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Supporting information for article:

Bending properties in the 4-halobenzonitrile crystals and C–halogen···N–C halogen bonds

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Cone correction: For cone correction, the number of hits within the angle range $\angle XNC = \theta \pm 5$ (where $\theta = 95 + 10n$ and $n = 0, 1, 2, \dots, 8$) and $\angle CXN = \theta \pm 5$ (where $\theta = 95 + 10n$ and $n = 0, 1, 2, \dots, 8$) were counted from the database search and this number of hits was then divided by $\sin\theta$ to obtain the cone corrected population at different angle ranges.

Table S1 Data for the C–I···N≡C interactions and $\angle INC = 90 - 180^\circ$.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
170-180	0.0872	29	19	333	56
160-170	0.2588	27	18	104	18
150-160	0.4226	25	16	59	10
140-150	0.5736	19	12	33	6
130-140	0.7071	14	9	20	3
120-130	0.8192	19	12	23	4
110-120	0.9063	13	8	14	2
100-110	0.9659	3	2	3	1
90-100	0.9962	5	3	5	1

Table S2 Data for the C–I...N≡C interactions and $\angle\text{CIN} = 90 - 180^\circ$.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
170-180	0.0872	105	68	1204	88
160-170	0.2588	35	23	135	10
150-160	0.4226	7	5	17	1
140-150	0.5736	5	3	9	1
130-140	0.7071	0	0	0	0
120-130	0.8192	0	0	0	0
110-120	0.9063	0	0	0	0
100-110	0.9659	1	1	1	0
90-100	0.9962	1	1	1	0

Table S3 Data for C–Br...N≡C interactions and $\angle\text{BrNC} = 90 - 180^\circ$.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
170-180	0.0872	12	5	138	26
160-170	0.2588	26	10	100	19
150-160	0.4226	16	6	38	7
140-150	0.5736	23	9	40	8
130-140	0.7071	28	11	40	8
120-130	0.8192	47	19	57	11
110-120	0.9063	45	18	50	10
100-110	0.9659	33	13	34	7
90-100	0.9962	24	9	24	5

Table S4 Data for the C–Br...N≡C interactions and $\angle\text{CBrN} = 90 - 180^\circ$.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
170-180	0.0872	97	38	1112	68
160-170	0.2588	103	41	398	24
150-160	0.4226	44	17	104	6
140-150	0.5736	8	3	14	1
130-140	0.7071	1	0	1	0
120-130	0.8192	1	0	1	0
110-120	0.9063	0	0	0	0
100-110	0.9659	0	0	0	0
90-100	0.9962	0	0	0	0

Table S5 Data for C–Cl...N≡C interactions and $\angle\text{CINC} = 90 - 180^\circ$.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
170-180	0.0872	7	2	80	15
160-170	0.2588	20	7	77	14
150-160	0.4226	26	9	62	12
140-150	0.5736	36	12	63	12
130-140	0.7071	44	14	62	12
120-130	0.8192	50	16	61	11
110-120	0.9063	56	18	62	12
100-110	0.9659	35	12	36	7
90-100	0.9962	30	10	30	6

Table S6 Data for the C–Cl···N≡C interactions and $\angle\text{CCIN} = 90 - 180^\circ$.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = $n/\text{Sin } \theta$	% Of hits After Cone Correction
170-180	0.0872	91	30	1044	62
160-170	0.2588	117	38	452	27
150-160	0.4226	51	17	121	7
140-150	0.5736	20	7	35	2
130-140	0.7071	6	2	8	1
120-130	0.8192	8	3	10	1
110-120	0.9063	0	0	0	0
100-110	0.9659	7	2	7	0
90-100	0.9962	5	2	5	0

Table S7 Percentage of interatomic contact surface area obtained from Crystal Explorer

Contacts	PERCENTAGE		
	X = I	X = Br	X = Cl
X···X	0.2	0.2	0.1
X···C	5.1	4.2	3.8
X···H	23.4	25.1	25.2
X···N	7.4	4.5	3.6
C···C	7.9	12.4	12.7
C···H	21	11.7	12.1
H···H	12.3	15.3	14.3
N···C	0.7	1.5	1.5
N···H	21.5	25.1	26.8
N···N	0.6	0	0

