

Supporting information to the article

Weak interactions in chain polymers $[M(\mu-X)_2L_2]_\infty$ (M = Zn, Cd; X = Cl, Br; L = substituted pyridine) - an electron density study

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Selected SORTAV output with merging results and redundancies for 1 - 5.

comp1.dat

CONDITIONS LIMITING POSSIBLE REFLECTIONS:

OKL,K=2N

HOL,H=2N

CRYSTAL CLASS POINT GROUP: -4M2

LAUE POINT GROUP: 4/MMM

LATTICE PARAMETERS:

A	B	C	ALPHA	BETA	GAMMA
13.7958	13.7958	3.6371	90.000	90.000	90.000

PROPORTIONALITY FACTOR, PP, FOR SIGNAL-PROPORTIONAL UNCERTAINTY ESTIMATES FOR CALCULATING RECIPROCAL-VARIANCE WEIGHTS FOR INTERFRAME SCALING, EMPIRICAL ABSORPTION ANISOTROPY CORRECTION, AND/OR EXPERIMENTALLY WEIGHTED DATA AVERAGING:

$$\text{VAR}(YI) = \text{SIGMA}(YI)**2 + (P*YMEAN)**2$$
$$P = 0.100E-01$$

EQUIVALENT DATA AVERAGING VARIABLES:

PTGP = XTAL POINT GROUP FOR EQUIVALENT REFLECTIONS AVERAGING
IW = 1
JW = 2
ZMAX = 6.0

AVERAGING FORMULAE:

$$YMEAN = \text{SUM}(W*Y)/\text{SUM}(W)$$
$$ESD = \text{SQRT}\{\text{SUM}[W*\text{SIGMA}(Y)**2]/\text{SUM}(W)\}$$
$$RMSD = \text{SQRT}\{[N/(N - 1)]*\text{SUM}[W*(Y - YMEAN)]/\text{SUM}(W)\}$$

WEIGHTS FOR AVERAGING:

$$W = WI*WJ$$

WHERE

$$\text{IF } IW = 0, \quad WI = 1$$
$$\text{IF } IW = 1, \quad WI = 1/\text{SIGMA}(Y)**2$$
$$\text{IF } JW = 0, \quad WJ = 1$$

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IF JW = 1, WJ = EXP(-0.5*Z**2)
IF JW = 2, WJ = [1 - (Z/ZMAX)**2]**2, IF ABS(Z) .LT. ZMAX
           = 0, IF ABS(Z) .GE. ZMAX
Z = [Y - MEDIAN(Y)]/SIGMA
IF IW = 0, SIGMA = MAX(MEDIAN[SIGMA(Y)], 1.25*MEDIAN{ABS[Y - MEDIAN(Y)]}*SQRT[N/(N - 1)])
IF IW = 1, SIGMA = SIGMA(Y)

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THRESHOLD VALUES FOR LISTING OUTLIER MEASUREMENTS:

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RMSD/ESD .GT. QLIMIT = 4.00
ABS(YI - YMEAN)/ESD .GT. ZLIMIT = 4.00

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PRINTED REFLECTIONS LIST:

LIST DISCORDANT MEASUREMENT SAMPLES WITH:

- (1) ONE OR MORE REJECTED MEASUREMENTS OR
- (2) RMSD/ESD .GT. QLIMIT
AND ONE OR MORE MEASUREMENTS WITH
ABS(Y - YMEAN)/ESD .GT. ZLIMIT.

COMPILE SIN(THETA)/LAMBDA DISTRIBUTION STATISTICS FOR VALUES OF
YMEAN/MAX(ESD, RMSD) .GE. QPRINT = 3.00

1-----
PROGRAM SORTAV/DATAIN. , . comp1

M = 54173 MEASUREMENTS READ FROM THE INPUT REFLECTION DATA FILE
N = 52786 ACCEPTED MEASUREMENTS WILL BE SORTED AND AVERAGED

N1 = 0 MEASUREMENTS REJECTED BECAUSE THEY APPEAR IN THE INPUT REJECTION LIST
N2 = 1386 ADDITIONAL MEASUREMENTS REJECTED BECAUSE SYMMETRY FORBIDDEN
N3 = 0 " " " " SIN(TH)/L .LT. SMIN1 = 0.000 OR .GT. SMAX1 = 9.000
N4 = 1 " " " " IH = IK = IL = 0
N5 = 0 " " " " ABS(IH), ABS(IK), OR ABS(IL) .GT. 500
N6 = 0 " " " " SIGMA(YMEAS) .LE. 0
N7 = 0 " " " " YMEAS .LT. -4*SIGMA(YMEAS)
N8 = 0 " " " " ISCALE .LT. 1 OR .GT. NSCALE

MILLER INDEX LIMITS OF THE ACCEPTED MEASUREMENTS:

HMIN KMIN LMIN

0 0 -8

HMAX KMAX LMAX
31 22 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE CRYSTAL CLASS POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 -8

HMAX KMAX LMAX
31 22 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE LAUE POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 0

HMAX KMAX LMAX
31 22 8

DATA RESOLUTION LIMITS:

SMIN = 0.051
SMAX = 1.144 RECIPROCAL ANGSTROMS

DMAX = $1/(2*SMIN)$ = 9.76 ANGSTROMS
DMIN = $1/(2*SMAX)$ = 0.44 ANGSTROMS

NTOTAL = 52786 TOTAL MEASUREMENTS

1-----
PROGRAM SORTAV/YMERGE. , . comp1

DATA MERGING STATISTICS (ADJUSTED FOR MEASUREMENT MULTIPLICITY):

NORMALIZED MEAN ABSOLUTE DEVIATION

$R1 = \langle \sqrt{N/(N-1)} * ABS(Y - YMEAN) \rangle / \langle Y \rangle$
= $SUM(H) \sqrt{N/(N-1)} * SUM(I) ABS(Y - YMEAN) / SUM(H) SUM(I) ABS(Y)$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION

$$R2 = \sqrt{\langle [N/(N-1)]*(Y - YMEAN)**2 \rangle / \langle Y**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) [(Y - YMEAN)**2] / \text{SUM}(H) \text{SUM}(I) Y**2}$$

NORMALIZED WEIGHTED ROOT-MEAN-SQUARE DEVIATION

$$RW = \sqrt{\langle [N/(N-1)]*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 \rangle / \langle [Y/\text{SIGMA}(Y)]**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W*[Y/\text{SIGMA}(Y)]**2}$$

STANDARDIZED ROOT-MEAN-SQUARE DEVIATION

$$Z = \sqrt{\langle \text{CHISQ} \rangle * N / (N - M)}, \quad \langle \text{CHISQ} \rangle = \text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W$$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION, OR POOLED COEFFICIENT OF VARIATION

$$V = \langle \text{RMSD} \rangle / \langle YMEAN \rangle$$

$$= \text{SUM}(H) \sqrt{\{ [N/(N-1)]* \text{SUM}(I) W*(Y - YMEAN)**2 / \text{SUM}(I) W \} / \text{SUM}(H) YMEAN}$$

WHERE $W = W_I * W_J$ $W_I = 1$ OR $W_J = 1$ OR

$W_I = 1/\text{SIGMA}(Y)**2$ $W_J = \text{EXP}(-0.5*Z**2)$ OR

$W_J = \{1 - \text{MIN}[1, (Z/ZMAX)**2]\}**2$, IN WHICH $Z = (Y - YMEAN)/\text{SIGMA}(Y)$

DATA CLASSES:

INTENSITY SIGNIFICANCE $Q = YMEAN/\text{MAX}(\text{ESD}, \text{RMSD})$

DIFFRACTION RESOLUTION $D = 1/(2*S)$ (ANGSTROM), $S = \text{SIN}(\text{THETA})/\text{LAMBDA}$ (ANGSTROM**-1)

CUMULATIVE INTENSITY-SIGNIFICANCE SUBSETS (Q .GE. QMIN)

NO OUTLIER REJECTION OR DOWN-WEIGHTING

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	52746	4308	12.2	0.0465	0.0464	0.0369	0.963	0.064
Q > 0	52746	4308	12.2	0.0465	0.0464	0.0369	0.963	0.064
Q > 1	51277	4154	12.3	0.0445	0.0451	0.0368	0.973	0.061
Q > 2	47670	3782	12.6	0.0404	0.0417	0.0363	0.996	0.054
Q > 3	44459	3473	12.8	0.0378	0.0397	0.0359	1.018	0.050
Q > 4	41451	3184	13.0	0.0360	0.0386	0.0355	1.043	0.047
Q > 6	35956	2676	13.4	0.0330	0.0367	0.0348	1.092	0.043

OUTLIERS DOWN-WEIGHTED OR REJECTED (HERE AND IN ALL THE FOLLOWING TABLES)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	52700	4308	12.2	0.0462	0.0451	0.0275	0.938	0.058
Q > 0	52700	4308	12.2	0.0462	0.0451	0.0275	0.938	0.058
Q > 1	51231	4154	12.3	0.0442	0.0437	0.0275	0.939	0.055
Q > 2	47624	3782	12.6	0.0401	0.0402	0.0274	0.943	0.050
Q > 3	44414	3473	12.8	0.0374	0.0381	0.0273	0.950	0.046
Q > 4	41406	3184	13.0	0.0356	0.0369	0.0271	0.958	0.044
Q > 6	35911	2676	13.4	0.0327	0.0349	0.0268	0.977	0.039

ACENTRIC AND CENTRIC REFLECTION SUBSETS

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ACENTRIC HKL	45615	3769	12.1	0.0477	0.0475	0.0280	0.916	0.061
CENTRIC HKL	7085	539	13.1	0.0389	0.0366	0.0258	1.047	0.043

RESOLUTION SHELLS (SMIN .LT. S .LE. SMAX) (DMAX .GT. D .GE. DMIN)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
D > 10	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
10 > D > 8	5	1	5.0	0.0133	0.0158	0.0134	1.371	0.014
8 > D > 6	16	2	8.0	0.0215	0.0327	0.0195	1.433	0.022
6 > D > 4	17	2	8.5	0.0185	0.0235	0.0178	1.792	0.018
4 > D > 3.5	14	2	7.0	0.0214	0.0330	0.0181	1.518	0.015
3.5 > D > 3	80	9	8.9	0.0164	0.0197	0.0166	1.171	0.017
3 > D > 2.5	104	10	10.4	0.0141	0.0175	0.0176	1.486	0.014
2.5 > D > 2	206	19	10.8	0.0147	0.0213	0.0164	1.256	0.016
2 > D > 1.5	801	68	11.8	0.0170	0.0204	0.0184	1.156	0.018
1.5 > D > 1	3628	254	14.3	0.0214	0.0253	0.0232	1.168	0.023
1 > D > 0.75	8748	497	17.6	0.0305	0.0344	0.0299	1.006	0.033
0.75 > D > 0.5	28345	2055	13.8	0.0526	0.0575	0.0391	0.776	0.064
0.5 > D > 0.4	10736	1389	7.7	0.1238	0.1386	0.0851	0.722	0.130
0.4 > D > 0.35	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
0.35 > D	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000

comp2.dat

CONDITIONS LIMITING POSSIBLE REFLECTIONS:

OKL,K=2N

HOL,H=2N

CRYSTAL CLASS POINT GROUP: -4M2

LAUE POINT GROUP: 4/MMM

LATTICE PARAMETERS:

A	B	C	ALPHA	BETA	GAMMA
13.8260	13.8260	3.7044	90.000	90.000	90.000

PROPORTIONALITY FACTOR, PP, FOR SIGNAL-PROPORTIONAL UNCERTAINTY ESTIMATES FOR CALCULATING RECIPROCAL-VARIANCE WEIGHTS FOR INTERFRAME SCALING, EMPIRICAL ABSORPTION ANISOTROPY CORRECTION, AND/OR EXPERIMENTALLY WEIGHTED DATA AVERAGING:

$$\text{VAR}(YI) = \text{SIGMA}(YI)**2 + (P*YMEAN)**2$$
$$P = 0.100E-01$$

EQUIVALENT DATA AVERAGING VARIABLES:

PTGP = XTAL POINT GROUP FOR EQUIVALENT REFLECTIONS AVERAGING

IW = 1

JW = 2

ZMAX = 6.0

AVERAGING FORMULAE:

$$YMEAN = \text{SUM}(W*Y)/\text{SUM}(W)$$
$$ESD = \text{SQRT}\{\text{SUM}[W*\text{SIGMA}(Y)**2]/\text{SUM}(W)\}$$
$$RMSD = \text{SQRT}\{[N/(N - 1)]*\text{SUM}[W*(Y - YMEAN)]/\text{SUM}(W)\}$$

WEIGHTS FOR AVERAGING:

$$W = WI*WJ$$

WHERE

IF IW = 0, WI = 1

IF IW = 1, WI = 1/SIGMA(Y)**2

IF JW = 0, WJ = 1

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IF JW = 1, WJ = EXP(-0.5*Z**2)
IF JW = 2, WJ = [1 - (Z/ZMAX)**2]**2, IF ABS(Z) .LT. ZMAX
           = 0, IF ABS(Z) .GE. ZMAX
Z = [Y - MEDIAN(Y)]/SIGMA
IF IW = 0, SIGMA = MAX(MEDIAN[SIGMA(Y)], 1.25*MEDIAN{ABS[Y - MEDIAN(Y)]}*SQRT[N/(N - 1)])
IF IW = 1, SIGMA = SIGMA(Y)

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THRESHOLD VALUES FOR LISTING OUTLIER MEASUREMENTS:

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RMSD/ESD .GT. QLIMIT = 4.00
ABS(YI - YMEAN)/ESD .GT. ZLIMIT = 4.00

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PRINTED REFLECTIONS LIST:

LIST DISCORDANT MEASUREMENT SAMPLES WITH:

- (1) ONE OR MORE REJECTED MEASUREMENTS OR
- (2) RMSD/ESD .GT. QLIMIT
AND ONE OR MORE MEASUREMENTS WITH
ABS(Y - YMEAN)/ESD .GT. ZLIMIT.

COMPILE SIN(THETA)/LAMBDA DISTRIBUTION STATISTICS FOR VALUES OF
YMEAN/MAX(ESD, RMSD) .GE. QPRINT = 3.00

1-----
PROGRAM SORTAV/DATAIN. , . comp2

M = 36384 MEASUREMENTS READ FROM THE INPUT REFLECTION DATA FILE
N = 35322 ACCEPTED MEASUREMENTS WILL BE SORTED AND AVERAGED

N1 = 0 MEASUREMENTS REJECTED BECAUSE THEY APPEAR IN THE INPUT REJECTION LIST
N2 = 1061 ADDITIONAL MEASUREMENTS REJECTED BECAUSE SYMMETRY FORBIDDEN
N3 = 0 " " " " SIN(TH)/L .LT. SMIN1 = 0.000 OR .GT. SMAX1 = 9.000
N4 = 1 " " " " IH = IK = IL = 0
N5 = 0 " " " " ABS(IH), ABS(IK), OR ABS(IL) .GT. 500
N6 = 0 " " " " SIGMA(YMEAS) .LE. 0
N7 = 0 " " " " YMEAS .LT. -4*SIGMA(YMEAS)
N8 = 0 " " " " ISCALE .LT. 1 OR .GT. NSCALE

MILLER INDEX LIMITS OF THE ACCEPTED MEASUREMENTS:

HMIN KMIN LMIN

0 0 -8

HMAX KMAX LMAX
31 21 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE CRYSTAL CLASS POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 -8

HMAX KMAX LMAX
31 21 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE LAUE POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 0

HMAX KMAX LMAX
31 21 8

DATA RESOLUTION LIMITS:

SMIN = 0.051
SMAX = 1.145 RECIPROCAL ANGSTROMS

DMAX = $1/(2 \cdot \text{SMIN}) = 9.78$ ANGSTROMS
DMIN = $1/(2 \cdot \text{SMAX}) = 0.44$ ANGSTROMS

NTOTAL = 35322 TOTAL MEASUREMENTS

1-----
PROGRAM SORTAV/YMERGE. , . comp2

DATA MERGING STATISTICS (ADJUSTED FOR MEASUREMENT MULTIPLICITY):

NORMALIZED MEAN ABSOLUTE DEVIATION

$R1 = \frac{\langle \sqrt{N/(N-1)} \cdot \text{ABS}(Y - Y_{\text{MEAN}}) \rangle}{\langle Y \rangle}$
= $\frac{\text{SUM}(H) \sqrt{N/(N-1)} \cdot \text{SUM}(I) \text{ABS}(Y - Y_{\text{MEAN}})}{\text{SUM}(H) \text{SUM}(I) \text{ABS}(Y)}$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION

$$R2 = \sqrt{\langle [N/(N-1)]*(Y - YMEAN)**2 \rangle / \langle Y**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) [(Y - YMEAN)**2] / \text{SUM}(H) \text{SUM}(I) Y**2}$$

NORMALIZED WEIGHTED ROOT-MEAN-SQUARE DEVIATION

$$RW = \sqrt{\langle [N/(N-1)]*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 \rangle / \langle [Y/\text{SIGMA}(Y)]**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W*[Y/\text{SIGMA}(Y)]**2}$$

STANDARDIZED ROOT-MEAN-SQUARE DEVIATION

$$Z = \sqrt{\langle \text{CHISQ} \rangle * N / (N - M)}, \quad \langle \text{CHISQ} \rangle = \text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W$$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION, OR POOLED COEFFICIENT OF VARIATION

$$V = \langle \text{RMSD} \rangle / \langle YMEAN \rangle$$

$$= \text{SUM}(H) \sqrt{\{ [N/(N-1)]* \text{SUM}(I) W*(Y - YMEAN)**2 / \text{SUM}(I) W \} / \text{SUM}(H) YMEAN}$$

WHERE $W = W_I * W_J$ $W_I = 1$ OR $W_J = 1$ OR

$W_I = 1/\text{SIGMA}(Y)**2$ $W_J = \text{EXP}(-0.5*Z**2)$ OR

$W_J = \{1 - \text{MIN}[1, (Z/ZMAX)**2]\}**2$, IN WHICH $Z = (Y - YMEAN)/\text{SIGMA}(Y)$

DATA CLASSES:

INTENSITY SIGNIFICANCE $Q = YMEAN/\text{MAX}(\text{ESD}, \text{RMSD})$

DIFFRACTION RESOLUTION $D = 1/(2*S)$ (ANGSTROM), $S = \text{SIN}(\text{THETA})/\text{LAMBDA}$ (ANGSTROM**-1)

CUMULATIVE INTENSITY-SIGNIFICANCE SUBSETS (Q .GE. QMIN)

NO OUTLIER REJECTION OR DOWN-WEIGHTING

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	35041	4004	8.8	0.0579	0.0634	0.0474	1.419	0.093
Q > 0	35041	4004	8.8	0.0579	0.0634	0.0474	1.419	0.093
Q > 1	33444	3691	9.1	0.0541	0.0608	0.0473	1.446	0.084
Q > 2	30711	3208	9.6	0.0486	0.0558	0.0471	1.496	0.071
Q > 3	28480	2829	10.1	0.0456	0.0534	0.0468	1.541	0.065
Q > 4	26865	2554	10.5	0.0438	0.0518	0.0466	1.573	0.061
Q > 6	24168	2114	11.4	0.0416	0.0501	0.0463	1.639	0.056

OUTLIERS DOWN-WEIGHTED OR REJECTED (HERE AND IN ALL THE FOLLOWING TABLES)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	34913	4004	8.7	0.0572	0.0609	0.0316	1.291	0.078
Q > 0	34913	4004	8.7	0.0572	0.0609	0.0316	1.291	0.078
Q > 1	33316	3691	9.0	0.0533	0.0581	0.0315	1.290	0.070
Q > 2	30583	3208	9.5	0.0477	0.0528	0.0315	1.292	0.061
Q > 3	28352	2829	10.0	0.0447	0.0502	0.0315	1.297	0.055
Q > 4	26738	2554	10.5	0.0429	0.0485	0.0314	1.301	0.052
Q > 6	24042	2114	11.4	0.0406	0.0466	0.0313	1.314	0.047

ACENTRIC AND CENTRIC REFLECTION SUBSETS

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ACENTRIC HKL	30102	3520	8.6	0.0597	0.0647	0.0326	1.274	0.081
CENTRIC HKL	4811	484	9.9	0.0449	0.0458	0.0284	1.357	0.058

RESOLUTION SHELLS (SMIN .LT. S .LE. SMAX) (DMAX .GT. D .GE. DMIN)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
D > 10	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
10 > D > 8	4	1	4.0	0.0437	0.0537	0.0435	1.274	0.048
8 > D > 6	26	2	13.0	0.0280	0.0310	0.0329	1.298	0.027
6 > D > 4	25	2	12.5	0.0207	0.0281	0.0181	1.701	0.018
4 > D > 3.5	24	2	12.0	0.0590	0.0589	0.0468	1.410	0.043
3.5 > D > 3	124	9	13.8	0.0229	0.0282	0.0247	1.403	0.023
3 > D > 2.5	167	10	16.7	0.0233	0.0292	0.0215	1.702	0.020
2.5 > D > 2	328	19	17.3	0.0240	0.0288	0.0242	1.516	0.024
2 > D > 1.5	1181	70	16.9	0.0241	0.0290	0.0250	1.528	0.024
1.5 > D > 1	4139	260	15.9	0.0313	0.0376	0.0289	1.399	0.031
1 > D > 0.75	8697	507	17.2	0.0458	0.0543	0.0395	1.255	0.048
0.75 > D > 0.5	16062	2085	7.7	0.0789	0.0915	0.0514	0.968	0.091
0.5 > D > 0.4	4136	1037	4.0	0.1850	0.2212	0.0903	0.670	0.166
0.4 > D > 0.35	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
0.35 > D	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000

comp3.dat

CONDITIONS LIMITING POSSIBLE REFLECTIONS:

OKL,K=2N

HOL,H=2N

CRYSTAL CLASS POINT GROUP: -4M2

LAUE POINT GROUP: 4/MMM

LATTICE PARAMETERS:

A	B	C	ALPHA	BETA	GAMMA
14.4457	14.4457	3.9345	90.000	90.000	90.000

PROPORTIONALITY FACTOR, PP, FOR SIGNAL-PROPORTIONAL UNCERTAINTY ESTIMATES FOR CALCULATING RECIPROCAL-VARIANCE WEIGHTS FOR INTERFRAME SCALING, EMPIRICAL ABSORPTION ANISOTROPY CORRECTION, AND/OR EXPERIMENTALLY WEIGHTED DATA AVERAGING:

$$\text{VAR}(YI) = \text{SIGMA}(YI)**2 + (P*YMEAN)**2$$
$$P = 0.100E-01$$

EQUIVALENT DATA AVERAGING VARIABLES:

PTGP = XTAL POINT GROUP FOR EQUIVALENT REFLECTIONS AVERAGING

IW = 1

JW = 2

ZMAX = 6.0

AVERAGING FORMULAE:

$$YMEAN = \text{SUM}(W*Y)/\text{SUM}(W)$$
$$ESD = \text{SQRT}\{\text{SUM}[W*\text{SIGMA}(Y)**2]/\text{SUM}(W)\}$$
$$RMSD = \text{SQRT}\{[N/(N - 1)]*\text{SUM}[W*(Y - YMEAN)]/\text{SUM}(W)\}$$

WEIGHTS FOR AVERAGING:

$$W = WI*WJ$$

WHERE

IF IW = 0, WI = 1

IF IW = 1, WI = 1/SIGMA(Y)**2

IF JW = 0, WJ = 1

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IF JW = 1, WJ = EXP(-0.5*Z**2)
IF JW = 2, WJ = [1 - (Z/ZMAX)**2]**2, IF ABS(Z) .LT. ZMAX
           = 0, IF ABS(Z) .GE. ZMAX
Z = [Y - MEDIAN(Y)]/SIGMA
IF IW = 0, SIGMA = MAX(MEDIAN[SIGMA(Y)], 1.25*MEDIAN{ABS[Y - MEDIAN(Y)]}*SQRT[N/(N - 1)])
IF IW = 1, SIGMA = SIGMA(Y)

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THRESHOLD VALUES FOR LISTING OUTLIER MEASUREMENTS:

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-----
RMSD/ESD .GT. QLIMIT = 4.00
ABS(YI - YMEAN)/ESD .GT. ZLIMIT = 4.00

```

PRINTED REFLECTIONS LIST:

LIST DISCORDANT MEASUREMENT SAMPLES WITH:

- (1) ONE OR MORE REJECTED MEASUREMENTS OR
- (2) RMSD/ESD .GT. QLIMIT
AND ONE OR MORE MEASUREMENTS WITH
ABS(Y - YMEAN)/ESD .GT. ZLIMIT.

COMPILE SIN(THETA)/LAMBDA DISTRIBUTION STATISTICS FOR VALUES OF
YMEAN/MAX(ESD, RMSD) .GE. QPRINT = 3.00

1-----
PROGRAM SORTAV/DATAIN. , . comp3

M = 47030 MEASUREMENTS READ FROM THE INPUT REFLECTION DATA FILE
N = 45936 ACCEPTED MEASUREMENTS WILL BE SORTED AND AVERAGED

N1 = 0 MEASUREMENTS REJECTED BECAUSE THEY APPEAR IN THE INPUT REJECTION LIST
N2 = 1093 ADDITIONAL MEASUREMENTS REJECTED BECAUSE SYMMETRY FORBIDDEN
N3 = 0 " " " " SIN(TH)/L .LT. SMIN1 = 0.000 OR .GT. SMAX1 = 9.000
N4 = 1 " " " " IH = IK = IL = 0
N5 = 0 " " " " ABS(IH), ABS(IK), OR ABS(IL) .GT. 500
N6 = 0 " " " " SIGMA(YMEAS) .LE. 0
N7 = 0 " " " " YMEAS .LT. -4*SIGMA(YMEAS)
N8 = 0 " " " " ISCALE .LT. 1 OR .GT. NSCALE

MILLER INDEX LIMITS OF THE ACCEPTED MEASUREMENTS:

HMIN KMIN LMIN

0 0 -8

HMAX KMAX LMAX
32 23 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE CRYSTAL CLASS POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 -8

HMAX KMAX LMAX
32 23 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE LAUE POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 0

HMAX KMAX LMAX
32 23 8

DATA RESOLUTION LIMITS:

SMIN = 0.049
SMAX = 1.146 RECIPROCAL ANGSTROMS

DMAX = $1/(2*SMIN)$ = 10.21 ANGSTROMS
DMIN = $1/(2*SMAX)$ = 0.44 ANGSTROMS

NTOTAL = 45936 TOTAL MEASUREMENTS

1-----
PROGRAM SORTAV/YMERGE. , . comp3

DATA MERGING STATISTICS (ADJUSTED FOR MEASUREMENT MULTIPLICITY):

NORMALIZED MEAN ABSOLUTE DEVIATION

$R1 = \frac{\langle \sqrt{N/(N-1)} * ABS(Y - YMEAN) \rangle}{\langle Y \rangle}$
= $\frac{SUM(H) \sqrt{N/(N-1)} * SUM(I) ABS(Y - YMEAN)}{SUM(H) SUM(I) ABS(Y)}$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION

$$R2 = \sqrt{\langle [N/(N-1)]*(Y - YMEAN)**2 \rangle / \langle Y**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) [(Y - YMEAN)**2] / \text{SUM}(H) \text{SUM}(I) Y**2}$$

NORMALIZED WEIGHTED ROOT-MEAN-SQUARE DEVIATION

$$RW = \sqrt{\langle [N/(N-1)]*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 \rangle / \langle [Y/\text{SIGMA}(Y)]**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W*[Y/\text{SIGMA}(Y)]**2}$$

STANDARDIZED ROOT-MEAN-SQUARE DEVIATION

$$Z = \sqrt{\langle \text{CHISQ} \rangle * N / (N - M)}, \quad \langle \text{CHISQ} \rangle = \text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W$$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION, OR POOLED COEFFICIENT OF VARIATION

$$V = \langle \text{RMSD} \rangle / \langle YMEAN \rangle$$

$$= \text{SUM}(H) \sqrt{\{ [N/(N-1)]* \text{SUM}(I) W*(Y - YMEAN)**2 / \text{SUM}(I) W \} / \text{SUM}(H) YMEAN}$$

WHERE $W = W_I * W_J$ $W_I = 1$ OR $W_J = 1$ OR

$W_I = 1/\text{SIGMA}(Y)**2$ $W_J = \text{EXP}(-0.5*Z**2)$ OR

$W_J = \{1 - \text{MIN}[1, (Z/ZMAX)**2]\}**2$, IN WHICH $Z = (Y - YMEAN)/\text{SIGMA}(Y)$

DATA CLASSES:

INTENSITY SIGNIFICANCE $Q = YMEAN/\text{MAX}(\text{ESD}, \text{RMSD})$

DIFFRACTION RESOLUTION $D = 1/(2*S)$ (ANGSTROM), $S = \text{SIN}(\text{THETA})/\text{LAMBDA}$ (ANGSTROM**-1)

CUMULATIVE INTENSITY-SIGNIFICANCE SUBSETS (Q .GE. QMIN)

NO OUTLIER REJECTION OR DOWN-WEIGHTING

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	45902	5113	9.0	0.0685	0.0671	0.0389	0.767	0.095
Q > 0	45902	5113	9.0	0.0685	0.0671	0.0389	0.767	0.095
Q > 1	40942	4408	9.3	0.0570	0.0586	0.0381	0.795	0.077
Q > 2	35203	3677	9.6	0.0467	0.0487	0.0371	0.832	0.061
Q > 3	31154	3160	9.9	0.0420	0.0447	0.0364	0.865	0.054
Q > 4	27537	2711	10.2	0.0388	0.0422	0.0357	0.901	0.049
Q > 6	22539	2135	10.6	0.0350	0.0393	0.0348	0.963	0.043

OUTLIERS DOWN-WEIGHTED OR REJECTED (HERE AND IN ALL THE FOLLOWING TABLES)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	45891	5113	9.0	0.0684	0.0668	0.0286	0.899	0.085
Q > 0	45891	5113	9.0	0.0684	0.0668	0.0286	0.899	0.085
Q > 1	40931	4408	9.3	0.0569	0.0583	0.0286	0.902	0.070
Q > 2	35192	3677	9.6	0.0466	0.0483	0.0284	0.912	0.057
Q > 3	31143	3160	9.9	0.0419	0.0443	0.0283	0.923	0.051
Q > 4	27526	2711	10.2	0.0387	0.0418	0.0281	0.937	0.046
Q > 6	22528	2135	10.6	0.0349	0.0388	0.0278	0.964	0.041

ACENTRIC AND CENTRIC REFLECTION SUBSETS

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ACENTRIC HKL	40689	4526	9.0	0.0726	0.0715	0.0304	0.879	0.091
CENTRIC HKL	5202	587	8.9	0.0461	0.0453	0.0241	0.990	0.057

RESOLUTION SHELLS (SMIN .LT. S .LE. SMAX) (DMAX .GT. D .GE. DMIN)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
D > 10	3	1	3.0	0.7834	0.8316	0.2411	1.014	0.376
10 > D > 8	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
8 > D > 6	15	2	7.5	0.0148	0.0150	0.0220	1.138	0.015
6 > D > 4	27	3	9.0	0.0206	0.0292	0.0173	1.553	0.017
4 > D > 3.5	29	4	7.3	0.0198	0.0265	0.0197	1.197	0.023
3.5 > D > 3	52	7	7.4	0.0152	0.0187	0.0191	1.389	0.018
3 > D > 2.5	116	13	8.9	0.0175	0.0215	0.0196	1.241	0.017
2.5 > D > 2	239	24	10.0	0.0202	0.0253	0.0214	1.309	0.021
2 > D > 1.5	716	77	9.3	0.0210	0.0253	0.0228	1.213	0.022
1.5 > D > 1	3161	301	10.5	0.0273	0.0319	0.0264	1.069	0.029
1 > D > 0.75	8086	591	13.7	0.0411	0.0440	0.0349	0.909	0.045
0.75 > D > 0.5	24629	2427	10.1	0.0823	0.0887	0.0452	0.648	0.095
0.5 > D > 0.4	8818	1663	5.3	0.1901	0.2080	0.0993	0.556	0.186
0.4 > D > 0.35	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
0.35 > D	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000

comp4.dat

CONDITIONS LIMITING POSSIBLE REFLECTIONS:

NONE

CRYSTAL CLASS POINT GROUP: 2/M

LAUE POINT GROUP: 2/M

LATTICE PARAMETERS:

A	B	C	ALPHA	BETA	GAMMA
20.0345	20.4024	3.8561	90.000	98.518	90.000

PROPORTIONALITY FACTOR, PP, FOR SIGNAL-PROPORTIONAL UNCERTAINTY ESTIMATES FOR CALCULATING RECIPROCAL-VARIANCE WEIGHTS FOR INTERFRAME SCALING, EMPIRICAL ABSORPTION ANISOTROPY CORRECTION, AND/OR EXPERIMENTALLY WEIGHTED DATA AVERAGING:

$$\begin{aligned} \text{VAR}(YI) &= \text{SIGMA}(YI)**2 + (P*YMEAN)**2 \\ P &= 0.100E-01 \end{aligned}$$

EQUIVALENT DATA AVERAGING VARIABLES:

PTGP = XTAL POINT GROUP FOR EQUIVALENT REFLECTIONS AVERAGING
IW = 1
JW = 2
ZMAX = 6.0

AVERAGING FORMULAE:

$$\begin{aligned} YMEAN &= \text{SUM}(W*Y)/\text{SUM}(W) \\ \text{ESD} &= \text{SQRT}\{\text{SUM}[W*\text{SIGMA}(Y)**2]/\text{SUM}(W)\} \\ \text{RMSD} &= \text{SQRT}\{[N/(N-1)]*\text{SUM}[W*(Y-YMEAN)]/\text{SUM}(W)\} \end{aligned}$$

WEIGHTS FOR AVERAGING:

$$W = WI*WJ$$

WHERE

$$\begin{aligned} \text{IF } IW = 0, \quad WI &= 1 \\ \text{IF } IW = 1, \quad WI &= 1/\text{SIGMA}(Y)**2 \\ \text{IF } JW = 0, \quad WJ &= 1 \\ \text{IF } JW = 1, \quad WJ &= \text{EXP}(-0.5*Z**2) \end{aligned}$$

```

IF JW = 2, WJ = [1 - (Z/ZMAX)**2]**2, IF ABS(Z) .LT. ZMAX
           = 0, IF ABS(Z) .GE. ZMAX
Z = [Y - MEDIAN(Y)]/SIGMA
IF IW = 0, SIGMA = MAX(MEDIAN[SIGMA(Y)], 1.25*MEDIAN{ABS[Y - MEDIAN(Y)]}*SQRT[N/(N - 1)])
IF IW = 1, SIGMA = SIGMA(Y)

```

THRESHOLD VALUES FOR LISTING OUTLIER MEASUREMENTS:

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-----
RMSD/ESD .GT. QLIMIT = 4.00
ABS(YI - YMEAN)/ESD .GT. ZLIMIT = 4.00

```

PRINTED REFLECTIONS LIST:

LIST DISCORDANT MEASUREMENT SAMPLES WITH:

- (1) ONE OR MORE REJECTED MEASUREMENTS OR
 - (2) RMSD/ESD .GT. QLIMIT
- AND ONE OR MORE MEASUREMENTS WITH
ABS(Y - YMEAN)/ESD .GT. ZLIMIT.

COMPILE SIN(THETA)/LAMBDA DISTRIBUTION STATISTICS FOR VALUES OF
YMEAN/MAX(ESD, RMSD) .GE. QPRINT = 3.00

1-----
PROGRAM SORTAV/DATAIN. , . comp4

M = 39548 MEASUREMENTS READ FROM THE INPUT REFLECTION DATA FILE
N = 39547 ACCEPTED MEASUREMENTS WILL BE SORTED AND AVERAGED

N1 = 0 MEASUREMENTS REJECTED BECAUSE THEY APPEAR IN THE INPUT REJECTION LIST
N2 = 0 ADDITIONAL MEASUREMENTS REJECTED BECAUSE SYMMETRY FORBIDDEN
N3 = 0 " " " " SIN(TH)/L .LT. SMIN1 = 0.000 OR .GT. SMAX1 = 9.000
N4 = 1 " " " " IH = IK = IL = 0
N5 = 0 " " " " ABS(IH), ABS(IK), OR ABS(IL) .GT. 500
N6 = 0 " " " " SIGMA(YMEAS) .LE. 0
N7 = 0 " " " " YMEAS .LT. -4*SIGMA(YMEAS)
N8 = 0 " " " " ISCALE .LT. 1 OR .GT. NSCALE

MILLER INDEX LIMITS OF THE ACCEPTED MEASUREMENTS:

HMIN KMIN LMIN
-44 0 0

HMAX KMAX LMAX
44 45 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE CRYSTAL CLASS POINT GROUP SYMMETRY:

HMIN KMIN LMIN
-44 0 0

HMAX KMAX LMAX
44 45 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE LAUE POINT GROUP SYMMETRY:

HMIN KMIN LMIN
-44 0 0

HMAX KMAX LMAX
44 45 8

DATA RESOLUTION LIMITS:

SMIN = 0.035
SMAX = 1.112 RECIPROCAL ANGSTROMS

DMAX = $1/(2*SMIN)$ = 14.21 ANGSTROMS
DMIN = $1/(2*SMAX)$ = 0.45 ANGSTROMS

NTOTAL = 39547 TOTAL MEASUREMENTS

PROGRAM SORTAV/YMERGE. , . comp4

DATA MERGING STATISTICS (ADJUSTED FOR MEASUREMENT MULTIPLICITY):

NORMALIZED MEAN ABSOLUTE DEVIATION

$R1 = \langle \sqrt{N/(N-1)} * \text{ABS}(Y - YMEAN) \rangle / \langle Y \rangle$
= $\text{SUM}(H) \sqrt{N/(N-1)} * \text{SUM}(I) \text{ABS}(Y - YMEAN) / \text{SUM}(H) \text{SUM}(I) \text{ABS}(Y)$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION

$R2 = \sqrt{\langle [N/(N-1)] * (Y - YMEAN)**2 \rangle / \langle Y**2 \rangle}$
= $\sqrt{\text{SUM}(H) [N/(N-1)] * \text{SUM}(I) [(Y - YMEAN)**2] / \text{SUM}(H) \text{SUM}(I) Y**2}$

NORMALIZED WEIGHTED ROOT-MEAN-SQUARE DEVIATION

$$RW = \sqrt{\frac{[N/(N-1)] * [(Y - YMEAN)/SIGMA(Y)]^2}{[Y/SIGMA(Y)]^2}}$$

$$= \sqrt{\frac{\sum(H) [N/(N-1)] * \sum(I) W * [(Y - YMEAN)/SIGMA(Y)]^2 / \sum(H) \sum(I) W * [Y/SIGMA(Y)]^2}{}}$$

STANDARDIZED ROOT-MEAN-SQUARE DEVIATION

$$Z = \sqrt{[<CHISQ> * N / (N - M)]}, \quad <CHISQ> = \sum(H) [N / (N - 1)] * \sum(I) W * [(Y - YMEAN) / SIGMA(Y)]^2 / \sum(H) \sum(I) W$$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION, OR POOLED COEFFICIENT OF VARIATION

$$V = <RMSD> / <YMEAN>$$

$$= \sum(H) \sqrt{[N / (N - 1)] * \sum(I) W * (Y - YMEAN)^2 / \sum(I) W} / \sum(H) YMEAN$$

WHERE $W = W_I * W_J$ $W_I = 1$ OR $W_J = 1$ OR
 $W_I = 1 / SIGMA(Y)^2$ $W_J = \exp(-0.5 * Z^2)$ OR
 $W_J = \{1 - \min[1, (Z/ZMAX)^2]\}^2$, IN WHICH $Z = (Y - YMEAN) / SIGMA(Y)$

DATA CLASSES:

 INTENSITY SIGNIFICANCE $Q = YMEAN / \max(ESD, RMSD)$
 DIFFRACTION RESOLUTION $D = 1 / (2 * S)$ (ANGSTROM), $S = \sin(\theta) / \lambda$ (ANGSTROM⁻¹)

CUMULATIVE INTENSITY-SIGNIFICANCE SUBSETS (Q .GE. QMIN)

 NO OUTLIER REJECTION OR DOWN-WEIGHTING

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	38622	7613	5.1	0.0579	0.0574	0.0371	0.920	0.085
Q > 0	38622	7613	5.1	0.0579	0.0574	0.0371	0.920	0.085
Q > 1	35330	6710	5.3	0.0505	0.0520	0.0366	0.946	0.072
Q > 2	31357	5725	5.5	0.0429	0.0446	0.0359	0.978	0.058
Q > 3	28568	5042	5.7	0.0393	0.0417	0.0353	1.005	0.052
Q > 4	26062	4456	5.8	0.0369	0.0400	0.0348	1.033	0.048
Q > 6	22290	3585	6.2	0.0339	0.0378	0.0339	1.080	0.043

OUTLIERS DOWN-WEIGHTED OR REJECTED (HERE AND IN ALL THE FOLLOWING TABLES)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	38611	7613	5.1	0.0578	0.0571	0.0282	1.001	0.076
Q > 0	38611	7613	5.1	0.0578	0.0571	0.0282	1.001	0.076
Q > 1	35319	6710	5.3	0.0504	0.0518	0.0282	1.000	0.065
Q > 2	31346	5725	5.5	0.0428	0.0443	0.0280	1.007	0.054
Q > 3	28557	5042	5.7	0.0392	0.0413	0.0279	1.014	0.049
Q > 4	26051	4456	5.8	0.0368	0.0396	0.0277	1.022	0.045
Q > 6	22279	3585	6.2	0.0337	0.0374	0.0273	1.039	0.040

ACENTRIC AND CENTRIC REFLECTION SUBSETS

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ACENTRIC HKL	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
CENTRIC HKL	38611	7613	5.1	0.0578	0.0571	0.0282	1.001	0.076

RESOLUTION SHELLS (SMIN .LT. S .LE. SMAX) (DMAX .GT. D .GE. DMIN)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
D > 10	21	2	10.5	0.7772	0.7054	0.2608	0.702	0.318
10 > D > 8	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
8 > D > 6	23	3	7.7	0.0101	0.0113	0.0132	0.657	0.012
6 > D > 4	32	5	6.4	0.0224	0.0303	0.0204	1.359	0.021
4 > D > 3.5	63	9	7.0	0.0184	0.0248	0.0185	1.169	0.017
3.5 > D > 3	114	17	6.7	0.0161	0.0223	0.0178	1.101	0.018
3 > D > 2.5	181	23	7.9	0.0184	0.0224	0.0205	1.234	0.019
2.5 > D > 2	390	47	8.3	0.0228	0.0267	0.0239	1.296	0.023
2 > D > 1.5	1378	158	8.7	0.0218	0.0252	0.0225	1.109	0.024
1.5 > D > 1	4918	584	8.4	0.0297	0.0330	0.0276	1.059	0.032
1 > D > 0.75	10036	1140	8.8	0.0462	0.0486	0.0376	0.946	0.051
0.75 > D > 0.5	17738	4249	4.2	0.0860	0.0934	0.0479	0.726	0.094
0.5 > D > 0.4	3717	1376	2.7	0.1887	0.2122	0.1027	0.660	0.175
0.4 > D > 0.35	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
0.35 > D	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000

comp5.dat

CONDITIONS LIMITING POSSIBLE REFLECTIONS:

OKL,K=2N

HOL,H=2N

CRYSTAL CLASS POINT GROUP: -4M2

LAUE POINT GROUP: 4/MMM

LATTICE PARAMETERS:

A	B	C	ALPHA	BETA	GAMMA
14.3513	14.3513	3.9082	90.000	90.000	90.000

PROPORTIONALITY FACTOR, PP, FOR SIGNAL-PROPORTIONAL UNCERTAINTY ESTIMATES FOR CALCULATING RECIPROCAL-VARIANCE WEIGHTS FOR INTERFRAME SCALING, EMPIRICAL ABSORPTION ANISOTROPY CORRECTION, AND/OR EXPERIMENTALLY WEIGHTED DATA AVERAGING:

$$\text{VAR}(YI) = \text{SIGMA}(YI)**2 + (P*YMEAN)**2$$
$$P = 0.100E-01$$

EQUIVALENT DATA AVERAGING VARIABLES:

PTGP = XTAL POINT GROUP FOR EQUIVALENT REFLECTIONS AVERAGING

IW = 1

JW = 2

ZMAX = 6.0

AVERAGING FORMULAE:

$$YMEAN = \text{SUM}(W*Y) / \text{SUM}(W)$$
$$ESD = \text{SQRT}\{\text{SUM}[W*\text{SIGMA}(Y)**2] / \text{SUM}(W)\}$$
$$RMSD = \text{SQRT}\{[N / (N - 1)] * \text{SUM}[W*(Y - YMEAN)] / \text{SUM}(W)\}$$

WEIGHTS FOR AVERAGING:

$$W = WI*WJ$$

WHERE

IF IW = 0, WI = 1

IF IW = 1, WI = 1/SIGMA(Y)**2

IF JW = 0, WJ = 1

```

IF JW = 1, WJ = EXP(-0.5*Z**2)
IF JW = 2, WJ = [1 - (Z/ZMAX)**2]**2, IF ABS(Z) .LT. ZMAX
           = 0, IF ABS(Z) .GE. ZMAX
Z = [Y - MEDIAN(Y)]/SIGMA
IF IW = 0, SIGMA = MAX(MEDIAN[SIGMA(Y)], 1.25*MEDIAN{ABS[Y - MEDIAN(Y)]}*SQRT[N/(N - 1)])
IF IW = 1, SIGMA = SIGMA(Y)

```

THRESHOLD VALUES FOR LISTING OUTLIER MEASUREMENTS:

```

-----
RMSD/ESD .GT. QLIMIT = 4.00
ABS(YI - YMEAN)/ESD .GT. ZLIMIT = 4.00

```

PRINTED REFLECTIONS LIST:

LIST DISCORDANT MEASUREMENT SAMPLES WITH:

- (1) ONE OR MORE REJECTED MEASUREMENTS OR
- (2) RMSD/ESD .GT. QLIMIT
AND ONE OR MORE MEASUREMENTS WITH
ABS(Y - YMEAN)/ESD .GT. ZLIMIT.

COMPILE SIN(THETA)/LAMBDA DISTRIBUTION STATISTICS FOR VALUES OF
YMEAN/MAX(ESD, RMSD) .GE. QPRINT = 3.00

1-----
PROGRAM SORTAV/DATAIN. , . comp5

M = 43527 MEASUREMENTS READ FROM THE INPUT REFLECTION DATA FILE
N = 42318 ACCEPTED MEASUREMENTS WILL BE SORTED AND AVERAGED

N1 = 0 MEASUREMENTS REJECTED BECAUSE THEY APPEAR IN THE INPUT REJECTION LIST
N2 = 1208 ADDITIONAL MEASUREMENTS REJECTED BECAUSE SYMMETRY FORBIDDEN
N3 = 0 " " " " SIN(TH)/L .LT. SMIN1 = 0.000 OR .GT. SMAX1 = 9.000
N4 = 1 " " " " IH = IK = IL = 0
N5 = 0 " " " " ABS(IH), ABS(IK), OR ABS(IL) .GT. 500
N6 = 0 " " " " SIGMA(YMEAS) .LE. 0
N7 = 0 " " " " YMEAS .LT. -4*SIGMA(YMEAS)
N8 = 0 " " " " ISCALE .LT. 1 OR .GT. NSCALE

MILLER INDEX LIMITS OF THE ACCEPTED MEASUREMENTS:

HMIN KMIN LMIN

0 0 -8

HMAX KMAX LMAX
32 23 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE CRYSTAL CLASS POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 -8

HMAX KMAX LMAX
32 23 8

MILLER INDEX LIMITS OF THE DATA UNIQUE UNDER THE LAUE POINT GROUP SYMMETRY:

HMIN KMIN LMIN
0 0 0

HMAX KMAX LMAX
32 23 8

DATA RESOLUTION LIMITS:

SMIN = 0.049
SMAX = 1.149 RECIPROCAL ANGSTROMS

DMAX = $1/(2*SMIN)$ = 10.15 ANGSTROMS
DMIN = $1/(2*SMAX)$ = 0.44 ANGSTROMS

NTOTAL = 42318 TOTAL MEASUREMENTS

1-----
PROGRAM SORTAV/YMERGE. , . comp5

DATA MERGING STATISTICS (ADJUSTED FOR MEASUREMENT MULTIPLICITY):

NORMALIZED MEAN ABSOLUTE DEVIATION

$R1 = \langle \sqrt{N/(N-1)} * ABS(Y - YMEAN) \rangle / \langle Y \rangle$
= $SUM(H) \sqrt{N/(N-1)} * SUM(I) ABS(Y - YMEAN) / SUM(H) SUM(I) ABS(Y)$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION

$$R2 = \sqrt{\langle [N/(N-1)]*(Y - YMEAN)**2 \rangle / \langle Y**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) [(Y - YMEAN)**2] / \text{SUM}(H) \text{SUM}(I) Y**2}$$

NORMALIZED WEIGHTED ROOT-MEAN-SQUARE DEVIATION

$$RW = \sqrt{\langle [N/(N-1)]*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 \rangle / \langle [Y/\text{SIGMA}(Y)]**2 \rangle}$$

$$= \sqrt{\text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W*[Y/\text{SIGMA}(Y)]**2}$$

STANDARDIZED ROOT-MEAN-SQUARE DEVIATION

$$Z = \sqrt{\langle \text{CHISQ} \rangle * N / (N - M)}, \quad \langle \text{CHISQ} \rangle = \text{SUM}(H) [N/(N-1)]* \text{SUM}(I) W*[(Y - YMEAN)/\text{SIGMA}(Y)]**2 / \text{SUM}(H) \text{SUM}(I) W$$

NORMALIZED ROOT-MEAN-SQUARE DEVIATION, OR POOLED COEFFICIENT OF VARIATION

$$V = \langle \text{RMSD} \rangle / \langle YMEAN \rangle$$

$$= \text{SUM}(H) \sqrt{\{ [N/(N-1)]* \text{SUM}(I) W*(Y - YMEAN)**2 / \text{SUM}(I) W \} / \text{SUM}(H) YMEAN}$$

WHERE $W = W_I * W_J$ $W_I = 1$ OR $W_J = 1$ OR

$W_I = 1/\text{SIGMA}(Y)**2$ $W_J = \text{EXP}(-0.5*Z**2)$ OR

$W_J = \{1 - \text{MIN}[1, (Z/ZMAX)**2]\}**2$, IN WHICH $Z = (Y - YMEAN)/\text{SIGMA}(Y)$

DATA CLASSES:

INTENSITY SIGNIFICANCE $Q = YMEAN/\text{MAX}(\text{ESD}, \text{RMSD})$

DIFFRACTION RESOLUTION $D = 1/(2*S)$ (ANGSTROM), $S = \text{SIN}(\text{THETA})/\text{LAMBDA}$ (ANGSTROM**-1)

CUMULATIVE INTENSITY-SIGNIFICANCE SUBSETS (Q .GE. QMIN)

NO OUTLIER REJECTION OR DOWN-WEIGHTING

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	42276	5049	8.4	0.0476	0.0513	0.0478	0.893	0.081
Q > 0	42276	5049	8.4	0.0476	0.0513	0.0478	0.893	0.081
Q > 1	41340	4860	8.5	0.0457	0.0500	0.0475	0.897	0.077
Q > 2	39335	4497	8.7	0.0413	0.0456	0.0466	0.900	0.068
Q > 3	37435	4156	9.0	0.0377	0.0416	0.0453	0.895	0.059
Q > 4	35675	3863	9.2	0.0351	0.0384	0.0443	0.893	0.053
Q > 6	32755	3389	9.7	0.0319	0.0352	0.0424	0.887	0.046

OUTLIERS DOWN-WEIGHTED OR REJECTED (HERE AND IN ALL THE FOLLOWING TABLES)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ALL DATA	42275	5049	8.4	0.0476	0.0513	0.0460	0.883	0.067
Q > 0	42275	5049	8.4	0.0476	0.0513	0.0460	0.883	0.067
Q > 1	41339	4860	8.5	0.0457	0.0500	0.0459	0.882	0.064
Q > 2	39334	4497	8.7	0.0413	0.0456	0.0457	0.882	0.057
Q > 3	37435	4156	9.0	0.0377	0.0416	0.0453	0.878	0.051
Q > 4	35675	3863	9.2	0.0351	0.0384	0.0448	0.878	0.047
Q > 6	32755	3389	9.7	0.0319	0.0352	0.0437	0.874	0.042

ACENTRIC AND CENTRIC REFLECTION SUBSETS

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
ACENTRIC HKL	36679	4462	8.2	0.0498	0.0546	0.0458	0.875	0.070
CENTRIC HKL	5596	587	9.5	0.0368	0.0383	0.0468	0.926	0.051

RESOLUTION SHELLS (SMIN .LT. S .LE. SMAX) (DMAX .GT. D .GE. DMIN)

	NTERMS	NMEANS	<N>	R1	R2	RW	Z	V
D > 10	7	1	7.0	0.0448	0.0546	0.0494	1.377	0.051
10 > D > 8	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
8 > D > 6	19	2	9.5	0.0286	0.0326	0.0469	1.237	0.032
6 > D > 4	14	2	7.0	0.0356	0.0453	0.0388	1.099	0.040
4 > D > 3.5	29	4	7.3	0.0233	0.0321	0.0182	0.489	0.027
3.5 > D > 3	71	8	8.9	0.0205	0.0231	0.0430	0.882	0.024
3 > D > 2.5	147	13	11.3	0.0186	0.0269	0.0218	0.592	0.023
2.5 > D > 2	342	23	14.9	0.0190	0.0240	0.0585	1.168	0.023
2 > D > 1.5	1278	78	16.4	0.0191	0.0244	0.0393	0.868	0.023
1.5 > D > 1	4385	289	15.2	0.0211	0.0260	0.0361	0.814	0.025
1 > D > 0.75	8451	585	14.4	0.0282	0.0332	0.0407	0.843	0.032
0.75 > D > 0.5	19698	2383	8.3	0.0611	0.0738	0.0486	0.888	0.072
0.5 > D > 0.4	7834	1661	4.7	0.1766	0.2119	0.0796	0.949	0.156
0.4 > D > 0.35	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000
0.35 > D	0	0	0.0	0.0000	0.0000	0.0000	0.000	0.000

Supporting information to the article

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Weak interactions in chain polymers $[M(\mu-X)_2L_2]_\infty$ ($M = \text{Zn, Cd}$; $X = \text{Cl, Br}$; $L =$ substituted pyridine) - an electron density study

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Gradient trajectory plots for **2** and **4**.

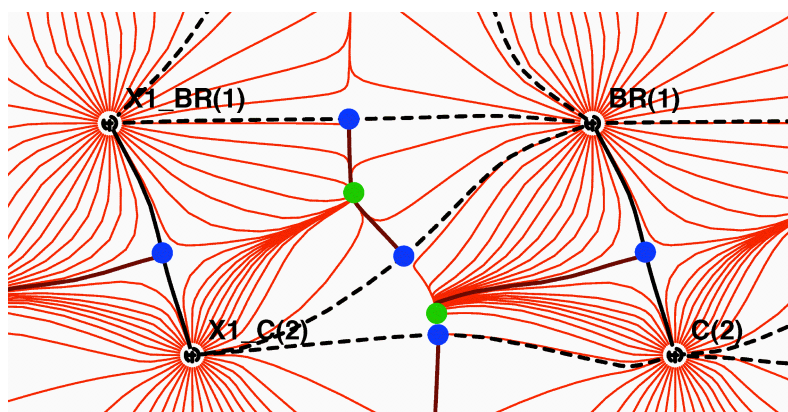


Figure S1. Bond paths between neighbouring pyridine rings along the polymer chain in **2**. Gradient trajectories (red), (3, -1) critical points (blue) and (3, 1) critical points (green) in the plane defined by C_{meta} of the pyridine ring, its halogen substituent, and the corresponding symmetry equivalent atoms defined by the symmetry operator $i = x, y, 1+z$.

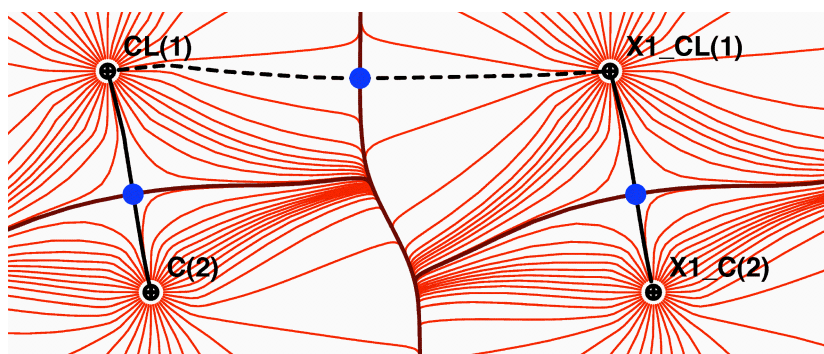


Figure S2. Bond paths between neighbouring pyridine rings along the polymer chain in one of the symmetrically independent strands in **4**. Gradient trajectories (red), (3, -1) and critical points (blue) in the plane defined by C_{meta} of the pyridine ring, its halogen substituent, and the corresponding symmetry equivalent atoms defined by the symmetry operator $i = x, y, 1+z$.

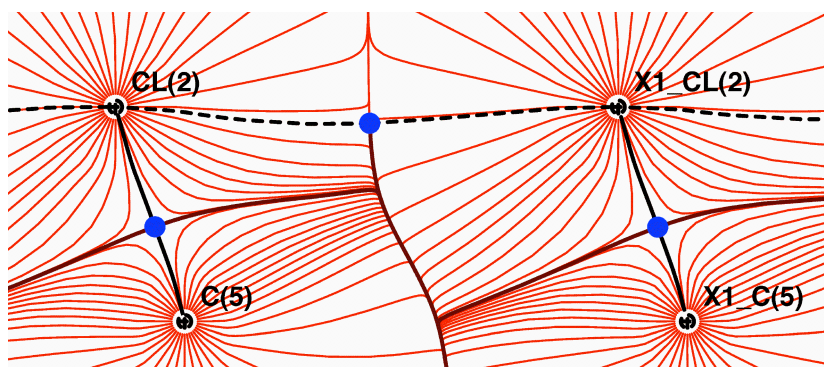


Figure S3. Bond paths between neighbouring pyridine rings along the polymer chain in the second of the symmetrically independent strands in **4**. Gradient trajectories (red), (3, -1) critical points (blue) in the plane defined by C_{meta} of the pyridine ring, its halogen substituent, and the corresponding symmetry equivalent atoms defined by the symmetry operator $i = x, y, 1+z$.