2—C1—C10	121.9 (4)	H41A—C41—H41C	109.5
C6—C1—C10	118.8 (5)	H41B—C41—H41C	109.5
C1—C2—C7	117.6 (4)	N3—C41—H41A	109.5
C3—C2—C1	120.0 (4)	N3—C41—H41B	109.5
C3—C2—C7	122.4 (5)	N3—C41—H41C	109.5
C2—C3—C4	121.9 (5)	H42A—C42—H42B	109.5
C2—C3—C18^{i}	118.8 (4)	H42A—C42—H42C	109.5
C4—C3—C18^{i}	119.3 (5)	H42B—C42—H42C	109.5
C3—C4—C8	120.4 (5)	N3—C42—H42A	109.5
C5—C4—C3	116.9 (5)	N3—C42—H42B	109.5
C5—C4—C8	122.7 (4)	N3—C42—H42C	109.5
C4—C5—C26^{ii}	120.5 (4)	N4—C43—H43	121.5
C6—C5—C4	122.8 (4)	O13—C43—H43	121.5
C6—C5—C26^{ii}	116.5 (4)	O13—C43—N4	116.9 (5)
C1—C6—C9	121.7 (5)	H44A—C44—H44B	109.5
C5—C6—C1	118.7 (5)	H44A—C44—H44C	109.5
C5—C6—C9	119.6 (4)	H44B—C44—H44C	109.5
C2—C7—H7A	109.5	N4—C44—H44A	109.5
C2—C7—H7B	109.5	N4—C44—H44B	109.5

C2—C7—H7C	109.5	N4—C44—H44C	109.5
H7A—C7—H7B	109.5	H45A—C45—H45B	109.5
H7A—C7—H7C	109.5	H45A—C45—H45C	109.5
H7B—C7—H7C	109.5	H45B—C45—H45C	109.5
C4—C8—H8A	110.4	N4—C45—H45A	109.5
C4—C8—H8B	109.2	N4—C45—H45B	109.5
C4—C8—H8C	108.8	N4—C45—H45C	109.5
H8A—C8—H8B	109.2	N5—C46—H46	114.8
H8A—C8—H8C	109.4	O14—C46—H46	114.8
H8B—C8—H8C	109.9	O14—C46—N5	130.4 (6)
C6—C9—H9A	109.5	H47A—C47—H47B	109.5
C6—C9—H9B	109.5	H47A—C47—H47C	109.5
C6—C9—H9C	109.5	H47B—C47—H47C	109.5
H9A—C9—H9B	109.5	N5—C47—H47A	109.5
H9A—C9—H9C	109.5	N5—C47—H47B	109.5
H9B—C9—H9C	109.5	N5—C47—H47C	109.5
C1—C10—H10A	110.2	H48A—C48—H48B	109.5
C1—C10—H10B	110.2	H48A—C48—H48C	109.5
H10A—C10—H10B	108.5	H48B—C48—H48C	109.5
O1—C10—C1	107.4 (4)	N5—C48—H48A	109.5
O1—C10—H10A	110.2	N5—C48—H48B	109.5
O1—C10—H10B	110.2	N5—C48—H48C	109.5
C16—C11—C12	120.1 (5)	N6—C49—H49	119.2
O1—C11—C12	115.8 (4)	O15—C49—H49	119.2
O1—C11—C16	124.1 (4)	O15—C49—N6	121.5 (5)
C11—C12—H12	120.0	H50A—C50—H50B	109.5
C13—C12—C11	120.0 (5)	H50A—C50—H50C	109.5
C13—C12—H12	120.0	H50B—C50—H50C	109.5
C12—C13—H13	119.9	N6—C50—H50A	109.5
C14—C13—C12	120.3 (4)	N6—C50—H50B	109.5
C14—C13—H13	119.9	N6—C50—H50C	109.5

C13—C14—C15	119.1 (4)	H51A—C51—H51B	109.5
C13—C14—C17	120.9 (4)	H51A—C51—H51C	109.5
C15—C14—C17	120.0 (4)	H51B—C51—H51C	109.5
C14—C15—H15	119.9	N6—C51—H51A	109.5
C16—C15—C14	120.3 (5)	N6—C51—H51B	109.5
C16—C15—H15	119.9	N6—C51—H51C	109.5
C11—C16—C15	120.2 (5)	C17—La1—La1^{iii}	59.02 (10)
C11—C16—H16	119.9	C33—La1—C17	122.80 (13)
C15—C16—H16	119.9	C33—La1—La1^{iii}	123.07 (11)
C14—C17—La1	172.0 (4)	O2—La1—C17	23.60 (12)
O2—C17—C14	118.9 (4)	O2—La1—C33	111.32 (13)
O2—C17—La1	53.3 (2)	O2—La1—La1^{iii}	82.62 (8)
O2—C17—O3	120.3 (4)	O2—La1—O3	47.96 (9)
O3—C17—C14	120.6 (4)	O2—La1—O8	134.30 (11)
O3—C17—La1	67.3 (2)	O2—La1—O9	91.06 (10)
C3^{i}—C18—H18A	110.7	O2—La1—O10	70.09 (11)
C3^{i}—C18—H18B	110.7	O2—La1—O11	138.56 (11)
H18A—C18—H18B	108.8	O3^{iii}—La1—C17	100.21 (12)
O4—C18—C3^{i}	105.0 (4)	O3—La1—C17	24.42 (11)
O4—C18—H18A	110.7	O3^{iii}—La1—C33	99.45 (12)
O4—C18—H18B	110.7	O3—La1—C33	131.34 (12)
C20—C19—C24	126.3 (5)	O3^{iii}—La1—La1^{iii}	41.32 (6)
C20—C19—O4	121.3 (4)	O3—La1—La1^{iii}	34.87 (6)
C24—C19—O4	112.5 (5)	O3^{iii}—La1—O2	123.71 (10)
C19—C20—H20	121.0	O3^{iii}—La1—O3	76.18 (9)
C19—C20—C21	118.1 (5)	O3^{iii}—La1—O5	74.94 (11)
C21—C20—H20	121.0	O3^{iii}—La1—O6^{iii}	77.31 (9)
C20—C21—H21	120.5	O3^{iii}—La1—O8	76.93 (9)
C22—C21—C20	119.0 (5)	O3^{iii}—La1—O9	124.55 (9)
C22—C21—H21	120.5	O3^{iii}—La1—O10	152.29 (11)
C21—C22—C23	119.9 (4)	O3^{iii}—La1—O11	87.92 (10)

C21—C22—C25	119.7 (5)	O5—La1—C17	67.17 (11)
C23—C22—C25	120.3 (4)	O5—La1—C33	67.23 (12)
C22—C23—H23	119.3	O5—La1—La1^{iii}	63.79 (7)
C22—C23—C24	121.4 (4)	O5—La1—O2	75.42 (11)
C24—C23—H23	119.3	O5—La1—O3	64.87 (9)
C19—C24—C23	115.3 (5)	O5—La1—O6^{iii}	130.71 (10)
C19—C24—H24	122.4	O5—La1—O8	71.96 (10)
C23—C24—H24	122.4	O5—La1—O9	74.53 (11)
O5—C25—C22	116.9 (4)	O5—La1—O10	132.54 (11)
O6—C25—C22	120.8 (4)	O5—La1—O11	144.16 (10)
O6—C25—O5	122.2 (4)	O6^{iii}—La1—C17	78.87 (11)
C5^{iv}—C26—H26A	110.6	O6^{iii}—La1—C33	158.14 (12)
C5^{iv}—C26—H26B	110.6	O6^{iii}—La1—La1^{iii}	68.39 (7)
H26A—C26—H26B	108.7	O6^{iii}—La1—O2	87.62 (10)
O7—C26—C5^{iv}	105.7 (4)	O6^{iii}—La1—O3	69.42 (9)
O7—C26—H26A	110.6	O6^{iii}—La1—O8	138.06 (10)
O7—C26—H26B	110.6	O6^{iii}—La1—O9	153.00 (11)
C28—C27—C32	119.9 (4)	O6^{iii}—La1—O10	79.68 (10)
O7—C27—C28	116.5 (4)	O6^{iii}—La1—O11	72.92 (9)
O7—C27—C32	123.4 (4)	O8—La1—C17	138.18 (12)
C27—C28—H28	120.2	O8—La1—C33	25.17 (12)
C27—C28—C29	119.6 (5)	O8—La1—La1^{iii}	109.60 (8)
C29—C28—H28	120.2	O8—La1—O3	133.56 (10)
C28—C29—H29	119.8	O9—La1—C17	108.82 (12)
C30—C29—C28	120.4 (5)	O9—La1—C33	25.44 (13)
C30—C29—H29	119.8	O9—La1—La1^{iii}	138.13 (8)
C29—C30—C33	119.5 (5)	O9—La1—O3	127.17 (10)
C31—C30—C29	119.2 (4)	O9—La1—O8	49.95 (10)
C31—C30—C33	121.2 (4)	O10—La1—C17	90.23 (12)
C30—C31—H31	118.9	O10—La1—C33	96.15 (12)
C30—C31—C32	122.3 (5)	O10—La1—La1^{iii}	138.62 (6)

C32—C31—H31	118.9	O10—La1—O3	109.70 (9)
C27—C32—H32	120.8	O10—La1—O8	111.73 (10)
C31—C32—C27	118.5 (5)	O10—La1—O9	74.55 (10)
C31—C32—H32	120.8	O10—La1—O11	70.61 (10)
C30—C33—La1	164.9 (4)	O11—La1—C17	148.14 (11)
O8—C33—C30	119.8 (4)	O11—La1—C33	85.41 (12)
O8—C33—La1	61.3 (2)	O11—La1—La1^{iii}	120.68 (7)
O8—C33—O9	119.4 (4)	O11—La1—O3	141.44 (9)
O9—C33—C30	120.8 (5)	O11—La1—O8	73.61 (10)
O9—C33—La1	60.6 (2)	O11—La1—O9	90.81 (11)
N1—C34—H34	117.4	C34—N1—C35	121.4 (4)
O10—C34—H34	117.4	C34—N1—C36	122.4 (4)
O10—C34—N1	125.2 (4)	C35—N1—C36	116.2 (4)
H35A—C35—H35B	109.5	C37—N2—C38	120.8 (4)
H35A—C35—H35C	109.5	C37—N2—C39	121.2 (4)
H35B—C35—H35C	109.5	C39—N2—C38	118.0 (4)
N1—C35—H35A	109.5	C40—N3—C41	126.2 (5)
N1—C35—H35B	109.5	C40—N3—C42	115.1 (5)
N1—C35—H35C	109.5	C42—N3—C41	118.5 (4)
H36A—C36—H36B	109.5	C43—N4—C44	139.2 (5)
H36A—C36—H36C	109.5	C43—N4—C45	105.0 (4)
H36B—C36—H36C	109.5	C44—N4—C45	115.9 (5)
N1—C36—H36A	109.5	C46—N5—C47	135.7 (5)
N1—C36—H36B	109.5	C46—N5—C48	113.7 (5)
N1—C36—H36C	109.5	C47—N5—C48	110.5 (5)
N2—C37—H37	118.4	C49—N6—C50	122.8 (5)
O11—C37—H37	118.4	C49—N6—C51	117.0 (4)
O11—C37—N2	123.1 (4)	C50—N6—C51	120.2 (4)
H38A—C38—H38B	109.5	C11—O1—C10	116.7 (4)
H38A—C38—H38C	109.5	C17—O2—La1	103.1 (3)
H38B—C38—H38C	109.5	C17—O3—La1^{iii}	164.0 (3)

N2—C38—H38A	109.5	C17—O3—La1	88.3 (3)
N2—C38—H38B	109.5	La1^{iii}—O3—La1	103.82 (9)
N2—C38—H38C	109.5	C19—O4—C18	115.7 (4)
H39A—C39—H39B	109.5	C25—O5—La1	142.2 (3)
H39A—C39—H39C	109.5	C25—O6—La1^{iii}	136.5 (3)
H39B—C39—H39C	109.5	C27—O7—C26	118.1 (4)
N2—C39—H39A	109.5	C33—O8—La1	93.6 (2)
N2—C39—H39B	109.5	C33—O9—La1	94.0 (3)
N2—C39—H39C	109.5	C34—O10—La1	131.8 (4)
N3—C40—H40	119.6	C37—O11—La1	125.2 (3)
O12—C40—H40	119.6	H1WA—O1W—H1WB	109.5
O12—C40—N3	120.8 (6)		
C1—C2—C3—C4	0.6 (8)	C22—C25—O6—La1^{iii}	175.5 (3)
C1—C2—C3—C18^{i}	−178.6 (4)	C23—C22—C25—O5	−179.7 (4)
C1—C10—O1—C11	−159.0 (4)	C23—C22—C25—O6	3.3 (6)
C2—C1—C6—C5	7.9 (7)	C24—C19—C20—C21	1.8 (8)
C2—C1—C6—C9	−172.4 (5)	C24—C19—O4—C18	−175.1 (4)
C2—C1—C10—O1	77.7 (6)	C25—C22—C23—C24	177.0 (4)
C2—C3—C4—C5	1.6 (8)	C26^{ii}—C5—C6—C1	179.8 (4)
C2—C3—C4—C8	−178.8 (5)	C26^{ii}—C5—C6—C9	0.1 (7)
C3—C4—C5—C6	1.0 (7)	C27—C28—C29—C30	0.9 (8)
C3—C4—C5—C26^{ii}	175.3 (4)	C28—C27—C32—C31	1.7 (8)
C3^{i}—C18—O4—C19	171.6 (4)	C28—C27—O7—C26	161.0 (5)
C4—C5—C6—C1	−5.8 (8)	C28—C29—C30—C31	−2.1 (8)
C4—C5—C6—C9	174.5 (4)	C28—C29—C30—C33	−179.0 (5)
C5^{iv}—C26—O7—C27	−151.3 (4)	C29—C30—C31—C32	3.3 (8)
C6—C1—C2—C3	−5.4 (7)	C29—C30—C33—La1	72.7 (15)
C6—C1—C2—C7	175.6 (4)	C29—C30—C33—O8	−17.2 (7)
C6—C1—C10—O1	−102.0 (5)	C29—C30—C33—O9	163.5 (5)
C7—C2—C3—C4	179.6 (5)	C30—C31—C32—C27	−3.1 (8)
C7—C2—C3—C18^{i}	0.3 (8)	C30—C33—O8—La1	162.8 (4)

C8—C4—C5—C6	−178.5 (5)	C30—C33—O9—La1	−162.6 (4)
C8—C4—C5—C26^{ii}	−4.3 (7)	C31—C30—C33—La1	−104.1 (14)
C10—C1—C2—C3	174.8 (5)	C31—C30—C33—O8	165.9 (5)
C10—C1—C2—C7	−4.2 (7)	C31—C30—C33—O9	−13.3 (8)
C10—C1—C6—C5	−172.3 (5)	C32—C27—C28—C29	−0.7 (8)
C10—C1—C6—C9	7.3 (7)	C32—C27—O7—C26	−14.1 (7)
C11—C12—C13—C14	−0.3 (8)	C33—C30—C31—C32	−179.9 (5)
C12—C11—C16—C15	0.3 (8)	La1—C17—O3—La1^{iii}	139.7 (9)
C12—C11—O1—C10	174.1 (4)	N1—C34—O10—La1	118.8 (5)
C12—C13—C14—C15	−0.5 (8)	N2—C37—O11—La1	−177.0 (4)
C12—C13—C14—C17	178.0 (5)	O1—C11—C12—C13	−179.2 (5)
C13—C14—C15—C16	1.1 (8)	O1—C11—C16—C15	179.8 (5)
C13—C14—C17—O2	−173.8 (5)	O2—C17—O3—La1	5.1 (4)
C13—C14—C17—O3	10.5 (7)	O2—C17—O3—La1^{iii}	144.8 (7)
C14—C15—C16—C11	−1.0 (8)	O3—C17—O2—La1	−5.9 (5)
C14—C17—O2—La1	178.4 (4)	O4—C19—C20—C21	−178.7 (4)
C14—C17—O3—La1	−179.2 (4)	O4—C19—C24—C23	−179.8 (4)
C14—C17—O3—La1^{iii}	−39.5 (11)	O5—C25—O6—La1^{iii}	−1.4 (7)
C15—C14—C17—O2	4.7 (7)	O6—C25—O5—La1	−33.1 (7)
C15—C14—C17—O3	−171.0 (4)	O7—C27—C28—C29	−176.0 (5)
C16—C11—C12—C13	0.4 (8)	O7—C27—C32—C31	176.7 (5)
C16—C11—O1—C10	−5.4 (8)	O8—C33—O9—La1	18.1 (5)
C17—C14—C15—C16	−177.4 (5)	O9—C33—O8—La1	−18.0 (5)
C18^{i}—C3—C4—C5	−179.2 (4)	O10—C34—N1—C35	−179.8 (5)
C18^{i}—C3—C4—C8	0.4 (7)	O10—C34—N1—C36	−0.3 (9)
C19—C20—C21—C22	−2.4 (7)	O11—C37—N2—C38	173.1 (5)
C20—C19—C24—C23	−0.3 (8)	O11—C37—N2—C39	−6.3 (8)
C20—C19—O4—C18	5.3 (7)	O12—C40—N3—C41	−17.0 (10)
C20—C21—C22—C23	1.6 (7)	O12—C40—N3—C42	168.6 (6)
C20—C21—C22—C25	−175.5 (4)	O13—C43—N4—C44	−142.9 (7)
C21—C22—C23—C24	−0.1 (7)	O13—C43—N4—C45	36.8 (7)

C21—C22—C25—O5	−2.6 (6)	O14—C46—N5—C47	164.4 (6)
C21—C22—C25—O6	−179.6 (4)	O14—C46—N5—C48	−15.2 (9)
C22—C23—C24—C19	−0.6 (7)	O15—C49—N6—C50	2.9 (8)
C22—C25—O5—La1	150.0 (3)	O15—C49—N6—C51	−180.0 (5)

Symmetry code(s): (i) −*x*+2, −*y*, −*z*; (ii) *x*+1, *y*+1, *z*; (iii) −*x*+1, −*y*, −*z*+1; (iv) *x*−1, *y*−1, *z*.