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Table A1. Experimental Parameters for the Crystal Structure Determinatiuon of Sodium Iron Hydroxy Phosphate, "SIHP", $Na_3Fe(PO_4)_2 \cdot Na_{1.55}H_{0.45}O$, and Maricite.

	SIHP	MARICITE
Empirical Formula	$Na_3Fe(PO_4)_2 \cdot Na_{1.55}H_{0.45}O$	$NaFePO_4$
Formula Weight	366.85	173.81
Crystal Color	red, irregular	colorless, plate
Crystal Dimensions (mm)	0.100 x 0.050 x 0.400	0.400 x 0.300 x 0.100
Crystal System	Orthorhombic	Orthorhombic
No. Reflections Used for Unit Determination (2θ range)	19 (44.3-49.2°)	14 (47.5-49.5°)
Omega Scan Peak Width at Half Height	0.33	0.39
Lattice Parameters	a = 14.698 Å b = 15.522 Å c = 7.114 Å V = 1623 Å	a = 8.990 Å b = 6.862 Å c = 5.047 Å V = 311.3 Å
Space Group	Ibam (#72)	Pnma (#62)
Z Value	8	4
D_{calc}	3.002 g cm^{-3}	3.708 g cm^{-3}
F_{000}	1428	336
μ (MoKα)	25.11 cm^{-1}	53.17 cm^{-1}
Diffractometer	Rigaku AFC6S	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å)	MoKα (λ = 0.71069 Å)
Temperature	26 °C	26 °C
Take off Angle	6.0 °C	6.0 °C
Detector Aperture	4.5 mm horizontal 3.0 mm vertical	4.3 mm horizontal 3.0 mm vertical
Crystal to Detector Distance	40 cm	40 cm
Scan Type	ω-2θ	ω-2θ

Scan Rate	4.0 °/min (in omega) (2 rescans)	4.0 °/min (in omega) (4 rescans)
Scan Width	$(1.31 + 0.35 \tan\theta)$ °	$(1.84 + 0.35 \tan\theta)$ °
$2\theta_{max}$	50.1 °	50.0 °
No. of Reflections Measured	Total: 848	Total: 3.58
Corrections	Lorentz-polarization absorption (trans. factors: 0.87-1.00); secondary extinction (coefficient: 0.30529E-06)	Lorentz-polarization absorption (trans. factors: 0.53-1.00) secondary extinction (coefficient: 0.30964E-05)

Table A2. Structure Solution and Refinement*

Structure Solution	Direct Methods	Direct Methods
Refinement	Full-matrix least-squares	Full-matrix least-squares
Function Minimized	Σ w $(\|F_o\| - \|F_c\|)^2$	Σ w $(\|F_o\| - \|F_c\|)^2$
Least-Squares Weights*	$w = 4F_o^2/\sigma^2(F_o^2)$	$w = 4F_o^2/\sigma^2(F_o^2)$
p-factor	0.01	0.01
Anomalous Dispersion	All non-hydrogen atoms	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	593	272
No. Variables	97	41
Reflection/Parameter Ratio	6.11	6.63
Residuals: R; R_w	0.034; 0.036	0.026; 0.031
Goodness of Fit Indicator	2.48	2.69
Max Shift/Error in Final Cycle	0.00	0.00
Maximum Peak in Final Diff. Map	0.45 $e^-/Å^3$	0.61 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-0.74 $e^-/Å^3$	-0.51 $e^-/Å^3$

* $\sigma^2(F_o^2) = [S^2(C+R^2B) + (pF_o^2)^2]/Lp^2$
S = Scan rate
C = Total Integrated Peak Count
R = Ratio of Scan Time to background counting time.
B = Total Background Count
Lp = Lorentz-polarization factor
p = p-factor

Standard deviation of an observation of unit weight: $[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_v)]^{1/2}$
where: N_o = number of observations; N_v = number of variables

Table A3. Intramolecular Bond Angles in SIHP*

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Fe(1)	O(1)	180.00	O(7)	Fe(1)	H(1)	21.24
O(1)	Fe(1)	O(4)	87.8(1)	H(1)	Fe(1)	H(1)	180.00
O(1)	Fe(1)	O(4)	92.2(1)	O(1)	P(1)	O(1)	109.8(3)
O(1)	Fe(1)	O(7)	88.0(2)	O(1)	P(1)	O(2)	111.4(2)
O(1)	Fe(1)	O(7)	92.0(2)	O(1)	P(1)	O(3)	106.6(2)
O(1)	Fe(1)	H(1)	67.59	O(1)	P(1)	O(2)	111.4(2)
O(1)	Fe(1)	H(1)	112.41	O(1)	P(1)	O(3)	106.6(2)
O(1)	Fe(1)	O(4)	92.2(1)	O(2)	P(1)	O(3)	110.7(3)
O(1)	Fe(1)	O(4)	87.8(1)	O(4)	P(2)	O(4)	110.8(3)
O(1)	Fe(1)	O(7)	92.0(2)	O(4)	P(2)	O(5)	107.5(2)
O(1)	Fe(1)	O(7)	88.0(2)	O(4)	P(2)	O(6)	110.1(2)
O(1)	Fe(1)	H(1)	112.41	O(4)	P(2)	O(5)	107.5(2)
O(1)	Fe(1)	H(1)	67.59	O(4)	P(2)	O(6)	110.1(2)
O(4)	Fe(1)	O(4)	180.00	O(5)	P(2)	O(6)	110.8(3)
O(4)	Fe(1)	O(7)	93.4(2)	O(1)	Na(1)	O(1)	141.0(2)
O(4)	Fe(1)	O(7)	86.6(2)	O(1)	Na(1)	O(6)	101.7(1)
O(4)	Fe(1)	H(1)	86.90	O(1)	Na(1)	O(6)	103.1(1)
O(4)	Fe(1)	H(1)	93.10	O(1)	Na(1)	O(6)	103.1(1)
O(4)	Fe(1)	O(7)	86.6(2)	O(1)	Na(1)	O(6)	101.7(1)
O(4)	Fe(1)	O(7)	93.4(2)	O(6)	Na(1)	O(6)	100.0(2)
O(4)	Fe(1)	H(1)	93.10	Na(2)	Na(2)	O(3)	88.3(2)
O(4)	Fe(1)	H(1)	86.90	Na(2)	Na(2)	O(3)	88.3(2)
O(7)	Fe(1)	O(7)	180.00	O(3)	Na(2)	O(3)	176.6(3)
O(7)	Fe(1)	H(1)	21.24	O(2)	Na(3)	O(2)	100.5(2)
O(7)	Fe(1)	H(1)	158.76	O(2)	Na(3)	O(4)	125.3(1)
O(7)	Fe(1)	H(1)	158.76	O(2)	Na(3)	O(4)	88.9(1)

Table A3 (Continued). Intramolecular Bond Angles in SIHP*

atom	atom	atom	angle	atom	atom	atom	angle
O(2)	Na(3)	O(4)	88.9(1)	O(1)	Na(6)	O(7)	73.2(1)
O(2)	Na(3)	O(4)	125.3(1)	O(1)	Na(6)	H(1)	72.35
O(4)	Na(3)	O(4)	128.1(2)	O(2)	Na(6)	O(3)	103.2(3)
O(4)	Na(4)	O(4)	142.9(2)	O(2)	Na(6)	O(7)	102.5(2)
O(4)	Na(4)	O(5)	94.7(1)	O(2)	Na(6)	H(1)	106.44
O(4)	Na(4)	O(6)	107.3(1)	O(3)	Na(6)	O(7)	154.2(3)
O(4)	Na(4)	O(7)	71.7(1)	O(3)	Na(6)	H(1)	150.32
O(4)	Na(4)	O(5)	94.7(1)	O(7)	Na(6)	H(1)	3.89
O(4)	Na(4)	O(6)	107.3(1)	Fe(1)	O(1)	P(1)	133.0(2)
O(4)	Na(4)	O(7)	71.7(1)	Fe(1)	O(1)	Na(1)	119.8(2)
O(5)	Na(4)	O(6)	96.1(2)	Fe(1)	O(1)	Na(6)	93.4(2)
O(5)	Na(4)	O(7)	114.8(2)	Fe(1)	O(1)	O(3)	162.5(2)
O(6)	Na(4)	O(7)	149.1(2)	Fe(1)	O(1)	H(1)	61.30
O(5)	Na(5)	O(5)	93.6(2)	P(1)	O(1)	Na(1)	97.5(2)
O(5)	Na(5)	O(5)	87.5(2)	P(1)	O(1)	Na(6)	123.9(2)
O(5)	Na(5)	O(5)	168.5(2)	P(1)	O(1)	O(3)	36.6(1)
O(5)	Na(5)	O(5)	168.5(2)	P(1)	O(1)	H(1)	147.05
O(5)	Na(5)	O(5)	87.5(2)	Na(1)	O(1)	Na(6)	77.3(1)
O(5)	Na(5)	O(5)	93.6(2)	Na(1)	O(1)	O(3)	62.1(1)
O(1)	Na(6)	O(1)	138.0(3)	Na(1)	O(1)	H(1)	95.74
O(1)	Na(6)	O(2)	105.6(1)	Na(6)	O(1)	O(3)	103.7(1)
O(1)	Na(6)	O(3)	99.7(1)	Na(6)	O(1)	H(1)	32.21
O(1)	Na(6)	O(7)	73.2(1)	O(3)	O(1)	H(1)	135.96
O(1)	Na(6)	H(1)	72.35	P(1)	O(2)	Na(3)	115.7(2)
O(1)	Na(6)	O(2)	105.6(1)	P(1)	O(2)	Na(3)	115.7(2)
O(1)	Na(6)	O(3)	99.7(1)	P(1)	O(2)	Na(6)	136.3(3)

Table A3 (Continued). Intramolecular Bond Angles in SIHP*

atom	atom	atom	angle	atom	atom	atom	angle
Na(3)	O(2)	Na(3)	97.3(2)	Na(3)	O(4)	O(5)	65.4(1)
Na(3)	O(2)	Na(6)	91.8(2)	Na(4)	O(4)	O(5)	108.9(2)
Na(3)	O(2)	Na(6)	91.8(2)	P(2)	O(5)	Na(4)	171.4(3)
P(1)	O(3)	Na(2)	92.1(2)	P(2)	O(5)	Na(5)	99.0(2)
P(1)	O(3)	Na(2)	92.1(2)	P(2)	O(5)	Na(5)	99.0(2)
P(1)	O(3)	Na(6)	170.3(4)	P(2)	O(5)	O(4)	36.4(1)
P(1)	O(3)	O(1)	36.7(1)	P(2)	O(5)	O(4)	36.4(1)
P(1)	O(3)	O(1)	36.7(1)	Na(4)	O(5)	Na(5)	86.9(1)
Na(2)	O(3)	Na(2)	96.2(2)	Na(4)	O(5)	Na(5)	86.9(1)
Na(2)	O(3)	Na(6)	94.4(2)	Na(4)	O(5)	O(4)	138.7(2)
Na(2)	O(3)	O(1)	128.1(2)	Na(4)	O(5)	O(4)	138.7(2)
Na(2)	O(3)	O(1)	81.8(2)	Na(5)	O(5)	Na(5)	92.5(2)
Na(2)	O(3)	Na(6)	94.4(2)	Na(5)	O(5)	O(4)	87.6(1)
Na(2)	O(3)	O(1)	81.8(2)	Na(5)	O(5)	O(4)	134.3(2)
Na(2)	O(3)	O(1)	128.1(2)	Na(5)	O(5)	O(4)	134.3(2)
Na(6)	O(3)	O(1)	137.5(2)	Na(5)	O(5)	O(4)	87.6(1)
Na(6)	O(3)	O(1)	137.5(2)	O(4)	O(5)	O(4)	61.6(2)
O(1)	O(3)	O(1)	61.5(2)	P(2)	O(6)	Na(1)	116.1(2)
Fe(1)	O(4)	P(2)	135.6(2)	P(2)	O(6)	Na(1)	116.1(2)
Fe(1)	O(4)	Na(3)	108.4(1)	P(2)	O(6)	Na(4)	144.5(3)
Fe(1)	O(4)	Na(4)	90.4(2)	Na(1)	O(6)	Na(1)	96.2(2)
Fe(1)	O(4)	O(5)	158.2(2)	Na(1)	O(6)	Na(4)	86.1(2)
P(2)	O(4)	Na(3)	99.3(2)	Na(1)	O(6)	Na(4)	86.1(2)
P(2)	O(4)	Na(4)	127.3(2)	Fe(1)	O(7)	Fe(1)	129.8(2)
P(2)	O(4)	O(5)	36.1(1)	Fe(1)	O(7)	Na(4)	96.5(2)
Na(3)	O(4)	Na(4)	83.8(1)	Fe(1)	O(7)	Na(6)	104.2(2)

Table A3 (Continued). Intramolecular Bond Angles in SIHP*

atom	atom	atom	angle	atom	atom	atom	angle
Fe(1)	O(7)	H(1)	101.87				
Fe(1)	O(7)	Na(4)	96.5(2)				
Fe(1)	O(7)	Na(6)	104.2(2)				
Fe(1)	O(7)	H(1)	101.87				
Na(4)	O(7)	Na(6)	129.2(2)				
Na(4)	O(7)	H(1)	135.44				
Na(6)	O(7)	H(1)	6.21				
Fe(1)	H(1)	Fe(1)	101.64				
Fe(1)	H(1)	Na(6)	126.40				
Fe(1)	H(1)	O(1)	51.11				
Fe(1)	H(1)	O(1)	147.37				
Fe(1)	H(1)	O(7)	56.89				
Fe(1)	H(1)	Na(6)	126.40				
Fe(1)	H(1)	O(1)	147.37				
Fe(1)	H(1)	O(1)	51.11				
Fe(1)	H(1)	O(7)	56.89				
Na(6)	H(1)	O(1)	75.44				
Na(6)	H(1)	O(1)	75.44				
Na(6)	H(1)	O(7)	169.90				
O(1)	H(1)	O(1)	142.96				
O(1)	H(1)	O(7)	106.36				
O(1)	H(1)	O(7)	106.36				

* Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table A4. Intramolecular Distances in SIHP*

atom	atom	distance	ADC*	atom	atom	distance	ADC*
Fe(1)	P(1)	3.290(1)	1	P(1)	O(2)	1.512(5)	1
Fe(1)	P(1)	3.290(1)	55410	P(1)	O(3)	1.540(5)	1
Fe(1)	P(2)	3.323(2)	1	P(1)	O(7)	3.444(5)	10
Fe(1)	P(2)	3.323(2)	10	P(2)	Na(1)	3.355(3)	1
Fe(1)	Na(4)	3.165(3)	1	P(2)	Na(1)	3.355(3)	6
Fe(1)	Na(4)	3.165(3)	55410	P(2)	Na(3)	3.133(3)	1
Fe(1)	Na(6)	3.283(4)	1	P(2)	Na(3)	3.133(3)	6
Fe(1)	Na(6)	3.283(4)	10	P(2)	Na(5)	3.099(2)	1
Fe(1)	O(1)	2.036(3)	1	P(2)	Na(5)	3.099(2)	56505
Fe(1)	O(1)	2.036(3)	13	P(2)	O(4)	1.547(4)	1
Fe(1)	O(4)	2.037(3)	1	P(2)	O(4)	1.547(4)	6
Fe(1)	O(4)	2.037(3)	13	P(2)	O(5)	1.536(5)	1
Fe(1)	O(7)	1.964(2)	1	P(2)	O(6)	1.526(5)	1
Fe(1)	O(7)	1.964(2)	10	P(2)	O(7)	3.376(5)	1
Fe(1)	H(1)	2.295	1	P(2)	H(1)	3.298	1
Fe(1)	H(1)	2.295	10	Na(1)	Na(2)	3.406(3)	55606
P(1)	Na(1)	3.067(2)	1	Na(1)	Na(2)	3.406(3)	66605
P(1)	Na(1)	3.067(2)	55606	Na(1)	Na(4)	3.210(4)	1
P(1)	Na(2)	2.890(3)	1	Na(1)	Na(4)	3.210(4)	56504

Table A4(Continued). Intramolecular Distances in SIHP*

atom	atom	distance	ADC*	atom	atom	distance	ADC*
P(1)	Na(2)	2.890(3)	55606	Na(1)	Na(6)	3.067(4)	1
P(1)	Na(2)	3.410(4)	66502	Na(1)	Na(6)	3.067(4)	56504
P(1)	Na(2)	3.410(4)	66605	Na(1)	O(1)	2.457(3)	1
P(1)	Na(3)	3.316(2)	10	Na(1)	O(1)	2.457(3)	56504
P(1)	Na(3)	3.316(2)	13	Na(1)	O(3)	2.544(4)	1
P(1)	O(1)	1.545(4)	1	Na(1)	O(3)	2.544(4)	56504
P(1)	O(1)	1.545(4)	55606	Na(1)	O(4)	3.192(4)	1
Na(1)	O(4)	3.192(4)	56504	Na(3)	O(5)	2.685(4)	1
Na(1)	O(6)	2.390(4)	1	Na(3)	O(5)	2.685(4)	3
Na(1)	O(6)	2.390(4)	56504	Na(3)	O(7)	3.367(4)	10
Na(2)	Na(2)	0.87(1)	66502	Na(3)	O(7)	3.367(4)	45512
Na(2)	Na(6)	2.897(4)	55601	Na(3)	H(1)	3.249	10
Na(2)	Na(6)	3.417(5)	56504	Na(3)	H(1)	3.249	45512
Na(2)	Na(6)	2.897(4)	65503	Na(4)	Na(5)	3.269(3)	1
Na(2)	Na(6)	3.417(5)	66602	Na(4)	Na(5)	3.269(3)	56605
Na(2)	O(1)	3.184(4)	55606	Na(4)	O(1)	3.062(5)	1
Na(2)	O(1)	3.184(4)	65508	Na(4)	O(1)	3.062(5)	55606
Na(2)	O(2)	2.805(6)	1	Na(4)	O(4)	2.409(4)	1
Na(2)	O(2)	2.805(6)	65603	Na(4)	O(4)	2.409(4)	55606

Table A4 (Continued). Intramolecular Distances in SIHP*

atom	atom	distance	ADC*	atom	atom	distance	ADC*
Na(2)	O(3)	2.390(4)	1	Na(4)	O(5)	2.286(6)	3
Na(2)	O(3)	2.518(4)	56604	Na(4)	O(6)	2.310(6)	56504
Na(2)	O(3)	2.390(4)	65603	Na(4)	O(7)	2.269(6)	10
Na(2)	O(3)	2.518(4)	66502	Na(4)	H(1)	2.935	10
Na(3)	Na(4)	3.269(4)	1	Na(5)	O(4)	3.424(3)	1
Na(3)	Na(4)	3.269(4)	3	Na(5)	O(4)	3.424(3)	3
Na(3)	Na(6)	3.317(4)	10	Na(5)	O(4)	3.424(3)	56502
Na(3)	Na(6)	3.317(4)	45512	Na(5)	O(4)	3.424(3)	56504
Na(3)	O(1)	3.183(4)	13	Na(5)	O(5)	2.463(4)	1
Na(3)	O(1)	3.183(4)	45515	Na(5)	O(5)	2.463(4)	3
Na(3)	O(2)	2.369(4)	45612	Na(5)	O(5)	2.463(4)	56502
Na(3)	O(2)	2.369(4)	55410	Na(5)	O(5)	2.463(4)	56504
Na(3)	O(4)	2.487(4)	1	Na(5)	O(6)	3.046(5)	1
Na(3)	O(4)	2.487(4)	3	Na(5)	O(6)	3.046(5)	3
Na(5)	O(6)	3.046(5)	56502	O(4)	O(5)	3.453(5)	3
Na(5)	O(6)	3.046(5)	56504	O(4)	O(6)	2.519(5)	1
Na(6)	O(1)	2.456(4)	1	O(4)	O(7)	2.914(5)	1
Na(6)	O(1)	2.456(4)	6	O(4)	O(7)	2.743(5)	10
Na(6)	O(2)	2.250(7)	65503	O(4)	H(1)	2.985	1

Table A4 (Continued). Intramolecular Distances in SIHP*

atom	atom	distance	ADC*	atom	atom	distance	ADC*
Na(6)	O(3)	2.265(5)	56504	O(4)	H(1)	3.150	10
Na(6)	O(6)	3.483(8)	1	O(5)	O(5)	3.41(1)	56502
Na(6)	O(7)	2.194(6)	1	O(5)	O(6)	2.520(7)	1
Na(6)	H(1)	1.353	1	O(5)	O(6)	3.418(7)	56502
O(1)	O(1)	2.528(8)	55606	O(7)	H(1)	0.849	1
O(1)	O(2)	2.525(6)	1	O(2)	H(1)	2.935	65503
O(1)	O(3)	2.474(5)	1	O(3)	O(3)	3.27(1)	66502
O(1)	O(4)	2.824(5)	1	O(3)	O(6)	3.414(8)	56504
O(1)	O(4)	2.935(5)	13	O(4)	O(4)	2.546(8)	6
O(1)	O(7)	2.779(5)	1	O(4)	O(5)	2.485(5)	1
O(1)	O(7)	2.877(5)	10				
O(1)	H(1)	2.418	1				
O(2)	O(3)	2.511(7)	1				
O(2)	O(4)	3.403(6)	10				
O(2)	O(4)	3.403(6)	13				
O(2)	O(7)	3.467(7)	65503				

* Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses. ADC, " atom designator codes"

Table A5. Anisotropic Thermal parameters, U_{ij}, for SIHP

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	0.0101(5)	0.0090(5)	0.0142(5)	0.0011(5)	-0.0009(4)	-0.0017(5)
P(1)	0.019(1)	0.011(1)	0.010(1)	-0.0053(8)	0	0
P(2)	0.012(1)	0.013(1)	0.010(1)	0.0044(8)	0	0
Na(1)	0.028(2)	0.034(2)	0.029(2)	0	0	0.007(2)
Na(2)	0.024(3)	0.030(4)	0.024(3)	0	-0.011(3)	0
Na(3)	0.035(2)	0.032(2)	0.025(2)	0	0.013(2)	0
Na(4)	0.037(2)	0.033(2)	0.034(2)	0.003(2)	0	0
Na(5)	0.076(4)	0.018(2)	0.026(3)	0	0	0
Na(6)	0.027(4)	0.012(3)	0.023(4)	-0.005(2)	0	0
O(1)	0.030(2)	0.014(2)	0.015(2)	-0.012(2)	-0.003(2)	0.000(2)
O(2)	0.022(3)	0.028(3)	0.026(3)	-0.001(2)	0	0
O(3)	0.029(3)	0.012(3)	0.016(3)	-0.009(2)	0	0
O(4)	0.018(2)	0.021(2)	0.012(2)	0.009(2)	-0.001(2)	0.002(2)
O(5)	0.016(3)	0.033(3)	0.015(3)	0.008(2)	0	0
O(6)	0.035(3)	0.017(3)	0.025(3)	-0.003(2)	0	0
O(7)	0.014(2)	0.018(3)	0.009(2)	0.000(2)	0	0
H(1)	0.0173					

Table A6. Structure Factors for SIHP: 10|F|o vs 10|F|c page 1

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
^^^^^^^	h =	0	^^^^^^^		3	0	228	267	9	15	4	24	67	50*
					3	2	455	411	9	16	1	280	311	13
0	2	356	418	8	3	4	58	60	38*	16	3	216	184	15
0	6	1303	1281	12	3	6	6	57	43*	17	0	507	516	16
0	8	2178	2179	17	3	8	93	19	37*	17	2	308	341	14
2	0	1547	1531	9	4	1	66	28	34*	18	1	0	8	51*
2	2	1933	1993	11	4	3	262	269	13					
2	4	367	405	11	4	5	47	31	42*	^^^^^^^	h =	2	^^^^^^^	
2	6	557	542	13	4	7	99	43	46*					
2	8	219	190	14	5	0	339	369	9	0	0	1629	1658	9
4	0	136	54	9	5	2	1284	1304	10	0	2	2014	1976	12
4	2	4484	4690	24	5	4	416	420	11	0	4	321	368	12
4	4	1073	1058	11	5	6	346	343	17	0	6	445	449	13
4	6	3104	3196	19	5	8	236	220	15	0	8	140	140	22
4	8	403	450	18	6	1	615	644	8	1	1	1402	1343	9
6	0	263	163	11	6	3	167	143	11	1	3	675	685	9
6	2	116	91	13	6	5	388	394	14	1	5	934	926	11
6	4	1262	1233	11	6	7	141	65	19	1	7	379	409	17
6	6	863	880	13	7	0	651	633	9	2	0	1625	1625	9
6	8	989	958	16	7	2	95	64	17	2	2	1005	1056	8
8	0	5572	5349	29	7	4	297	295	15	2	4	837	852	10
8	2	66	76	30*	7	6	105	134	25	2	6	472	439	13
8	4	3706	3742	21	8	1	137	122	11	2	8	462	453	16
8	6	168	176	17	8	3	36	60	39*	3	1	1799	1671	11
10	0	1276	1258	11	8	5	106	91	37*	3	3	950	893	9
10	2	1702	1679	13	8	7	130	101	23	3	5	959	976	11
10	4	256	269	12	9	0	821	859	10	3	7	667	680	14
10	6	506	505	17	9	2	200	222	10	4	0	1711	1705	10
12	0	697	723	11	9	4	747	733	12	4	2	423	334	9
12	2	2875	2925	18	9	6	0	63	50*	4	4	1541	1561	12
12	4	151	138	16	10	1	179	184	11	4	6	416	387	14
12	6	1497	1474	16	10	3	342	350	14	4	8	853	839	15
14	0	1658	1672	14	10	5	199	169	14	5	1	884	849	8
14	2	510	471	13	10	7	103	45	52*	5	3	851	839	10
14	4	1507	1493	15	11	0	389	406	12	5	5	807	833	12
16	0	1535	1532	15	11	2	0	12	41*	5	7	238	270	14
16	2	79	85	48*	11	4	97	40	37*	6	0	760	794	8
16	4	1469	1465	16	11	6	252	284	14	6	2	167	187	10
18	0	81	156	51*	12	1	102	189	37*	6	4	1019	1030	11
					12	3	312	282	11	6	6	577	587	14
^^^^^^^	h =	1	^^^^^^^		12	5	178	206	16	7	1	582	617	9
					13	0	75	73	35*	7	3	419	380	11
1	2	75	138	32*	13	2	700	683	13	7	5	168	176	14
1	4	53	61	37*	13	4	48	96	48*	7	7	192	218	18
1	6	0	60	45*	13	6	409	399	19	8	0	1402	1421	11
1	8	84	2	48*	14	1	221	209	12	8	2	1010	1022	10
2	1	195	277	8	14	3	86	39	46*	8	4	910	903	12
2	3	68	32	26*	14	5	228	219	15	8	6	520	556	16
2	5	94	108	36*	15	0	292	319	14	9	1	765	743	10
2	7	7	61	48*	15	2	0	8	48*	9	3	213	198	10

Table A6 (Cont.). Structure Factors for SIHP: 10|F|o vs 10|F|c page 2

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
9	5	544	577	14	5	4	291	318	11	0	8	325	336	14
9	7	332	346	14	5	6	475	478	15	1	1	596	597	8
10	0	1333	1339	11	5	8	216	188	16	1	3	1709	1682	12
10	2	665	674	11	6	1	408	358	10	1	5	58	93	43*
10	4	685	709	13	6	3	178	151	11	1	7	372	348	16
10	6	188	191	16	6	5	213	222	12	2	0	1652	1673	10
11	1	769	778	11	6	7	74	77	38*	2	2	175	114	9
11	3	1395	1405	13	7	0	234	204	9	2	4	1459	1469	12
11	5	514	537	15	7	2	462	480	10	2	6	428	440	15
12	0	1167	1169	12	7	4	125	145	17	2	8	836	799	15
12	2	1001	989	12	7	6	29	53	47*	3	1	301	251	11
12	4	840	847	13	8	1	394	392	11	3	3	160	164	11
12	6	549	519	16	8	3	574	581	11	3	5	0	120	45*
13	1	145	138	16	8	5	114	173	25	3	7	47	27	47*
13	3	85	21	44*	8	7	0	221	56*	4	0	5559	5442	29
13	5	0	45	52*	9	0	1344	1308	11	4	2	1944	1849	12
14	0	491	464	13	9	2	474	496	11	4	4	3204	3331	19
14	2	514	510	14	9	4	613	612	13	4	6	307	325	13
14	4	555	546	15	9	6	0	4	48*	4	8	1528	1463	16
15	1	146	158	18	10	1	278	254	14	5	1	318	280	11
15	3	412	438	17	10	3	92	39	36*	5	3	948	935	10
16	0	790	806	14	10	5	221	224	14	5	5	295	307	12
16	2	671	671	15	11	0	505	547	12	5	7	0	21	51*
16	4	724	745	16	11	2	105	131	21	6	0	1717	1698	11
17	1	0	12	50*	11	4	95	80	25*	6	2	1595	1603	12
17	3	169	175	19	11	6	367	385	14	6	4	524	550	12
18	0	806	809	15	12	1	43	18	42*	6	6	494	453	15
					12	3	0	47	44*	7	1	797	797	9
^^^^^^^	h =	3	^^^^^^^		12	5	73	48	41*	7	3	292	265	13
					13	0	772	792	12	7	5	492	503	14
1	0	65	49	33*	13	2	438	469	15	7	7	280	271	14
1	2	640	698	8	13	4	463	431	15	8	0	632	617	10
1	4	0	42	38*	14	1	134	138	18	8	2	3988	3984	22
1	6	187	178	13	14	3	95	130	49*	8	4	186	179	13
1	8	120	8	40*	14	5	0	111	52*	8	6	2119	2120	16
2	1	0	94	35*	15	0	609	652	14	9	1	0	28	39*
2	3	469	485	9	15	2	14	88	48*	9	3	605	598	12
2	5	0	31	41*	15	4	160	160	19	9	5	0	48	47*
2	7	0	34	47*	16	1	140	158	20	9	7	165	144	19
3	0	234	267	11	16	3	114	126	44*	10	0	1149	1137	11
3	2	92	40	16	17	0	80	99	51*	10	2	160	164	13
3	4	138	139	14	17	2	0	73	52*	10	4	1226	1191	13
3	6	0	2	47*	18	1	156	147	21	10	6	347	389	14
3	8	0	10	54*						11	1	95	69	37*
4	1	42	31	35*	^^^^^^^	h =	4	^^^^^^^		11	3	433	439	14
4	3	274	299	10						11	5	190	159	16
4	5	0	47	43*	0	0	63	138	35*	12	0	2638	2641	17
4	7	101	28	42*	0	2	4964	5045	26	12	2	237	245	11
5	0	317	215	10	0	4	823	817	10	12	4	2351	2327	17
5	2	489	449	10	0	6	3272	3242	20	12	6	99	90	31*

Table A6 (Cont.). Structure Factors for SIHP: 10|F|o vs 10|F|c page 3

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
13	1	158	168	16	9	2	0	27	40*	5	5	76	24	42*
13	3	54	57	47*	9	4	316	330	13	5	7	110	93	47*
13	5	63	126	51*	9	6	123	95	24	6	0	1647	1652	12
14	0	145	170	18	10	1	406	393	12	6	2	1453	1463	12
14	2	1175	1153	14	10	3	202	222	12	6	4	484	471	13
14	4	175	196	17	10	5	342	348	14	6	6	280	277	12
15	1	365	375	17	11	0	162	183	14	7	1	487	445	11
15	3	84	38	50*	11	2	97	125	40*	7	3	871	839	11
16	0	283	299	14	11	4	352	325	17	7	5	391	400	16
16	2	1674	1688	16	11	6	48	65	54*	7	7	465	477	19
17	1	95	94	51*	12	1	0	113	45*	8	0	824	799	10
18	0	940	895	15	12	3	221	199	13	8	2	938	923	11
					12	5	130	134	23	8	4	719	713	13
^^^^^^^	h =	5	^^^^^^^		13	0	173	190	15	8	6	598	575	15
					13	2	479	456	14	9	1	544	553	12
1	0	107	49	14	13	4	0	26	50*	9	3	600	640	13
1	2	1260	1229	10	14	1	322	291	12	9	5	462	456	15
1	4	312	296	13	14	3	103	97	47*	10	0	197	172	12
1	6	288	302	12	15	0	109	13	41*	10	2	404	389	14
1	8	214	196	15	15	2	270	255	12	10	4	683	666	14
2	1	74	80	36*	15	4	0	99	52*	10	6	722	759	16
2	3	196	225	10	16	1	121	204	43*	11	1	529	521	13
2	5	0	14	44*	16	3	223	229	16	11	3	654	691	14
2	7	87	24	30*	17	0	76	154	55*	11	5	400	429	19
3	0	680	654	8	17	2	411	383	17	12	0	457	460	14
3	2	602	621	9						12	2	907	885	12
3	4	123	105	16	^^^^^^^	h =	6	^^^^^^^		12	4	606	585	14
3	6	552	542	14						13	1	66	106	48*
3	8	125	135	43*	0	0	1548	1455	11	13	3	281	282	12
4	1	377	366	11	0	2	729	759	9	13	5	146	134	24
4	3	151	169	12	0	4	406	385	12	14	0	505	518	15
4	5	246	251	11	0	6	1212	1197	13	14	2	930	926	14
4	7	0	21	48*	1	1	591	555	9	14	4	318	292	14
5	0	107	103	15	1	3	166	143	11	15	1	455	494	16
5	2	77	85	38*	1	5	602	602	12	15	3	369	388	13
5	4	65	104	43*	1	7	304	337	15	16	0	1082	1090	14
5	6	97	12	43*	2	0	424	470	10	16	2	697	695	16
6	1	682	711	9	2	2	784	811	9	17	1	218	231	15
6	3	192	210	11	2	4	795	795	11					
6	5	391	369	15	2	6	848	836	14	^^^^^^^	h =	7	^^^^^^^	
6	7	205	184	15	3	1	107	48	15					
7	0	431	424	10	3	3	330	299	12	1	0	1305	1322	10
7	2	864	880	10	3	5	204	200	13	1	2	67	32	38*
7	4	85	81	44*	3	7	308	322	14	1	4	589	603	12
7	6	176	182	16	4	0	1747	1753	12	1	6	177	189	16
8	1	475	455	11	4	2	1335	1321	11	2	1	192	176	9
8	3	258	257	12	4	4	486	504	12	2	3	412	386	11
8	5	273	225	13	4	6	311	285	13	2	5	166	173	16
8	7	123	117	26	5	1	363	351	11	2	7	117	21	40*
9	0	647	645	11	5	3	264	308	11	3	0	361	376	12

Table A6 (Cont.). Structure Factors for SIHP: 10|F|o vs 10|F|c page 4

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
3	2	0	31	39*	1	1	470	452	12					
3	4	197	168	11	1	3	490	492	11	^^^^^^^	h =	9	^^^^^^^	
3	6	360	347	17	1	5	305	319	12					
4	1	663	619	10	1	7	93	22	51*	1	0	808	814	11
4	3	265	249	11	2	0	622	632	10	1	2	65	132	43*
4	5	365	347	14	2	2	1522	1522	12	1	4	625	634	13
4	7	74	127	55*	2	4	483	493	14	1	6	52	20	49*
5	0	406	375	11	2	6	898	890	14	2	1	94	36	19
5	2	1111	1123	11	3	1	136	187	14	2	3	608	628	12
5	4	0	20	44*	3	3	320	340	15	2	5	182	187	15
5	6	358	331	13	3	5	105	97	37*	2	7	93	17	50*
6	1	566	556	10	3	7	196	165	17	3	0	998	978	11
6	3	0	83	44*	4	0	376	374	12	3	2	282	259	11
6	5	335	336	12	4	2	4168	4221	23	3	4	517	514	14
6	7	80	175	54*	4	4	72	85	44*	3	6	34	29	49*
7	0	347	371	13	4	6	2200	2213	17	4	1	142	167	15
7	2	214	215	11	5	1	188	183	11	4	3	612	614	12
7	4	94	110	25*	5	3	709	735	12	4	5	69	26	39*
7	6	0	11	50*	5	5	242	252	12	4	7	0	122	55*
8	1	0	70	42*	5	7	139	131	23	5	0	635	669	11
8	3	314	321	16	6	0	1176	1161	11	5	2	0	38	43*
8	5	0	49	47*	6	2	918	919	11	5	4	304	334	12
9	0	803	803	11	6	4	866	869	13	5	6	157	148	20
9	2	85	69	44*	6	6	508	534	16	6	1	0	3	42*
9	4	860	824	13	7	1	493	512	12	6	3	140	110	16
9	6	154	204	21	7	3	55	89	36*	6	5	72	44	37*
10	1	405	418	13	7	5	449	416	16	7	0	523	517	12
10	3	584	598	13	8	0	2700	2718	17	7	2	84	90	42*
10	5	194	198	17	8	2	123	97	19	7	4	525	556	15
11	0	273	311	13	8	4	2365	2361	17	7	6	0	86	54*
11	2	288	300	13	8	6	192	220	18	8	1	0	14	43*
11	4	0	49	50*	9	1	81	55	43*	8	3	434	483	16
12	1	290	295	13	9	3	285	284	13	8	5	0	86	50*
12	3	115	122	39*	9	5	40	17	43*	9	0	78	62	45*
12	5	216	265	17	10	0	0	67	44*	9	2	69	40	46*
13	0	236	257	13	10	2	1414	1414	14	9	4	87	17	48*
13	2	793	761	14	10	4	199	201	15	10	1	104	36	22
13	4	94	151	52*	11	1	513	524	14	10	3	164	154	16
14	1	130	121	21	11	3	73	12	46*	10	5	125	43	23
14	3	134	126	24	11	5	482	457	18	11	0	223	201	13
15	0	235	261	15	12	0	110	115	40*	11	2	559	573	15
15	2	166	166	19	12	2	2175	2219	16	11	4	120	97	24
16	1	74	123	52*	12	4	108	105	28*	12	1	53	169	42*
					13	1	343	355	17	12	3	240	231	14
^^^^^^^	h =	8	^^^^^^^		13	3	0	150	52*	13	0	288	302	14
					14	0	1404	1399	15	13	2	57	62	49*
0	0	4260	4275	23	14	2	436	439	16	13	4	116	127	52*
0	2	423	408	11	15	1	224	205	15	14	1	0	18	51*
0	4	3253	3272	19	15	3	0	16	51*	14	3	123	150	24
0	6	215	220	14	16	0	1396	1399	15	15	0	94	7	38*

Table A6 (Cont.). Structure Factors for SIHP: 10|F|o vs 10|F|c page 5

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
15	2	77	77	51*	15	1	597	594	16	0	6	1484	1455	16
										1	1	172	357	26
^^^^^^^	h =	10	^^^^^^^		^^^^^^^	h =	11	^^^^^^^		1	3	571	565	14
										1	5	205	154	14
0	0	506	528	12	1	0	189	185	13	2	0	971	968	12
0	2	1353	1374	12	1	2	216	197	11	2	2	1093	1089	13
0	4	73	68	45*	1	4	130	150	21	2	4	703	685	14
0	6	558	554	15	1	6	350	345	14	2	6	610	603	17
1	1	653	691	14	2	1	94	104	43*	3	1	777	803	13
1	3	1015	1038	12	2	3	215	207	12	3	3	564	565	15
1	5	425	440	15	2	5	77	50	49*	3	5	614	581	15
2	0	1099	1094	11	3	0	805	842	12	4	0	2176	2207	15
2	2	1193	1193	12	3	2	362	391	15	4	2	101	87	25
2	4	626	620	13	3	4	73	92	47*	4	4	1976	1975	16
2	6	532	536	16	3	6	255	237	14	5	1	457	470	15
3	1	517	482	12	4	1	155	179	15	5	3	521	528	15
3	3	658	641	12	4	3	0	40	47*	5	5	321	305	14
3	5	414	444	16	4	5	169	171	18	6	0	468	440	15
4	0	417	398	13	5	0	498	489	13	6	2	999	992	13
4	2	450	448	13	5	2	94	147	46*	6	4	567	569	15
4	4	565	581	14	5	4	420	409	16	7	1	271	268	12
4	6	451	449	17	5	6	137	148	25	7	3	31	85	49*
5	1	390	387	15	6	1	518	517	13	7	5	288	257	13
5	3	645	686	13	6	3	384	337	15	8	0	159	185	19
5	5	309	318	14	6	5	344	350	13	8	2	1963	1978	16
6	0	268	256	12	7	0	191	197	14	8	4	89	47	41*
6	2	708	696	12	7	2	26	64	47*	9	1	226	244	14
6	4	630	613	14	7	4	151	161	18	9	3	104	53	52*
6	6	843	845	15	8	1	624	629	14	10	0	1294	1328	15
7	1	664	666	12	8	3	486	520	14	10	2	666	659	15
7	3	651	667	13	8	5	389	400	19	10	4	878	843	16
7	5	534	548	16	9	0	442	476	15	11	1	602	565	15
8	0	99	67	41*	9	2	751	736	14	11	3	360	309	14
8	2	962	980	13	9	4	0	115	52*	12	0	1374	1376	15
8	4	240	234	14	10	1	141	111	19	12	2	218	230	16
9	1	0	52	45*	10	3	0	60	49*	13	1	177	172	19
9	3	513	535	15	11	0	233	225	13					
9	5	0	26	54*	11	2	70	103	50*	^^^^^^^	h =	13	^^^^^^^	
10	0	773	760	13	11	4	0	95	54*					
10	2	901	872	14	12	1	0	19	50*	1	0	0	234	65*
10	4	490	475	16	12	3	112	78	45*	1	2	560	543	14
11	1	508	502	14	13	0	317	293	15	1	4	0	19	50*
11	3	313	306	14	13	2	181	176	18	2	1	0	18	46*
12	0	1105	1130	14	14	1	235	238	16	2	3	421	412	16
12	2	731	705	15						2	5	81	127	53*
12	4	636	647	17	^^^^^^^	h =	12	^^^^^^^		3	0	750	738	13
13	1	71	128	52*						3	2	361	387	18
13	3	37	83	52*	0	0	583	622	13	3	4	281	254	12
14	0	595	565	16	0	2	2706	2735	17	4	1	274	279	12
14	2	727	718	15	0	4	0	102	50*	4	3	0	91	48*

Table A6 (Cont.). Structure Factors for SIHP: 10|F|o vs 10|F|c page 6

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
4	5	263	254	13	1	0	394	405	18					
5	0	0	24	46*	1	2	56	21	51*					
5	2	175	177	17	1	4	246	206	15					
5	4	88	77	41*	2	1	0	29	50*					
6	1	111	86	43*	2	3	387	384	14					
6	3	232	239	14	3	0	377	323	18					
7	0	144	150	19	3	2	168	161	18					
7	2	412	404	19	3	4	75	87	53*					
7	4	114	22	46*	4	1	0	16	49*					
8	1	242	234	13	4	3	254	261	14					
8	3	0	96	53*	5	0	95	107	51*					
9	0	34	109	51*	5	2	375	331	19					
9	2	227	226	15	6	1	79	61	49*					
10	1	234	198	15	6	3	181	182	18					
10	3	116	92	51*	7	0	311	318	15					
11	0	333	309	15	7	2	0	9	52*					
11	2	88	67	43*	8	1	217	195	16					
12	1	167	133	19	9	0	206	177	17					
^^^^^^^ h = 14 ^^^^^^^					^^^^^^^ h = 16 ^^^^^^^									
0	0	889	902	13	0	0	1407	1431	15					
0	2	68	141	42*	0	2	51	115	53*					
0	4	815	807	14	1	1	27	271	62*					
1	1	0	6	57*	1	3	254	236	14					
1	3	179	185	16	2	0	766	764	16					
1	5	66	51	50*	2	2	642	652	17					
2	0	676	682	14	3	1	255	230	13					
2	2	778	784	14	3	3	177	129	18					
2	4	675	623	14	4	0	222	281	17					
3	1	388	402	16	4	2	1369	1357	15					
3	3	456	464	16	5	1	67	29	43*					
4	0	300	263	14	6	0	1234	1215	15					
4	2	563	522	14	6	2	467	474	18					
4	4	325	286	12	7	1	264	219	15					
5	1	261	274	13										
5	3	540	580	17	^^^^^^^ h = 17 ^^^^^^^									
6	0	682	688	15										
6	2	923	891	15	1	0	419	405	21					
6	4	482	485	17	2	1	97	95	41*					
7	1	437	433	16	3	0	0	124	57*					
7	3	245	234	14										
8	0	970	993	15										
8	2	420	363	18										
9	1	107	4	49*										
10	0	783	774	16										
10	2	586	552	16										
^^^^^^^ h = 15 ^^^^^^^														