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Supporting information for article:

Three new quinuclidine-based structures: second harmonic generation response for 1,2-bis(1-azoniabicyclo[2.2.2]octan-3-ylidene)hydrazine dichloride

Liang Qiao, Xiao-Gang Chen, Ji-Xing Gao and Yong Ai

Supporting information

Table S1 Selected geometric parameters (Å, °) for **3**

N1—C1	1.4716 (15)	C2—C3	1.5025 (16)
N1—C7	1.4721 (16)	C3—C4	1.5341 (17)
N1—C6	1.4730 (16)	C3—C5	1.5394 (18)
N2—C2	1.2771 (16)	C4—C7	1.5453 (19)
N2—N3	1.4105 (15)	C5—C6	1.5419 (18)
C1—C2	1.5068 (16)		
C1—N1—C7	108.21 (9)	C2—C3—C4	107.91 (10)
C1—N1—C6	108.95 (10)	C2—C3—C5	107.89 (9)
C7—N1—C6	109.38 (10)	C4—C3—C5	107.74 (10)
C2—N2—N3	115.50 (10)	C3—C4—C7	108.22 (10)
N1—C1—C2	110.36 (9)	C3—C5—C6	108.27 (10)
N2—C2—C3	121.30 (11)	N1—C6—C5	112.18 (10)
N2—C2—C1	126.65 (11)	N1—C7—C4	112.22 (10)
C3—C2—C1	112.05 (10)		

Table S2 Selected geometric parameters (Å, °) for **4**

N1—C1	1.4643 (15)	C2—C3	1.4996 (16)
N1—C7	1.4656 (17)	C3—C4	1.5296 (19)
N1—C6	1.4670 (17)	C3—C5	1.5335 (18)
N2—C2	1.2693 (16)	C4—C7	1.5294 (19)
N2—N2 ⁱ	1.418 (2)	C5—C6	1.5291 (19)

C1—C2	1.5060 (16)		
C1—N1—C7	108.05 (10)	C2—C3—C4	107.90 (10)
C1—N1—C6	108.64 (10)	C2—C3—C5	106.63 (11)
C7—N1—C6	108.75 (10)	C4—C3—C5	108.14 (11)
C2—N2—N2 ⁱ	114.53 (11)	C7—C4—C3	108.79 (11)
N1—C1—C2	110.70 (10)	C6—C5—C3	108.32 (10)
N2—C2—C3	121.63 (11)	N1—C6—C5	112.91 (11)
N2—C2—C1	126.47 (11)	N1—C7—C4	112.50 (10)
C3—C2—C1	111.88 (10)		

Symmetry code: (i) $-x+3/2, -y+1/2, z$.

Table S3 Selected geometric parameters (Å, °) for **5**

C1—C2	1.497 (3)	C3—C6	1.535 (3)
C1—C3	1.495 (3)	C4—C6	1.526 (3)
C1—N2	1.274 (2)	C4—N1	1.495 (3)
C10—C12	1.534 (3)	C5—C7	1.515 (3)
C10—C14	1.529 (3)	C7—N1	1.502 (3)
C11—C12	1.510 (4)	C8—C9	1.500 (3)
C11—N4	1.492 (3)	C8—C10	1.493 (3)
C13—C14	1.512 (4)	C8—N3	1.270 (2)
C13—N4	1.496 (3)	C9—N4	1.484 (3)
C2—N1	1.493 (2)	N2—N3	1.422 (2)
C3—C5	1.538 (3)		
C1—N2—N3	111.58 (16)	C8—N3—N2	112.44 (16)
C1—C3—C5	106.34 (16)	C8—C10—C12	106.39 (16)
C1—C3—C6	108.16 (17)	C8—C10—C14	108.17 (17)
C10—C8—C9	112.82 (15)	C9—N4—C13	110.78 (18)

C11—N4—C13	109.2 (2)	C9—N4—C11	109.40 (18)
C11—C12—C10	109.67 (18)	N1—C7—C5	109.55 (17)
C13—C14—C10	109.86 (18)	N1—C4—C6	109.60 (16)
C14—C10—C12	108.75 (16)	N1—C2—C1	107.94 (16)
C2—N1—C7	109.73 (16)	N2—C1—C2	124.61 (18)
C2—N1—C4	110.42 (15)	N2—C1—C3	122.24 (17)
C3—C1—C2	113.10 (15)	N3—C8—C9	124.25 (18)
C4—N1—C7	109.99 (18)	N3—C8—C10	122.87 (18)
C4—C6—C3	109.64 (17)	N4—C13—C14	109.97 (18)
C6—C3—C5	108.96 (17)	N4—C11—C12	110.24 (18)
C7—C5—C3	110.02 (18)	N4—C9—C8	108.17 (18)
