

Supporting information

An Empirical Correction for the Low Energy Contamination of Mirror Focused X-ray Data

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S1. Theoretical validation

S2. $k_{3\lambda}$ determination

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S6. Data for Figure 4

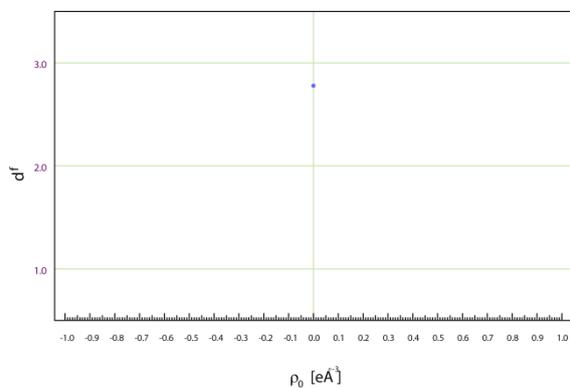
S7. Intensity comparison

S1. Theoretical validation

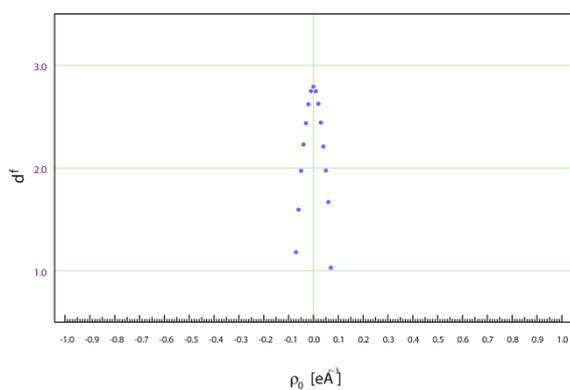
To visualize the effect of low energy contamination theoretical hkl were generated from the calculated structure factors of compound **1**. These hkl were then artificially contaminated by the addition of a certain fraction of the structure factor of all reflections hkl to their corresponding $3h3k3l$ reflections (fractions added: 0.2 % and 1.0 %). The differences between the model and the given data were calculated. Of course, this only adds a sharp peak of wavelength 3λ while in practice the blurred streaks of low energy photons contaminate as well.

Table S1 Comparison of the fractal dimension against residual density after artificial addition of contamination to theoretical data. The difference Fourier was calculated using 72x64x64 grid points, a σ -cutoff of 0 and a resolution of 0.40 Å.

0.0 % contamination



0.2 % contamination



1.0 % contamination

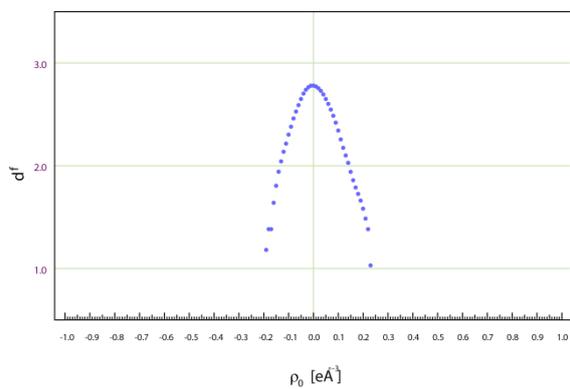
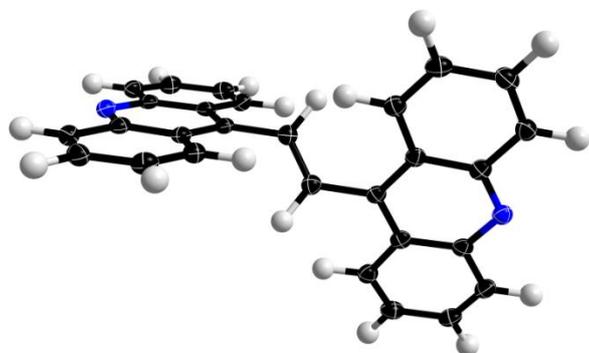


Table S2 Selected quality indicators after artificial addition of contamination to theoretical data.

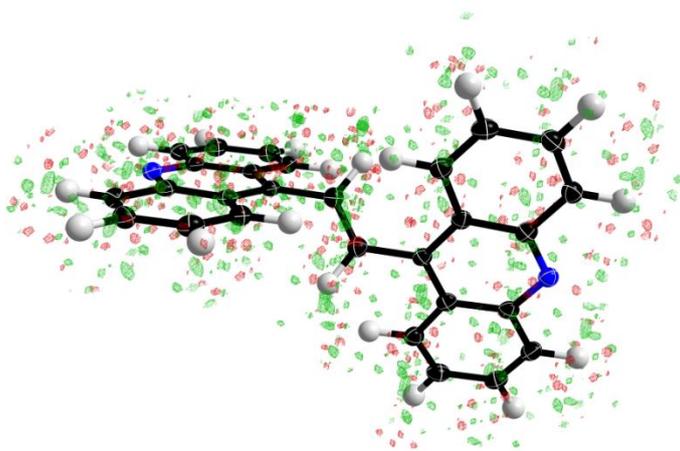
contamination [%]	0.0	0.2	1.0
Rw(F ²)	0.0	0.0019	0.0096
R(F ²)	0.0	0.0011	0.0054
residual density peak	0.001	0.074	0.238
residual density hole	-0.001	-0.074	-0.197
<i>N</i> (1) – <i>C</i> (1) [Å]	1.346758	1.346758	1.346758
<i>e</i> _{gross} [e]	0.00	13.96	36.88
<i>d</i> ^f (ρ_0):	2.7720	2.7909	2.7805
$\rho_{min}(d = 2)$ [eÅ ⁻³):	-0.0028	-0.0488	-0.1341
$\rho_{max}(d = 2)$ [eÅ ⁻³):	0.0028	0.0488	0.1430

Table S3 Residual densities calculated for the same model against different un-/contaminated data.

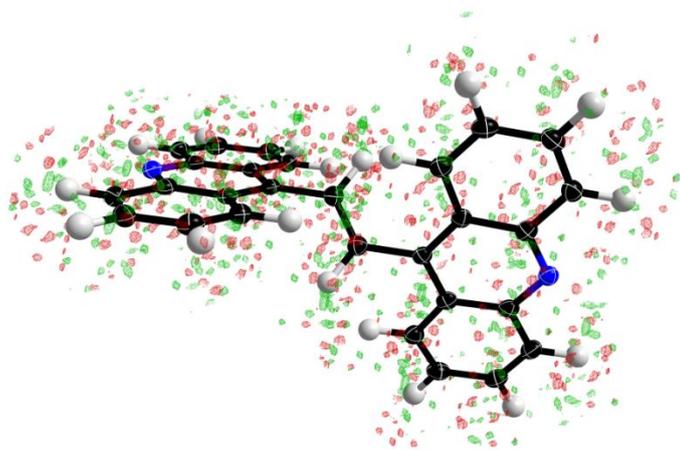
contamination: 0.0 %, map Level 0.001 e·Å⁻³



contamination: 0.2 %, map Level 0.048 e·Å⁻³

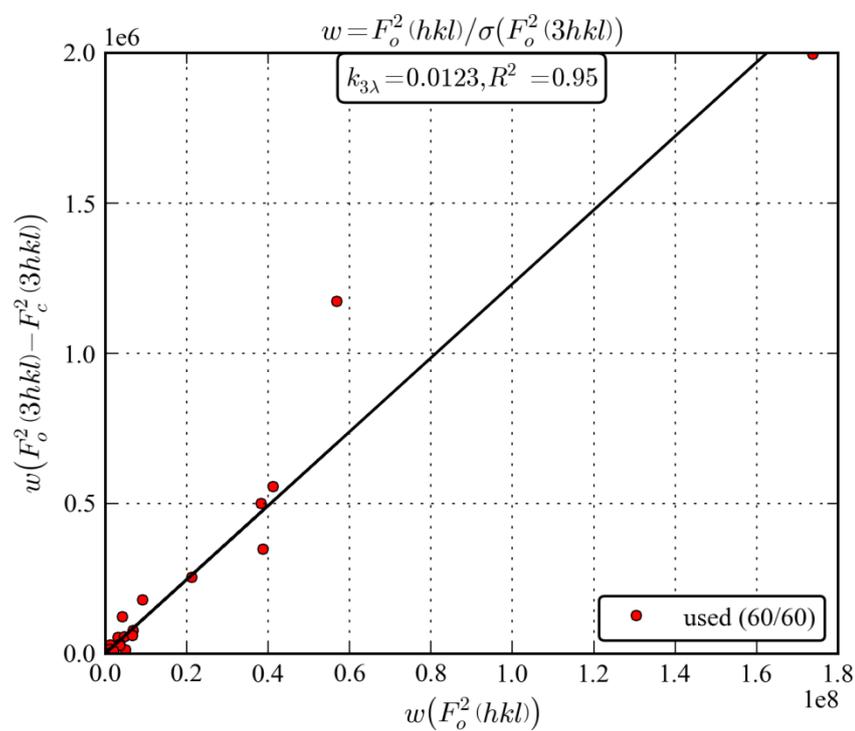


contamination: 1.0 %, map Level 0.137 e·Å⁻³

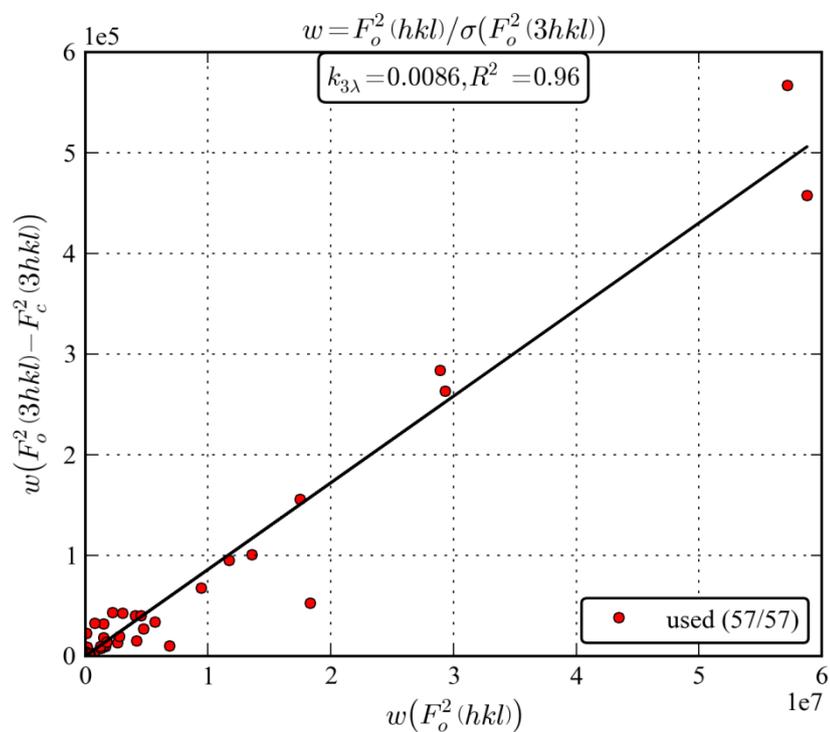


S2. $k_{3\lambda}$ determinationTable S4 plots for $k_{3\lambda}$ determination for structures 1 to 6

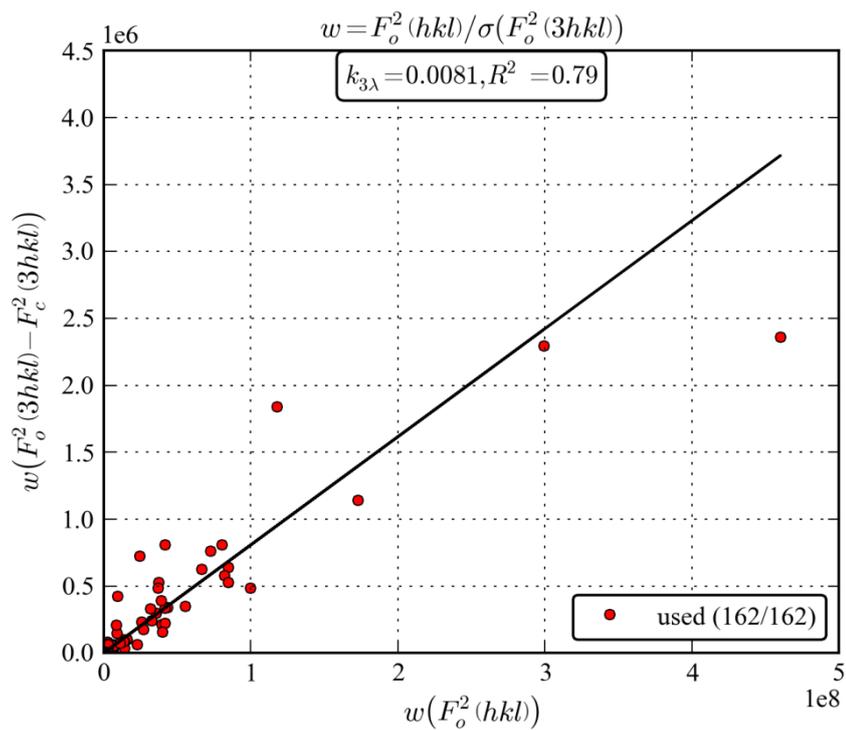
1



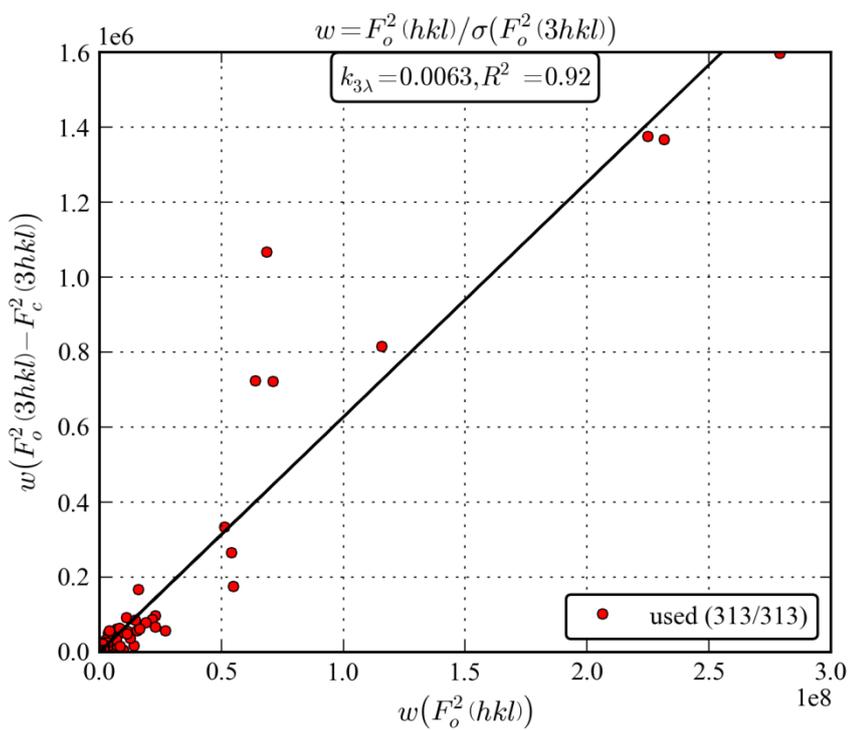
2



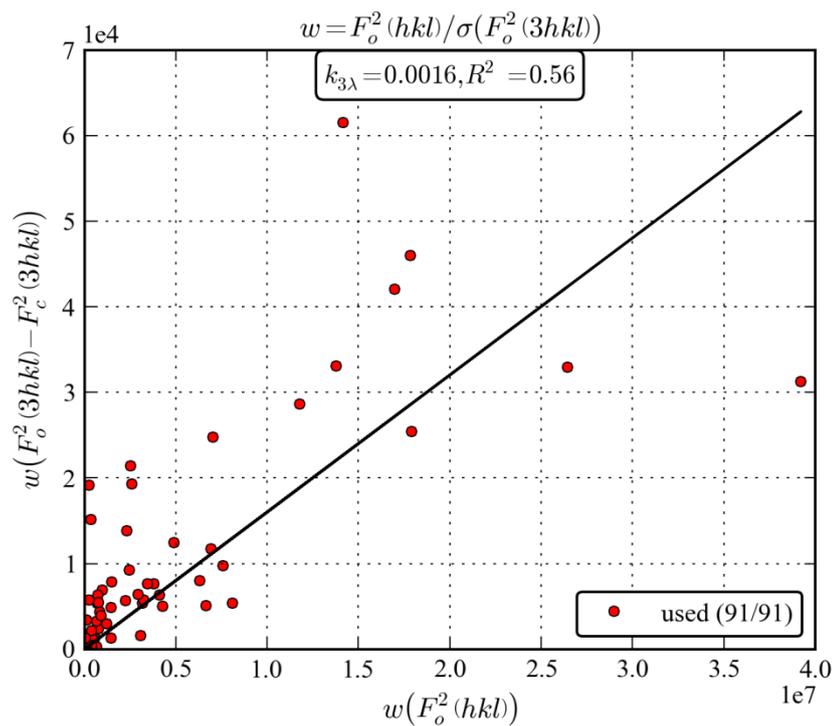
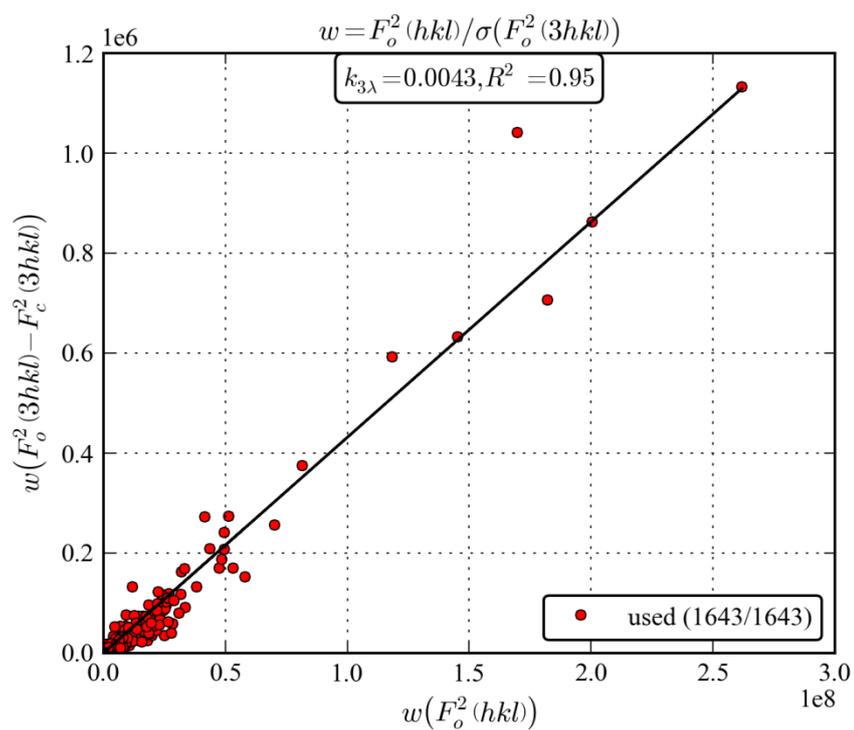
3



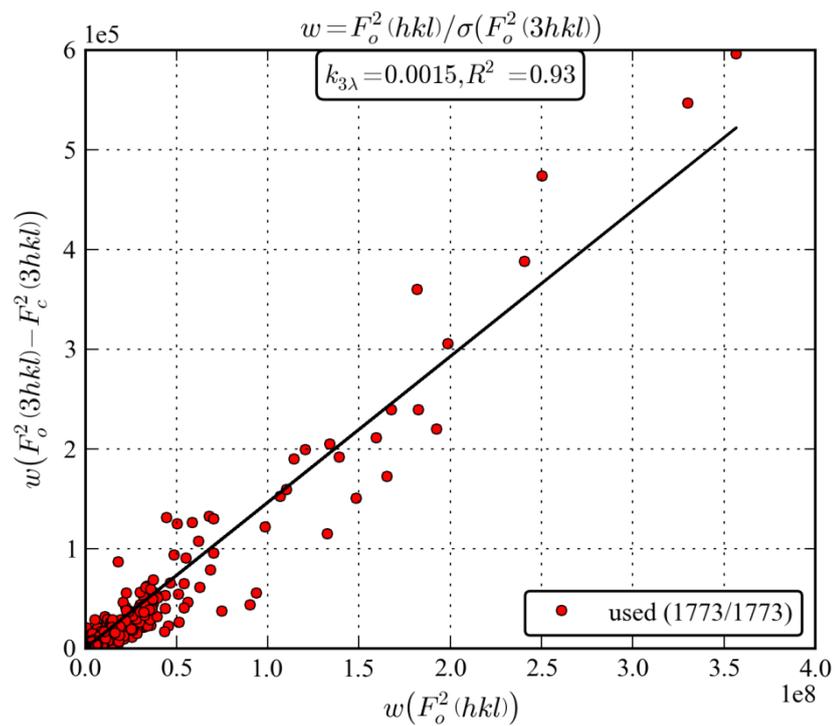
4



5

6 (μS)

6 (TXS)



S3. Crystallographic data**Table S5** Crystallographic data for compound **1**.

Empirical formula	C ₂₈ H ₁₈ N ₂		
Formula weight	382.44		
Temperature [K]	100(2)		
Wavelength [Å]	0.71073		
Crystal system	Monoclinic		
Space group	C2/c		
Z	4		
Density (calculated) [Mg/m ³]	1.383		
Absorption coefficient [mm ⁻¹]	0.081		
F(000)	800		
Crystal size [mm]	0.320 x 0.250 x 0.100		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F ²		
data correction	unfiltered, uncorrected	filtered	corrected (<i>k_{twin}</i>)
a [Å]	13.5559(13)	13.5537(16)	13.5559 (13)
b [Å]	12.2134(12)	12.2132(15)	12.2134 (12)
c [Å]	12.6643(12)	12.6619(15)	12.6643 (12)
β [°]	118.8339(17)	118.836(2)	118.8339 (17)
Volume [Å ³]	1836.8(3)	1836.1(4)	1836.8(3)
θ range for data collection [°]	2.392 to 25.500	2.392 to 25.556	2.392 to 25.500
Reflections collected	14302	14259	14302
Independent reflections	1697 [R(int) = 0.0254]	1707 [R(int) = 0.0262]	1697 [R(int) = 0.0253]
Completeness to θ = 25.242°	99.9 %	100.0 %	99.9 %
Max. and min. transmission	0.7452 and 0.7094	0.7452 and 0.7060	0.7452 and 0.7094
Data / restraints / parameters	1697 / 123 / 136	1707 / 123 / 136	1697 / 123 / 137
Goodness-of-fit on F ²	1.115	1.097	1.093
Final R indices [I>2σ(I)]	R1 = 0.0429 wR2 = 0.1237	R1 = 0.0393 wR2 = 0.1070	R1 = 0.0396 wR2 = 0.1081
R indices (all data)	R1 = 0.0463 wR2 = 0.1265	R1 = 0.0428 wR2 = 0.1105	R1 = 0.0435 wR2 = 0.1113
Largest diff. peak/hole [e·Å ⁻³]	0.239 / -0.199	0.270 / -0.194	0.274 / -0.178

Table S6 Crystallographic data for compound **2**.

Empirical formula	C ₁₂ H ₄ N ₄		
Formula weight	204.19		
Temperature [K]	100(2)		
Wavelength [Å]	0.71073		
Crystal system	Monoclinic		
Space group	C2/c		
Z	4		
Density (calculated) [Mg/m ³]	1.356		
Absorption coefficient [mm ⁻¹]	0.088		
F(000)	416		
Crystal size [mm]	0.180 x 0.130 x 0.060		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F ²		
data correction	unfiltered, uncorrected	filtered	corrected (<i>k_{twin}</i>)
a [Å]	8.896(2)	8.8840(12)	8.896(2)
b [Å]	6.9130(19)	6.9036(9)	6.9130(19)
c [Å]	16.439(5)	16.421(2)	16.439(5)
β [°]	98.290(3)	98.241(2)	98.290(3)
Volume [Å ³]	1000.5(5)	996.7(2)	1000.5(5)
θ range for data collection [°]	2.504 to 30.680	2.507 to 30.728	2.504 to 30.680
Reflections collected	10353	10375	10353
Independent reflections	1543 [R(int) = 0.0153]	1545 [R(int) = 0.0155]	1543 [R(int) = 0.0154]
Completeness to θ = 25.242°	99.9 %	100.0 %	99.9 %
Max. and min. transmission	0.7461 and 0.7182	0.7461 and 0.7184	0.7461 and 0.7182
Data / restraints / parameters	1543 / 0 / 73	1545 / 0 / 73	1543 / 0 / 74
Goodness-of-fit on F ²	1.090	1.084	1.087
Final R indices [I>2σ(I)]	R1 = 0.0360	R1 = 0.0338	R1 = 0.0338
	wR2 = 0.1059	wR2 = 0.0966	wR2 = 0.0943
R indices (all data)	R1 = 0.0377	R1 = 0.0362	R1 = 0.0357
	wR2 = 0.1075	wR2 = 0.0992	wR2 = 0.0963
Largest diff. peak/hole [e·Å ⁻³]	0.469 / -0.164	0.465 / -0.192	0.464 / -0.173

Table S7 Crystallographic data for compound **3**.

Empirical formula	C ₁₈ H ₁₇ CuO ₆		
Formula weight	392.86		
Temperature [K]	100(2)		
Wavelength [Å]	0.71073		
Crystal system	Monoclinic		
Space group	C2/c		
Z	8		
Density (calculated) [Mg/m ³]	1.538		
Absorption coefficient [mm ⁻¹]	1.318		
F(000)	1616		
Crystal size [mm]	0.140 x 0.100 x 0.050		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F ²		
data correction	unfiltered, uncorrected	filtered	corrected (<i>k_{twin}</i>)
a [Å]	9.7935(7)	9.7936(7)	9.7935(7)
b [Å]	19.0055(13)	18.9973(12)	19.0055(13)
c [Å]	18.2997(13)	18.2982(12)	18.2997(13)
β [°]	94.7996(11)	94.8400(10)	94.7996(11)
Volume [Å ³]	3394.2(4)	3392.3(4)	3394.2(4)
θ range for data collection [°]	2.143 to 28.426	2.144 to 28.332	2.143 to 28.426
Reflections collected	29203	29137	29203
Independent reflections	4282 [R(int) = 0.0282]	4233 [R(int) = 0.0329]	4282 [R(int) = 0.0280]
Completeness to θ = 25.242°	100.0 %	100.0 %	100.0 %
Max. and min. transmission	0.7457 and 0.6951	0.7457 and 0.6935	0.7457 and 0.6951
Data / restraints / parameters	4282 / 652 / 300	4233 / 652 / 300	4282 / 652 / 301
Goodness-of-fit on F ²	1.069	1.034	1.033
Final R indices [I>2σ(I)]	R1 = 0.0273	R1 = 0.0276	R1 = 0.0260
	wR2 = 0.0676	wR2 = 0.0642	wR2 = 0.0619
R indices (all data)	R1 = 0.0342	R1 = 0.0380	R1 = 0.0328
	wR2 = 0.0704	wR2 = 0.0681	wR2 = 0.0650
Largest diff. peak/hole [e·Å ⁻³]	0.390 and -0.281	0.338 and -0.294	0.359 and -0.297

Table S8 Crystallographic data for compound **4**.

Empirical formula	$C_{34}H_{26}MgN_4O_4$		
Formula weight	578.90		
Temperature [K]	100(2)		
Wavelength [Å]	0.71073		
Crystal system	Monoclinic		
Space group	$P2_1/n$		
Z	4		
Density (calculated) [Mg/m ³]	1.361		
Absorption coefficient [mm ⁻¹]	0.111		
F(000)	1208		
Crystal size [mm]	0.190 x 0.150 x 0.110		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F^2		
data correction	unfiltered, uncorrected	filtered	corrected (k_{twin})
a [Å]	11.3068(12)	11.3182(14)	11.3068(12)
b [Å]	14.9595(16)	14.9745(18)	14.9595(16)
c [Å]	16.7252(17)	16.744(2)	16.7252(17)
β [°]	93.0500(15)	93.044(2)	93.0500(15)
Volume [Å ³]	2825.0(5)	2833.9(6)	2825.0(5)
θ range for data collection [°]	1.828 to 30.615	1.826 to 30.816	1.828 to 30.615
Reflections collected	36155	36495	36155
Independent reflections	8694 [R(int) = 0.0265]	8866 [R(int) = 0.0310]	8694 [R(int) = 0.0264]
Completeness to $\theta = 25.242^\circ$	99.9 %	100.0 %	99.9 %
Max. and min. transmission	0.7461 and 0.6883	0.7461 and 0.6789	0.7461 and 0.6883
Data / restraints / parameters	8694 / 408 / 392	8866 / 408 / 392	8694 / 408 / 393
Goodness-of-fit on F^2	1.030	1.034	1.017
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0407	R1 = 0.0403	R1 = 0.0399
	wR2 = 0.1090	wR2 = 0.1046	wR2 = 0.1030
R indices (all data)	R1 = 0.0483	R1 = 0.0499	R1 = 0.0475
	wR2 = 0.1149	wR2 = 0.1112	wR2 = 0.1091
Largest diff. peak/hole [$e \cdot \text{Å}^{-3}$]	0.533 / -0.250	0.447 / -0.255	0.534 / -0.248

Table S9 Crystallographic data for compound **5**.

Empirical formula	C ₁₁ H ₁₀ O ₂ S		
Formula weight	206.25		
Temperature [K]	293(2)		
Wavelength [Å]	0.71073		
Crystal system	Orthorhombic		
Space group	P2 ₁ 2 ₁ 2 ₁		
Z	4		
Density (calculated) [Mg/m ³]	1.381		
Absorption coefficient [mm ⁻¹]	0.294		
F(000)	432		
Crystal size [mm]	0.250 x 0.250 x 0.250		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F ²		
data correction	unfiltered, uncorrected	filtered	corrected (<i>k_{twin}</i>)
a [Å]	5.96330(10)	5.9641(2)	5.96330(10)
b [Å]	9.0417(2)	9.0419(2)	9.0417(2)
c [Å]	18.4007(4)	9.0419(2)	18.4007(4)
Volume [Å ³]	992.14(3)	992.40(5)	992.14(3)
θ range for data collection [°]	2.214 to 28.308	2.213 to 28.283	2.214 to 28.308
Reflections collected	15091	15101	15091
Independent reflections	2456 [R(int) = 0.0199]	2453 [R(int) = 0.0199]	2456 [R(int) = 0.0199]
Completeness to θ = 25.242°	100.0 %	100.0 %	100.0 %
Max. and min. transmission	0.7457 and 0.7096	0.7457 and 0.7124	0.7457 and 0.7096
Data / restraints / parameters	2456 / 0 / 129	2453 / 0 / 129	2456 / 0 / 130
Goodness-of-fit on F ²	1.089	1.105	1.078
Final R indices [I > 2σ(I)]	R1 = 0.0254 wR2 = 0.0674	R1 = 0.0252 wR2 = 0.0667	R1 = 0.0249 wR2 = 0.0661
R indices (all data)	R1 = 0.0262 wR2 = 0.0680	R1 = 0.0261 wR2 = 0.0674	R1 = 0.0256 wR2 = 0.0668
Largest diff. peak/hole [e·Å ⁻³]	0.219 and -0.197	0.210 and -0.187	0.218 and -0.184
Absolute structure parameter	0.034(14)	0.049(16)	0.035(15)

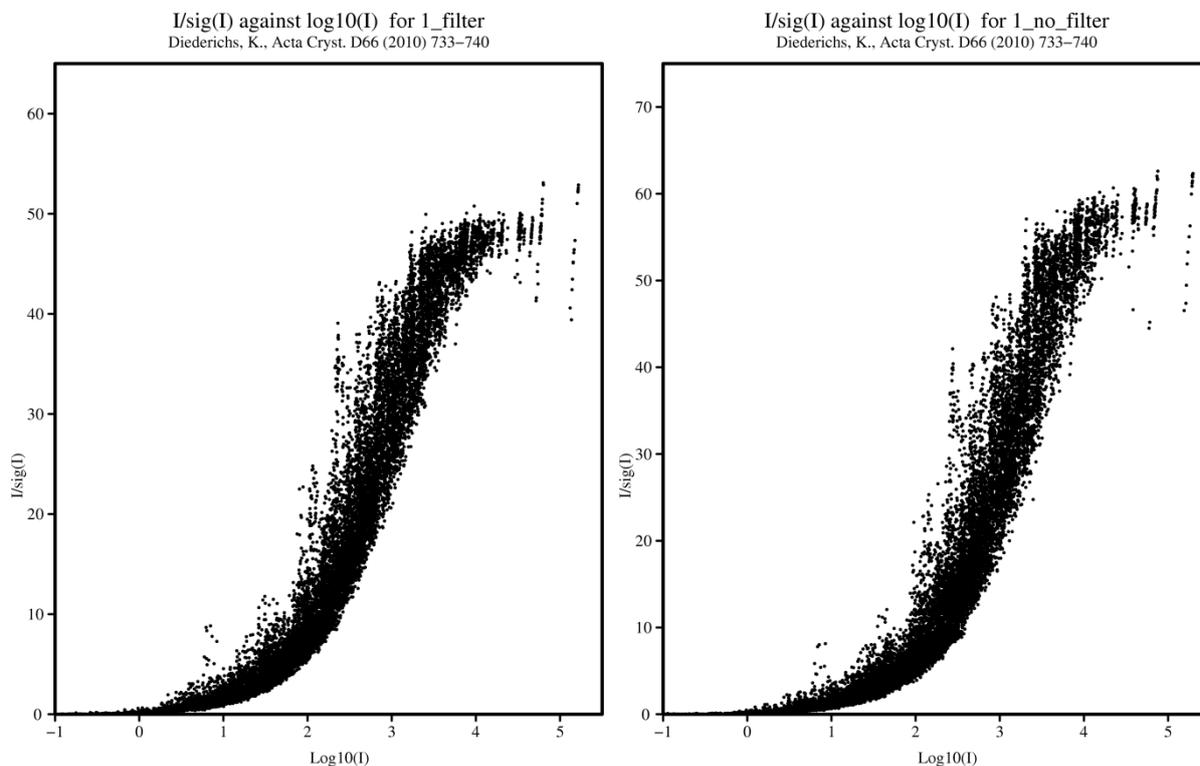
Table S10 Crystallographic data for compound **6**.

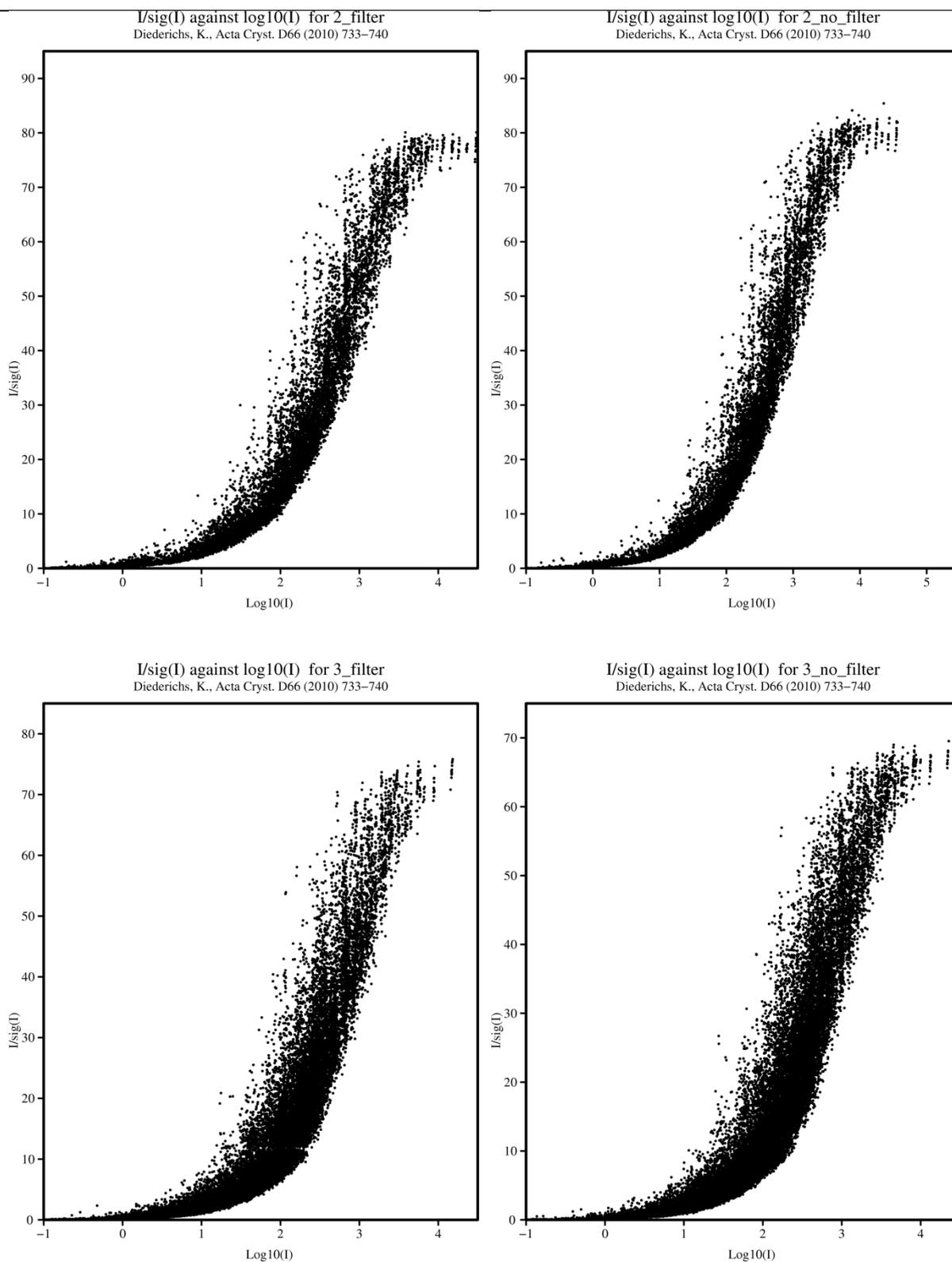
Empirical formula	C ₂₆ H ₁₉ PS	
Formula weight	394.44	
Temperature [K]	100(2)	
Wavelength [Å]	0.71073	
Crystal system	Triclinic	
Space group	<i>P</i> $\bar{1}$	
Z	4	
Density (calculated) [Mg/m ³]	1.328	
Absorption coefficient [mm ⁻¹]	0.254	
F(000)	824	
Crystal size [mm]	0.100 x 0.100 x 0.150	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
a [Å]	10.215(2)	
b [Å]	12.322(2)	
c [Å]	17.351(3)	
α [°]	101.57(2)	
β [°]	91.25(2)	
γ [°]	112.02(2)	
Volume [Å ³]	1972.2(7)	
θ range for data collection [°]	1.205 to 52.955	
Reflections collected	272253	
Independent reflections	45758 [R(int) = 0.0149]	
Completeness to $\theta = 25.242^\circ$	99.8 %	
Max. and min. transmission	0.7504 and 0.7163	
Data / restraints / parameters	45758 / 0 / 815	
data correction	unfiltered, uncorrected	corrected ($k_{3,\lambda}$)
Goodness-of-fit on F ²	1.67	1.398
Final R indices [I>2sigma(I)]	0.021	0.020
R indices (all data)	0.021	0.020
Largest diff. peak/hole [e·Å ⁻³]	0.291 and -0.208	0.295 and -0.207

S4. Systematic errors

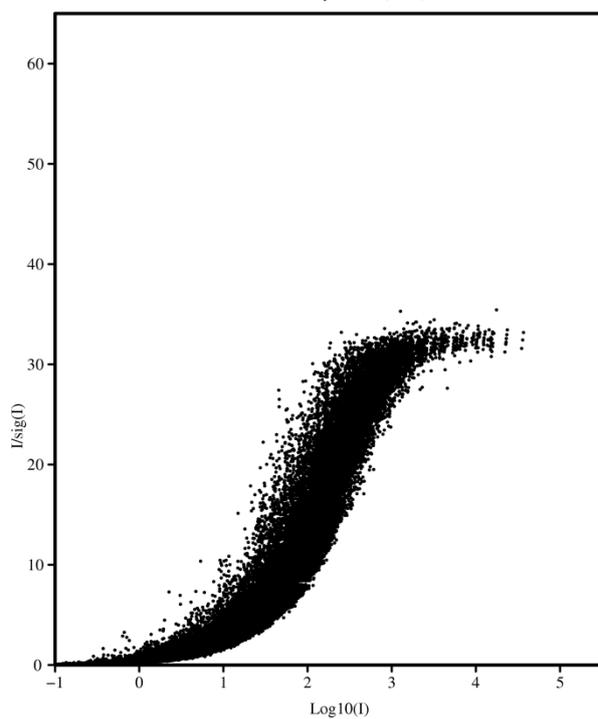
In 2010, Diederichs suggested an indicator which is calculated for the unmerged data after the data reduction to be used to estimate the systematic instrument error of the X-ray source. The value of this indicator is the highest $[I/\sigma(I)]$ value the given experimental setup can produce.

Table S11 Systematic errors.

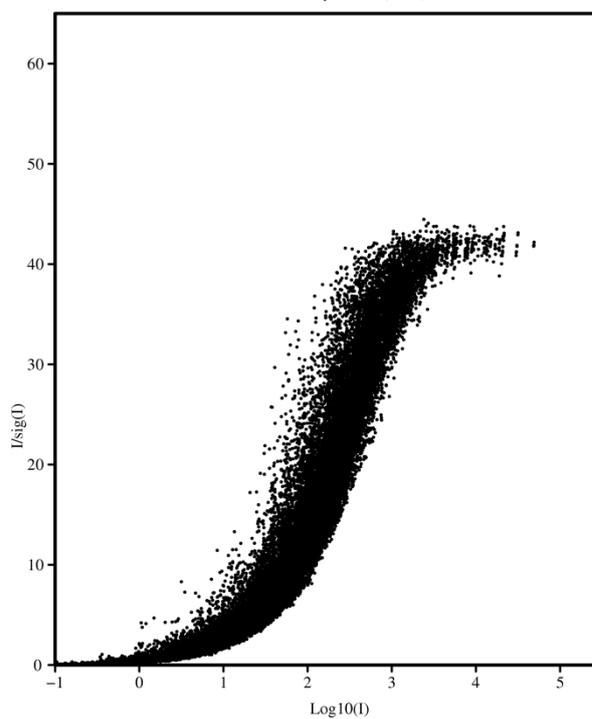




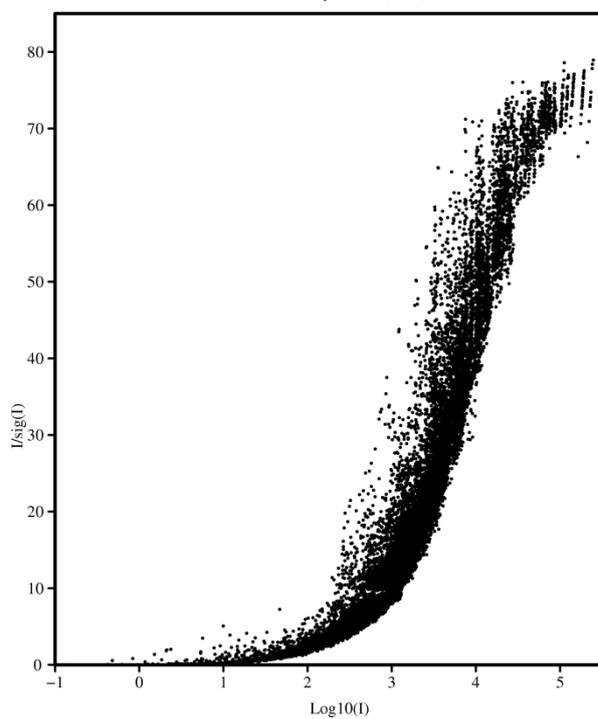
$I/\sigma(I)$ against $\log_{10}(I)$ for 4_filter
Diederichs, K., Acta Cryst. D66 (2010) 733–740



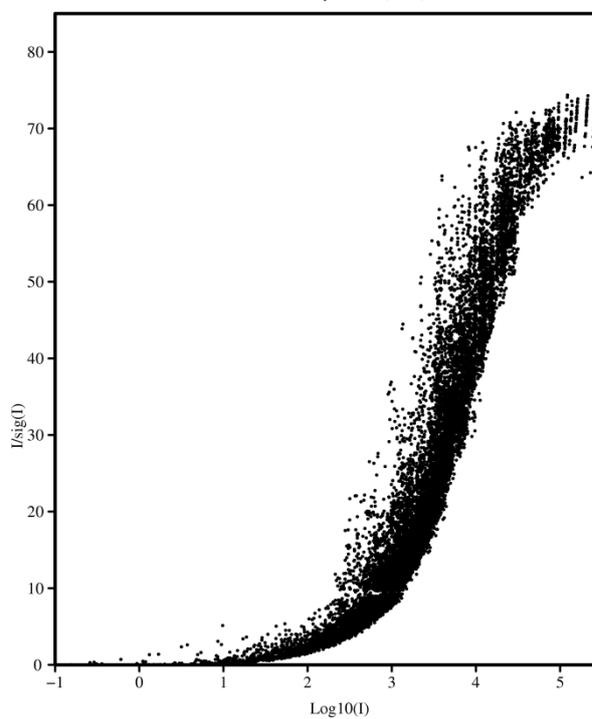
$I/\sigma(I)$ against $\log_{10}(I)$ for 4_no_filter
Diederichs, K., Acta Cryst. D66 (2010) 733–740



$I/\sigma(I)$ against $\log_{10}(I)$ for 5_filter
Diederichs, K., Acta Cryst. D66 (2010) 733–740



$I/\sigma(I)$ against $\log_{10}(I)$ for 5_no_filter
Diederichs, K., Acta Cryst. D66 (2010) 733–740



S5. $k_{3\lambda}$ default values**Table S12** Comparison of quality indicators for models derived from data individually corrected or corrected with a *default value* of 1% for selected structures.

Formula Sum	$\Delta(C - C)$ [Å]	R1	k
C ₂₈ H ₃₈ N ₄	0.0020	0.0443	0.0075
	0.0020	0.0444	0.0100
C ₁₄ H ₂₃ N ₃	0.0016	0.0417	0.0170
	0.0016	0.0421	0.0100
C ₁₅ H ₁₀ N ₂ O ₂	0.0016	0.0368	0.0150
	0.0016	0.0374	0.0100
C ₃₄ H ₂₆ MgN ₄ O ₄	0.0018	0.0412	0.0120
	0.0018	0.0413	0.0100
C ₇₀ H ₈₄ N ₄ O ₂ Si ₂	0.0022	0.0430	0.0042
	0.0023	0.0435	0.0100
C ₁₆ H ₁₅ N ₃ OS	0.0041	0.0339	0.0079
	0.0041	0.0339	0.0100
C ₁₄ H ₉ N ₃ S ₂	0.0046	0.0312	0.0075
	0.0046	0.0311	0.0100
C ₁₈₈ H ₁₅₂ Al ₁₀ Cl ₁₀ N ₂₀ O ₂₀	0.0029	0.0398	0.0097
	0.0029	0.0398	0.0100
C ₁₆ H ₁₂ AlClN ₂ S ₂	0.0034	0.0397	0.0136
	0.0034	0.0399	0.0100
C ₁₉ H ₃₁ GeKN ₂ OS ₂	0.0033	0.0303	0.0063
	0.0033	0.0304	0.0100

S6. Data for Figure 4

Table S13 Data for Figure 4: Transmission-ratio versus $k_{3\lambda}$ for a collection of different structures.

Formula sum	Space group	<i>e.s.d.</i> (C–C) [Å]	R1	wR2	transmission ratio	BASF	<i>e.s.d.</i> (BASF)	source
C ₂₃ H ₂₄ O ₂	<i>C2/c</i>	0.0017	0.0333	0.0881	0.940561	0.00988	0.00036	I μ S
C ₁₄ H ₂₇ N ₃	<i>C2/c</i>	0.0036	0.0542	0.1607	0.909787	0.01015	0.00055	I μ S
C ₂₈ H ₄₄ Li ₂ N ₆	<i>P2₁/n</i>	0.0019	0.0408	0.1113	0.955869	0.00886	0.00037	I μ S
C ₇₃ H ₁₀₀ Cl ₄ Li ₂ O ₈ S ₆ Zn ₄	<i>P$\bar{1}$</i>	0.0054	0.0380	0.1012	0.897611	0.00484	0.00022	I μ S
C ₃₀ H ₁₇ N O ₄	<i>P2₁/c</i>	0.0020	0.0411	0.1056	0.954667	0.01050	0.00041	I μ S
C ₁₇ H ₁₄ O ₂	<i>P2₁/c</i>	0.0015	0.0387	0.1104	0.956702	0.01092	0.00043	I μ S
C ₁₂ H ₁₈ N ₂ O ₆	<i>P2₁2₁2₁</i>	0.0023	0.034	0.0879	0.771880	0.01075	0.00049	I μ S
C ₂₁ H ₁₆ O	<i>Pbca</i>	0.0000	0.0643	0.1764	0.834809	0.01159	0.00070	I μ S
C ₂₁ H ₁₈ O	<i>P2₁/n</i>	0.0017	0.0380	0.0976	0.939370	0.00680	0.00017	I μ S
C ₁₇ H ₁₆ N ₄	<i>P$\bar{1}$</i>	0.0017	0.0403	0.1111	0.913504	0.00766	0.00047	I μ S
C ₁₅ H ₁₀ N ₂ O ₂	<i>P2₁/c</i>	0.0016	0.0367	0.1006	0.934844	0.01294	0.00041	I μ S
C ₁₈₈ H ₁₅₂ Al ₁₀ Cl ₁₀ N ₂₀ O ₂₀	<i>C2/m</i>	0.0029	0.0393	0.1015	0.947411	0.01064	0.00043	I μ S
C ₁₆ H ₁₂ Al Cl N ₂ S ₂	<i>P$\bar{1}$</i>	0.0034	0.0396	0.0990	0.925543	0.01511	0.00082	I μ S
C ₁₅ H ₁₀ N ₂ O S	<i>P$\bar{1}$</i>	0.0017	0.0343	0.0896	0.975204	0.00955	0.00058	I μ S
C ₁₆ H ₁₅ N ₃ O S	<i>P2₁</i>	0.0041	0.0338	0.0848	0.925305	0.00730	0.00038	I μ S
C ₁₇ H ₁₄ N ₂ O ₂	<i>P$\bar{1}$</i>	0.0021	0.0380	0.0979	0.925305	0.00766	0.00036	I μ S
C ₁₄ H ₉ N ₃ S ₂	<i>P2₁</i>	0.0046	0.0310	0.0804	0.943252	0.01064	0.00085	I μ S
C ₇₁ H ₆₀ N ₁₂ S ₈	<i>P$\bar{1}$</i>	0.0024	0.0350	0.0880	0.955338	0.00623	0.00037	I μ S
C ₁₆ H ₁₆ Br Li N ₄	<i>P2₁/c</i>	0.0020	0.0194	0.0510	0.896043	0.00559	0.00033	I μ S
C ₂₈ H ₃₈ N ₄	<i>P2₁/n</i>	0.0020	0.0446	0.1264	0.918814	0.00642	0.00043	I μ S
C ₇₀ H ₈₄ N ₄ O ₂ Si ₂	<i>P2₁/n</i>	0.0022	0.0425	0.1063	0.925171	0.00355	0.00023	I μ S
C ₁₉ H ₃₁ Ge K N ₂ O S ₂	<i>P2₁/c</i>	0.0033	0.0302	0.0706	0.908006	0.00532	0.00030	I μ S
C ₂₅ H ₃₉ Cl ₂ N ₃ Si	<i>P2₁/c</i>	0.0019	0.0305	0.0803	0.910139	0.00339	0.00021	I μ S
C ₂₂ H ₅₁ Cl N ₂ Si ₆	<i>P2₁/c</i>	0.0030	0.0402	0.1025	0.916723	0.00565	0.00030	I μ S
C ₈ H ₁₄ Br ₂ S ₂	<i>P2₁/c</i>	0.0030	0.0223	0.0468	0.781950	0.00784	0.00038	I μ S
C ₉₁ H ₈₈ O ₂₀	<i>P2₁/c</i>	0.0020	0.0409	0.1190	0.921797	0.00275	0.00010	I μ S
C ₂₁ H ₁₈ O	<i>Cc</i>	0.0033	0.0360	0.0824	0.910408	0.00808	0.00061	I μ S
C ₁₀ H ₆ N ₂	<i>P2₁/n</i>	0.0018	0.0344	0.0932	0.910408	0.01352	0.00067	I μ S
C ₃₄ H ₂₆ Mg N ₄ O ₄	<i>P2₁/n</i>	0.0019	0.0416	0.1105	0.922799	0.00903	0.00025	I μ S
C ₂₁ H ₂₅ P S	<i>P2₁/c</i>	0.0021	0.0361	0.0876	0.948095	0.00647	0.00028	I μ S

C ₅₂ H ₈₂ Cl ₂ N ₈ Si ₄	<i>P2₁/n</i>	0.0034	0.0373	0.1041	0.844316	0.00628	0.00028	IμS
C ₆₇ H ₁₀₀ N ₈ O ₆ Si ₄	<i>P2₁/n</i>	0.0030	0.0423	0.1053	0.919909	0.00718	0.00024	IμS
C ₁₄ H ₂₃ N ₃	<i>Pbca</i>	0.0015	0.0410	0.1221	0.919909	0.01393	0.00046	IμS
C ₂₂ H ₂₆ O ₈	<i>P2₁/n</i>	0.0012	0.0368	0.1037	0.947192	0.00213	0.00020	TXS
C ₃₂ H ₂₆ B F ₁₀ N O P	<i>C2/c</i>	0.0010	0.0372	0.1178	0.959487	0.00157	0.00006	TXS
C ₃₂ H ₂₇ B F ₁₀ N P	<i>P2₁/n</i>	0.0006	0.0367	0.1236	0.964414	0.00158	0.00004	TXS
C ₂₀ H ₁₄ S ₂	<i>P2₁/n</i>	0.0030	0.0444	0.1166	0.931303	0.00339	0.00035	TXS
C ₂₆ H ₃₄ N ₄	<i>P2₁/c</i>	0.0016	0.0385	0.1109	0.963380	0.00315	0.00025	TXS
C ₂₆ H ₃₄ N ₄	<i>P2₁/c</i>	0.0013	0.0417	0.1202	0.942478	0.00323	0.00029	TXS
C ₁₀ H ₁₄ N ₂ O ₅	<i>P2₁/c</i>	0.0018	0.0335	0.0800	0.941524	0.00299	0.00022	TXS
C ₁₀ H ₁₀ S ₂	<i>P2₁/n</i>	0.0024	0.0328	0.0826	0.877650	0.00311	0.00025	TXS
C ₃₀ H ₂₈ N ₂ O ₄	<i>P$\bar{1}$</i>	0.0021	0.0420	0.1032	0.920714	0.00300	0.00022	TXS
C ₁₂ H ₁₁ N O	<i>C2/c</i>	0.0020	0.0383	0.0935	0.952509	0.00419	0.00044	TXS
C ₂₄ H ₂₆ O ₆	<i>Pbca</i>	0.0020	0.0397	0.1051	0.827609	0.00271	0.00029	TXS
C ₄₂ H ₄₉ Cl N ₂ O Si	<i>P2₁/c</i>	0.0031	0.0404	0.1259	0.841095	0.00376	0.00029	TXS
C ₇₀ H ₈₄ N ₄ O ₂ Si ₂	<i>P2₁/n</i>	0.0022	0.0424	0.1066	0.925171	0.00355	0.00023	TXS
C ₂₅ H ₃₉ Cl ₂ N ₃ Si	<i>P2₁/c</i>	0.0019	0.0305	0.0804	0.910139	0.00339	0.00021	TXS
C ₁₇ H ₁₉ Al N ₂	<i>Pbca</i>	0.0029	0.0446	0.1051	0.788407	0.00280	0.00027	TXS
C ₂₄ H ₁₂ F ₁₂ O ₃	<i>C2/c</i>	0.0030	0.0489	0.1161	0.767404	0.00256	0.00034	TXS
C ₉₁ H ₈₈ O ₂₀	<i>P2₁/c</i>	0.0020	0.0411	0.1196	0.921797	0.00276	0.00010	TXS
C ₆ H ₉ Br O ₄	<i>P2₁2₁</i>	0.0030	0.0114	0.0305	0.692555	0.00209	0.00039	TXS
C ₂₁ H ₄₁ N ₃ Si ₃	<i>P$\bar{1}$</i>	0.0018	0.0303	0.0826	0.958820	0.00187	0.00015	TXS
H ₄ Na ₂ O ₆ W	<i>Pbca</i>	0.0000	0.0146	0.0329	0.717586	0.00127	0.00006	TXS
C ₄ Co Sc ₃	<i>Immm</i>	0.0006	0.0118	0.0329	0.821709	0.00073	0.00014	TXS
C ₁₃ H ₁₀ F ₃ I O ₃ S	<i>P2₁/c</i>	0.0042	0.0201	0.0473	0.913603	0.00448	0.00035	TXS
C ₃₃ H ₄₁ I ₃ N ₂ Pd	<i>P2₁/n</i>	0.0047	0.0229	0.0504	0.908640	0.00242	0.00022	TXS
C ₂₆ H ₅₂ N ₂ Rb ₂ Si ₄	<i>C2/c</i>	0.0030	0.0303	0.0645	0.741322	0.00117	0.00025	TXS
C _{12.46} H ₄₈ K ₂ N _{5.54} Si ₄	<i>P2₁/n</i>	0.0000	0.0218	0.0580	0.912798	0.00243	0.00018	TXS
C ₁₈ H ₃₀ Cs ₂ O ₄	<i>Pbca</i>	0.0038	0.0243	0.0599	0.568556	0.00021	0.00012	TXS
C ₅ H ₈ Cs N	<i>Pnma</i>	0.0030	0.0180	0.0412	0.374883	0.00015	0.00010	TXS
C ₃₄ H ₄₆ N ₄ O ₂ Rb ₂	<i>Pbca</i>	0.0050	0.0330	0.0858	0.701503	0.00216	0.00037	TXS
C ₃₄ H ₂₆ Mg N ₄ O ₄	<i>P2₁/n</i>	0.0016	0.0399	0.1091	0.922530	0.00515	0.00023	TXS
C ₁₂ H ₄ N ₄	<i>C2/c</i>	0.0011	0.0338	0.0963	0.962606	0.00816	0.00047	TXS
C ₁₈ H ₁₇ Cu O ₆	<i>C2/c</i>	0.0026	0.0260	0.0650	0.932144	0.00760	0.00029	TXS
C ₂₈ H ₁₈ N ₂	<i>C2/c</i>	0.0021	0.0396	0.1113	0.951959	0.01167	0.00070	TXS
C ₁₁ H ₁₀ O ₂ S	<i>P2₁2₁</i>	0.0024	0.0249	0.0668	0.951589	0.00184	0.00023	TXS

S7. Intensity comparison**Table S14** Comparison of the significances and the raw intensities of the filtered and the unfiltered data for all investigated compounds. Filter: Aluminium foil, thickness 100 μm .

		XPREP		SAINT	
		I/ σ	Δ (%)	$\langle I \rangle$	Δ (%)
1	no filter	48.11 [*]	3.51	1904.95	16.87
	filter [#]	46.42		1583.56	
2	no filter	61.12	5.96	288.47	26.47
	filter	57.48		212.11	
3	no filter	36.39	13.38	700.42	15.64
	filter	31.52		590.84	
4	no filter	25.40	19.21	327.04	32.63
	filter	20.52		220.34	
5	no filter	69.57	0.86	7318.76	9.75
	filter	68.97		6605.07	

[#] 3 layers were needed to block the contamination (300 μm)

^{*} exposure time reduced (from 30s to 20s) to avoid detector saturation