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Does the size of a crystal matter in an X-ray crystal structure analysis of a small molecule?

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Table S1 **Refinement of $C_7H_8FN_3$ ($P2_1/c$ space group; μ = 0.36 mm^{-1})**

Unit cell (Å, °)	11.9470(8) 5.5093(3) 12.4564(7) 91.712(6)	11.9525(8) 5.5111(3) 12.4566(7) 91.699(5)	11.9359(7) 5.5005(3) 12.4375(7) 91.776(5)	11.9533(8) 5.5087(4) 12.4688(8) 91.699(6)
Volume (Å^3)	819.51(8)	820.17(8)	816.17(8)	820.7(1)
Size, mm	0.71x0.36x0.18	0.47x0.40x0.17	0.34x0.28x0.17	0.30x0.25x0.15
Crystal *vol*., mm^3	0.0396	0.0241	0.0117	0.0090
Eqiv. *r*, mm	0.21	0.18	0.14	0.13
min./max. trans. (Multi-scan T_{min})	0.846 – 0.942 (0.788)	0.874 – 0.945 (0.799)	0.910 – 0.945 (0.869)	0.915 – 0.952 (0.920)
No. reflns.	1892	1892	1881	1894
Av. R_{eqiv}, $\sigma(I/I_{net})$	0.035, 0.040	0.037, 0.040	0.041, 0.043	0.041, 0.048
No. $I>2\sigma(I)$ reflns.	1536	1513	1475	1475
Av. R_{eqiv}, $\sigma(I/I_{net})$	27.58	27.58	27.54	27.58
$2\theta_{max}$	0.035	0.036	0.036	0.037
R	$(0.0336P)^2$+0.4252*P*	$(0.0383P)^2$+0.3747*P*	$(0.0424P)^2$+0.3065*P*	$(0.0367P)^2$+0.3187*P*
Weighting	-0.26 – 0.26	-0.24 – 0.28	-0.27 – 0.32	-0.26 – 0.26
e map, min./max.				

Table S2 **Refinement of $C_{20}H_{25}Br$ ($P2_12_12_1$ space group; μ = 2.72 mm^{-1})**

Unit cell (Å, °)	5.6130(4) 8.5301(5) 31.435(2)	5.6011(3) 8.5219(4) 31.474(1)	5.6104(4) 8.5238(4) 31.496(2)	5.6112(4) 8.5333(4) 31.439(1)
Volume (Å^3)	1505.1(2)	1502.3(1)	1506.2(2)	1505.4(1)
Size, mm	0.85x0.36x0.22	0.51x0.39x0.23	0.44x0.28x0.22	0.25x0.20x0.20
Crystal *vol*., mm^3	0.0536	0.0293	0.0153	0.0073
Eqiv. *r*, mm	0.23	0.19	0.15	0.12
min./max. trans. (Multi-scan T_{min})	0.251 – 0.601 (0.252)	0.392 – 0.619 (0.696)	0.460 – 0.633 (0.759)	0.598 – 0.647 (0.869)
No. reflns.	3488	3479	3486	3454
Av. R_{eqiv}, $\sigma(I/I_{net})$	0.044, 0.078	0.034, 0.042	0.047, 0.068	0.047, 0.068
No. $I>2\sigma(I)$ reflns.	3007	3169	3018	3005
$2\theta_{max}$	27.57	27.59	27.60	27.60
R	0.048	0.035	0.047	0.047
Weighting	$(0.0335P)^2$	$(0.0336P)^2$+0.9819*P*	$(0.0332P)^2$+1.2196*P*	$(0.0332P)^2$+1.2196*P*
Flack parameter	0.01(1)	0.01(1)	0.02(2)	0.02(2)
e map, min./max.	-0.84 – 1.06	-0.67 – 0.96	-0.96 – 1.13	-0.97 – 1.15

Table S3 **Refinement of $Cu(H_2O)_2(C_6H_{12}N_4)(C_7H_3N_2O_6)_2{\cdot}2H_2O$ (*C*2/*c* space group; μ = 0.97 mm^{-1})**

Unit cell (Å, °)	23.002(1)	23.015(1)	23.014(1)	23.025(1)
	8.9753(4)	8.9752(3)	8.9745(5)	8.9728(5)
	12.3386(5)	12.3404(5)	12.3423(6)	12.3325(7)
	98.041(4)	98.108(3)	98.069(5)	98.120(5)
Volume (Å^3)	2522.3(2)	2523.6(2)	2524.0(2)	2522.4(2)
Size, mm	0.85x0.66x0.38	0.59x0.46x0.38	0.25x0.22x0.14	0.19x0.16x0.08
Crystal *vol*., mm^3	0.1531	0.0627	0.0522	0.0123
Eqiv. *r*, mm	0.33	0.25	0.11	0.07
min./max. trans.	0.516 – 0.730	0.658 – 0.751	0.826 – 0.899	0.879 – 0.946
(Multi-scan T_{min})	(0.544)	(0.861)	(0.804)	(0.869)
No. reflns.	2912	2911	2914	2914
Av. R_{eqiv}, $\sigma(I/I_{net})$	0.041, 0.034	0.032, 0.025	0.038, 0.036	0.048, 0.040
No. $I>2\sigma(I)$ reflns.	2556	2641	2496	2414
$2\theta_{max}$	27.61	27.58	27.57	27.59
R	0.029	0.028	0.031	0.032
Weighting	$(0.0373P)^2+2.2802P$	$(0.0400P)^2+2.7080P$	$(0.0374P)^2+4.1601P$	$(0.0341P)^2+3.9381P$
e map, min./max.	-0.48 – 0.43	-0.76 – 0.32	-0.57 – 0.39	-0.38 – 0.41

Table S4 **Refinement of $[SnCl(H_2O)(C_6H_5)_3(C_{10}H_8N_2)]_2$ (*C*2/*c* space group; μ = 1.19 mm^{-1})**

Unit cell (Å, °)	15.5966(7)	15.5993(5)	15.5742(4)	15.5844(7)
	16.1294(6)	16.1284(4)	16.1161(4)	16.1120(5)
	20.4387(9)	20.4476(7)	20.4181(6)	20.4375(9)
	108.891(5)	108.849(4)	108.879(3)	108.872(5)
Volume (Å^3)	4864.7(4)	4868.6(3)	4849.2(2)	4855.9(3)
Size, mm	0.91x0.63x0.13	0.61x0.55x0.13	0.33x0.26x0.15	0.22x0.18x0.14
Crystal *vol*., mm^3	0.0426	0.0284	0.0096	0.0036
Eqiv. *r*, mm	0.22	0.19	0.13	0.09
min./max. trans.	0.501 – 0.857	0.565 – 0.875	0.765 – 0.856	0.804 – 0.874
(Multi-scan T_{min})	(0.595)	(0.634)	(0.836)	(0.842)
No. reflns.	5635	5640	5610	5627
Av. R_{eqiv}, $\sigma(I/I_{net})$	0.034, 0.032	0.038, 0.026	0.034, 0.023	0.061, 0.044
No. $I>2\sigma(I)$ reflns.	4651	4804	4855	4352
$2\theta_{max}$	27.60	27.61	27.58	27.60
R	0.028	0.028	0.026	0.033
Weighting	$(0.0432P)^2+6.3326P$	$(0.0453P)^2+5.7910P$	$(0.0440P)^2+7.5426P$	$(0.0420P)^2+8.9852P$
e map, min./max.	-0.67 – 2.56	-0.70 – 2.96	-0.40 – 2.68	-0.65 – 2.96

Table S5 **Refinement of $Pb(NO_3)_2(C_3H_9N_3S)$ ($P2_1/n$ space group; μ = 16.4 mm^{-1})**

Unit cell (Å, °)	5.3641(2) 13.8966(6) 14.2315(6) 100.132(4)	5.3460(2) 13.8593(5) 14.1995(6) 100.138(4)	5.3522(2) 13.8783(6) 14.2186(6) 100.048(4)	5.3522(2) 13.8826(6) 14.2217(6) 100.075(4)
Volume ($Å^3$)	1044.31(7)	1035.64(7)	1039.95(7)	1040.41(7)
Size, mm	0.61x0.28x0.10	0.34x0.27x0.09	0.25x0.23x0.10	0.32x0.08x0.06
Crystal *vol*., mm^3	0.0127	0.0061	0.0037	0.0012
Eqiv. *r*, mm	0.14	0.11	0.10	0.07
min./max. trans. (Multi-scan T_{min})	0.026 – 0.259 (0.006)	0.034 – 0.282 (0.095)	0.062 – 0.281 (0.266)	0.112 – 0.423 (0.360)
No. reflns.	2366	2384	2394	2396
Av. R_{eqiv}, $\sigma(I/I_{net})$	0.048, 0.044	0.062, 0.046	0.051, 0.042	0.042, 0.040
No. $I>2\sigma(I)$ reflns.	2129	2144	2110	2092
$2\theta_{max}$	27.58	27.58	27.57	27.58
R	0.029	0.027	0.023	0.040
Weighting	$(0.0346P)^2$	$(0.0272P)^2$	$(0.0196P)^2$	$(0.0171P)^2$
e map, min./max.	-3.54 – 0.93	-2.27 – 1.13	-1.48 – 0.94	-0.93 – 1.14

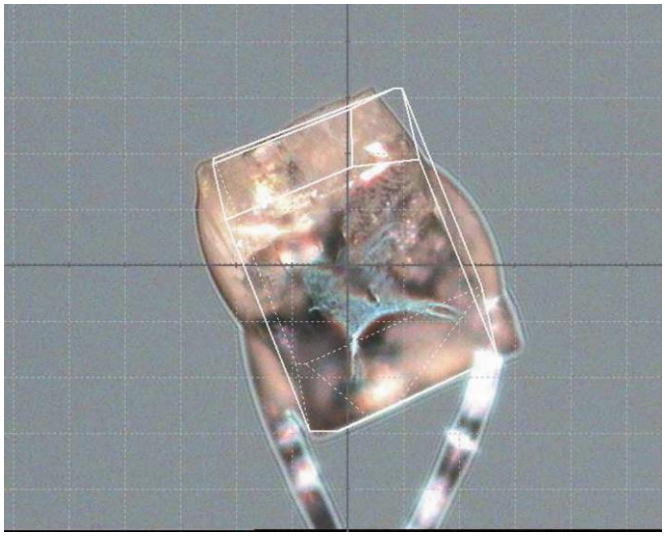

Figure S1 The huge crystal used for measuring (I). One square grid is 0.1 x 0.1 mm.

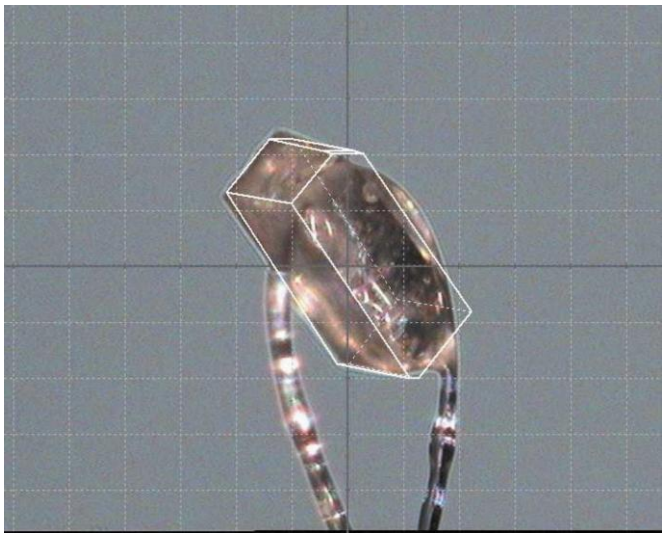

Figure S2 The large crystal used for measuring (I). One square grid is 0.1 x 0.1 mm.

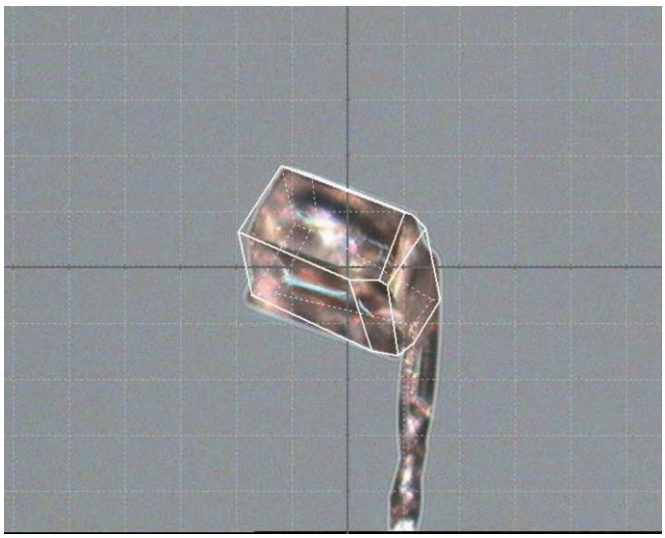

Figure S3 The medium crystal used for measuring (I). One square grid is 0.1 x 0.1 mm.

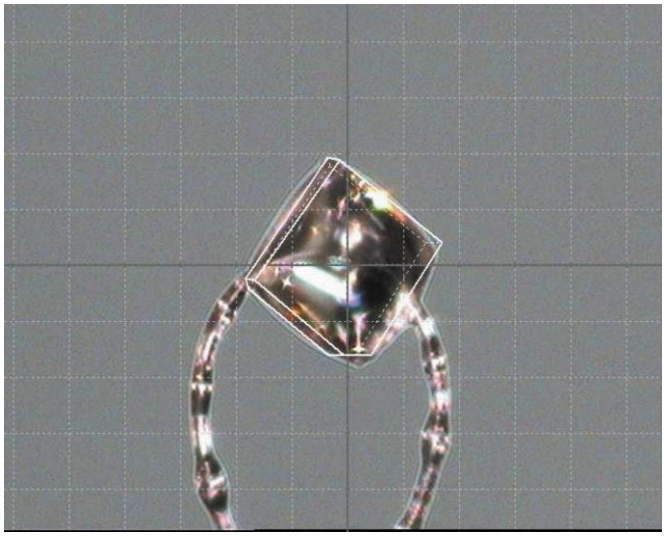

Figure S4 The small crystal used for measuring (I). One square grid is 0.1 x 0.1 mm.

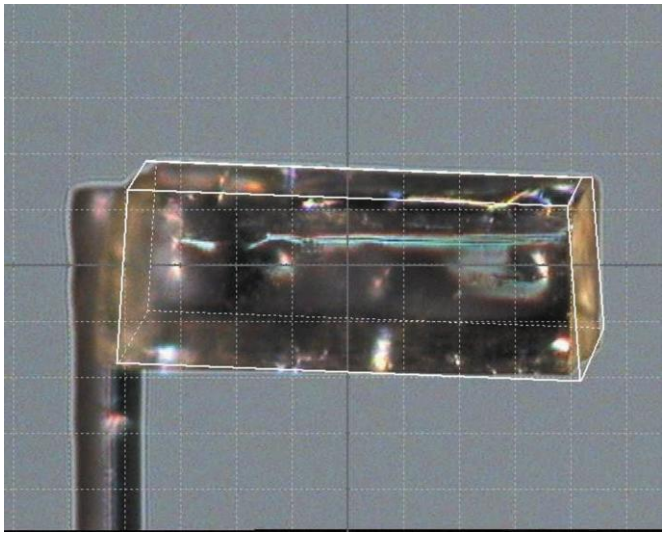

Figure S5 The huge crystal used for measuring (II). One square grid is 0.1 x 0.1 mm.

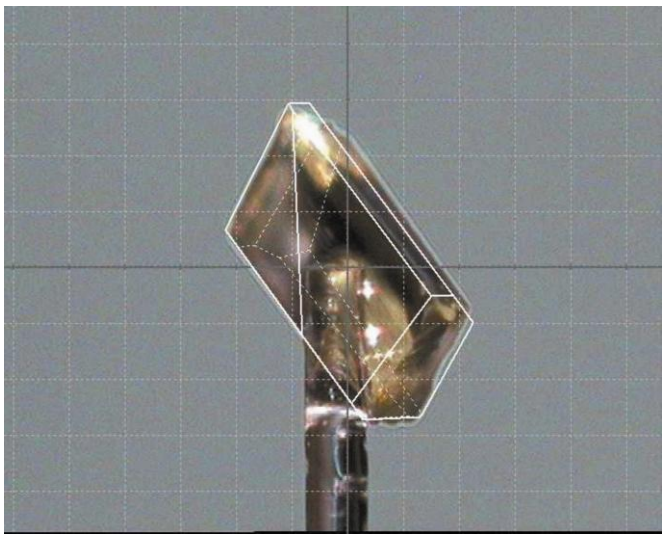

Figure S6 The large crystal used for measuring (II). One square grid is 0.1 x 0.1 mm.

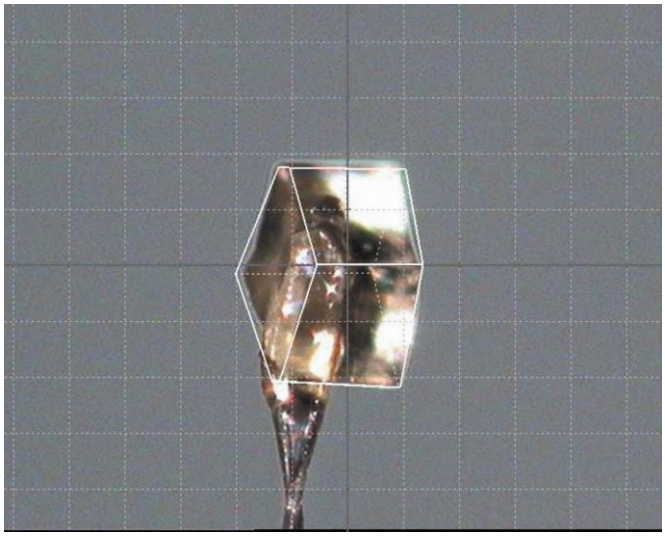

Figure S7 The medium crystal used for measuring (II). One square grid is 0.1 x 0.1 mm.

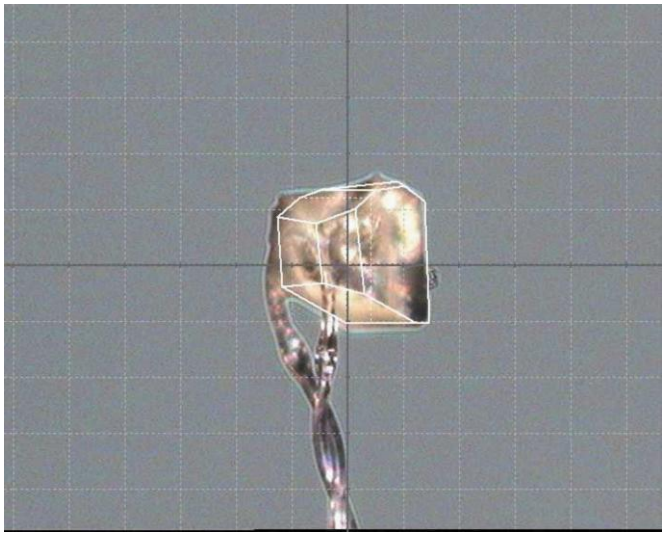

Figure S8 The small crystal used for measuring (II). One square grid is 0.1 x 0.1 mm.

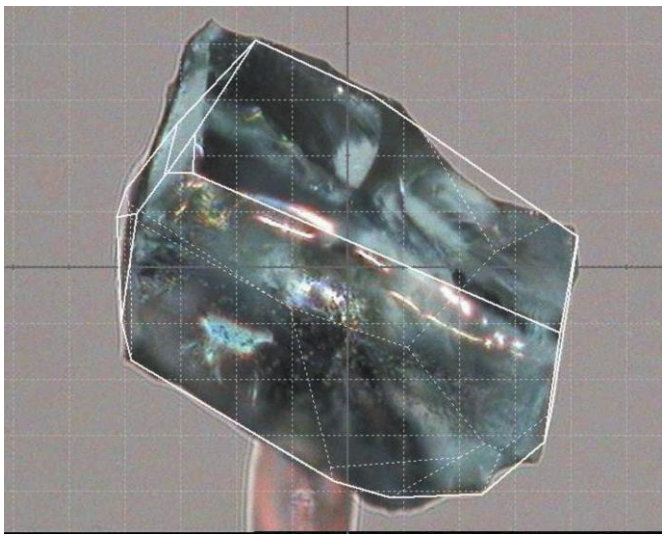

Figure S9 The huge crystal used for measuring (III). One square grid is 0.1 x 0.1 mm.

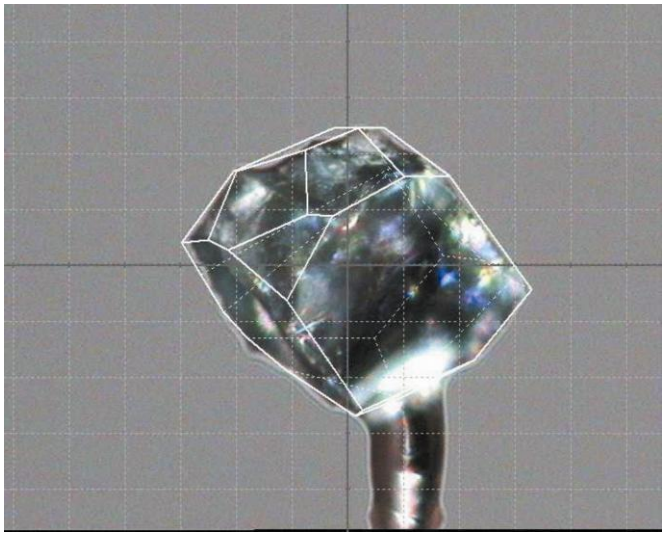

Figure S10 The large crystal used for measuring (III). One square grid is 0.1 x 0.1 mm.

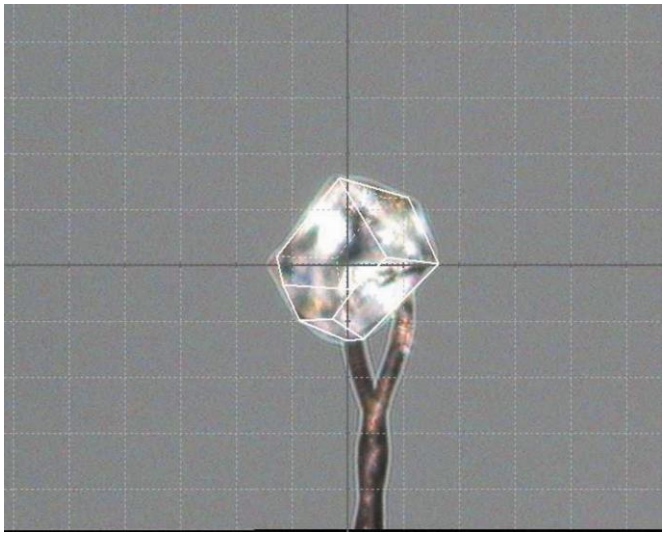

Figure S11 The medium crystal used for measuring (III). One square grid is 0.1 x 0.1 mm.

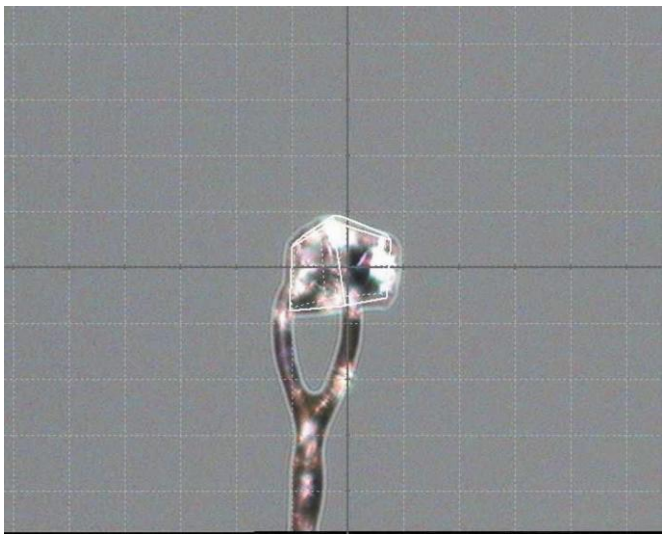

Figure S12 The small crystal used for measuring (III). One square grid is 0.1 x 0.1 mm.

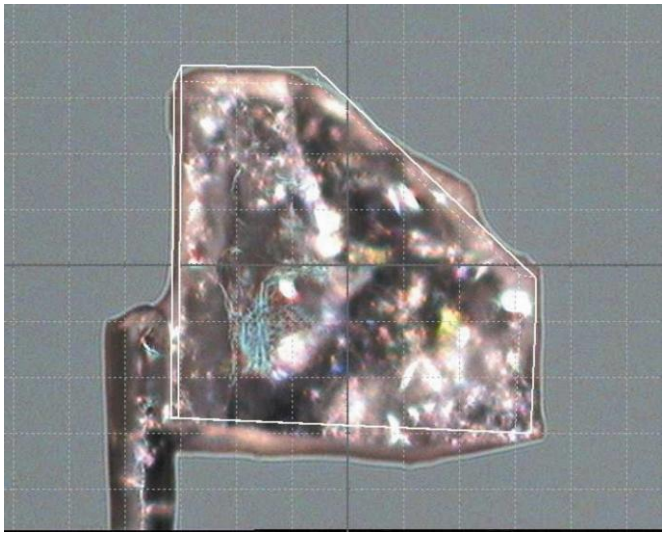

Figure S13 The huge crystal used for measuring (IV). One square grid is 0.1 x 0.1 mm.

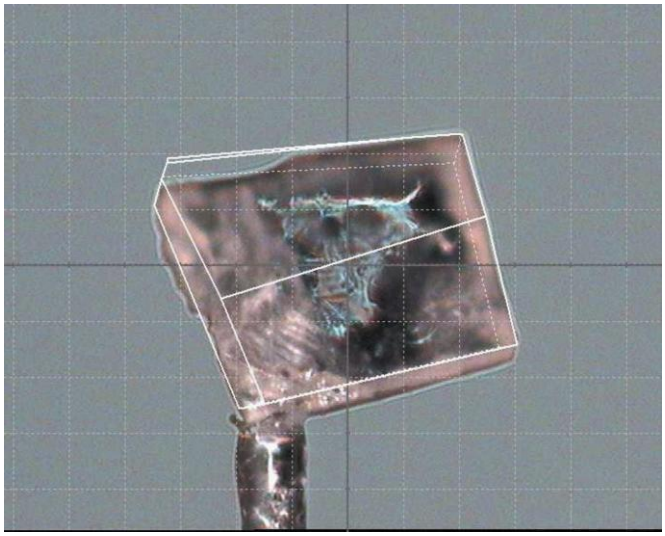

Figure S14 The large crystal used for measuring (IV). One square grid is 0.1 x 0.1 mm.

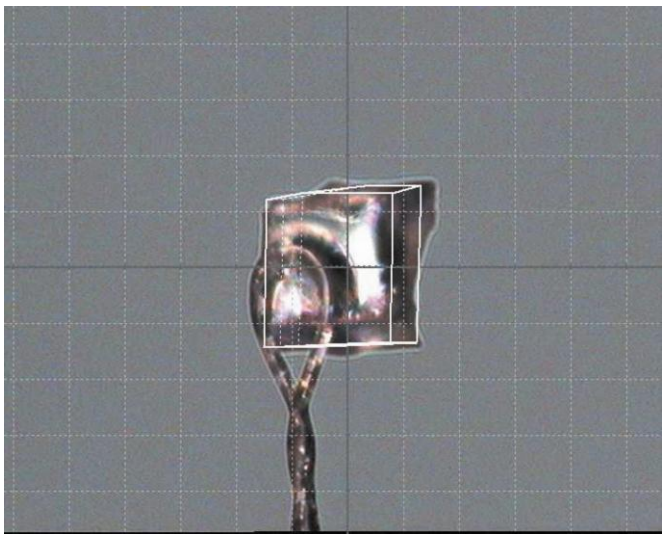

Figure S15 The medium crystal used for measuring (IV). One square grid is 0.1 x 0.1 mm.

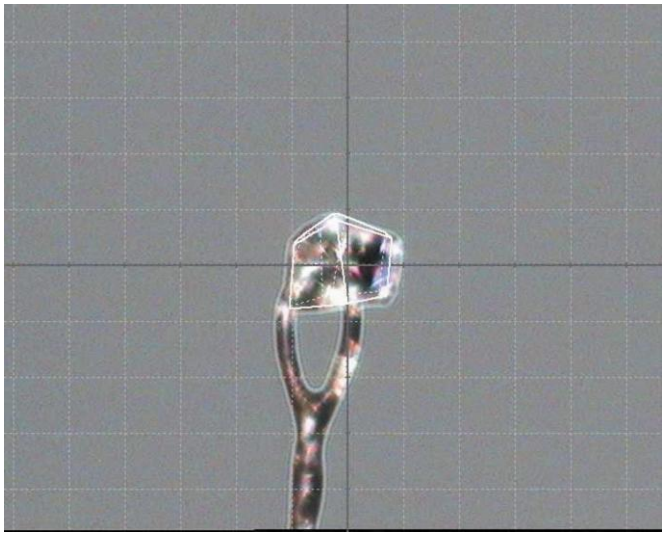

Figure S16 The small crystal used for measuring (IV). One square grid is 0.1 x 0.1 mm.

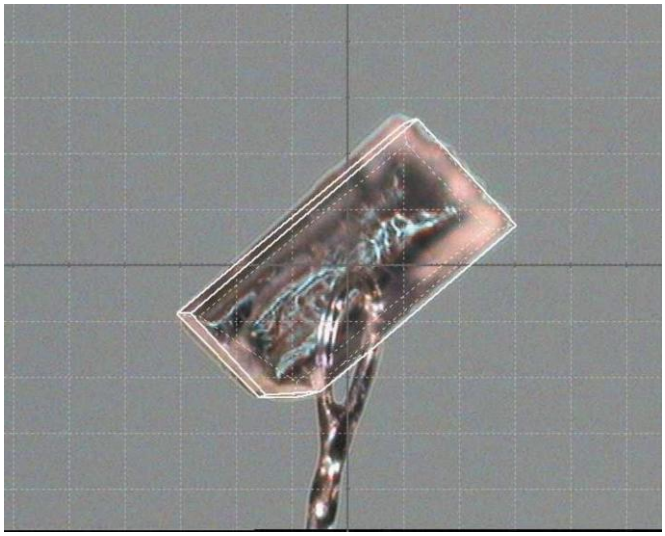

Figure S17 The huge crystal used for measuring (V). One square grid is 0.1 x 0.1 mm.

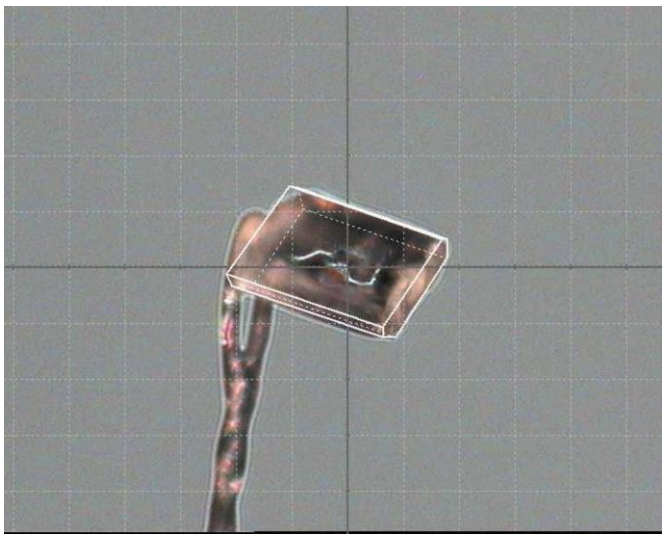

Figure S18 The large crystal used for measuring (V). One square grid is 0.1 x 0.1 mm.

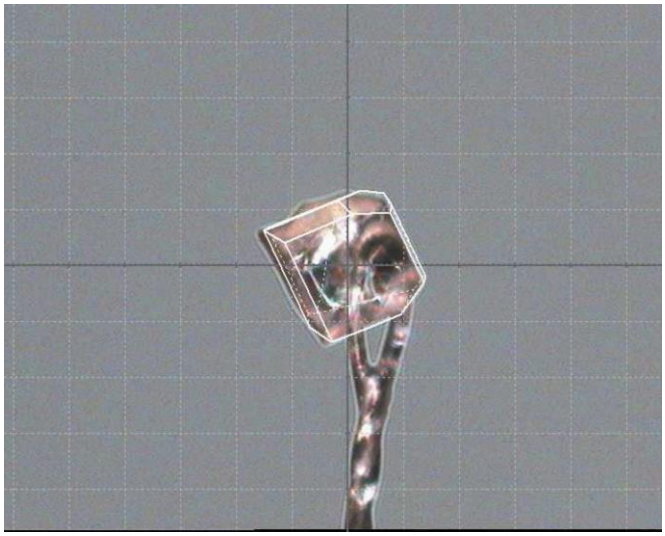

Figure S19 The medium crystal used for measuring (V). One square grid is 0.1 x 0.1 mm.

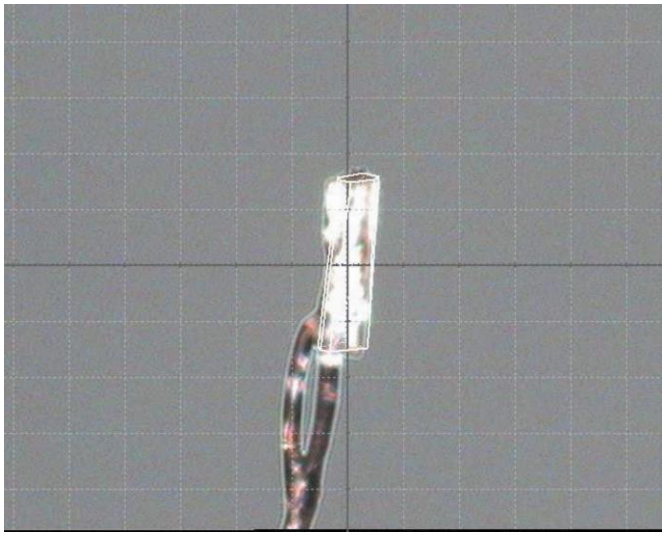

Figure S20 The small crystal used for measuring (V). One square grid is 0.1 x 0.1 mm.

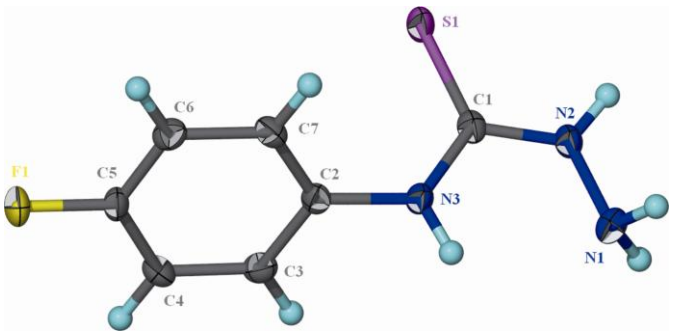

Figure S21 70% Probability *ORTEP* (Barbour, 2001) plot of the refinement of the crystal structure of (I) from measurements on the huge crystal shown in Figure **S1**.

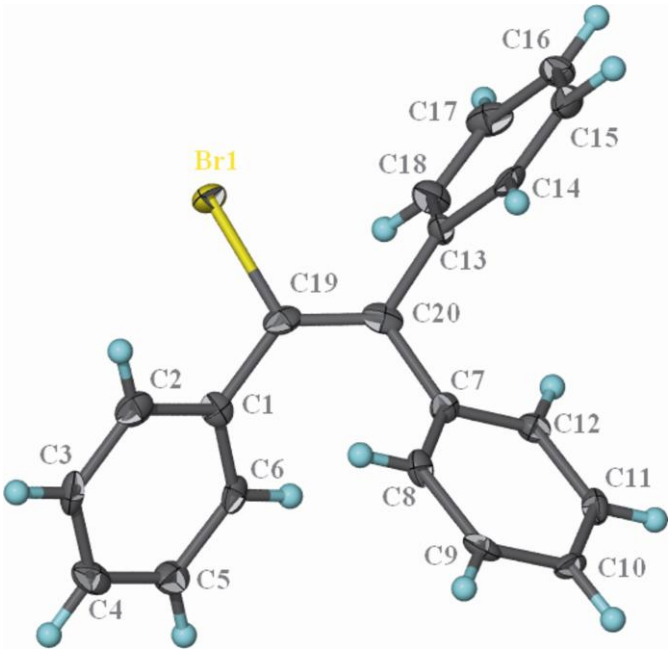

Figure S22 70% Probability *ORTEP* (Barbour, 2001) plot of the refinement of the crystal structure of (II) from measurements on the huge crystal shown in Figure **S5**.

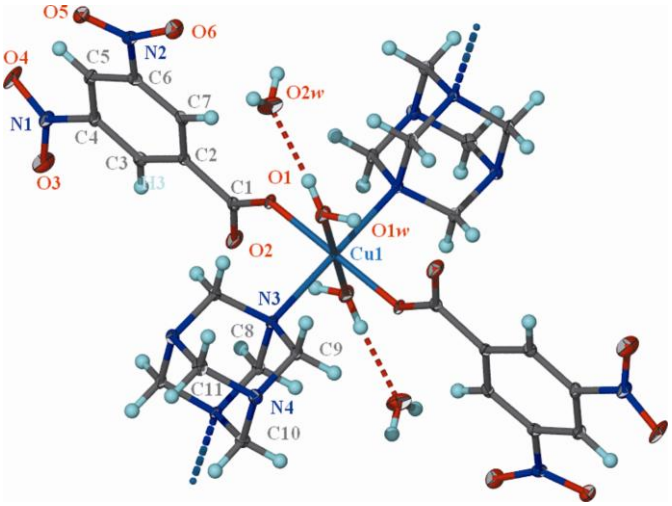

Figure S23 70% Probability *ORTEP* (Barbour, 2001) plot of the refinement of the crystal structure of (III) from measurements on the huge crystal shown in Figure **S9**.

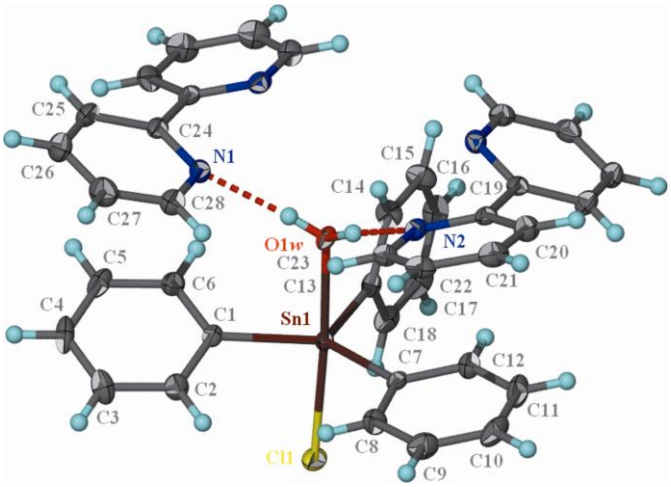

Figure S24 70% Probability *ORTEP* (Barbour, 2001) plot of the refinement of the crystal structure of (IV) from measurements on the huge crystal shown in Figure **S13**.

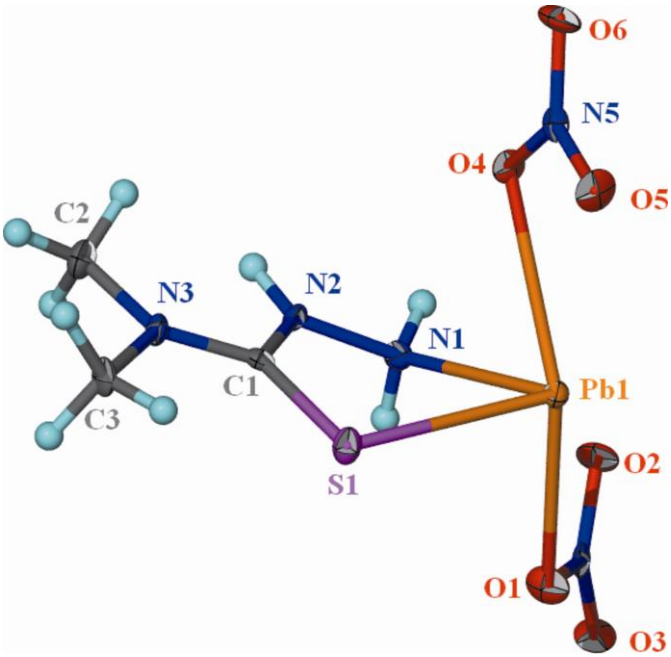

Figure S25 70% Probability *ORTEP* (Barbour, 2001) plot of the refinement of the crystal structure of (V) from measurements on the huge crystal shown in Figure **S17.**