

Crystal Structure and Theoretical Investigation of Thiobarbituric Acid Derivatives as Nonlinear Optical (NLO) Materials

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A. Geometry parameters for crystals

A1. Geometric parameters (Å, °) of 1

S1—C10	1.663 (2)	C4—H4A	0.9500
N1—C5	1.337 (3)	C5—C6	1.506 (3)
N1—C1	1.338 (3)	C6—H6A	0.9900
N2—C7	1.308 (3)	C6—H6B	0.9900
N2—C6	1.463 (3)	C7—C8	1.396 (3)
N2—H2A	0.93 (3)	C7—H7A	0.9500
N3—C10	1.382 (3)	C8—C9	1.434 (3)
N3—C9	1.407 (3)	C8—C11	1.435 (3)
N3—C14	1.483 (3)	C12—C13	1.515 (3)
N4—C10	1.389 (3)	C12—H12A	0.9900
N4—C11	1.407 (3)	C12—H12B	0.9900

N4—C12	1.482 (3)	C13—H13A	0.9800
O1—C9	1.233 (3)	C13—H13B	0.9800
O2—C11	1.228 (3)	C13—H13C	0.9800
C1—C2	1.387 (3)	C14—C15	1.516 (3)
C1—H1B	0.9500	C14—H14A	0.9900
C2—C3	1.382 (4)	C14—H14B	0.9900
C2—H2B	0.9500	C15—H15A	0.9800
C3—C4	1.387 (3)	C15—H15B	0.9800
C3—H3A	0.9500	C15—H15C	0.9800
C4—C5	1.389 (3)		
C5—N1—C1	117.2 (2)	C7—C8—C11	117.21 (19)
C7—N2—C6	122.22 (18)	C9—C8—C11	121.4 (2)
C7—N2—H2A	122.1 (19)	O1—C9—N3	119.88 (19)
C6—N2—H2A	115.7 (19)	O1—C9—C8	123.6 (2)
C10—N3—C9	124.51 (18)	N3—C9—C8	116.48 (19)
C10—N3—C14	119.89 (18)	N3—C10—N4	116.69 (19)
C9—N3—C14	115.60 (17)	N3—C10—S1	121.98 (16)
C10—N4—C11	124.52 (18)	N4—C10—S1	121.33 (16)
C10—N4—C12	119.96 (18)	O2—C11—N4	118.97 (19)
C11—N4—C12	115.36 (17)	O2—C11—C8	124.8 (2)
N1—C1—C2	123.7 (2)	N4—C11—C8	116.21 (18)
N1—C1—H1B	118.1	N4—C12—C13	111.23 (17)
C2—C1—H1B	118.1	N4—C12—H12A	109.4
C3—C2—C1	118.5 (2)	C13—C12—H12A	109.4
C3—C2—H2B	120.8	N4—C12—H12B	109.4
C1—C2—H2B	120.8	C13—C12—H12B	109.4
C2—C3—C4	118.6 (2)	H12A—C12—H12B	108.0
C2—C3—H3A	120.7	C12—C13—H13A	109.5

C4—C3—H3A	120.7	C12—C13—H13B	109.5
C3—C4—C5	118.9 (2)	H13A—C13—H13B	109.5
C3—C4—H4A	120.5	C12—C13—H13C	109.5
C5—C4—H4A	120.5	H13A—C13—H13C	109.5
N1—C5—C4	123.1 (2)	H13B—C13—H13C	109.5
N1—C5—C6	117.5 (2)	N3—C14—C15	110.99 (18)
C4—C5—C6	119.45 (19)	N3—C14—H14A	109.4
N2—C6—C5	111.26 (17)	C15—C14—H14A	109.4
N2—C6—H6A	109.4	N3—C14—H14B	109.4
C5—C6—H6A	109.4	C15—C14—H14B	109.4
N2—C6—H6B	109.4	H14A—C14—H14B	108.0
C5—C6—H6B	109.4	C14—C15—H15A	109.5
H6A—C6—H6B	108.0	C14—C15—H15B	109.5
N2—C7—C8	126.23 (19)	H15A—C15—H15B	109.5
N2—C7—H7A	116.9	C14—C15—H15C	109.5
C8—C7—H7A	116.9	H15A—C15—H15C	109.5
C7—C8—C9	121.3 (2)	H15B—C15—H15C	109.5
C5—N1—C1—C2	−0.2 (3)	C11—C8—C9—N3	2.2 (3)
N1—C1—C2—C3	1.0 (3)	C9—N3—C10—N4	−2.1 (3)
C1—C2—C3—C4	−0.8 (3)	C14—N3—C10—N4	178.14 (16)
C2—C3—C4—C5	−0.2 (3)	C9—N3—C10—S1	177.48 (15)
C1—N1—C5—C4	−0.9 (3)	C14—N3—C10—S1	−2.3 (3)
C1—N1—C5—C6	177.60 (18)	C11—N4—C10—N3	4.7 (3)
C3—C4—C5—N1	1.1 (3)	C12—N4—C10—N3	179.82 (16)
C3—C4—C5—C6	−177.36 (18)	C11—N4—C10—S1	−174.93 (14)
C7—N2—C6—C5	175.89 (18)	C12—N4—C10—S1	0.2 (3)
N1—C5—C6—N2	10.9 (3)	C10—N4—C11—O2	176.05 (18)
C4—C5—C6—N2	−170.54 (18)	C12—N4—C11—O2	0.7 (3)

C6—N2—C7—C8	178.31 (19)	C10—N4—C11—C8	−3.6 (3)
N2—C7—C8—C9	−1.7 (3)	C12—N4—C11—C8	−178.99 (16)
N2—C7—C8—C11	−178.97 (19)	C7—C8—C11—O2	−2.4 (3)
C10—N3—C9—O1	179.98 (18)	C9—C8—C11—O2	−179.6 (2)
C14—N3—C9—O1	−0.3 (3)	C7—C8—C11—N4	177.28 (17)
C10—N3—C9—C8	−1.2 (3)	C9—C8—C11—N4	0.0 (3)
C14—N3—C9—C8	178.60 (16)	C10—N4—C12—C13	−91.1 (2)
C7—C8—C9—O1	3.9 (3)	C11—N4—C12—C13	84.4 (2)
C11—C8—C9—O1	−178.98 (19)	C10—N3—C14—C15	−92.6 (2)
C7—C8—C9—N3	−174.95 (17)	C9—N3—C14—C15	87.6 (2)

A2. Geometric parameters (Å, °) of 2

S1—C12	1.6718 (13)	C3—H3B	0.9900
O1—C3	1.4284 (17)	C4—H4A	0.9900
O1—C1	1.4315 (16)	C4—H4B	0.9900
O2—C9	1.2230 (16)	C5—C6	1.5101 (19)
O3—C15	1.2352 (15)	C5—H5A	0.9900
N1—C4	1.4632 (17)	C5—H5B	0.9900
N1—C5	1.4674 (17)	C6—H6A	0.9900
N1—C2	1.4680 (17)	C6—H6B	0.9900
N2—C7	1.3062 (17)	C7—C8	1.3963 (18)
N2—C6	1.4648 (17)	C7—H7A	0.9500
N2—H2A	0.88 (2)	C8—C15	1.4282 (17)
N3—C12	1.3770 (16)	C8—C9	1.4396 (17)
N3—C9	1.4135 (16)	C10—C11	1.5131 (18)
N3—C10	1.4851 (15)	C10—H10A	0.9900
N4—C12	1.3800 (16)	C10—H10B	0.9900
N4—C15	1.4054 (16)	C11—H11A	0.9800
N4—C13	1.4818 (15)	C11—H11B	0.9800

C1—C2	1.5206 (19)	C11—H11C	0.9800
C1—H1A	0.9900	C13—C14	1.5151 (18)
C1—H1B	0.9900	C13—H13A	0.9900
C2—H2B	0.9900	C13—H13B	0.9900
C2—H2C	0.9900	C14—H14A	0.9800
C3—C4	1.507 (2)	C14—H14B	0.9800
C3—H3A	0.9900	C14—H14C	0.9800
C3—O1—C1	108.48 (10)	N2—C6—H6A	109.5
C4—N1—C5	109.53 (10)	C5—C6—H6A	109.5
C4—N1—C2	108.32 (10)	N2—C6—H6B	109.5
C5—N1—C2	112.21 (11)	C5—C6—H6B	109.5
C7—N2—C6	122.15 (11)	H6A—C6—H6B	108.1
C7—N2—H2A	117.7 (12)	N2—C7—C8	125.95 (12)
C6—N2—H2A	119.7 (12)	N2—C7—H7A	117.0
C12—N3—C9	124.60 (10)	C8—C7—H7A	117.0
C12—N3—C10	119.98 (10)	C7—C8—C15	121.28 (11)
C9—N3—C10	115.35 (10)	C7—C8—C9	117.36 (11)
C12—N4—C15	124.05 (10)	C15—C8—C9	121.35 (11)
C12—N4—C13	120.12 (10)	O2—C9—N3	119.51 (11)
C15—N4—C13	115.82 (10)	O2—C9—C8	124.77 (12)
O1—C1—C2	111.22 (11)	N3—C9—C8	115.71 (11)
O1—C1—H1A	109.4	N3—C10—C11	111.95 (10)
C2—C1—H1A	109.4	N3—C10—H10A	109.2
O1—C1—H1B	109.4	C11—C10—H10A	109.2
C2—C1—H1B	109.4	N3—C10—H10B	109.2
H1A—C1—H1B	108.0	C11—C10—H10B	109.2
N1—C2—C1	110.18 (11)	H10A—C10—H10B	107.9
N1—C2—H2B	109.6	C10—C11—H11A	109.5

C1—C2—H2B	109.6	C10—C11—H11B	109.5
N1—C2—H2C	109.6	H11A—C11—H11B	109.5
C1—C2—H2C	109.6	C10—C11—H11C	109.5
H2B—C2—H2C	108.1	H11A—C11—H11C	109.5
O1—C3—C4	111.21 (11)	H11B—C11—H11C	109.5
O1—C3—H3A	109.4	N3—C12—N4	117.17 (11)
C4—C3—H3A	109.4	N3—C12—S1	121.75 (9)
O1—C3—H3B	109.4	N4—C12—S1	121.08 (9)
C4—C3—H3B	109.4	N4—C13—C14	112.13 (10)
H3A—C3—H3B	108.0	N4—C13—H13A	109.2
N1—C4—C3	110.96 (11)	C14—C13—H13A	109.2
N1—C4—H4A	109.4	N4—C13—H13B	109.2
C3—C4—H4A	109.4	C14—C13—H13B	109.2
N1—C4—H4B	109.4	H13A—C13—H13B	107.9
C3—C4—H4B	109.4	C13—C14—H14A	109.5
H4A—C4—H4B	108.0	C13—C14—H14B	109.5
N1—C5—C6	112.27 (11)	H14A—C14—H14B	109.5
N1—C5—H5A	109.2	C13—C14—H14C	109.5
C6—C5—H5A	109.2	H14A—C14—H14C	109.5
N1—C5—H5B	109.2	H14B—C14—H14C	109.5
C6—C5—H5B	109.2	O3—C15—N4	119.44 (11)
H5A—C5—H5B	107.9	O3—C15—C8	123.65 (11)
N2—C6—C5	110.69 (11)	N4—C15—C8	116.89 (11)
C3—O1—C1—C2	−59.70 (14)	C15—C8—C9—N3	2.06 (17)
C4—N1—C2—C1	−56.24 (14)	C12—N3—C10—C11	−88.50 (14)
C5—N1—C2—C1	−177.28 (11)	C9—N3—C10—C11	88.58 (13)
O1—C1—C2—N1	59.41 (14)	C9—N3—C12—N4	5.84 (17)
C1—O1—C3—C4	59.60 (14)	C10—N3—C12—N4	−177.37 (10)

C5—N1—C4—C3	179.29 (11)	C9—N3—C12—S1	−173.72 (9)
C2—N1—C4—C3	56.61 (14)	C10—N3—C12—S1	3.07 (15)
O1—C3—C4—N1	−59.58 (15)	C15—N4—C12—N3	−2.94 (17)
C4—N1—C5—C6	166.79 (11)	C13—N4—C12—N3	177.95 (10)
C2—N1—C5—C6	−72.88 (14)	C15—N4—C12—S1	176.62 (9)
C7—N2—C6—C5	−167.11 (12)	C13—N4—C12—S1	−2.49 (15)
N1—C5—C6—N2	−58.13 (15)	C12—N4—C13—C14	92.14 (14)
C6—N2—C7—C8	−172.57 (12)	C15—N4—C13—C14	−87.03 (13)
N2—C7—C8—C15	−0.6 (2)	C12—N4—C15—O3	−178.85 (11)
N2—C7—C8—C9	178.35 (12)	C13—N4—C15—O3	0.29 (16)
C12—N3—C9—O2	174.92 (11)	C12—N4—C15—C8	−0.01 (17)
C10—N3—C9—O2	−2.00 (17)	C13—N4—C15—C8	179.13 (10)
C12—N3—C9—C8	−5.39 (17)	C7—C8—C15—O3	−1.91 (19)
C10—N3—C9—C8	177.69 (10)	C9—C8—C15—O3	179.20 (11)
C7—C8—C9—O2	2.80 (19)	C7—C8—C15—N4	179.31 (11)
C15—C8—C9—O2	−178.27 (12)	C9—C8—C15—N4	0.42 (17)
C7—C8—C9—N3	−176.87 (10)		

A3. Geometric parameters (Å, °) of 3

S1—C9	1.6571 (15)	N4—C9	1.3885 (19)
N1—C5	1.3278 (19)	N4—C10	1.403 (2)
N1—C1	1.333 (2)	N4—C11	1.4808 (19)
C1—C2	1.384 (2)	C10—C7	1.434 (2)
C1—H1	0.9500	C8—C7	1.446 (2)
O1—C8	1.2268 (19)	C7—C6	1.385 (2)
O2—C10	1.2348 (19)	C6—H6	0.9500
N2—C6	1.325 (2)	C11—C12	1.516 (2)
N2—C5	1.411 (2)	C11—H11A	0.9900
N2—H2A	0.89 (2)	C11—H11B	0.9900

C2—C3	1.382 (2)	C12—H12A	0.9800
C2—H2	0.9500	C12—H12B	0.9800
N3—C9	1.3815 (19)	C12—H12C	0.9800
N3—C8	1.406 (2)	C13—C14	1.516 (2)
N3—C13	1.4851 (18)	C13—H13A	0.9900
C3—C4	1.379 (2)	C13—H13B	0.9900
C3—H3	0.9500	C14—H14A	0.9800
C4—C5	1.392 (2)	C14—H14B	0.9800
C4—H4	0.9500	C14—H14C	0.9800
C5—N1—C1	116.65 (13)	O1—C8—C7	124.44 (14)
N1—C1—C2	123.82 (15)	N3—C8—C7	115.58 (13)
N1—C1—H1	118.1	C6—C7—C10	121.86 (14)
C2—C1—H1	118.1	C6—C7—C8	117.20 (13)
C6—N2—C5	123.60 (13)	C10—C7—C8	120.92 (14)
C6—N2—H2A	115.4 (13)	N2—C6—C7	125.03 (14)
C5—N2—H2A	120.9 (13)	N2—C6—H6	117.5
C3—C2—C1	118.13 (15)	C7—C6—H6	117.5
C3—C2—H2	120.9	N4—C11—C12	111.68 (13)
C1—C2—H2	120.9	N4—C11—H11A	109.3
C9—N3—C8	124.92 (12)	C12—C11—H11A	109.3
C9—N3—C13	119.55 (12)	N4—C11—H11B	109.3
C8—N3—C13	115.40 (12)	C12—C11—H11B	109.3
C4—C3—C2	119.57 (14)	H11A—C11—H11B	107.9
C4—C3—H3	120.2	C11—C12—H12A	109.5
C2—C3—H3	120.2	C11—C12—H12B	109.5
C3—C4—C5	117.29 (14)	H12A—C12—H12B	109.5
C3—C4—H4	121.4	C11—C12—H12C	109.5
C5—C4—H4	121.4	H12A—C12—H12C	109.5

C9—N4—C10	123.81 (12)	H12B—C12—H12C	109.5
C9—N4—C11	119.66 (13)	N3—C13—C14	111.73 (13)
C10—N4—C11	116.50 (12)	N3—C13—H13A	109.3
N1—C5—C4	124.52 (14)	C14—C13—H13A	109.3
N1—C5—N2	116.89 (13)	N3—C13—H13B	109.3
C4—C5—N2	118.59 (13)	C14—C13—H13B	109.3
O2—C10—N4	119.64 (14)	H13A—C13—H13B	107.9
O2—C10—C7	123.35 (15)	C13—C14—H14A	109.5
N4—C10—C7	116.98 (13)	C13—C14—H14B	109.5
N3—C9—N4	116.70 (13)	H14A—C14—H14B	109.5
N3—C9—S1	121.84 (11)	C13—C14—H14C	109.5
N4—C9—S1	121.46 (11)	H14A—C14—H14C	109.5
O1—C8—N3	119.96 (13)	H14B—C14—H14C	109.5
C5—N1—C1—C2	−0.2 (2)	C11—N4—C9—S1	1.07 (19)
N1—C1—C2—C3	1.0 (3)	C9—N3—C8—O1	170.63 (14)
C1—C2—C3—C4	−0.6 (3)	C13—N3—C8—O1	−5.3 (2)
C2—C3—C4—C5	−0.4 (2)	C9—N3—C8—C7	−10.5 (2)
C1—N1—C5—C4	−1.0 (2)	C13—N3—C8—C7	173.55 (13)
C1—N1—C5—N2	179.01 (13)	O2—C10—C7—C6	4.6 (2)
C3—C4—C5—N1	1.2 (2)	N4—C10—C7—C6	−173.48 (14)
C3—C4—C5—N2	−178.74 (14)	O2—C10—C7—C8	−176.71 (14)
C6—N2—C5—N1	−3.6 (2)	N4—C10—C7—C8	5.2 (2)
C6—N2—C5—C4	176.42 (14)	O1—C8—C7—C6	1.2 (2)
C9—N4—C10—O2	173.05 (14)	N3—C8—C7—C6	−177.57 (13)
C11—N4—C10—O2	−5.0 (2)	O1—C8—C7—C10	−177.46 (15)
C9—N4—C10—C7	−8.8 (2)	N3—C8—C7—C10	3.7 (2)
C11—N4—C10—C7	173.17 (13)	C5—N2—C6—C7	−179.50 (14)
C8—N3—C9—N4	7.5 (2)	C10—C7—C6—N2	−2.0 (2)

C13—N3—C9—N4	−176.72 (13)	C8—C7—C6—N2	179.28 (14)
C8—N3—C9—S1	−172.77 (11)	C9—N4—C11—C12	−86.12 (17)
C13—N3—C9—S1	3.03 (19)	C10—N4—C11—C12	92.04 (17)
C10—N4—C9—N3	2.8 (2)	C9—N3—C13—C14	−90.59 (17)
C11—N4—C9—N3	−179.18 (13)	C8—N3—C13—C14	85.60 (17)
C10—N4—C9—S1	−176.95 (11)		

A. Computational chemistry

B1. Optimized geometry co-ordinates of crystal 1.

0 1

S(PDBName=S1,ResName=UNK,ResNum=1)	−4.59125700	1.01388500	−
0.46000100			
N(PDBName=N1,ResName=UNK,ResNum=1)	4.42233800	0.79622500	
0.56217300			
N(PDBName=N2,ResName=UNK,ResNum=1)	1.85765600	−0.53443900	
0.99021200			
N(PDBName=N3,ResName=UNK,ResNum=1)	−2.03288500	1.20630300	
0.30170400			
N(PDBName=N4,ResName=UNK,ResNum=1)	−2.76830200	−0.94546300	−
0.36533900			
O(PDBName=O1,ResName=UNK,ResNum=1)	0.14217500	1.55301700	
0.92487100			
O(PDBName=O2,ResName=UNK,ResNum=1)	−1.35137000	−2.74224300	−
0.29274300			
C(PDBName=C1,ResName=UNK,ResNum=1)	5.35300900	1.41802200	−
0.16384700			
H(PDBName=H1B,ResName=UNK,ResNum=1)	5.47170000	2.48154600	
0.02127800			
C(PDBName=C2,ResName=UNK,ResNum=1)	6.14703200	0.76897200	−
1.10885300			
H(PDBName=H2B,ResName=UNK,ResNum=1)	6.89223300	1.32097400	−
1.66861600			
C(PDBName=C3,ResName=UNK,ResNum=1)	5.95346700	−0.59321800	−
1.30917600			
H(PDBName=H3A,ResName=UNK,ResNum=1)	6.54702100	−1.13652700	−
2.03565600			

C(PDBName=C4,ResName=UNK,ResNum=1) 0.56287700	4.97724900	-1.24959200	-
H(PDBName=H4A,ResName=UNK,ResNum=1) 0.69894700	4.79296700	-2.30904500	-
C(PDBName=C5,ResName=UNK,ResNum=1) 0.36246800	4.23693500	-0.51406400	
C(PDBName=C6,ResName=UNK,ResNum=1) 1.21737400	3.15944700	-1.15246100	
H(PDBName=H6A,ResName=UNK,ResNum=1) 1.00749900	3.07638600	-2.21984300	
H(PDBName=H6B,ResName=UNK,ResNum=1) 2.27206900	3.42869000	-1.03331400	
C(PDBName=C7,ResName=UNK,ResNum=1) 0.57928500	0.78470800	-1.18941500	
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.41444000	0.88895100	-2.25806700	
C(PDBName=C8,ResName=UNK,ResNum=1) 0.34160900	-0.46954000	-0.64300300	
C(PDBName=C9,ResName=UNK,ResNum=1) 0.54564300	-0.72287600	0.75765500	
C(PDBName=C10,ResName=UNK,ResNum=1) 0.16137000	-3.06153200	0.39473100	-
C(PDBName=C11,ResName=UNK,ResNum=1) 0.11486200	-1.51094200	-1.54146800	-
C(PDBName=C12,ResName=UNK,ResNum=1) 0.85891800	-3.81838700	-1.86990600	-
H(PDBName=H12A,ResName=UNK,ResNum=1) 1.43670200	-3.29909000	-2.63127900	-
H(PDBName=H12B,ResName=UNK,ResNum=1) 1.51240900	-4.46872900	-1.29497800	-
C(PDBName=C13,ResName=UNK,ResNum=1) 0.27404900	-4.61359100	-2.51395200	
H(PDBName=H13A,ResName=UNK,ResNum=1) 0.14737800	-5.36337500	-3.18946800	-
H(PDBName=H13B,ResName=UNK,ResNum=1) 0.86629400	-5.13360700	-1.75886800	
H(PDBName=H13C,ResName=UNK,ResNum=1) 0.92551000	-3.96027800	-3.09793200	

C(PDBName=C14,ResName=UNK,ResNum=1)	-2.27124100	2.64956000	
0.54965700			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-1.60378800	2.92821800	
1.36218400			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-3.30332800	2.75009500	
0.87404400			
C(PDBName=C15,ResName=UNK,ResNum=1)	-1.99932600	3.51097400	-
0.68099500			
H(PDBName=H15A,ResName=UNK,ResNum=1)	-2.18263500	4.56094300	-
0.43599100			
H(PDBName=H15B,ResName=UNK,ResNum=1)	-2.65971700	3.23553500	-
1.50512900			
H(PDBName=H15C,ResName=UNK,ResNum=1)	-0.96027000	3.41517600	-
1.00262500			
H(PDBName=H2A,ResName=UNK,ResNum=1)	1.75242600	0.47307000	
1.12675600			
1 24 1.0			
2 8 1.5 16 1.5			
3 17 1.0 20 2.0 40 1.0			
4 23 1.0 24 1.0 33 1.0			
5 24 1.0 25 1.0 26 1.0			
6 23 2.0			
7 25 2.0			
8 9 1.0 10 1.5			
9			
10 11 1.0 12 1.5			
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12 13 1.0 14 1.5			
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14 15 1.0 16 1.5			
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16 17 1.0			
17 18 1.0 19 1.0			
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20 21 1.0 22 1.5			
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22 23 1.5 25 1.0			

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 26 27 1.0 28 1.0 29 1.0
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 29 30 1.0 31 1.0 32 1.0
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 33 34 1.0 35 1.0 36 1.0
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 36 37 1.0 38 1.0 39 1.0
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B2. Optimized geometry co-ordinates of crystal 2.

0 1

S(PDBName=S1,ResName=UNK,ResNum=1)	4.68484700	1.66907600	
0.26490200			
O(PDBName=O1,ResName=UNK,ResNum=1)	-5.87797800	1.58231100	
0.09949800			
O(PDBName=O2,ResName=UNK,ResNum=1)	2.53632500	-2.80075100	
0.08379000			
O(PDBName=O3,ResName=UNK,ResNum=1)	-0.22797000	0.99605500	
0.41892300			
N(PDBName=N1,ResName=UNK,ResNum=1)	-4.03028100	-0.55256100	-
0.29642000			
N(PDBName=N2,ResName=UNK,ResNum=1)	-1.33570000	-1.46842800	
0.28600200			
N(PDBName=N3,ResName=UNK,ResNum=1)	3.44124500	-0.70199600	
0.21398600			
N(PDBName=N4,ResName=UNK,ResNum=1)	2.05075500	1.20922400	
0.38292200			
C(PDBName=C1,ResName=UNK,ResNum=1)	-5.38150900	0.83826800	
1.20459000			

H(PDBName=H1A,ResName=UNK,ResNum=1) 1.95222700	-6.17634600	0.82548000	
H(PDBName=H1B,ResName=UNK,ResNum=1) 1.62977000	-4.50133100	1.34155100	
C(PDBName=C2,ResName=UNK,ResNum=1) 0.79281500	-5.01148000	-0.58320100	
H(PDBName=H2B,ResName=UNK,ResNum=1) 1.65651200	-4.58930000	-1.10496300	
H(PDBName=H2C,ResName=UNK,ResNum=1) 0.48651400	-5.92552400	-1.12439200	
C(PDBName=C3,ResName=UNK,ResNum=1) 0.95395300	-4.92117700	1.63043800	-
H(PDBName=H3A,ResName=UNK,ResNum=1) 0.61544600	-4.01893200	2.15885900	-
H(PDBName=H3B,ResName=UNK,ResNum=1) 1.76424800	-5.38155800	2.19796900	-
C(PDBName=C4,ResName=UNK,ResNum=1) 1.42425400	-4.54728300	0.22912400	-
H(PDBName=H4A,ResName=UNK,ResNum=1) 1.87742900	-5.43413300	-0.24988000	-
H(PDBName=H4B,ResName=UNK,ResNum=1) 2.19171500	-3.77101800	0.29979200	-
C(PDBName=C5,ResName=UNK,ResNum=1) 0.68263000	-3.55473300	-1.87772000	-
H(PDBName=H5A,ResName=UNK,ResNum=1) 1.68744900	-3.12917400	-1.80902300	-
H(PDBName=H5B,ResName=UNK,ResNum=1) 0.72417300	-4.37078900	-2.62047600	-
C(PDBName=C6,ResName=UNK,ResNum=1) 0.26845600	-2.46704500	-2.38539500	
H(PDBName=H6A,ResName=UNK,ResNum=1) 1.28297200	-2.86626000	-2.49343100	
H(PDBName=H6B,ResName=UNK,ResNum=1) 0.05134200	-2.11964300	-3.37061200	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.23128500	-0.06671200	-1.83394300	
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.15632300	0.14123500	-2.89767500	

C(PDBName=C8,ResName=UNK,ResNum=1)	1.03339700	-0.98520900	
0.26028600			
C(PDBName=C9,ResName=UNK,ResNum=1)	2.34556400	-1.59526100	
0.17925100			
C(PDBName=C10,ResName=UNK,ResNum=1)	4.77845000	-1.33951100	
0.12738300			
H(PDBName=H10A,ResName=UNK,ResNum=1)	4.68052800	-2.30597700	
0.61683100			
H(PDBName=H10B,ResName=UNK,ResNum=1)	5.46759600	-0.71436700	
0.68814400			
C(PDBName=C11,ResName=UNK,ResNum=1)	5.25090600	-1.51927800	-
1.31313800			
H(PDBName=H11A,ResName=UNK,ResNum=1)	6.23330800	-1.99977500	-
1.31525900			
H(PDBName=H11B,ResName=UNK,ResNum=1)	5.34453200	-0.55622100	-
1.81810100			
H(PDBName=H11C,ResName=UNK,ResNum=1)	4.56207300	-2.15586400	-
1.87207500			
C(PDBName=C12,ResName=UNK,ResNum=1)	3.33214000	0.67818700	
0.28807300			
C(PDBName=C13,ResName=UNK,ResNum=1)	1.85495900	2.67678600	
0.47703200			
H(PDBName=H13A,ResName=UNK,ResNum=1)	2.70774100	3.07834900	
1.01702000			
H(PDBName=H13B,ResName=UNK,ResNum=1)	0.95036600	2.82204800	
1.06327000			
C(PDBName=C14,ResName=UNK,ResNum=1)	1.71466400	3.33833000	-
0.89185400			
H(PDBName=H14A,ResName=UNK,ResNum=1)	1.56449800	4.41381200	-
0.76229500			
H(PDBName=H14B,ResName=UNK,ResNum=1)	0.85351600	2.93864700	-
1.43127200			
H(PDBName=H14C,ResName=UNK,ResNum=1)	2.61544300	3.19214600	-
1.49046900			
C(PDBName=C15,ResName=UNK,ResNum=1)	0.87400800	0.44008200	
0.35964000			
H(PDBName=H2A,ResName=UNK,ResNum=1)	-1.52442900	-0.46598000	
0.35225100			

1 38 1.0

2 9 1.0 15 1.0

3 30 2.0

4 46 2.0

5 12 1.0 18 1.0 21 1.0

6 24 1.0 27 2.0 47 1.0

7 30 1.0 31 1.0 38 1.0

8 38 1.0 39 1.0 46 1.0

9 10 1.0 11 1.0 12 1.0

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12 13 1.0 14 1.0

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15 16 1.0 17 1.0 18 1.0

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21 22 1.0 23 1.0 24 1.0

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27 28 1.0 29 1.5

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29 30 1.0 46 1.5

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31 32 1.0 33 1.0 34 1.0

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34 35 1.0 36 1.0 37 1.0

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39 40 1.0 41 1.0 42 1.0

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42 43 1.0 44 1.0 45 1.0

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B3. Optimized geometry co-ordinates of crystal 3.

0 1

S(PDBName=S1,ResName=UNK,ResNum=1) -4.50204200 0.41287600

0.04698200

N(PDBName=N1,ResName=UNK,ResNum=1) 4.04871100 -1.12786600 -

0.14907400

C(PDBName=C1,ResName=UNK,ResNum=1) 5.36375800 -1.36161100 -

0.17029700

H(PDBName=H1,ResName=UNK,ResNum=1) 5.65708000 -2.39550800 -

0.32492500

O(PDBName=O1,ResName=UNK,ResNum=1) -0.57644400 -2.58178200 -

0.42067400

O(PDBName=O2,ResName=UNK,ResNum=1) 0.18117500 2.01206800

0.30959400

H(PDBName=H2A,ResName=UNK,ResNum=1) 1.91033400 1.31649400

0.20462200

N(PDBName=N2,ResName=UNK,ResNum=1) 2.26115300 0.36628900

0.06054500

C(PDBName=C2,ResName=UNK,ResNum=1) 6.32381400 -0.36751500 -

0.00782100

H(PDBName=H2,ResName=UNK,ResNum=1) 7.37799100 -0.61238200 -

0.03320200

N(PDBName=N3,ResName=UNK,ResNum=1) -2.32645100 -1.12162000 -

0.22692400

C(PDBName=C3,ResName=UNK,ResNum=1) 5.88447200 0.94211900

0.18696900

H(PDBName=H3,ResName=UNK,ResNum=1) 0.31821500	6.59475600	1.75023700	
C(PDBName=C4,ResName=UNK,ResNum=1) 0.21146900	4.52256800	1.20413200	
H(PDBName=H4,ResName=UNK,ResNum=1) 0.36006600	4.14182600	2.20777600	
N(PDBName=N4,ResName=UNK,ResNum=1) 0.20692000	-1.94309700	1.17824800	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.03764000	3.64590800	0.12507900	
C(PDBName=C10,ResName=UNK,ResNum=1) 0.15882500	-0.55231400	1.02708400	
C(PDBName=C9,ResName=UNK,ResNum=1) 0.00671500	-2.85042500	0.13963700	
C(PDBName=C8,ResName=UNK,ResNum=1) 0.24611000	-0.94693500	-1.43208400	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.05780900	-0.04375200	-0.30639500	-
C(PDBName=C6,ResName=UNK,ResNum=1) 0.08988200	1.31314300	-0.56474300	-
H(PDBName=H6,ResName=UNK,ResNum=1) 0.24446300	1.65333600	-1.58151200	-
C(PDBName=C11,ResName=UNK,ResNum=1) 0.46732100	-2.43133100	2.55611900	
H(PDBName=H11A,ResName=UNK,ResNum=1) 1.10326900	-1.68369900	3.02486600	
H(PDBName=H11B,ResName=UNK,ResNum=1) 1.01286100	-3.36613100	2.46272400	
C(PDBName=C12,ResName=UNK,ResNum=1) 0.81332800	-2.62493300	3.36375100	-
H(PDBName=H12A,ResName=UNK,ResNum=1) 1.35787500	-1.68410000	3.46669800	-
H(PDBName=H12B,ResName=UNK,ResNum=1) 0.55854800	-2.98017000	4.36611400	-
H(PDBName=H12C,ResName=UNK,ResNum=1) 1.46185400	-3.36794200	2.89642500	-
C(PDBName=C13,ResName=UNK,ResNum=1) 0.45146100	-3.23370000	-2.27505200	-

H(PDBName=H13A,ResName=UNK,ResNum=1)	-2.69952800	-2.94996700	-
1.11653600			
H(PDBName=H13B,ResName=UNK,ResNum=1)	-4.11833500	-1.89258900	-
0.95280000			
C(PDBName=C14,ResName=UNK,ResNum=1)	-3.60501600	-2.99019700	
0.84495400			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-4.26370500	-3.83292000	
0.61742600			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-4.13520000	-2.32070700	
1.52472900			
H(PDBName=H14C,ResName=UNK,ResNum=1)	-2.71543400	-3.38135300	
1.34255700			

1 19 1.0

2 3 1.5 17 1.5

3 4 1.0 9 1.5

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5 20 2.0

6 18 2.0

7 8 1.0

8 17 1.0 22 1.5

9 10 1.0 12 1.5

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11 19 1.0 20 1.0 31 1.0

12 13 1.0 14 1.5

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14 15 1.0 17 1.5

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16 18 1.0 19 1.0 24 1.0

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18 21 1.5

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21 22 2.0

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 31 32 1.0 33 1.0 34 1.0
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 34 35 1.0 36 1.0 37 1.0
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B4. Optimized geometry co-ordinates of transition state (TS) for crystal **1**.

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C	-0.52332800	0.90825000	-0.16958100
C	-0.30778200	-0.52324200	-0.29840400
C	-1.43152600	-1.39276800	-0.60045900
C	-2.92613600	0.41950500	0.17417900
S	-4.45051900	0.92714600	0.65319900
O	0.36265400	1.74226100	-0.28482600
O	-1.30418500	-2.51517700	-1.07067100
N	-1.84034800	1.28607000	0.17546200
N	-2.70256300	-0.88018100	-0.26371300
C	-2.02644100	2.71940400	0.50602600
H	-1.07825100	3.05680000	0.91981300
H	-2.79823900	2.77393000	1.26936900
C	-2.40264900	3.56056300	-0.71147900
H	-1.62002700	3.51622900	-1.47144300
H	-3.34642800	3.22307800	-1.14374800
H	-2.52364400	4.60452200	-0.40865900
C	-3.83338600	-1.82771500	-0.41413600
H	-4.71164400	-1.24024500	-0.66778100
H	-3.57195300	-2.47357800	-1.24990200
C	-4.07691200	-2.65740000	0.84415700
H	-3.19837500	-3.25651100	1.09414900
H	-4.33057800	-2.01799900	1.69147700
H	-4.91282500	-3.34126200	0.67195400

C	1.02609900	-0.97472500	-0.78269000
H	1.43550200	-0.97547100	-1.78877800
C	3.01329000	-1.91607800	0.31631900
H	3.15982300	-2.60475900	-0.51964800
N	1.63902100	-1.38872000	0.26339500
C	4.03752100	-0.80077900	0.23728000
C	4.81255700	-0.43900600	1.33853200
C	5.00099100	0.81450900	-1.07144900
C	5.72342400	0.60576800	1.19845000
H	4.70324100	-0.95957500	2.28274300
C	5.82130700	1.24838200	-0.03023800
H	5.04622300	1.29210900	-2.04560900
H	6.34002300	0.91268600	2.03556100
H	6.51161300	2.06866200	-0.18463300
N	4.13001500	-0.18786200	-0.94798500
H	3.11093000	-2.47177800	1.24842500
H	0.50010300	-1.03099900	0.85033100

1 2 1.0 6 2.0 8 1.0

2 3 1.0 24 1.0

3 7 2.0 9 1.0

4 5 1.0 8 1.0 9 1.0

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8 10 1.0

9 17 1.0

10 11 1.0 12 1.0 13 1.0

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20 21 1.0 22 1.0 23 1.0

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 24 25 1.0 28 2.0
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 26 27 1.0 28 1.0 29 1.0 39 1.0
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 29 30 1.5 38 1.5
 30 32 1.5 33 1.0
 31 34 1.5 35 1.0 38 1.5
 32 34 1.5 36 1.0
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 34 37 1.0
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B5. Optimized geometry co-ordinates of transition state (TS) for crystal 2.

0 1

C	1.78068200	-1.26892100	-0.08143200
C	1.09238100	0.01048600	-0.08433400
C	1.82641400	1.21740400	-0.42291800
C	3.90758700	-0.01796200	0.08892400
C	-0.35603300	-0.00604100	-0.42646200
H	-0.81769100	-0.11901500	-1.40308100
N	-0.97233800	0.14334400	0.68564200
H	0.27527500	0.18257800	1.15331100
N	3.17441500	-1.19885700	0.12256900
N	3.22280800	1.14794800	-0.23381100
C	3.85557800	-2.49823800	0.34014500
H	3.11831300	-3.14742700	0.80838600
H	4.67393500	-2.31699200	1.03238000
C	4.36403800	-3.12327500	-0.95650500
H	5.09503900	-2.47564400	-1.44386300

H	4.85253900	-4.07588500	-0.73293900
H	3.53844600	-3.31870300	-1.64371200
C	3.95571400	2.42532900	-0.41199800
H	4.94565100	2.17789200	-0.78554000
H	3.40774100	2.97982700	-1.17109400
C	4.04552100	3.23603900	0.87837300
H	4.58574700	4.16702000	0.68503000
H	3.05074500	3.49502900	1.24788200
H	4.58487800	2.68453100	1.65030300
S	5.55476800	-0.00466500	0.39477900
O	1.20753600	-2.34474600	-0.18550200
O	1.28607500	2.24724700	-0.80368700
C	-2.40921700	0.20531300	0.94775100
H	-2.59736400	1.13448000	1.49158700
H	-2.63214000	-0.61352500	1.63690200
C	-3.30266500	0.14938300	-0.29585300
H	-3.08754900	-0.76166600	-0.88193100
H	-3.06606900	1.00650500	-0.93303500
C	-5.54423200	0.78553800	-1.00253900
C	-5.26504100	-1.04987800	0.52437000
C	-6.98610600	0.92114400	-0.52622800
H	-5.15949300	1.77229500	-1.27675700
C	-6.71669000	-0.87337000	0.95791200
H	-5.21518500	-1.80748900	-0.27901000
H	-7.62954700	1.25892000	-1.34021300
H	-6.76428300	-0.21794100	1.83972100
O	-7.50683900	-0.32948700	-0.09155000
N	-4.71287200	0.23219900	0.07222200
H	-5.51993100	0.14660100	-1.90405800
H	-7.03672000	1.65182000	0.29392500
H	-7.15953700	-1.83781000	1.21176300
H	-4.68492800	-1.42501000	1.37190200

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B6. Optimized geometry co-ordinates of transition state (TS) for crystal 3.

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C	-0.70928000	1.10658800	-0.71278400
C	-0.00912800	-0.11116200	-0.34403100
C	-0.76171300	-1.33298400	-0.12237700
C	-2.77682900	0.07113500	0.16969300
C	1.38003400	-0.26182100	-0.85739600
H	1.74151600	-0.51786500	-1.84788800
N	2.13773300	-0.01482100	0.15390300
H	0.98460400	0.15201600	0.76276200
N	-2.07336900	1.15029300	-0.35101800
N	-2.11410400	-1.14887100	0.23492400
C	-2.74745100	2.45417000	-0.56460200
H	-3.79010900	2.24345100	-0.78673500
H	-2.27067700	2.89691800	-1.43671700
C	-2.62225400	3.38343400	0.64015500
H	-1.57431800	3.60192100	0.85787000
H	-3.12526600	4.32983300	0.42268800
H	-3.09063600	2.94487300	1.52300300
C	-2.83519100	-2.37275500	0.66056200
H	-2.08326200	-3.02494100	1.10041200
H	-3.54979600	-2.07300500	1.42290800
C	-3.53490400	-3.07845800	-0.49852800
H	-4.04331000	-3.97202400	-0.12554200
H	-4.28396900	-2.43067400	-0.95743200
H	-2.81321600	-3.39021600	-1.25612700
S	-4.36833800	0.22816400	0.67124300
O	-0.16499400	2.05860000	-1.25478600
O	-0.26628000	-2.45002800	-0.17785200
C	3.55884400	-0.01570700	0.18810300
C	4.18605000	0.28445300	1.39617800
C	5.57693800	0.28099900	1.42045100
H	3.59626000	0.50992000	2.27543000

C	5.53661300	-0.30483000	-0.90171000
C	6.26939200	-0.01892300	0.25118800
H	6.10847800	0.50850900	2.33692500
H	6.04039700	-0.54347000	-1.83323600
H	7.35190700	-0.03270600	0.22575100
N	4.20378000	-0.30468700	-0.93956000

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B7. Geometry co-ordinates for NLO properties for crystal 1 (Gaseous).

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S(PDBName=S1,ResName=UNK,ResNum=1)	4.59114300	1.01387300	
0.46019700			
N(PDBName=N1,ResName=UNK,ResNum=1)	-4.42262600	0.79616700	-
0.56236200			
N(PDBName=N2,ResName=UNK,ResNum=1)	-1.85766000	-0.53433300	-
0.99065500			
N(PDBName=N3,ResName=UNK,ResNum=1)	2.03286700	1.20630800	-
0.30180700			
N(PDBName=N4,ResName=UNK,ResNum=1)	2.76817600	-0.94546200	
0.36530700			
O(PDBName=O1,ResName=UNK,ResNum=1)	-0.14231400	1.55316900	-
0.92452300			
O(PDBName=O2,ResName=UNK,ResNum=1)	1.35129100	-2.74228300	
0.29222700			
C(PDBName=C1,ResName=UNK,ResNum=1)	-5.35319200	1.41789400	
0.16389000			
H(PDBName=H1B,ResName=UNK,ResNum=1)	-5.47212000	2.48137800	-
0.02130800			
C(PDBName=C2,ResName=UNK,ResNum=1)	-6.14668200	0.76882400	
1.10930000			
H(PDBName=H2B,ResName=UNK,ResNum=1)	-6.89171600	1.32076200	
1.66935500			
C(PDBName=C3,ResName=UNK,ResNum=1)	-5.95274200	-0.59330900	
1.30976000			
H(PDBName=H3A,ResName=UNK,ResNum=1)	-6.54589200	-1.13660900	
2.03658000			
C(PDBName=C4,ResName=UNK,ResNum=1)	-4.97671800	-1.24960000	
0.56315500			

H(PDBName=H4A,ResName=UNK,ResNum=1) 0.69927200	-4.79218700	-2.30900600	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.36257800	-4.23688600	-0.51403100	-
C(PDBName=C6,ResName=UNK,ResNum=1) 1.21771900	-3.15949300	-1.15230500	-
H(PDBName=H6A,ResName=UNK,ResNum=1) 1.00797400	-3.07639400	-2.21970600	-
H(PDBName=H6B,ResName=UNK,ResNum=1) 2.27236500	-3.42882100	-1.03299000	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.57961900	-0.78476100	-1.18933300	-
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.41493300	-0.88902200	-2.25800900	-
C(PDBName=C8,ResName=UNK,ResNum=1) 0.34178700	0.46946500	-0.64295500	-
C(PDBName=C9,ResName=UNK,ResNum=1) 0.54556800	0.72281100	0.75775100	-
C(PDBName=C10,ResName=UNK,ResNum=1) 0.16134100	3.06147400	0.39469600	
C(PDBName=C11,ResName=UNK,ResNum=1) 0.11451500	1.51087000	-1.54149700	
C(PDBName=C12,ResName=UNK,ResNum=1) 0.85913600	3.81815400	-1.86991900	
H(PDBName=H12A,ResName=UNK,ResNum=1) 1.43694400	3.29874600	-2.63120000	
H(PDBName=H12B,ResName=UNK,ResNum=1) 1.51261800	4.46844000	-1.29492800	
C(PDBName=C13,ResName=UNK,ResNum=1) 0.27366100	4.61347900	-2.51411700	-
H(PDBName=H13A,ResName=UNK,ResNum=1) 0.14794600	5.36325600	-3.18953000	
H(PDBName=H13B,ResName=UNK,ResNum=1) 0.86595900	5.13352500	-1.75909500	-
H(PDBName=H13C,ResName=UNK,ResNum=1) 0.92508000	3.96024500	-3.09822300	-
C(PDBName=C14,ResName=UNK,ResNum=1) 0.54977800	2.27134200	2.64954800	-

H(PDBName=H14A,ResName=UNK,ResNum=1) 1.36243300	1.60405600	2.92824500	-
H(PDBName=H14B,ResName=UNK,ResNum=1) 0.87396400	3.30350100	2.74997500	-
C(PDBName=C15,ResName=UNK,ResNum=1) 0.68080300	1.99933500	3.51102700	
H(PDBName=H15A,ResName=UNK,ResNum=1) 0.43574300	2.18272500	4.56096900	
H(PDBName=H15B,ResName=UNK,ResNum=1) 1.50501200	2.65963900	3.23560200	
H(PDBName=H15C,ResName=UNK,ResNum=1) 1.00232300	0.96024200	3.41530500	
H(PDBName=H2A,ResName=UNK,ResNum=1) 1.12709200	-1.75237100	0.47318900	-

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B8. Geometry co-ordinates for NLO properties for crystal **1** (ACN).

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S(PDBName=S1,ResName=UNK,ResNum=1)	4.61894800	1.12769000	
0.28424800			
N(PDBName=N1,ResName=UNK,ResNum=1)	-4.20658400	0.73481200	-
0.44080900			
N(PDBName=N2,ResName=UNK,ResNum=1)	-1.85217000	-0.72309400	-
0.68715100			
N(PDBName=N3,ResName=UNK,ResNum=1)	2.00191000	1.19870500	-
0.28534200			
N(PDBName=N4,ResName=UNK,ResNum=1)	2.87104300	-0.90456200	
0.34831800			
O(PDBName=O1,ResName=UNK,ResNum=1)	-0.22401900	1.44903600	-
0.75721900			
O(PDBName=O2,ResName=UNK,ResNum=1)	1.53299000	-2.76015000	
0.41268600			
C(PDBName=C1,ResName=UNK,ResNum=1)	-5.20189700	1.48463600	
0.04655200			
H(PDBName=H1B,ResName=UNK,ResNum=1)	-5.12030800	2.55500700	-
0.11592400			

C(PDBName=C2,ResName=UNK,ResNum=1) 0.72597800	-6.29573300	0.95391400	
H(PDBName=H2B,ResName=UNK,ResNum=1) 1.09768700	-7.07635400	1.60588500	
C(PDBName=C3,ResName=UNK,ResNum=1) 0.91393100	-6.35071400	-0.42432600	
H(PDBName=H3A,ResName=UNK,ResNum=1) 1.44262500	-7.18067000	-0.87835700	
C(PDBName=C4,ResName=UNK,ResNum=1) 0.41824800	-5.31572000	-1.21292200	
H(PDBName=H4A,ResName=UNK,ResNum=1) 0.55335200	-5.32071900	-2.28793300	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.25590600	-4.26531400	-0.59001100	-
C(PDBName=C6,ResName=UNK,ResNum=1) 0.86290200	-3.13474500	-1.39748600	-
H(PDBName=H6A,ResName=UNK,ResNum=1) 0.41624900	-3.07924400	-2.38976500	-
H(PDBName=H6B,ResName=UNK,ResNum=1) 1.93533900	-3.32391500	-1.52375300	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.34298900	-0.73542500	-1.32257300	-
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.15810100	-0.78846000	-2.39050200	-
C(PDBName=C8,ResName=UNK,ResNum=1) 0.19483100	0.51565100	-0.71387500	-
C(PDBName=C9,ResName=UNK,ResNum=1) 0.43120800	0.69485700	0.68811800	-
C(PDBName=C10,ResName=UNK,ResNum=1) 0.10675600	3.08630200	0.43784300	
C(PDBName=C11,ResName=UNK,ResNum=1) 0.20012400	1.62021500	-1.55290700	
C(PDBName=C12,ResName=UNK,ResNum=1) 0.77683900	3.99175500	-1.77873500	
H(PDBName=H12A,ResName=UNK,ResNum=1) 1.41544500	3.55219400	-2.54075700	
H(PDBName=H12B,ResName=UNK,ResNum=1) 1.36547400	4.66815100	-1.16644400	

C(PDBName=C13,ResName=UNK,ResNum=1)	4.71976500	-2.42297700	-
0.40010900			
H(PDBName=H13A,ResName=UNK,ResNum=1)	5.52203000	-3.06240400	-
0.02214100			
H(PDBName=H13B,ResName=UNK,ResNum=1)	5.16478700	-1.66676500	-
1.04941400			
H(PDBName=H13C,ResName=UNK,ResNum=1)	4.04120200	-3.04215300	-
0.99023700			
C(PDBName=C14,ResName=UNK,ResNum=1)	2.15874000	2.64746100	-
0.56970600			
H(PDBName=H14A,ResName=UNK,ResNum=1)	1.43481700	2.88277300	-
1.34586200			
H(PDBName=H14B,ResName=UNK,ResNum=1)	3.16092300	2.78803800	-
0.96333700			
C(PDBName=C15,ResName=UNK,ResNum=1)	1.92537300	3.51951200	
0.66105100			
H(PDBName=H15A,ResName=UNK,ResNum=1)	2.04524900	4.57079900	
0.38587500			
H(PDBName=H15B,ResName=UNK,ResNum=1)	2.64506900	3.29008100	
1.44904100			
H(PDBName=H15C,ResName=UNK,ResNum=1)	0.91542000	3.38404800	
1.05302800			
H(PDBName=H2A,ResName=UNK,ResNum=1)	-1.81316200	0.28300900	-
0.85370800			

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B9. Geometry co-ordinates for NLO properties for crystal **1** (CHCl₃).

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S(PDBName=S1,ResName=UNK,ResNum=1)	4.61112200	1.11161700	
0.32681700			
N(PDBName=N1,ResName=UNK,ResNum=1)	-4.26332600	0.73432800	-
0.51196900			
N(PDBName=N2,ResName=UNK,ResNum=1)	-1.85428900	-0.69442000	-
0.75063700			
N(PDBName=N3,ResName=UNK,ResNum=1)	2.00580700	1.20163200	-
0.28760800			

N(PDBName=N4,ResName=UNK,ResNum=1)	2.85292500	-0.91125200	
0.35192400			
O(PDBName=O1,ResName=UNK,ResNum=1)	-0.20954400	1.46416800	-
0.80117600			
O(PDBName=O2,ResName=UNK,ResNum=1)	1.50140600	-2.75809200	
0.38835800			
C(PDBName=C1,ResName=UNK,ResNum=1)	-5.24543900	1.46743200	
0.02135000			
H(PDBName=H1B,ResName=UNK,ResNum=1)	-5.21360400	2.53315200	-
0.18367600			
C(PDBName=C2,ResName=UNK,ResNum=1)	-6.26805100	0.92575200	
0.79772400			
H(PDBName=H2B,ResName=UNK,ResNum=1)	-7.04258500	1.56471300	
1.20345500			
C(PDBName=C3,ResName=UNK,ResNum=1)	-6.26033700	-0.44500600	
1.03613500			
H(PDBName=H3A,ResName=UNK,ResNum=1)	-7.03330300	-0.90664400	
1.63956000			
C(PDBName=C4,ResName=UNK,ResNum=1)	-5.23575600	-1.21656300	
0.49285900			
H(PDBName=H4A,ResName=UNK,ResNum=1)	-5.19243500	-2.28531800	
0.66631200			
C(PDBName=C5,ResName=UNK,ResNum=1)	-4.26058900	-0.58381200	-
0.27765400			
C(PDBName=C6,ResName=UNK,ResNum=1)	-3.13848800	-1.36460600	-
0.93296200			
H(PDBName=H6A,ResName=UNK,ResNum=1)	-3.07201100	-2.37265100	-
0.52378500			
H(PDBName=H6B,ResName=UNK,ResNum=1)	-3.34443400	-1.45007800	-
2.00619600			
C(PDBName=C7,ResName=UNK,ResNum=1)	-0.74302800	-1.30065900	-
0.39188500			
H(PDBName=H7A,ResName=UNK,ResNum=1)	-0.80382600	-2.36854900	-
0.20743200			
C(PDBName=C8,ResName=UNK,ResNum=1)	0.50782300	-0.70261700	-
0.22707400			
C(PDBName=C9,ResName=UNK,ResNum=1)	0.69954500	0.70004600	-
0.45922000			

C(PDBName=C10,ResName=UNK,ResNum=1)	3.08159000	0.43285300	
0.12041100			
C(PDBName=C11,ResName=UNK,ResNum=1)	1.60180000	-1.55185400	
0.18247200			
C(PDBName=C12,ResName=UNK,ResNum=1)	3.96276600	-1.79350500	
0.79123000			
H(PDBName=H12A,ResName=UNK,ResNum=1)	3.50830700	-2.56188300	
1.41176700			
H(PDBName=H12B,ResName=UNK,ResNum=1)	4.63083000	-1.18920200	
1.39773300			
C(PDBName=C13,ResName=UNK,ResNum=1)	4.70953100	-2.42674100	-
0.37990200			
H(PDBName=H13A,ResName=UNK,ResNum=1)	5.50344100	-3.07294000	
0.00440600			
H(PDBName=H13B,ResName=UNK,ResNum=1)	5.16861400	-1.66420000	-
1.01166600			
H(PDBName=H13C,ResName=UNK,ResNum=1)	4.03899500	-3.03791800	-
0.98742900			
C(PDBName=C14,ResName=UNK,ResNum=1)	2.17568500	2.65101300	-
0.55970100			
H(PDBName=H14A,ResName=UNK,ResNum=1)	1.46302500	2.89589400	-
1.34348200			
H(PDBName=H14B,ResName=UNK,ResNum=1)	3.18501000	2.78796600	-
0.93653000			
C(PDBName=C15,ResName=UNK,ResNum=1)	1.92958400	3.51529300	
0.67415100			
H(PDBName=H15A,ResName=UNK,ResNum=1)	2.05945200	4.56806300	
0.40898700			
H(PDBName=H15B,ResName=UNK,ResNum=1)	2.63747100	3.27602600	
1.46981400			
H(PDBName=H15C,ResName=UNK,ResNum=1)	0.91270300	3.38309600	
1.04907000			
H(PDBName=H2A,ResName=UNK,ResNum=1)	-1.80612600	0.31182600	-
0.91700700			
1 24 1.0			
2 8 1.5 16 1.5			
3 17 1.0 20 2.0 40 1.0			

4 23 1.0 24 1.0 33 1.0

5 24 1.0 25 1.0 26 1.0

6 23 2.0

7 25 2.0

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B10. Geometry co-ordinates for NLO properties for crystal **1** (MeOH).

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S(PDBName=S1,ResName=UNK,ResNum=1)	4.61011000	1.22370900	
0.14491900			
N(PDBName=N1,ResName=UNK,ResNum=1)	-4.05968000	0.66360500	-
0.29918900			
N(PDBName=N2,ResName=UNK,ResNum=1)	-1.84973600	-0.85632800	-
0.41724200			
N(PDBName=N3,ResName=UNK,ResNum=1)	1.95726500	1.19763900	-
0.26894300			
N(PDBName=N4,ResName=UNK,ResNum=1)	2.93680200	-0.87028200	
0.31428100			
O(PDBName=O1,ResName=UNK,ResNum=1)	-0.30721100	1.37922700	-
0.58366000			
O(PDBName=O2,ResName=UNK,ResNum=1)	1.67484100	-2.78259900	
0.43513600			
C(PDBName=C1,ResName=UNK,ResNum=1)	-5.06931600	1.50142700	-
0.02174600			
H(PDBName=H1B,ResName=UNK,ResNum=1)	-4.85886800	2.56145900	-
0.14697400			
C(PDBName=C2,ResName=UNK,ResNum=1)	-6.32524900	1.07272300	
0.40335500			
H(PDBName=H2B,ResName=UNK,ResNum=1)	-7.10859800	1.79356300	
0.61359200			
C(PDBName=C3,ResName=UNK,ResNum=1)	-6.53896100	-0.29835000	
0.55433300			
H(PDBName=H3A,ResName=UNK,ResNum=1)	-7.50028400	-0.67614800	
0.88989900			
C(PDBName=C4,ResName=UNK,ResNum=1)	-5.49521700	-1.17822600	
0.27550600			
H(PDBName=H4A,ResName=UNK,ResNum=1)	-5.62198200	-2.25081800	
0.38770000			
C(PDBName=C5,ResName=UNK,ResNum=1)	-4.27299100	-0.65061400	-
0.15112700			
C(PDBName=C6,ResName=UNK,ResNum=1)	-3.11843800	-1.56631800	-
0.52021600			
H(PDBName=H6A,ResName=UNK,ResNum=1)	-3.09743800	-2.44796000	
0.12641900			

H(PDBName=H6B,ResName=UNK,ResNum=1)	-3.25485800	-1.92134600	-
1.55165100			
C(PDBName=C7,ResName=UNK,ResNum=1)	-0.69018100	-1.42176300	-
0.15851300			
H(PDBName=H7A,ResName=UNK,ResNum=1)	-0.69103700	-2.49458200	
0.01630900			
C(PDBName=C8,ResName=UNK,ResNum=1)	0.54510600	-0.76691200	-
0.08746500			
C(PDBName=C9,ResName=UNK,ResNum=1)	0.65639700	0.64328900	-
0.32627400			
C(PDBName=C10,ResName=UNK,ResNum=1)	3.09017000	0.47737500	
0.05909600			
C(PDBName=C11,ResName=UNK,ResNum=1)	1.70179400	-1.56826200	
0.23104900			
C(PDBName=C12,ResName=UNK,ResNum=1)	4.10439200	-1.71035900	
0.67693200			
H(PDBName=H12A,ResName=UNK,ResNum=1)	3.71910100	-2.48593100	
1.33729300			
H(PDBName=H12B,ResName=UNK,ResNum=1)	4.79820500	-1.08049100	
1.22960400			
C(PDBName=C13,ResName=UNK,ResNum=1)	4.77715200	-2.33570100	-
0.54352600			
H(PDBName=H13A,ResName=UNK,ResNum=1)	5.62102400	-2.95371500	-
0.21723400			
H(PDBName=H13B,ResName=UNK,ResNum=1)	5.15806500	-1.56643900	-
1.22166800			
H(PDBName=H13C,ResName=UNK,ResNum=1)	4.07585600	-2.97466200	-
1.08845500			
C(PDBName=C14,ResName=UNK,ResNum=1)	2.03642300	2.65035000	-
0.56089500			
H(PDBName=H14A,ResName=UNK,ResNum=1)	1.25492100	2.85103700	-
1.29250100			
H(PDBName=H14B,ResName=UNK,ResNum=1)	3.00741100	2.83540600	-
1.01511800			
C(PDBName=C15,ResName=UNK,ResNum=1)	1.83512200	3.51047200	
0.68498000			
H(PDBName=H15A,ResName=UNK,ResNum=1)	1.89458000	4.56917400	
0.40914800			

H(PDBName=H15B,ResName=UNK,ResNum=1)	2.60693900	3.30772000	
1.43326800			
H(PDBName=H15C,ResName=UNK,ResNum=1)	0.85226100	3.32780600	
1.12961500			
H(PDBName=H2A,ResName=UNK,ResNum=1)	-1.86786300	0.15632400	-
0.56504900			

1 24 1.0

2 8 1.5 16 1.5

3 17 1.0 20 2.0 40 1.0

4 23 1.0 24 1.0 33 1.0

5 24 1.5 25 1.0 26 1.0

6 23 2.0

7 25 2.0

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B11. Geometry co-ordinates for NLO properties for crystal 2 (Gaseous).

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S(PDBName=S1,ResName=UNK,ResNum=1)	-4.68442600	1.66922500	-
0.26507200			
O(PDBName=O1,ResName=UNK,ResNum=1)	5.87675600	1.58284500	-
0.09989600			
O(PDBName=O2,ResName=UNK,ResNum=1)	-2.53628300	-2.80078400	-
0.08399100			
O(PDBName=O3,ResName=UNK,ResNum=1)	0.22837200	0.99584300	-
0.41844200			
N(PDBName=N1,ResName=UNK,ResNum=1)	4.02995500	-0.55267300	
0.29647500			
N(PDBName=N2,ResName=UNK,ResNum=1)	1.33587100	-1.46888700	-
0.28591500			
N(PDBName=N3,ResName=UNK,ResNum=1)	-3.44100000	-0.70193300	-
0.21406300			
N(PDBName=N4,ResName=UNK,ResNum=1)	-2.05033200	1.20918200	-
0.38276000			
C(PDBName=C1,ResName=UNK,ResNum=1)	5.38084400	0.83816600	-
1.20480000			
H(PDBName=H1A,ResName=UNK,ResNum=1)	6.17584400	0.82547200	-
1.95227400			
H(PDBName=H1B,ResName=UNK,ResNum=1)	4.50050100	1.34086200	-
1.63034800			
C(PDBName=C2,ResName=UNK,ResNum=1)	5.01139900	-0.58332200	-
0.79255000			
H(PDBName=H2B,ResName=UNK,ResNum=1)	4.58959100	-1.10564500	-
1.65610100			

H(PDBName=H2C,ResName=UNK,ResNum=1) 0.48581600	5.92563000	-1.12395100	-
C(PDBName=C3,ResName=UNK,ResNum=1) 0.95336800	4.91974900	1.63095100	
H(PDBName=H3A,ResName=UNK,ResNum=1) 0.61451100	4.01732100	2.15884000	
H(PDBName=H3B,ResName=UNK,ResNum=1) 1.76352300	5.37975300	2.19900100	
C(PDBName=C4,ResName=UNK,ResNum=1) 1.42414700	4.54641100	0.22964600	
H(PDBName=H4A,ResName=UNK,ResNum=1) 1.87762100	5.43341600	-0.24878900	
H(PDBName=H4B,ResName=UNK,ResNum=1) 2.19142300	3.76995600	0.30023900	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.68300100	3.55479700	-1.87789400	
H(PDBName=H5A,ResName=UNK,ResNum=1) 1.68787800	3.12938700	-1.80914200	
H(PDBName=H5B,ResName=UNK,ResNum=1) 0.72450300	4.37101400	-2.62046100	
C(PDBName=C6,ResName=UNK,ResNum=1) 0.26792500	2.46713400	-2.38595600	-
H(PDBName=H6A,ResName=UNK,ResNum=1) 1.28236300	2.86644100	-2.49440300	-
H(PDBName=H6B,ResName=UNK,ResNum=1) 0.05230600	2.11967100	-3.37101300	
C(PDBName=C7,ResName=UNK,ResNum=1) 0.23117000	0.06684900	-1.83421700	-
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.15626300	-0.14126400	-2.89793000	-
C(PDBName=C8,ResName=UNK,ResNum=1) 0.26018700	-1.03317500	-0.98535800	-
C(PDBName=C9,ResName=UNK,ResNum=1) 0.17932500	-2.34540200	-1.59530900	-
C(PDBName=C10,ResName=UNK,ResNum=1) 0.12764200	-4.77825800	-1.33933100	-
H(PDBName=H10A,ResName=UNK,ResNum=1) 0.61709000	-4.68036000	-2.30580600	-

H(PDBName=H10B,ResName=UNK,ResNum=1) 0.68845400	-5.46729200	-0.71409800	-
C(PDBName=C11,ResName=UNK,ResNum=1) 1.31283200	-5.25091200	-1.51907600	
H(PDBName=H11A,ResName=UNK,ResNum=1) 1.31479300	-6.23334900	-1.99950300	
H(PDBName=H11B,ResName=UNK,ResNum=1) 1.81778200	-5.34454000	-0.55600600	
H(PDBName=H11C,ResName=UNK,ResNum=1) 1.87185100	-4.56219000	-2.15572100	
C(PDBName=C12,ResName=UNK,ResNum=1) 0.28809300	-3.33177300	0.67824000	-
C(PDBName=C13,ResName=UNK,ResNum=1) 0.47692200	-1.85439000	2.67671000	-
H(PDBName=H13A,ResName=UNK,ResNum=1) 1.01697100	-2.70710200	3.07835700	-
H(PDBName=H13B,ResName=UNK,ResNum=1) 1.06310200	-0.94973000	2.82184800	-
C(PDBName=C14,ResName=UNK,ResNum=1) 0.89194900	-1.71412300	3.33831900	
H(PDBName=H14A,ResName=UNK,ResNum=1) 0.76232100	-1.56389100	4.41378600	
H(PDBName=H14B,ResName=UNK,ResNum=1) 1.43144500	-0.85303800	2.93860200	
H(PDBName=H14C,ResName=UNK,ResNum=1) 1.49049400	-2.61497300	3.19222500	
C(PDBName=C15,ResName=UNK,ResNum=1) 0.35934200	-0.87364900	0.43993900	-
H(PDBName=H2A,ResName=UNK,ResNum=1) 0.35209500	1.52480900	-0.46646800	-

1 38 1.0

2 9 1.0 15 1.0

3 30 2.0

4 46 2.0

5 12 1.0 18 1.0 21 1.0

6 24 1.0 27 2.0 47 1.0

7 30 1.0 31 1.0 38 1.0

8 38 1.0 39 1.0 46 1.0

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B12. Geometry co-ordinates for NLO properties for crystal 2 (ACN).

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S(PDBName=S1,ResName=UNK,ResNum=1)	-4.72444800	1.65198200	-
0.23561900			
O(PDBName=O1,ResName=UNK,ResNum=1)	5.94023100	1.56548000	
0.00733500			
O(PDBName=O2,ResName=UNK,ResNum=1)	-2.52795200	-2.79776500	-
0.05531000			
O(PDBName=O3,ResName=UNK,ResNum=1)	0.19289500	1.01920700	-
0.50167100			
N(PDBName=N1,ResName=UNK,ResNum=1)	4.02318800	-0.54060800	
0.28635300			
N(PDBName=N2,ResName=UNK,ResNum=1)	1.32964300	-1.44879600	-
0.38257900			
N(PDBName=N3,ResName=UNK,ResNum=1)	-3.44900900	-0.70574500	-
0.17598600			
N(PDBName=N4,ResName=UNK,ResNum=1)	-2.08677900	1.21031500	-
0.40381800			
C(PDBName=C1,ResName=UNK,ResNum=1)	5.36911100	0.93376000	-
1.13976100			
H(PDBName=H1A,ResName=UNK,ResNum=1)	6.12916600	0.96155400	-
1.92178000			
H(PDBName=H1B,ResName=UNK,ResNum=1)	4.49296800	1.50526900	-
1.47590600			
C(PDBName=C2,ResName=UNK,ResNum=1)	4.96528300	-0.50447500	-
0.83933300			
H(PDBName=H2B,ResName=UNK,ResNum=1)	4.49827200	-0.93079000	-
1.73044300			
H(PDBName=H2C,ResName=UNK,ResNum=1)	5.86824000	-1.10055000	-
0.61632800			
C(PDBName=C3,ResName=UNK,ResNum=1)	5.02936300	1.53854800	
1.10854600			
H(PDBName=H3A,ResName=UNK,ResNum=1)	4.13771100	2.13144500	
0.86204500			

H(PDBName=H3B,ResName=UNK,ResNum=1) 1.94950300	5.54287000	2.00672700	
C(PDBName=C4,ResName=UNK,ResNum=1) 1.45613000	4.62269000	0.11239200	
H(PDBName=H4A,ResName=UNK,ResNum=1) 1.81420800	5.50906600	-0.44095100	
H(PDBName=H4B,ResName=UNK,ResNum=1) 2.26799700	3.89069000	0.13490000	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.58922500	3.54600200	-1.89071600	
H(PDBName=H5A,ResName=UNK,ResNum=1) 1.59326100	3.11446200	-1.88081700	
H(PDBName=H5B,ResName=UNK,ResNum=1) 0.59179300	4.36432300	-2.63003500	
C(PDBName=C6,ResName=UNK,ResNum=1) 0.39604700	2.47317800	-2.35785100	-
H(PDBName=H6A,ResName=UNK,ResNum=1) 1.41344300	2.87109300	-2.40688400	-
H(PDBName=H6B,ResName=UNK,ResNum=1) 0.12768000	2.12967800	-3.35779200	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.28717400	0.07442500	-1.81993500	-
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.20237000	-0.11566200	-2.88494900	-
C(PDBName=C8,ResName=UNK,ResNum=1) 0.28771500	-1.04162300	-0.97369700	-
C(PDBName=C9,ResName=UNK,ResNum=1) 0.16586700	-2.34011200	-1.58794900	-
C(PDBName=C10,ResName=UNK,ResNum=1) 0.04426000	-4.77752400	-1.35518000	-
H(PDBName=H10A,ResName=UNK,ResNum=1) 0.53301300	-4.68942800	-2.32209300	-
H(PDBName=H10B,ResName=UNK,ResNum=1) 0.59078900	-5.48899000	-0.74375900	-
C(PDBName=C11,ResName=UNK,ResNum=1) 1.41044600	-5.20662700	-1.52902700	
H(PDBName=H11A,ResName=UNK,ResNum=1) 1.44275000	-6.18103400	-2.02379500	

H(PDBName=H11B,ResName=UNK,ResNum=1)	-5.29836300	-0.56413500	
1.91251800			
H(PDBName=H11C,ResName=UNK,ResNum=1)	-4.49319100	-2.14739000	
1.95877400			
C(PDBName=C12,ResName=UNK,ResNum=1)	-3.35064300	0.66789600	-
0.27374800			
C(PDBName=C13,ResName=UNK,ResNum=1)	-1.90351400	2.67895900	-
0.52034900			
H(PDBName=H13A,ResName=UNK,ResNum=1)	-2.77406700	3.07011800	-
1.03779200			
H(PDBName=H13B,ResName=UNK,ResNum=1)	-1.02412600	2.82497700	-
1.14250100			
C(PDBName=C14,ResName=UNK,ResNum=1)	-1.71930800	3.35730000	
0.83484500			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-1.57968600	4.43127600	
0.68546400			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-0.83969000	2.96849200	
1.35152800			
H(PDBName=H14C,ResName=UNK,ResNum=1)	-2.59577900	3.21299200	
1.46932700			
C(PDBName=C15,ResName=UNK,ResNum=1)	-0.89958500	0.44672700	-
0.40464300			
H(PDBName=H2A,ResName=UNK,ResNum=1)	1.51525500	-0.44758900	-
0.44960100			

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B13. Geometry co-ordinates for NLO properties for crystal 2 (CHCl₃).

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S(PDBName=S1,ResName=UNK,ResNum=1) 0.24862200	-4.71948100	1.64865800	-
O(PDBName=O1,ResName=UNK,ResNum=1) 0.00276400	5.92876000	1.57204700	-
O(PDBName=O2,ResName=UNK,ResNum=1) 0.05438500	-2.52417100	-2.80009900	-
O(PDBName=O3,ResName=UNK,ResNum=1) 0.48619500	0.19826200	1.01710700	-
N(PDBName=N1,ResName=UNK,ResNum=1) 0.28478900	4.03029700	-0.54538000	
N(PDBName=N2,ResName=UNK,ResNum=1) 0.36531400	1.33363200	-1.44823200	-
N(PDBName=N3,ResName=UNK,ResNum=1) 0.18238500	-3.44659700	-0.70904200	-
N(PDBName=N4,ResName=UNK,ResNum=1) 0.40156700	-2.08172200	1.20928600	-
C(PDBName=C1,ResName=UNK,ResNum=1) 1.14608200	5.39617300	0.90547700	-
H(PDBName=H1A,ResName=UNK,ResNum=1) 1.90753600	6.17729600	0.92085900	-
H(PDBName=H1B,ResName=UNK,ResNum=1) 1.52158100	4.52295900	1.45684900	-
C(PDBName=C2,ResName=UNK,ResNum=1) 0.81730300	4.99940800	-0.52913900	-
H(PDBName=H2B,ResName=UNK,ResNum=1) 1.70737600	4.55854600	-0.98543700	-
H(PDBName=H2C,ResName=UNK,ResNum=1) 0.55584500	5.90328900	-1.10841600	-
C(PDBName=C3,ResName=UNK,ResNum=1) 1.07108400	4.98775800	1.56881100	
H(PDBName=H3A,ResName=UNK,ResNum=1) 0.78162300	4.09590500	2.14159400	
H(PDBName=H3B,ResName=UNK,ResNum=1) 1.91089000	5.47225600	2.06897300	
C(PDBName=C4,ResName=UNK,ResNum=1) 1.45124900	4.58754700	0.14865500	
H(PDBName=H4A,ResName=UNK,ResNum=1) 1.85257500	5.46965100	-0.38172700	

H(PDBName=H4B,ResName=UNK,ResNum=1) 2.23920800	3.83027800	0.18663200	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.60528600	3.54977100	-1.88877700	
H(PDBName=H5A,ResName=UNK,ResNum=1) 1.60871200	3.11694400	-1.86597700	
H(PDBName=H5B,ResName=UNK,ResNum=1) 0.61808700	4.36535500	-2.63157600	
C(PDBName=C6,ResName=UNK,ResNum=1) 0.37614600	2.47417500	-2.35944900	-
H(PDBName=H6A,ResName=UNK,ResNum=1) 1.39296900	2.87413300	-2.41518700	-
H(PDBName=H6B,ResName=UNK,ResNum=1) 0.10343800	2.12880800	-3.35812200	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.27733200	0.07508500	-1.81921100	-
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.19605900	-0.11783700	-2.88435300	-
C(PDBName=C8,ResName=UNK,ResNum=1) 0.28140600	-1.03855200	-0.97496700	-
C(PDBName=C9,ResName=UNK,ResNum=1) 0.16532100	-2.33914900	-1.59119500	-
C(PDBName=C10,ResName=UNK,ResNum=1) 0.05761100	-4.77598900	-1.35779700	-
H(PDBName=H10A,ResName=UNK,ResNum=1) 0.54069300	-4.68341900	-2.32734400	-
H(PDBName=H10B,ResName=UNK,ResNum=1) 0.61075400	-5.48350500	-0.74740000	-
C(PDBName=C11,ResName=UNK,ResNum=1) 1.39496400	-5.21463900	-1.52554000	
H(PDBName=H11A,ResName=UNK,ResNum=1) 1.42342400	-6.18966300	-2.01947400	
H(PDBName=H11B,ResName=UNK,ResNum=1) 1.89170000	-5.30970400	-0.55829300	
H(PDBName=H11C,ResName=UNK,ResNum=1) 1.94901300	-4.50512100	-2.14336000	
C(PDBName=C12,ResName=UNK,ResNum=1) 0.27899000	-3.34928500	0.66691100	-

C(PDBName=C13,ResName=UNK,ResNum=1)	-1.89937000	2.67806100	-
0.51600200			
H(PDBName=H13A,ResName=UNK,ResNum=1)	-2.76479900	3.06756600	-
1.04364800			
H(PDBName=H13B,ResName=UNK,ResNum=1)	-1.01120300	2.82481400	-
1.12565700			
C(PDBName=C14,ResName=UNK,ResNum=1)	-1.73383100	3.35688100	
0.84142500			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-1.59369100	4.43115200	
0.69405100			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-0.85967100	2.96966700	
1.36862400			
H(PDBName=H14C,ResName=UNK,ResNum=1)	-2.61911200	3.21215200	
1.46331000			
C(PDBName=C15,ResName=UNK,ResNum=1)	-0.89547000	0.44718700	-
0.39626100			
H(PDBName=H2A,ResName=UNK,ResNum=1)	1.52013100	-0.44644100	-
0.42895100			

1 38 1.0

2 9 1.0 15 1.0

3 30 2.0

4 46 2.0

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 39 40 1.0 41 1.0 42 1.0
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B14. Geometry co-ordinates for NLO properties for crystal 2 (MeOH).

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S(PDBName=S1,ResName=UNK,ResNum=1)	-4.72444800	1.65198300	-
0.23561800			
O(PDBName=O1,ResName=UNK,ResNum=1)	5.94023000	1.56548000	
0.00733500			
O(PDBName=O2,ResName=UNK,ResNum=1)	-2.52795200	-2.79776500	-
0.05531000			

O(PDBName=O3,ResName=UNK,ResNum=1) 0.50166900	0.19289600	1.01920700	-
N(PDBName=N1,ResName=UNK,ResNum=1) 0.28635300	4.02318800	-0.54060800	
N(PDBName=N2,ResName=UNK,ResNum=1) 0.38257800	1.32964300	-1.44879600	-
N(PDBName=N3,ResName=UNK,ResNum=1) 0.17598700	-3.44900900	-0.70574500	-
N(PDBName=N4,ResName=UNK,ResNum=1) 0.40381800	-2.08677900	1.21031500	-
C(PDBName=C1,ResName=UNK,ResNum=1) 1.13976000	5.36911200	0.93376000	-
H(PDBName=H1A,ResName=UNK,ResNum=1) 1.92177900	6.12916700	0.96155500	-
H(PDBName=H1B,ResName=UNK,ResNum=1) 1.47590600	4.49296800	1.50526800	-
C(PDBName=C2,ResName=UNK,ResNum=1) 0.83933300	4.96528400	-0.50447500	-
H(PDBName=H2B,ResName=UNK,ResNum=1) 1.73044300	4.49827400	-0.93079000	-
H(PDBName=H2C,ResName=UNK,ResNum=1) 0.61632700	5.86824100	-1.10055000	-
C(PDBName=C3,ResName=UNK,ResNum=1) 1.10854600	5.02936100	1.53854800	
H(PDBName=H3A,ResName=UNK,ResNum=1) 0.86204500	4.13770900	2.13144500	
H(PDBName=H3B,ResName=UNK,ResNum=1) 1.94950300	5.54286700	2.00672800	
C(PDBName=C4,ResName=UNK,ResNum=1) 1.45613000	4.62268900	0.11239200	
H(PDBName=H4A,ResName=UNK,ResNum=1) 1.81420800	5.50906500	-0.44095100	
H(PDBName=H4B,ResName=UNK,ResNum=1) 2.26799600	3.89068800	0.13489900	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.58922400	3.54600300	-1.89071700	
H(PDBName=H5A,ResName=UNK,ResNum=1) 1.59326100	3.11446400	-1.88081900	

H(PDBName=H5B,ResName=UNK,ResNum=1) 0.59179100	4.36432400	-2.63003500	
C(PDBName=C6,ResName=UNK,ResNum=1) 0.39604800	2.47317800	-2.35785100	-
H(PDBName=H6A,ResName=UNK,ResNum=1) 1.41344300	2.87109200	-2.40688200	-
H(PDBName=H6B,ResName=UNK,ResNum=1) 0.12768100	2.12967800	-3.35779300	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.28717400	0.07442400	-1.81993500	-
H(PDBName=H7A,ResName=UNK,ResNum=1) 0.20237200	-0.11566200	-2.88494900	-
C(PDBName=C8,ResName=UNK,ResNum=1) 0.28771500	-1.04162300	-0.97369700	-
C(PDBName=C9,ResName=UNK,ResNum=1) 0.16586700	-2.34011200	-1.58794900	-
C(PDBName=C10,ResName=UNK,ResNum=1) 0.04426100	-4.77752400	-1.35518000	-
H(PDBName=H10A,ResName=UNK,ResNum=1) 0.53301400	-4.68942900	-2.32209200	-
H(PDBName=H10B,ResName=UNK,ResNum=1) 0.59078900	-5.48899000	-0.74375800	-
C(PDBName=C11,ResName=UNK,ResNum=1) 1.41044500	-5.20662700	-1.52902700	
H(PDBName=H11A,ResName=UNK,ResNum=1) 1.44275000	-6.18103500	-2.02379400	
H(PDBName=H11B,ResName=UNK,ResNum=1) 1.91251900	-5.29836300	-0.56413600	
H(PDBName=H11C,ResName=UNK,ResNum=1) 1.95877300	-4.49319100	-2.14739100	
C(PDBName=C12,ResName=UNK,ResNum=1) 0.27374800	-3.35064300	0.66789600	-
C(PDBName=C13,ResName=UNK,ResNum=1) 0.52035000	-1.90351300	2.67895900	-
H(PDBName=H13A,ResName=UNK,ResNum=1) 1.03779300	-2.77406700	3.07011700	-
H(PDBName=H13B,ResName=UNK,ResNum=1) 1.14250300	-1.02412600	2.82497600	-

C(PDBName=C14,ResName=UNK,ResNum=1) 0.83484300	-1.71930800	3.35730100	
H(PDBName=H14A,ResName=UNK,ResNum=1) 0.68546100	-1.57968600	4.43127700	
H(PDBName=H14B,ResName=UNK,ResNum=1) 1.35152600	-0.83969000	2.96849300	
H(PDBName=H14C,ResName=UNK,ResNum=1) 1.46932500	-2.59577900	3.21299400	
C(PDBName=C15,ResName=UNK,ResNum=1) 0.40464200	-0.89958500	0.44672700	-
H(PDBName=H2A,ResName=UNK,ResNum=1) 0.44959900	1.51525500	-0.44758900	-

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B15. Geometry co-ordinates for NLO properties for crystal 3 (Gaseous).

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S(PDBName=S1,ResName=UNK,ResNum=1)	-4.50198600	0.41324600	
0.04549100			
N(PDBName=N1,ResName=UNK,ResNum=1)	4.04876500	-1.12792000	-
0.14948200			
C(PDBName=C1,ResName=UNK,ResNum=1)	5.36379900	-1.36166500	-
0.17108800			
H(PDBName=H1,ResName=UNK,ResNum=1)	5.65713600	-2.39552600	-
0.32604400			
O(PDBName=O1,ResName=UNK,ResNum=1)	-0.57659200	-2.58221100	-
0.41889200			
O(PDBName=O2,ResName=UNK,ResNum=1)	0.18130400	2.01196400	
0.30984100			

H(PDBName=H2A,ResName=UNK,ResNum=1) 0.20510200	1.91054000	1.31634100	
N(PDBName=N2,ResName=UNK,ResNum=1) 0.06097500	2.26120500	0.36613100	
C(PDBName=C2,ResName=UNK,ResNum=1) 0.00861500	6.32390900	-0.36757400	-
H(PDBName=H2,ResName=UNK,ResNum=1) 0.03434200	7.37810400	-0.61242500	-
N(PDBName=N3,ResName=UNK,ResNum=1) 0.22669700	-2.32644800	-1.12164600	-
C(PDBName=C3,ResName=UNK,ResNum=1) 0.18661600	5.88456700	0.94201100	
H(PDBName=H3,ResName=UNK,ResNum=1) 0.31788600	6.59486400	1.75014000	
C(PDBName=C4,ResName=UNK,ResNum=1) 0.21154800	4.52264800	1.20400800	
H(PDBName=H4,ResName=UNK,ResNum=1) 0.36052900	4.14196500	2.20764000	
N(PDBName=N4,ResName=UNK,ResNum=1) 0.20715200	-1.94302800	1.17821200	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.03764900	3.64597400	0.12493500	
C(PDBName=C10,ResName=UNK,ResNum=1) 0.15927200	-0.55221600	1.02700200	
C(PDBName=C9,ResName=UNK,ResNum=1) 0.00650000	-2.85042400	0.13974100	
C(PDBName=C8,ResName=UNK,ResNum=1) 0.24504800	-0.94696700	-1.43240000	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.05709900	-0.04370900	-0.30659500	-
C(PDBName=C6,ResName=UNK,ResNum=1) 0.08925100	1.31314700	-0.56491300	-
H(PDBName=H6,ResName=UNK,ResNum=1) 0.24372200	1.65333700	-1.58172200	-
C(PDBName=C11,ResName=UNK,ResNum=1) 0.46762500	-2.43120900	2.55610900	
H(PDBName=H11A,ResName=UNK,ResNum=1) 1.10405100	-1.68382400	3.02465500	

H(PDBName=H11B,ResName=UNK,ResNum=1)	-3.36630000	2.46267800	
1.01269000			
C(PDBName=C12,ResName=UNK,ResNum=1)	-2.62420900	3.36409800	-
0.81289700			
H(PDBName=H12A,ResName=UNK,ResNum=1)	-1.68314600	3.46712300	-
1.35705100			
H(PDBName=H12B,ResName=UNK,ResNum=1)	-2.97950700	4.36643900	-
0.55796900			
H(PDBName=H12C,ResName=UNK,ResNum=1)	-3.36701600	2.89699000	-
1.46185600			
C(PDBName=C13,ResName=UNK,ResNum=1)	-3.23377000	-2.27495200	-
0.45170000			
H(PDBName=H13A,ResName=UNK,ResNum=1)	-2.69925100	-2.95016300	-
1.11623000			
H(PDBName=H13B,ResName=UNK,ResNum=1)	-4.11795800	-1.89241100	-
0.95380500			
C(PDBName=C14,ResName=UNK,ResNum=1)	-3.60635900	-2.98976000	
0.84454500			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-4.26511300	-3.83235900	
0.61658000			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-4.13696900	-2.31999100	
1.52375200			
H(PDBName=H14C,ResName=UNK,ResNum=1)	-2.71731100	-3.38107100	
1.34301100			

1 19 1.0

2 3 1.5 17 1.5

3 4 1.0 9 1.5

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5 20 2.0

6 18 2.0

7 8 1.0

8 17 1.0 22 1.5

9 10 1.0 12 1.5

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11 19 1.0 20 1.0 31 1.0

12 13 1.0 14 1.5

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 16 18 1.0 19 1.0 24 1.0
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 22 23 1.0
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 34 35 1.0 36 1.0 37 1.0
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B16. Geometry co-ordinates for NLO properties for crystal **3** (ACN).

0 1

S(PDBName=S1,ResName=UNK,ResNum=1)	-4.51569200	0.37981400	
0.04676900			
N(PDBName=N1,ResName=UNK,ResNum=1)	4.04515300	-1.12195700	-
0.13222500			
C(PDBName=C1,ResName=UNK,ResNum=1)	5.36045500	-1.36751000	-
0.15481500			
H(PDBName=H1,ResName=UNK,ResNum=1)	5.64839700	-2.40440700	-
0.29566600			
O(PDBName=O1,ResName=UNK,ResNum=1)	-0.55044900	-2.56414700	-
0.43076700			

O(PDBName=O2,ResName=UNK,ResNum=1) 0.31737300	0.15219400	2.03336900	
H(PDBName=H2A,ResName=UNK,ResNum=1) 0.20864200	1.93566500	1.34626100	
N(PDBName=N2,ResName=UNK,ResNum=1) 0.06318300	2.26708500	0.39130600	
C(PDBName=C2,ResName=UNK,ResNum=1) 0.00890400	6.32722400	-0.37729500	-
H(PDBName=H2,ResName=UNK,ResNum=1) 0.03384400	7.37904900	-0.63120000	-
N(PDBName=N3,ResName=UNK,ResNum=1) 0.22585600	-2.31564700	-1.12460900	-
C(PDBName=C3,ResName=UNK,ResNum=1) 0.16846900	5.89981400	0.93837000	
H(PDBName=H3,ResName=UNK,ResNum=1) 0.28554000	6.61646200	1.74239300	
C(PDBName=C4,ResName=UNK,ResNum=1) 0.19329900	4.53879500	1.21213300	
H(PDBName=H4,ResName=UNK,ResNum=1) 0.32676000	4.16884000	2.22123700	
N(PDBName=N4,ResName=UNK,ResNum=1) 0.20747700	-1.96444600	1.17539800	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.03826000	3.65646800	0.13811500	
C(PDBName=C10,ResName=UNK,ResNum=1) 0.16268500	-0.56689200	1.03921500	
C(PDBName=C9,ResName=UNK,ResNum=1) 0.00721800	-2.84925400	0.12902900	
C(PDBName=C8,ResName=UNK,ResNum=1) 0.24830600	-0.93203100	-1.41307400	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.05542500	-0.04470400	-0.28412900	-
C(PDBName=C6,ResName=UNK,ResNum=1) 0.08618600	1.32062800	-0.53005900	-
H(PDBName=H6,ResName=UNK,ResNum=1) 0.24155800	1.66436400	-1.54463000	-
C(PDBName=C11,ResName=UNK,ResNum=1) 0.47055600	-2.46737800	2.54857000	

H(PDBName=H11A,ResName=UNK,ResNum=1)	-1.73038400	3.02112600	
1.11504700			
H(PDBName=H11B,ResName=UNK,ResNum=1)	-3.40134400	2.44623800	
1.01471800			
C(PDBName=C12,ResName=UNK,ResNum=1)	-2.66187300	3.36060500	-
0.80696600			
H(PDBName=H12A,ResName=UNK,ResNum=1)	-1.72122500	3.47264800	-
1.34979800			
H(PDBName=H12B,ResName=UNK,ResNum=1)	-3.02534900	4.35828400	-
0.54680800			
H(PDBName=H12C,ResName=UNK,ResNum=1)	-3.39642900	2.89147500	-
1.46404100			
C(PDBName=C13,ResName=UNK,ResNum=1)	-3.20906200	-2.28909200	-
0.45456600			
H(PDBName=H13A,ResName=UNK,ResNum=1)	-2.67387500	-2.95052800	-
1.13120200			
H(PDBName=H13B,ResName=UNK,ResNum=1)	-4.09946500	-1.91653700	-
0.95160300			
C(PDBName=C14,ResName=UNK,ResNum=1)	-3.56641400	-3.01986000	
0.83684200			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-4.21282200	-3.86986800	
0.60259700			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-4.10278900	-2.36434200	
1.52542400			
H(PDBName=H14C,ResName=UNK,ResNum=1)	-2.67164800	-3.40003500	
1.33360400			
1 19 1.0			
2 3 1.5 17 1.5			
3 4 1.0 9 1.5			
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5 20 2.0			
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 20 21 1.0
 21 22 1.5
 22 23 1.0
 23
 24 25 1.0 26 1.0 27 1.0
 25
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 27 28 1.0 29 1.0 30 1.0
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 31 32 1.0 33 1.0 34 1.0
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 34 35 1.0 36 1.0 37 1.0
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B17. Geometry co-ordinates for NLO properties for crystal **3** (CHCl₃).

0 1

S(PDBName=S1,ResName=UNK,ResNum=1)	-4.51160300	0.38898200	
0.05172000			
N(PDBName=N1,ResName=UNK,ResNum=1)	4.04596700	-1.12538000	-
0.12696500			
C(PDBName=C1,ResName=UNK,ResNum=1)	5.36109800	-1.36813200	-
0.14841300			
H(PDBName=H1,ResName=UNK,ResNum=1)	5.65004900	-2.40539700	-
0.28507800			

O(PDBName=O1,ResName=UNK,ResNum=1) 0.43120900	-0.55810800	-2.56856600	-
O(PDBName=O2,ResName=UNK,ResNum=1) 0.31449300	0.16081400	2.02763100	
H(PDBName=H2A,ResName=UNK,ResNum=1) 0.20599800	1.92897900	1.33787900	
N(PDBName=N2,ResName=UNK,ResNum=1) 0.06201700	2.26554600	0.38411000	
C(PDBName=C2,ResName=UNK,ResNum=1) 0.00644700	6.32624200	-0.37568400	-
H(PDBName=H2,ResName=UNK,ResNum=1) 0.03015400	7.37868800	-0.62741600	-
N(PDBName=N3,ResName=UNK,ResNum=1) 0.22719500	-2.31891200	-1.12325000	-
C(PDBName=C3,ResName=UNK,ResNum=1) 0.16554000	5.89596000	0.93982700	
H(PDBName=H3,ResName=UNK,ResNum=1) 0.27938000	6.61102400	1.74591300	
C(PDBName=C4,ResName=UNK,ResNum=1) 0.18903800	4.53467100	1.21075100	
H(PDBName=H4,ResName=UNK,ResNum=1) 0.31824800	4.16190800	2.21959700	
N(PDBName=N4,ResName=UNK,ResNum=1) 0.20796800	-1.95806300	1.17657700	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.03833000	3.65395100	0.13401700	
C(PDBName=C10,ResName=UNK,ResNum=1) 0.16129700	-0.56263100	1.03591800	
C(PDBName=C9,ResName=UNK,ResNum=1) 0.00856100	-2.84988100	0.13225000	
C(PDBName=C8,ResName=UNK,ResNum=1) 0.24935100	-0.93636800	-1.41819900	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.05660500	-0.04441000	-0.29023800	-
C(PDBName=C6,ResName=UNK,ResNum=1) 0.08723700	1.31866800	-0.53991400	-
H(PDBName=H6,ResName=UNK,ResNum=1) 0.24169600	1.66154900	-1.55518300	-

C(PDBName=C11,ResName=UNK,ResNum=1)	-2.45667800	2.55114800	
0.47070500			
H(PDBName=H11A,ResName=UNK,ResNum=1)	-1.71718100	3.02211400	
1.11378900			
H(PDBName=H11B,ResName=UNK,ResNum=1)	-3.39159600	2.45118100	
1.01396200			
C(PDBName=C12,ResName=UNK,ResNum=1)	-2.64954000	3.36282500	-
0.80735600			
H(PDBName=H12A,ResName=UNK,ResNum=1)	-1.70835300	3.47214400	-
1.34987700			
H(PDBName=H12B,ResName=UNK,ResNum=1)	-3.01020400	4.36191000	-
0.54830200			
H(PDBName=H12C,ResName=UNK,ResNum=1)	-3.38672500	2.89541100	-
1.46264200			
C(PDBName=C13,ResName=UNK,ResNum=1)	-3.21672500	-2.28385500	-
0.45763700			
H(PDBName=H13A,ResName=UNK,ResNum=1)	-2.68122100	-2.94819100	-
1.13146100			
H(PDBName=H13B,ResName=UNK,ResNum=1)	-4.10474600	-1.90697700	-
0.95615000			
C(PDBName=C14,ResName=UNK,ResNum=1)	-3.58030600	-3.01266100	
0.83315800			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-4.22991200	-3.86003800	
0.59786900			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-4.11643200	-2.35452200	
1.51934200			
H(PDBName=H14C,ResName=UNK,ResNum=1)	-2.68789300	-3.39737400	
1.33070600			
1 19 1.0			
2 3 1.5 17 1.5			
3 4 1.0 9 1.5			
4			
5 20 2.0			
6 18 2.0			
7 8 1.0			
8 17 1.0 22 1.5			
9 10 1.0 12 1.5			

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 11 19 1.0 20 1.0 31 1.0
 12 13 1.0 14 1.5
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 14 15 1.0 17 1.5
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 16 18 1.0 19 1.0 24 1.0
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 18 21 1.5
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 20 21 1.0
 21 22 1.5
 22 23 1.0
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 24 25 1.0 26 1.0 27 1.0
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 27 28 1.0 29 1.0 30 1.0
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 31 32 1.0 33 1.0 34 1.0
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 34 35 1.0 36 1.0 37 1.0
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B18. Geometry co-ordinates for NLO properties for crystal **3** (MeOH).

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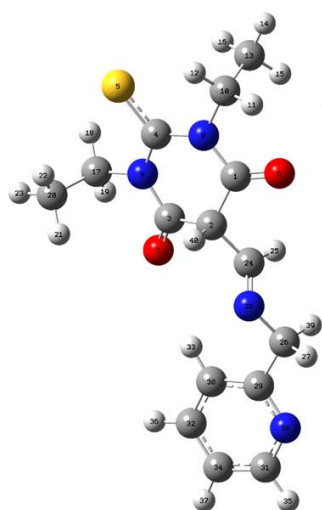
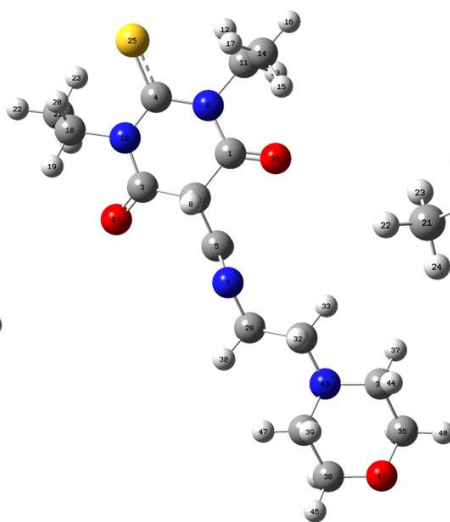
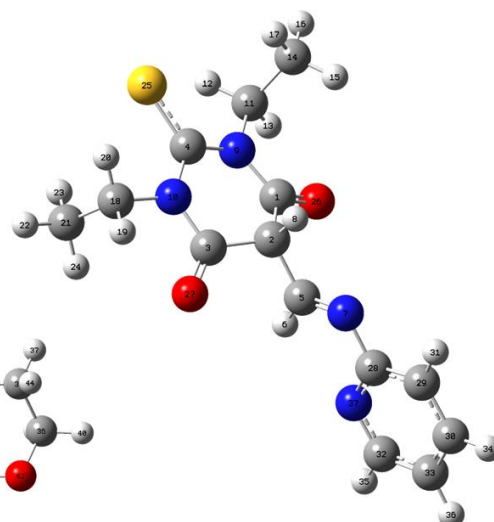
S(PDBName=S1,ResName=UNK,ResNum=1)	-4.51562200	0.37997400	
0.04687400			
N(PDBName=N1,ResName=UNK,ResNum=1)	4.04516400	-1.12203400	-
0.13204400			
C(PDBName=C1,ResName=UNK,ResNum=1)	5.36046300	-1.36754300	-
0.15462200			

H(PDBName=H1,ResName=UNK,ResNum=1) 0.29533100	5.64841800	-2.40445700	-
O(PDBName=O1,ResName=UNK,ResNum=1) 0.43078400	-0.55058300	-2.56421800	-
O(PDBName=O2,ResName=UNK,ResNum=1) 0.31734600	0.15234300	2.03327100	
H(PDBName=H2A,ResName=UNK,ResNum=1) 0.20860900	1.93555900	1.34611700	
N(PDBName=N2,ResName=UNK,ResNum=1) 0.06317700	2.26706000	0.39118000	
C(PDBName=C2,ResName=UNK,ResNum=1) 0.00886500	6.32720700	-0.37728000	-
H(PDBName=H2,ResName=UNK,ResNum=1) 0.03378300	7.37904200	-0.63115100	-
N(PDBName=N3,ResName=UNK,ResNum=1) 0.22588200	-2.31570500	-1.12458100	-
C(PDBName=C3,ResName=UNK,ResNum=1) 0.16832800	5.89975400	0.93839600	
H(PDBName=H3,ResName=UNK,ResNum=1) 0.28527300	6.61637700	1.74246200	
C(PDBName=C4,ResName=UNK,ResNum=1) 0.19313900	4.53873000	1.21211400	
H(PDBName=H4,ResName=UNK,ResNum=1) 0.32645600	4.16873200	2.22122500	
N(PDBName=N4,ResName=UNK,ResNum=1) 0.20749400	-1.96433700	1.17542200	
C(PDBName=C5,ResName=UNK,ResNum=1) 0.03826900	3.65642900	0.13803800	
C(PDBName=C10,ResName=UNK,ResNum=1) 0.16267700	-0.56681900	1.03915800	
C(PDBName=C9,ResName=UNK,ResNum=1) 0.00725000	-2.84926700	0.12908900	
C(PDBName=C8,ResName=UNK,ResNum=1) 0.24832400	-0.93210700	-1.41315700	-
C(PDBName=C7,ResName=UNK,ResNum=1) 0.05543200	-0.04470000	-0.28423300	-
C(PDBName=C6,ResName=UNK,ResNum=1) 0.08618700	1.32059600	-0.53022700	-

H(PDBName=H6,ResName=UNK,ResNum=1)	1.66431900	-1.54480900	-
0.24154300			
C(PDBName=C11,ResName=UNK,ResNum=1)	-2.46719300	2.54862000	
0.47056500			
H(PDBName=H11A,ResName=UNK,ResNum=1)	-1.73017200	3.02114100	
1.11505600			
H(PDBName=H11B,ResName=UNK,ResNum=1)	-3.40119100	2.44633000	
1.01468200			
C(PDBName=C12,ResName=UNK,ResNum=1)	-2.66162000	3.36066100	-
0.80696600			
H(PDBName=H12A,ResName=UNK,ResNum=1)	-1.72094800	3.47266100	-
1.34976500			
H(PDBName=H12B,ResName=UNK,ResNum=1)	-3.02505300	4.35836300	-
0.54682700			
H(PDBName=H12C,ResName=UNK,ResNum=1)	-3.39620800	2.89157300	-
1.46403500			
C(PDBName=C13,ResName=UNK,ResNum=1)	-3.20919800	-2.28899000	-
0.45465900			
H(PDBName=H13A,ResName=UNK,ResNum=1)	-2.67399400	-2.95046700	-
1.13124700			
H(PDBName=H13B,ResName=UNK,ResNum=1)	-4.09954700	-1.91634800	-
0.95173400			
C(PDBName=C14,ResName=UNK,ResNum=1)	-3.56669400	-3.01975100	
0.83671300			
H(PDBName=H14A,ResName=UNK,ResNum=1)	-4.21314800	-3.86971000	
0.60241200			
H(PDBName=H14B,ResName=UNK,ResNum=1)	-4.10308800	-2.36420500	
1.52525000			
H(PDBName=H14C,ResName=UNK,ResNum=1)	-2.67198200	-3.40001600	
1.33350600			
1 19 1.0			
2 3 1.5 17 1.5			
3 4 1.0 9 1.5			
4			
5 20 2.0			
6 18 2.0			
7 8 1.0			

8 17 1.0 22 1.5
9 10 1.0 12 1.5
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11 19 1.0 20 1.0 31 1.0
12 13 1.0 14 1.5
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14 15 1.0 17 1.5
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16 18 1.0 19 1.0 24 1.0
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18 21 1.5
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20 21 1.0
21 22 1.5
22 23 1.0
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24 25 1.0 26 1.0 27 1.0
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27 28 1.0 29 1.0 30 1.0
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31 32 1.0 33 1.0 34 1.0
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34 35 1.0 36 1.0 37 1.0
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B19. Optimized geometry of imine tautomer for all the three crystals (**1-3**)

**1****2****3**