Intramolecular Cyclopropanation of Glycals: Studies Toward the Synthesis of Canadensolide, Sporothriolide, and Xylovobide

Ming Yu, Vincent Lynch[+] and Brian L. Pagenkopf*

Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712

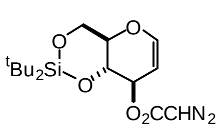
Pagenkopf@mail.utexas.edu

Experimental Section

All reactions were run under an atmosphere of argon unless otherwise indicated. Flasks were oven or flamed-dried and allowed to cool in dry box or desiccator prior to use. Solvents and reagents were purified by standard methods.[1]

Thin-layer chromatography (TLC) was performed on EM 250 Kieselgel 60 F254 silica gel plates. The plates were visualized by staining with I_2 on silica, CAM, ninhydrin, or potassium permanganate. Column chromatography was performed with EM Science Silica gel 60 according to the method of Still.[2]

The ^{1}H, ^{13}C, ^{31}F NMR data was obtained on a General Electric QE-300 spectrometer, a Varian Unity Plus 300 spectrometer, or a Varian INOVA 500. For ^{1}H NMR, chemical shifts are reported in parts per million (ppm) downfield from tetramethylsilane and are, in all cases, referenced to the residual proton resonance peaks: δ 7.24 for $CHCl_3$, δ 7.15 for benzene-d_6. The ^{13}C NMR chemical shifts were reported in ppm relative to the center peak of the multiplet for deuterated solvents: δ 77.0 (t) for $CDCl_3$, 128.0 (t) for benzene-d_6. ^{13}C and ^{19}F NMR spectra were routinely run with broadband ^{1}H decoupling. Chemical shifts for ^{19}F NMR are reported in ppm downfield from $CFCl_3$ as external standard. Coupling constants for all spectra are reported in Hertz (Hz). Infrared spectra were measured on a NEXUS 470 FT-IR spectrometer as thin films on sodium bromide plates and are recorded in units of cm^{-1}. HRMS were made with a VG analytical ZAB2-E instrument.



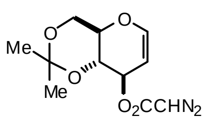
Diazo-acetic acid 2,2-di-*tert*-butyl-4,4a,8,8a-tetrahydro-1,3,5-trioxa-2-sila-naphthalen-8-yl ester (5a).
To a solution of glycal **4a** (288 mg, 1.0 mmol) and glyoxylic acid chloride *p*-toluenesulfonylhydrazone **10** (340 mg, 1.3 mmol) in CH_2Cl_2 (8 mL) and DMF (2 mL) cooled to 0 °C was added *N*,*N*-dimethylaniline (294 µL, 2.9 mmol) in one portion. The resulting solution was stirred 5 min and treated with Et_3N (750 µL, 5.4 mmol). The reaction mixture was stirred for an additional 10 min and H_2O (30 mL) and additional CH_2Cl_2 (10 mL) was added. The organic layer was separated and washed with H_2O (3 × 10 mL), saturated Na_2CO_3 solution (10 mL), and dried (Na_2SO_4). After filtration through

[+] Author for inquiries concerning the X-ray data.

[1] Armarego, W.L.F.; Perrin, D. D. *Purification of Laboratory Chemicals*; 4th Ed.; Oxford ; Boston : Butterworth Heinemann, 1996.

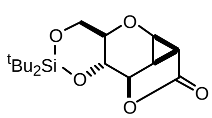
[2] Still, W. C.; Kahn, M.; Mitra, A. A. *J. Org. Chem*. **1978**, *43*, 2923-2925.

a pad of celite, the solvent was removed under reduced pressure. Purification of the residual oil by flash chromatography on silica gel with 10:1 hexanes-EtOAc for elution gave the title compound as light yellow syrup (325 mg, 92%). R_f 0.54 (EtOAc : hexanes = 1 : 5); IR (thin film):n = 3150, 2105, 1692, 1643 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 6.27 (dd, J = 6.1, 1.2 Hz, 1H), 5.41 (dt, J = 6.1, 1.9 Hz, 1H), 4.76 (s, 1H), 4.68 (dd, J = 6.1, 1.8 Hz, 1H), 4.15-4.00 (m, 2H), 3.93-3.78 (m, 2H), 1.01 (s, 9H), 0.97 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.8, 145.3, 101.0, 74.0, 73.2, 73.1, 66.1, 46.6, 27.7, 27.2, 23.0, 20.2; HRMS: m/z calcd for $C_{16}H_{27}N_2O_5Si$ ($M+1^+$): 355.1689, found: 355.1684.



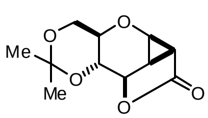
Diazo-acetic acid 2,2-dimethyl -4,4a,8,8a-tetrahydro-pyrano[3,2-*d*]dioxin-8-yl ester (5b).

The title compound **5b** was prepared according to the general procedure described above for the preparation of **5a,** starting with **4b** (102 mg, 0.54 mmol). Crude **5b** was purified by flash chromatography on silica gel with 10: 1 of hexanes-EtOAc for elution to give **5b** as a colorless syrup (122 mg, 88%). R_f 0.45 (EtOAc : hexanes = 1 : 3); IR (thin film):n = 3106, 2112, 1689, 1623 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 6.32 (dd, J = 6.1, 1.5 Hz, 1H), 5.41 (dd, J = 6.1, 1.8 Hz, 1 H), 4.79 (s, 1 H), 4.74 (dd, J = 6.0, 1.8 Hz, 1H), 4.01-3.90 (m, 2H), 3.86-3.77 (m, 2H), 1.49 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.6, 145.7, 101.2, 100.1, 70.2, 70.1, 70.0, 61.8, 46.6, 29.1, 19.2; HRMS: m/z calcd for $C_{11}H_{15}N_2O_5$ ($M+1^+$): 255.0981, found: 255.0971.



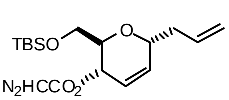
6,6-Di-*tert*-butyl-hexahydro-1,3,5,7-tetraoxa-6-sila-benzo[*g*]cyclopropa[*cd*]inden-2-one (6a).

To a refluxing solution of $Cu(TBS)_2$ complex **11** (7.5 mg, 5 mol %) in 60 mL of toluene was added **5a** (1.20 g, 3.38 mmol) in 20 mL of toluene over a period of 12 h via syringe pump. After the addition was complete, the reaction mixture was heated at reflux for additional 2 h, allowed to cool to rt, and the solvent was removed under reduced pressure. Purification of the residue by flash chromatography on silica gel (5:1 hexane-EtOAc to EtOAc gradient for elution) afforded a pale yellow solid (1.01 g, 92%). Recrystallization from EtOAc/hexane afforded the title compound as colorless needles (81%). mp (ethyl acetate-hexanes) 199.5-201.0 °C; R_f 0.52 (EtOAc : hexanes = 1 : 2); IR (KBr pellet):n 3035, 1790, 1466 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 4.91 (*app* d, J = 6.1 Hz, 1H), 4.34-4.29 (m, 2H), 3.92 (*app* d, J = 9.4 Hz, 1H), 3.79 (dd, J = 9.6, 10.8 Hz, 1H), 3.46 (ddd, J = 9.4, 5.3, 1.4 Hz, 1H), 2.57 (ddd, J = 12.1, 6.2, 6.0 Hz, 1H), 2.32 (dd, J = 6.7, 6.7 Hz, 1H), 1.01 (s, 9H), 0.97 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.1, 78.6, 76.3, 74.6, 67.2, 60.0, 28.9, 27.8, 27.5, 22.9, 22.8, 20.6; HRMS: m/z calcd for $C_{16}H_{27}O_5Si$ ($M+1^+$): 327.1628, found: 327.1618.



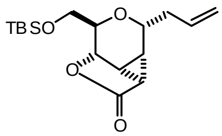
6,6-Dimethyl-hexahydro-1,3,5,7-tetraoxa-benzo[*g*]cyclopropa[*cd*]inden-2-one (6b).

The title compound **6b** was prepared according to the general procedure as described above for the preparation of **6a,** starting with **5b** (108 mg, 0.43 mmol). Crude **6b** was purified by flash chromatography on silica gel (4:1 hexanes-EtOAc to 100% EtOAc gradient elution) to give **6b** as a pale yellow oil (86 mg, 89%). R_f 0.55 (EtOAc : hexanes = 2 : 1); IR (thin film):n 1792 cm^{-1}; ^1H NMR (300 MHz, d_6-benzene): δ 4.39 (*app* d, J = 6.4 Hz, 1H), 3.74 (ddd, J = 10.1, 4.7, 0.5 Hz, 1H), 3.60 (*app* d, J = 10.1 Hz, 1H), 3.43-3.34 (m, 2H), 3.00 (ddd, J = 10.3, 10.3, 4.7 Hz, 1H), 1.55 (dd, J = 6.7, 6.7 Hz, 1H), 1.40 (ddd, J = 13.0, 6.7, 6.7 Hz, 1H), 1.36 (d, J = 0.4 Hz, 3H), 1.03 (d, J = 0.4 Hz, 3H); ^{13}C NMR (75 MHz, d_6-benzene): δ 169.9, 101.2, 76.2, 74.7, 73.1, 63.6, 62.1, 29.2, 29.1, 23.7, 19.1; HRMS: m/z calcd for $C_{11}H_{15}O_5$ ($M+1^+$): 227.0919, found: 227.0910.

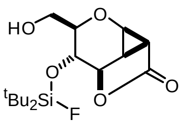


Diazo-acetic acid 6-allyl-2-(*tert*-butyl-dimethyl-silanyloxymethyl)-3,6-dihydro-2*H*-pyran-3-yl ester (8).

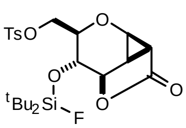
The title compound **8** was prepared according to the general procedure as described for the preparation of **5a,** starting with **7** (46mg, 0.16 mmol). Crude **8** was purified by flash chromatography on silica gel with 10: 1 of hexanes-EtOAc for elution to give a pale yellow syrup (48 mg, 86%). R_f 0.65 (EtOAc : Hexanes = 2 : 3); IR (thin film): v 3072, 2110, 1697, 1643 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 5.92-5.76 (m, 3H), 5.18-5.13 (m, 2H), 5.11-5.04 (m, 1H), 4.75 (s, 1H), 4.25-4.17 (m, 1H), 3.78 (ddd, J = 1.0, 5.3, 9.0 Hz, 1H), 3.72 (d, J = 5.3 Hz, 2H), 2.44-2.25 (m, 2H), 0.87 (s, 9H), 0.03 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.2, 134.2, 133.3, 123.6, 117.3, 73.3, 70.9, 65.8, 62.8, 46.3, 38.2, 25.9, 18.3, -5.4.
HRMS: m/z calcd for $C_{17}H_{28}N_2O_4Si$ ($M+1^+$): 353.1937, found 353.1936.



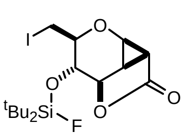
3-Allyl-5-(*tert*-butyl-dimethyl-silanyloxymethyl)-hexahydro-1,4-dioxa-cyclopropa[*cd*]inden-2-one (9).
The title compound **9** was prepared according to the general procedure as described above for the preparation of **6a**, starting with **8** (42 mg, 0.12mmol). Crude **9** was purified by flash chromatography on silica gel with hexanes-EtOAc (3:1 hexanes-EtOAc) for elution to give as a pale yellow oil (33 mg, 85%). R_f 0.3 (EtOAc : Hexanes = 3 : 1); IR (thin film): *v* 3073, 1763, 1643 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 5.89-5.75 (m, 1H), 5.19-5.05 (m, 2H), 4.72 (dd, *J* = 2.3, 4.4 Hz, 1H), 4.13 (dd, *J* = 6.7, 6.7, 3.4 Hz, 1H), 3.96-3.75 (m, 3H), 2.62 (dd, *J* = 6.8, 6.8 Hz, 1H), 2.45-2.26 (m, 2H), 2.14 (dd, *J* = 8.7, 6.7 Hz, 1H), 1.46 (ddd, *J* = 8.4, 8.4, 3.4 Hz, 1H), 0.88 (s, 9H), 0.06 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.0, 133.5, 117.9, 72.3, 71.1, 66.1, 60.1, 40.2, 25.8, 22.8, 22.44, 22.40, 18.1, -5.5; HRMS: m/z calcd. for $C_{17}H_{28}O_4Si$ ($M+1^+$): 325.1835, found: 325.1840.



5-(Di-*tert*-butyl-fluoro-silanyloxy)-4-hydroxymethyl-hexahydro-1,3-dioxa-cyclopropa[*cd*]inden-2-one (12).
To a rt solution of **6a** (300 mg, 0.92 mmol) in toluene (11 mL) was added allyltrimethylsilane (306 μL, 1.92 mmol) and $BF_3•Et_2O$ (207 μL, 1.78 mmol) sequentially. The reaction vessel was placed into an 85 °C oil bath and after 30 min TLC analysis of an aliquot indicated the reaction was complete. The reaction mixture was allowed to cool to rt and was treated with 5% aqueous Na_2CO_3 solution (3 mL). The organic layer was separated and washed with H_2O (3 × 10 mL), brine (5 mL) and dried ($MgSO_4$). After filtration through a small pad of celite, the solvent was removed under reduced pressure. Purification of the residue by flash chromatography on silica gel with 3:1 of hexanes-EtOAc for elution gave the title compound as a colorless oil (302 mg, 95%). R_f 0.62 (EtOAc : hexanes = 2 : 1); IR (thin film):*n* 3200-3450 (br), 3092, 1772 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 4.86 (dd, *J* = 5.6, 1.6 Hz, 1H), 4.18 (dd, *J* = 6.1, 6.1 Hz, 1H), 4.13 (dd, *J* = 6.0, 1.5 Hz, 1H), 3.88-3.81 (m, 1H), 3.65-3.51 (m, 2H), 2.54 (ddd, *J* = 5.8, 5.8, 5.8 Hz, 1H), 2.35 (dd, *J* = 6.4, 6.4 Hz, 1H), 2.1 (br s, 1H), 1.03 (s, 9H), 1.04 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 171.3 (C), 81.4 (CH), 76.1 (CH), 67.3 (CH), 63.0 (CH_2), 54.1 (CH), 26.8 (CH_3), 26.4 (CH), 20.8 (CH), 20.2 (d, *J* = 14.6 Hz, C), 20.0 (d, *J* = 14.6 Hz, C); ^{19}F NMR (470 MHz, $CDCl_3$): -159.9; HRMS: m/z calcd for $C_{16}H_{28}O_5FSi$ ($M+1^+$): 347.1690, found: 346.1688.

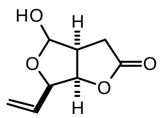


Toluene-4-sulfonic acid 5-(1-*tert*-butyl-1-fluoro-2,2-silanyloxy)-2-oxo-octahydro-cyclopropa[*cd*]inden-4-ylmethyl ester.
To a stirred, rt solution of **12** (270 mg, 0.78 mmol) and *p*-toluene sulfonyl chloride (186 mg, 0.98 mmol) in CH_2Cl_2 (6 mL) was added pyridine (2 mL, 24.7 mmol) in one portion. The resulting solution was stirred at rt for 20 h and then volatiles were removed in vacuo. The resulting residue was dissolved in EtOAc (30 mL) and the solution was washed with H_2O (2 × 4 mL), brine (10 mL), and dried ($MgSO_4$). After filtration through a pad of celite, the solvent was removed under reduced pressure. Purification of the residual oil by flash chromatography on silica gel using 4:1 of hexanes-EtOAc for elution provided the title compound as white solid (344 mg, 92%). The tosylate was used immediately in the next reaction. R_f 0.64 (EtOAc : hexanes = 1 : 1); ^1H NMR (300 MHz, $CDCl_3$): 7.74 (dd, *J* = 6.8, 1.7 Hz, 2H), 7.30 (dd, *J* = 6.7, 1.7 Hz, 2H), 4.85 (dd, *J* = 5.7, 1.5 Hz, 1H), 4.27 (dd, *J* = 11.0, 2.5 Hz, 1H), 4.13 (dd, *J* = 7.2, 1.5 Hz, 1H), 3.97-3.85 (m, 2H), 3.67 (ddd, *J* = 9.2, 6.8, 2.5 Hz, 1H), 2.54 (ddd, *J* = 6.0, 6.0, 6.0 Hz, 1H), 2.46 (s, 3H), 2.34 (dd, *J* = 6.4, 6.4 Hz, 1H), 1.07 (s, 9H), 1.12 (s, 9H).

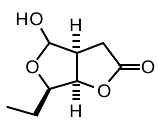


5-(*tert*-Butyl-hydroxy-isopropyl-silanyloxy)-4-iodomethyl-octahydro-cyclopropa[*cd*]inden-2-one (13).
A mixture of the tosylate prepared in the preceding reaction (344 mg, 0.71 mmol) and NaI (700 mg, 4.35 mmol, 6.1 equiv) in acetone (3.5 mL) was stirred in the dark at reflux temperature for 30 h. To the cooled reaction mixture solid $NaHCO_3$ (15 mg, 0.21 mmol) was added. After stirring for 10 min, the solvent was removed under reduced pressure. Water (8 mL) and EtOAc (30 mL) were added to residue and the organic layer was separated, washed with H_2O (8 mL) and dried ($MgSO_4$). After filtration through a pad of celite, the solvent was removed under reduced pressure. Purification of the residual oil by flash chromatography on silica gel with 6:1 hexanes-EtOAc for elution provided the title compound as a pale yellow syrup (300 mg, 92%). R_f 0.74 (EtOAc : hexanes = 1 : 1); IR ($CDCl_3$):*n* 3115, 1779 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 4.48 (dd, *J* = 5.6, 1.3 Hz, 1H), 4.22 (dd, *J* = 6.0, 6.0 Hz, 1H), 4.00 (dd, *J* = 6.3, 1.1 Hz, 1H), 3.49 (dd, *J*

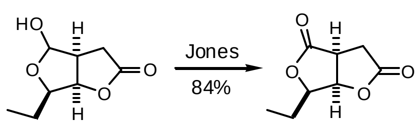
= 10.8, 2.7 Hz, 1H), 3.39 (ddd, J = 6.5, 6.5, 2.73 Hz, 1H), 3.13 (dd, J = 10.8, 7.8 Hz, 1H), 2.55 (ddd, J = 6.0, 6.0, 6.0 Hz, 1H); 2.35 (dd, J = 6.4, 6.4 Hz, 1H), 1.09 (d, J = 0.9 Hz, 9H), 1.03 (d, J = 0.9 Hz, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.2 (C), 80.7 (CH), 76.4 (CH), 71.5 (CH), 54.9 (CH), 26.8 (CH_3), 26.7 (CH_3), 26.6 (CH), 20.7(CH), 20.2 (d, J = 14.5 Hz, C), 20.0 (d, J = 14.5 Hz, C), 4.9 (CH_2); HRMS: m/z calcd for $C_{16}H_{27}O_4FSiI$ (M+1$^+$): 457.0707, found: 457.0700.



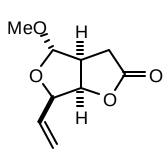
4-Hydroxy-6-vinyl-tetrahydro-furo[3,4-*b*]furan-2-one (16).
A 10 mL round-bottomed flask containing a suspension of Zn-Cu couple[3] (400 mg, 6.2 mmol) in THF (1.2 mL) was placed in a 60 °C oil bath. The reaction mixture was treated sequentially with Me_3SiCl (170 mL, 1.3 mmol) and $BrCH_2CH_2Br$ (150 µL, 1.7 mmol). After ethylene evolution ceased (about 5 min), the reaction mixture was allowed to cool to rt and a solution of iodide **13** (40 mg, 0.09 mmol) in 0.8 mL of THF was added. After 20 min the reaction appeared complete as determined by TLC, and the cloudy solution was decanted from the remaining zinc metal and transferred with the aid of additional THF (2 × 2 mL) into a plastic test tube containing HF•pyridine (20% HF, 5 mL) and THF (0.5 mL). After 2 min 10% aqueous H_2SO_4 (2 mL) was added, and the resulting mixture was extracted with EtOAc (4 × 1.5 mL). The combined organic layers were washed with H_2O (2 mL), saturated aqueous Na_2HCO_3 solution (2 × 1 mL), brine (1 mL) and dried ($MgSO_4$). Removal of volatile components under reduced pressure and purification of the resulting residue by flash chromatography on silica gel with 2:1 of hexanes-EtOAc for elution provided the title compound as a colorless oil (11.4 mg, 76%). To simplify characterization of the readily epimerizable hemiacetals, the olefin was reduced and the hemiacetal oxidized to the lactone **22** as described in the next two experiments. R_f 0.45 (EtOAc : hexanes = 3 : 1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 5.90 (ddd, J = 17.3, 10.4, 6.9 Hz, 1H), 5.46-5.41 (m, 2H), 5.28 (*app* s, 1H), 5.00 (dd, J = 6.9, 4.0 Hz, 1H), 4.57-4.50 (m,1H). 3.06-2.90 (m, 1H), 2.83 (dd, J = 8.5, 1.2 Hz, 1H), 2.50 (dd, J = 8.6, 3.9 Hz, 1H), 2.2 (br s, 1H).



6-Ethyl-4-hydroxyl-tetrahydro-furo[3,4-*b*]furan-2-one (17).
To a solution of **16** (25 mg, 0.145mmol) in 2.5 mL of ethanol at rt was added 5% Pd-C (ca. 3 mg). The reaction mixture was stirred under hydrogen atmosphere (balloon) for 3 h and then filtrated through a pad of celite. Removal of the solvent under reduced pressure afforded the title compound as colorless oil (24 mg, 96%). The product was used immediately in the following reaction. ^{1}H NMR (300 MHz, $CDCl_3$): δ 5.32 (s, 1H), 5.00 (dd, J = 4.9, 3.7 Hz, 1H), 4.15 (dt, J = 7.0, 4.9, Hz, 1H), 3.11-3.02 (m, 1 H), 2.83 (*app* dd, J = 18.6, 11.2 Hz, 1H), 2.61 (br s, 1H), 2.48 (dd, 1 H, J = 18.6, 3.6 Hz, 1H), 1.76-1.67 (m, 2H), 1.04-0.97 (m, 3H).



6-Ethyl-tetrahydro-furo[3,4-*b*]furan-2,4-dione (22).
To a rt solution of hemiacetal **17** from the preceding reaction (22 mg, 0.128 mmol) in acetone (1 mL) was added Jones' reagent[4] drop-wise until a brown color persisted. The resulting solution was then treated with *iso*-propanol (0.1 M in acetone) drop-wise until the solution became green-blue. To the reaction mixture was added H_2O (1 mL) and the volatile components were removed under reduced pressure. The residue was dissolved in EtOAc (5 mL), and washed with 5% aqueous Na_2CO_3 solution (2 × 1 mL), H_2O (1 mL), brine (5 mL) and dried ($MgSO_4$). The solution was filtered through celite and volatiles were removed under reduced pressure. Purification of the residual oil by flash chromatography on silica gel with 5 : 1 hexanes-EtOAc for elution afforded the title compound as a yellow oil (18 mg, 84%). R_f 0.70 (EtOAc : hexanes = 3 : 2); IR (thin film): ν 1772 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 5.08 (dd, J = 6.1, 3.9 Hz, 1H), 4.50 (td, J = 7.2, 3.7 Hz, 1H), 3.48 (*app* ddd, J = 10.1, 6.0, 4.0 Hz, 1H), 2.94-2.89 (m, 2H), 2.01-1.78 (m, 2H), 1.07 (t, J = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.0, 173.2, 83.6, 79.4, 41.8, 31.1, 22.2, 9.7; HRMS: m/z calcd for $C_8H_{11}O_4$ (M+1$^+$): 171.0657, found: 171.0665.



4-methoxy-6-vinyl-tetrahydro-furo[3,4-*b*]furan-2-one (19).
To a solution of hemiacetal **16** (11.4 mg, 66 µmol) in 0.5 mL of MeOH was added 10% aqueous H_2SO_4 (0.1 mL). The reaction mixture was stirred at rt for 6 h and subsequently concentrated under reduced pressure. The residue was dissolved in EtOAc (3 mL), which was

[3] LeGoff, E. J. *J. Org. Chem*. **1964**, *29*, 2048-2049.
[4] Bowden, K.; Halsall, T. G.; Jones, E. R. H.; Weedon, B. C. L. *J. Chem. Soc*. **1946**, 39-45.

then washed with aqueous Na_2CO_3 (2 × 0.5 mL), H_2O (0.5 mL), brine (1 mL) and dried (Na_2SO_4). After filtration through celite, the solvent was removed under reduced pressure to afford 12 mg, (99%) of the title compound as a mixture of diastereomers. Separation of the major diastereomer by flash chromatography on silica gel with 4: 1 hexanes-EtOAc for elution provided the title compound as a colorless oil (10 mg, 82%).

R_f 0.75 (EtOAc : hexanes = 1 : 1); IR (thin film): ν 1771, 1643 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 5.91 (ddd, *J* = 17.4, 10.4, 7.1 Hz, 1H), 5.55-5.35 (m, 2H), 4.95 (dd, *J* = 6.9, 3.9 Hz, 1H), 4.85 (*app* s, 1H), 4.51-4.47 (m, 1H), 3.27 (s, 3H), 3.09-3.04 (m, 1H), 2.80 (dd, *J* = 18.6, 11.2 Hz, 1H), 2.5 (dd, *J* = 18.5, 3.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.4, 131.2, 119.7, 109.2, 84.0, 80.6, 54.8, 45.9, 31.9; HRMS: m/z calcd for $C_8H_{11}O_4$ ($M+1^+$): 185.0814, found: 185.0806.

X-Ray Crystallographic Material

In the X-ray section, the compound 1 refers to **6a** in the manuscript.

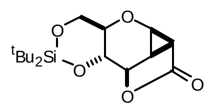


Table 1. Crystallographic Data for 1.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of 1.

Table 3. Bond Lengths (Å) and Angles (°) for the non-hydrogen atoms of 1.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of 1.

Table 5. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of 1.

Table 6. Observed and calculated structure factor amplitudes for 1. Values for Fo, Fc and σ(Fo) have been multiplied by 10.

Figure 1. View of 1 showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Most hydrogen atoms have been removed for clarity.

Figure 2. Unit cell packing diagram for 1. The view is approximately down the **a** axis.

X-ray Experimental for $C_{16}H_{26}O_5Si$: Crystals grew as colorless prisms by slow evaporation from ethyl acetate and hexanes. The data crystal had approximate dimensions; 0.30 x 0.20 x 0.14 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 634 frames of data were collected using ω-scans with a scan range of 0.9° and a counting time of 54 seconds per frame. The data were collected at –120 °C using a Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR92[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0799*P)^2 + (0.625*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.143, with R(F) equal to 0.0524 and a goodness of fit, S, = 1.135. The absolute configuration was determined by the method of Flack.[4] The Flack parameter was refined to 0.13(11). Definitions used for calculating R(F),$R_w(F^2)$ and the goodness of fit, S, are given below.[5] Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[6] All figures were generated using SHELXTL/PC.[7] Tables of positional and thermal parameters, bond lengths and angles, figures and lists of observed and calculated structure factors are located in tables 1 through 6.

Table 1. Crystal data and structure refinement for 1.

Empirical formula	$C_{16}H_{26}O_5Si$	
Formula weight	330.43	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 6.4313(1) Å	α= 90°.
	b = 11.6244(1) Å	β= 90°.
	c = 22.4048(3) Å	γ = 90°.
Volume	1674.98(4) $Å^3$	
Z	4	
Density (calculated)	1.310 Mg/m^3	
Absorption coefficient	0.214 mm^{-1}	
F(000)	712	
Crystal size	0.30 x 0.20 x 0.14 mm	
Theta range for data collection	3.30 to 27.50°.	
Index ranges	-8<=h<=8, -15<=k<=15, -29<=l<=28	
Reflections collected	13670	
Independent reflections	3846 [R(int) = 0.1062]	
Completeness to theta = 27.50°	99.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3846 / 0 / 200	
Goodness-of-fit on F^2	1.241	
Final R indices [I>2sigma(I)]	R1 = 0.0526, wR2 = 0.1413	
R indices (all data)	R1 = 0.0568, wR2 = 0.1428	
Absolute structure parameter	0.13(11)	
Largest diff. peak and hole	0.91 and -0.50 e.$Å^{-3}$ (near Si1)	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si1	2473(1)	2322(1)	3425(1)	20(1)
O2	4954(2)	2115(1)	3569(1)	22(1)
C3	5933(3)	1127(2)	3823(1)	22(1)
C4	4372(3)	155(2)	3887(1)	18(1)
O5	5236(2)	-745(2)	4254(1)	21(1)
C6	4004(4)	-1740(2)	4174(1)	22(1)
C7	2761(4)	-2209(2)	4689(1)	23(1)
C8	2493(4)	-1458(2)	5220(1)	20(1)
O9	1536(3)	-461(1)	5062(1)	22(1)
C10	1094(3)	-421(2)	4427(1)	19(1)
C11	2363(3)	588(2)	4171(1)	16(1)
O12	1225(2)	1207(1)	3728(1)	18(1)
O13	2950(3)	-1647(2)	5731(1)	27(1)
C14	1710(4)	-1586(2)	4178(1)	22(1)
C15	1999(4)	2222(2)	2589(1)	21(1)
C16	2648(5)	3329(2)	2261(1)	32(1)
C17	-275(4)	1943(3)	2453(1)	32(1)
C18	3367(5)	1241(3)	2344(1)	35(1)
C19	1670(4)	3685(2)	3811(1)	22(1)
C20	3090(4)	4704(2)	3655(1)	30(1)
C21	-593(4)	3996(2)	3635(2)	35(1)
C22	1765(6)	3501(2)	4488(1)	39(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

Si1-O2	1.6463(16)	C14-H14	0.96
Si1-O12	1.6692(16)	C15-C17	1.529(3)
Si1-C19	1.877(2)	C15-C16	1.539(4)
Si1-C15	1.901(3)	C15-C18	1.541(4)
O2-C3	1.427(3)	C16-H16A	0.96
C3-C4	1.518(3)	C16-H16B	0.96
C3-H3A	0.96	C16-H16C	0.96
C3-H3B	0.96	C17-H17A	0.96
C4-O5	1.442(3)	C17-H17B	0.96
C4-C11	1.525(3)	C17-H17C	0.96
C4-H4	0.96	C18-H18A	0.96
O5-C6	1.414(3)	C18-H18B	0.96
C6-C14	1.486(3)	C18-H18C	0.96
C6-C7	1.506(4)	C19-C22	1.532(4)
C6-H6	0.9601	C19-C20	1.536(3)
C7-C8	1.486(4)	C19-C21	1.551(4)
C7-C14	1.515(3)	C20-H20A	0.96
C7-H7	0.96	C20-H20B	0.96
C8-O13	1.203(3)	C20-H20C	0.96
C8-O9	1.359(3)	C21-H21A	0.96
O9-C10	1.452(3)	C21-H21B	0.96
C10-C14	1.517(3)	C21-H21C	0.96
C10-C11	1.539(3)	C22-H22A	0.96
C10-H10	0.96	C22-H22B	0.96
C11-O12	1.428(3)	C22-H22C	0.96
C11-H11	0.96		
O2-SI1-O12	105.81(9)	O2-C3-C4	110.19(18)
O2-SI1-C19	107.47(11)	O2-C3-H3A	110.0
O12-SI1-C19	109.63(10)	C4-C3-H3A	109.6
O2-Si1-C15	109.85(10)	O2-C3-H3B	109.3
O12-Si1-C15	106.03(10)	C4-C3-H3B	109.4
C19-Si1-C15	117.48(11)	H3A-C3-H3B	108.2
C3-O2-Si1	128.59(13)	O5-C4-C3	109.88(19)

O5-C4-C11	109.17(18)	C6-C14-C10	111.7(2)
C3-C4-C11	110.78(18)	C7-C14-C10	105.4(2)
O5-C4-H4	109.0	C6-C14-H14	121.7
C3-C4-H4	109.3	C7-C14-H14	121.2
C11-C4-H4	108.7	C10-C14-H14	121.0
C6-O5-C4	107.79(17)	C17-C15-C16	109.9(2)
O5-C6-C14	117.19(19)	C17-C15-C18	108.5(2)
O5-C6-C7	119.8(2)	C16-C15-C18	107.1(2)
C14-C6-C7	60.82(16)	C17-C15-SI1	111.32(18)
O5-C6-H6	115.6	C16-C15-SI1	112.07(18)
C14-C6-H6	116.0	C18-C15-SI1	107.74(17)
C7-C6-H6	116.3	C15-C16-H16A	109.3
C8-C7-C6	117.6(2)	C15-C16-H16B	109.3
C8-C7-C14	105.82(19)	H16A-C16-H16B	109.5
C6-C7-C14	58.96(16)	C15-C16-H16C	109.7
C8-C7-H7	119.1	H16A-C16-H16C	109.5
C6-C7-H7	120.0	H16B-C16-H16C	109.5
C14-C7-H7	119.3	C15-C17-H17A	109.8
O13-C8-O9	121.0(2)	C15-C17-H17B	109.4
O13-C8-C7	128.8(2)	H17A-C17-H17B	109.5
O9-C8-C7	110.2(2)	C15-C17-H17C	109.2
C8-O9-C10	111.82(18)	H17A-C17-H17C	109.5
O9-C10-C14	106.29(18)	H17B-C17-H17C	109.5
O9-C10-C11	106.55(18)	C15-C18-H18A	109.6
C14-C10-C11	113.89(19)	C15-C18-H18B	109.4
O9-C10-H10	109.9	H18A-C18-H18B	109.5
C14-C10-H10	109.9	C15-C18-H18C	109.5
C11-C10-H10	110.2	H18A-C18-H18C	109.5
O12-C11-C4	108.11(17)	H18B-C18-H18C	109.5
O12-C11-C10	111.75(17)	C22-C19-C20	108.1(2)
C4-C11-C10	110.67(18)	C22-C19-C21	108.8(2)
O12-C11-H11	108.8	C20-C19-C21	108.7(2)
C4-C11-H11	108.8	C22-C19-SI1	109.05(17)
C10-C11-H11	108.7	C20-C19-SI1	112.45(18)
C11-O12-SI1	115.31(13)	C21-C19-SI1	109.71(18)
C6-C14-C7	60.22(16)	C19-C20-H20A	109.3

C19-C20-H20B	109.8
H20A-C20-H20B	109.5
C19-C20-H20C	109.3
H20A-C20-H20C	109.5
H20B-C20-H20C	109.5
C19-C21-H21A	109.6
C19-C21-H21B	109.4
H21A-C21-H21B	109.5
C19-C21-H21C	109.4
H21A-C21-H21C	109.5
H21B-C21-H21C	109.5
C19-C22-H22A	109.6
C19-C22-H22B	109.1
H22A-C22-H22B	109.5
C19-C22-H22C	109.8
H22A-C22-H22C	109.5
H22B-C22-H22C	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
SI1	18(1)	21(1)	21(1)	2(1)	0(1)	0(1)
O2	14(1)	21(1)	31(1)	8(1)	-1(1)	-1(1)
C3	12(1)	27(1)	25(1)	9(1)	1(1)	1(1)
C4	17(1)	19(1)	18(1)	6(1)	1(1)	3(1)
O5	19(1)	20(1)	25(1)	7(1)	-1(1)	3(1)
C6	28(1)	17(1)	20(1)	0(1)	0(1)	5(1)
C7	30(1)	15(1)	23(1)	4(1)	-4(1)	-1(1)
C8	21(1)	19(1)	21(1)	6(1)	1(1)	-3(1)
O9	26(1)	19(1)	20(1)	5(1)	4(1)	2(1)
C10	17(1)	19(1)	22(1)	5(1)	-2(1)	-1(1)
C11	15(1)	16(1)	17(1)	3(1)	0(1)	0(1)
O12	16(1)	18(1)	20(1)	7(1)	-2(1)	1(1)
O13	34(1)	26(1)	22(1)	6(1)	-2(1)	-2(1)
C14	27(1)	17(1)	22(1)	2(1)	-6(1)	-4(1)
C15	24(1)	23(1)	18(1)	1(1)	-2(1)	-3(1)
C16	47(2)	29(1)	21(1)	3(1)	3(1)	-8(1)
C17	32(1)	38(1)	25(1)	2(1)	-9(1)	-7(1)
C18	46(2)	37(1)	22(1)	-8(1)	2(1)	10(1)
C19	28(1)	15(1)	23(1)	-2(1)	3(1)	1(1)
C20	37(1)	21(1)	33(1)	-2(1)	1(1)	-8(1)
C21	29(1)	28(1)	49(2)	-7(1)	1(1)	7(1)
C22	71(2)	25(1)	22(1)	-3(1)	9(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H3A	6503	1314	4206	26
H3B	7050	884	3568	26
H4	4057	-153	3500	22
H6	4535	-2295	3896	26
H7	2571	-3024	4731	27
H10	-364	-292	4364	23
H11	2707	1104	4491	19
H14	826	-1987	3902	27
H16A	2382	3242	1842	48
H16B	1857	3965	2413	48
H16C	4103	3470	2323	48
H17A	-476	1896	2029	47
H17B	-635	1220	2632	47
H17C	-1145	2539	2613	47
H18A	3155	1169	1922	52
H18B	4802	1411	2422	52
H18C	2996	532	2537	52
H20A	2621	5378	3863	45
H20B	4495	4534	3769	45
H20C	3034	4841	3232	45
H21A	-1001	4694	3832	53
H21B	-675	4100	3211	53
H21C	-1506	3383	3753	53
H22A	1352	4194	4689	59
H22B	836	2888	4595	59
H22C	3156	3301	4604	59

Table 6. Observed and calculated structure factors for 1 Page 1

h	k	l	10Fo	10Fc	10s
4	0	0	531	442	4
6	0	0	252	180	4
8	0	0	202	204	3
1	1	0	767	777	8
2	1	0	267	263	1
3	1	0	123	123	1
4	1	0	270	268	1
5	1	0	19	14	1
6	1	0	14	22	2
7	1	0	143	143	1
8	1	0	192	189	2
0	2	0	577	663	5
1	2	0	292	275	158
2	2	0	601	598	8
3	2	0	292	261	2
4	2	0	618	569	4
5	2	0	89	61	1
6	2	0	140	131	1
7	2	0	65	61	2
8	2	0	161	166	1
1	3	0	428	446	2
2	3	0	272	269	1
3	3	0	329	335	2
4	3	0	68	61	1
5	3	0	51	52	1
6	3	0	155	158	1
7	3	0	60	52	1
8	3	0	29	36	4
0	4	0	318	275	2
1	4	0	193	199	1
2	4	0	65	89	1
3	4	0	360	339	7
4	4	0	469	454	5
5	4	0	220	150	7
6	4	0	151	154	1
7	4	0	147	136	2
8	4	0	67	76	2
1	5	0	328	324	2
2	5	0	545	535	3
3	5	0	76	89	1
4	5	0	76	66	1
5	5	0	143	148	1
6	5	0	106	102	1
7	5	0	62	66	1
0	6	0	59	39	1
1	6	0	12	0	2
2	6	0	111	81	1
3	6	0	183	190	1
4	6	0	239	239	3
5	6	0	216	201	13
6	6	0	121	122	1
7	6	0	185	179	2
1	7	0	328	341	2
2	7	0	330	332	2
3	7	0	346	371	2
4	7	0	67	67	1
5	7	0	84	90	2
6	7	0	56	57	1
7	7	0	120	122	1
0	8	0	86	110	2
1	8	0	54	56	54
2	8	0	232	244	5
3	8	0	176	182	1
4	8	0	88	80	2
5	8	0	0	15	1
6	8	0	134	136	1
7	8	0	29	27	4
1	9	0	148	152	1
2	9	0	35	32	2
3	9	0	168	180	1
4	9	0	55	56	1
5	9	0	228	228	2
6	9	0	56	55	2
0	10	0	255	275	3
1	10	0	244	250	2
2	10	0	429	446	3
3	10	0	112	122	1
4	10	0	24	22	3
5	10	0	8	9	8
6	10	0	39	37	6
1	11	0	364	357	4
2	11	0	0	6	1
3	11	0	264	262	6
4	11	0	5	7	5
5	11	0	159	155	2
0	12	0	134	130	3
1	12	0	26	21	3

h	k	l	10Fo	10Fc	10s
2	12	0	29	24	9
3	12	0	81	85	1
4	12	0	130	133	1
5	12	0	18	9	18
1	13	0	216	201	3
2	13	0	42	40	2
3	13	0	278	260	3
4	13	0	62	61	3
0	14	0	22	29	7
1	14	0	0	13	1
2	14	0	24	30	7
3	14	0	92	95	2
1	0	1	36	34	1
2	0	1	545	550	4
3	0	1	325	298	2
4	0	1	139	128	1
5	0	1	15	12	1
6	0	1	181	186	1
7	0	1	39	36	2
8	0	1	69	69	3
-8	1	1	118	102	14
-7	1	1	176	147	5
-6	1	1	64	55	11
-5	1	1	171	154	4
-4	1	1	105	33	3
-3	1	1	910	788	8
-2	1	1	365	271	91
2	1	1	388	274	88
3	1	1	898	786	8
4	1	1	104	34	1
5	1	1	171	156	4
6	1	1	77	56	6
7	1	1	180	149	5
8	1	1	127	103	8
-8	2	1	91	90	1
-7	2	1	86	89	1
-6	2	1	49	53	1
-5	2	1	211	219	1
-4	2	1	87	83	1
-3	2	1	237	224	1
-2	2	1	243	243	1
-1	2	1	853	859	9
0	2	1	264	284	1
1	2	1	853	859	7
2	2	1	242	241	1
3	2	1	236	223	1
4	2	1	85	82	1
5	2	1	212	219	1
6	2	1	52	53	1
7	2	1	86	88	1
8	2	1	91	90	1
-8	3	1	135	132	3
-7	3	1	169	155	5
-6	3	1	82	62	3
-5	3	1	263	258	3
-4	3	1	223	225	4
-3	3	1	420	377	11
-2	3	1	179	133	21
-1	3	1	460	447	9
0	3	1	30	30	1
1	3	1	455	452	3
2	3	1	177	134	23
3	3	1	448	381	8
4	3	1	224	224	6
5	3	1	268	260	5
6	3	1	76	62	3
7	3	1	169	155	4
8	3	1	137	133	2
-8	4	1	46	49	3
-7	4	1	69	68	1
-6	4	1	62	66	1
-5	4	1	168	169	1
-4	4	1	244	256	1
-3	4	1	81	68	1
-2	4	1	450	428	2
-1	4	1	392	363	2
0	4	1	392	420	2
1	4	1	394	364	2
2	4	1	448	426	2
3	4	1	81	67	1
4	4	1	243	255	1
5	4	1	166	169	1
6	4	1	63	66	1
7	4	1	66	68	2
8	4	1	51	49	3
-7	5	1	61	59	5
-6	5	1	195	197	2

h	k	l	10Fo	10Fc	10s
-5	5	1	231	232	2
-4	5	1	533	528	18
-3	5	1	171	172	2
-2	5	1	409	405	5
-1	5	1	119	134	1
0	5	1	63	84	1
1	5	1	119	135	1
2	5	1	410	404	2
3	5	1	166	172	1
4	5	1	533	529	4
5	5	1	231	232	1
6	5	1	200	197	2
7	5	1	67	59	4
-7	6	1	89	84	1
-6	6	1	50	49	1
-5	6	1	221	232	1
-4	6	1	364	378	2
-3	6	1	241	251	1
-2	6	1	170	166	1
-1	6	1	37	42	1
0	6	1	191	205	1
1	6	1	37	42	1
2	6	1	173	168	1
3	6	1	242	251	1
4	6	1	366	377	2
5	6	1	221	233	1
6	6	1	51	51	2
7	6	1	84	83	1
-7	7	1	98	105	2
-6	7	1	104	105	1
-5	7	1	83	83	4
-4	7	1	142	148	1
-3	7	1	228	234	1
-2	7	1	168	167	1
-1	7	1	176	173	1
0	7	1	602	612	4
1	7	1	176	175	1
2	7	1	170	168	1
3	7	1	225	231	1
4	7	1	141	149	1
5	7	1	88	85	1
6	7	1	103	106	2
7	7	1	99	103	2
-7	8	1	45	47	3
-6	8	1	90	88	1
-5	8	1	14	10	14
-4	8	1	136	140	1
-3	8	1	74	78	1
-2	8	1	250	258	2
-1	8	1	454	469	3
0	8	1	445	458	3
1	8	1	456	469	3
2	8	1	250	258	1
3	8	1	70	78	1
4	8	1	136	142	1
5	8	1	17	10	8
6	8	1	87	86	1
7	8	1	41	48	3
-6	9	1	56	55	2
-5	9	1	60	67	1
-4	9	1	64	67	1
-3	9	1	51	59	9
-2	9	1	23	25	3
-1	9	1	279	290	8
0	9	1	135	137	6
1	9	1	280	291	2
2	9	1	22	26	2
3	9	1	56	61	6
4	9	1	55	66	1
5	9	1	60	68	1
6	9	1	52	54	4
-6	10	1	100	104	1
-5	10	1	40	41	3
-4	10	1	119	124	1
-3	10	1	55	53	1
-2	10	1	186	191	8
-1	10	1	51	51	4
0	10	1	392	392	11
1	10	1	50	49	1
2	10	1	187	194	4
3	10	1	49	51	2
4	10	1	120	125	1
5	10	1	41	40	4
6	10	1	105	104	2
-5	11	1	158	160	1
-4	11	1	41	37	3
-3	11	1	100	98	1

h	k	l	10Fo	10Fc	10s
-2	11	1	121	123	1
-1	11	1	147	156	2
0	11	1	264	271	3
1	11	1	147	155	1
2	11	1	119	123	1
3	11	1	95	98	1
4	11	1	41	36	2
5	11	1	159	161	1
-5	12	1	100	99	2
-4	12	1	158	151	3
-3	12	1	72	61	3
-2	12	1	285	278	4
-1	12	1	35	25	9
0	12	1	145	138	5
1	12	1	28	26	4
2	12	1	286	276	3
3	12	1	67	62	2
4	12	1	154	152	4
5	12	1	98	98	2
-4	13	1	63	61	3
-3	13	1	64	71	3
-2	13	1	22	24	6
-1	13	1	117	120	1
0	13	1	25	21	7
1	13	1	116	120	1
2	13	1	28	24	4
3	13	1	71	71	2
4	13	1	61	61	3
-3	14	1	119	115	3
-2	14	1	115	109	5
-1	14	1	44	39	3
0	14	1	5	3	4
1	14	1	40	37	6
2	14	1	122	108	4
3	14	1	121	117	2
0	15	1	20	17	6
2	0	2	380	196	4
3	0	2	530	251	5
4	0	2	229	203	1
5	0	2	51	61	1
6	0	2	33	13	2
7	0	2	214	200	2
8	0	2	34	12	5
-8	1	2	121	122	2
-7	1	2	87	88	1
-6	1	2	156	160	1
-5	1	2	117	127	1
-4	1	2	29	27	1
-3	1	2	232	218	1
-2	1	2	483	480	3
-1	1	2	532	537	3
1	1	2	530	537	3
2	1	2	483	480	3
3	1	2	232	218	1
4	1	2	30	27	1
5	1	2	117	127	1
6	1	2	155	160	1
7	1	2	91	89	1
8	1	2	117	122	1
-8	2	2	161	142	6
-7	2	2	117	105	2
-6	2	2	150	125	5
-5	2	2	216	204	11
-4	2	2	292	258	39
-3	2	2	217	210	56
-2	2	2	309	254	18
-1	2	2	207	214	207
0	2	2	755	777	8
1	2	2	192	217	191
2	2	2	309	251	24
3	2	2	245	213	49
4	2	2	300	260	38
5	2	2	214	203	8
6	2	2	150	127	2
7	2	2	121	105	3
8	2	2	156	141	9
-8	3	2	116	122	2
-7	3	2	121	124	1
-6	3	2	35	33	1
-5	3	2	223	223	1
-4	3	2	104	106	1
-3	3	2	255	252	1
-2	3	2	122	111	1
-1	3	2	452	439	2
0	3	2	241	260	1
1	3	2	452	438	2
2	3	2	122	113	1

h	k	l	10Fo	10Fc	10s
3	3	2	255	253	1
4	3	2	103	105	1
5	3	2	223	222	1
6	3	2	36	32	2
7	3	2	123	124	1
8	3	2	118	121	3
-8	4	2	39	38	4
-7	4	2	138	135	2
-6	4	2	97	90	10
-5	4	2	493	485	13
-4	4	2	320	296	14
-3	4	2	334	329	36
-2	4	2	265	255	12
-1	4	2	488	531	13
0	4	2	194	206	1
1	4	2	498	532	7
2	4	2	261	256	10
3	4	2	328	326	33
4	4	2	323	298	19
5	4	2	497	487	12
6	4	2	93	91	13
7	4	2	132	135	1
8	4	2	44	38	3
-7	5	2	93	91	1
-6	5	2	67	67	1
-5	5	2	138	139	1
-4	5	2	233	238	1
-3	5	2	159	169	1
-2	5	2	422	418	2
-1	5	2	253	243	1
0	5	2	288	300	1
1	5	2	251	243	1
2	5	2	423	415	2
3	5	2	158	168	1
4	5	2	233	237	1
5	5	2	139	140	1
6	5	2	65	67	1
7	5	2	94	92	1
-7	6	2	203	188	8
-6	6	2	115	121	1
-5	6	2	133	136	6
-4	6	2	292	294	3
-3	6	2	542	540	7
-2	6	2	297	294	1
-1	6	2	246	264	2
0	6	2	192	185	1
1	6	2	247	268	6
2	6	2	297	295	2
3	6	2	534	541	5
4	6	2	287	293	3
5	6	2	135	136	5
6	6	2	118	120	2
7	6	2	193	187	6
-7	7	2	27	29	16
-6	7	2	96	97	1
-5	7	2	174	177	1
-4	7	2	388	403	3
-3	7	2	169	182	1
-2	7	2	249	267	1
-1	7	2	277	278	2
0	7	2	521	531	4
1	7	2	280	279	1
2	7	2	249	268	1
3	7	2	170	183	1
4	7	2	389	403	2
5	7	2	175	177	1
6	7	2	91	94	2
7	7	2	29	29	4
-7	8	2	59	59	5
-6	8	2	29	30	5
-5	8	2	49	48	2
-4	8	2	63	64	1
-3	8	2	107	120	5
-2	8	2	204	214	1
-1	8	2	247	262	3
0	8	2	255	253	2
1	8	2	243	260	5
2	8	2	204	213	1
3	8	2	104	118	1
4	8	2	63	63	3
5	8	2	43	47	2
6	8	2	30	29	5
7	8	2	64	61	3
-6	9	2	86	89	2
-5	9	2	0	14	1
-4	9	2	136	141	1
-3	9	2	113	120	1

h	k	l	10Fo	10Fc	10s
-2	9	2	140	138	1
-1	9	2	368	377	3
0	9	2	293	296	2
1	9	2	370	377	2
2	9	2	136	137	3
3	9	2	118	121	1
4	9	2	135	142	1
5	9	2	22	15	4
6	9	2	88	89	3
-6	10	2	52	57	2
-5	10	2	36	39	3
-4	10	2	86	90	1
-3	10	2	41	41	2
-2	10	2	95	102	2
-1	10	2	189	200	9
0	10	2	267	280	2
1	10	2	191	200	1
2	10	2	94	101	1
3	10	2	39	41	2
4	10	2	83	89	1
5	10	2	39	39	2
6	10	2	51	57	2
-5	11	2	49	48	2
-4	11	2	184	177	2
-3	11	2	160	160	3
-2	11	2	137	139	2
-1	11	2	125	126	2
0	11	2	165	168	1
1	11	2	126	128	2
2	11	2	139	139	2
3	11	2	155	159	1
4	11	2	189	178	2
5	11	2	52	49	3
-5	12	2	37	34	5
-4	12	2	15	19	14
-3	12	2	93	95	2
-2	12	2	143	145	1
-1	12	2	78	83	2
0	12	2	12	6	11
1	12	2	80	83	1
2	12	2	138	146	1
3	12	2	90	96	1
4	12	2	10	19	10
5	12	2	30	34	6
-4	13	2	207	198	4
-3	13	2	152	148	2
-2	13	2	147	135	4
-1	13	2	55	48	7
0	13	2	158	152	1
1	13	2	61	48	4
2	13	2	143	136	4
3	13	2	151	147	5
4	13	2	207	198	3
-3	14	2	42	35	4
-2	14	2	71	77	3
-1	14	2	38	40	3
0	14	2	43	38	4
1	14	2	41	40	5
2	14	2	77	77	2
3	14	2	43	35	6
0	15	2	79	75	2
1	0	3	347	350	2
2	0	3	169	184	1
3	0	3	764	752	5
4	0	3	116	109	1
5	0	3	26	30	1
6	0	3	26	32	2
7	0	3	42	31	2
8	0	3	94	97	2
-8	1	3	209	204	7
-7	1	3	37	30	2
-6	1	3	207	197	12
-5	1	3	139	122	7
-4	1	3	411	381	5
-3	1	3	137	100	3
-2	1	3	682	617	30
-1	1	3	449	401	46
1	1	3	462	400	44
2	1	3	700	613	28
3	1	3	135	101	4
4	1	3	406	381	9
5	1	3	140	122	8
6	1	3	216	196	11
7	1	3	38	31	3
8	1	3	207	203	10
-8	2	3	88	94	2
-7	2	3	96	96	1

h	k	l	10Fo	10Fc	10s
-6	2	3	236	232	1
-5	2	3	104	104	1
-4	2	3	169	168	1
-3	2	3	58	71	1
-2	2	3	638	636	4
-1	2	3	612	632	4
0	2	3	495	501	4
1	2	3	609	631	5
2	2	3	635	636	4
3	2	3	58	72	1
4	2	3	169	168	1
5	2	3	103	104	1
6	2	3	234	232	2
7	2	3	95	96	1
8	2	3	89	95	2
-8	3	3	151	153	5
-7	3	3	68	60	5
-6	3	3	153	146	5
-5	3	3	164	107	16
-4	3	3	578	532	34
-3	3	3	326	294	9
-2	3	3	450	442	35
-1	3	3	316	275	23
0	3	3	148	86	12
1	3	3	321	275	22
2	3	3	460	441	41
3	3	3	327	296	13
4	3	3	593	533	31
5	3	3	158	106	13
6	3	3	161	145	2
7	3	3	67	60	4
8	3	3	153	154	5
-8	4	3	51	45	3
-7	4	3	74	79	1
-6	4	3	108	106	1
-5	4	3	285	293	2
-4	4	3	141	145	1
-3	4	3	520	525	3
-2	4	3	401	388	2
-1	4	3	517	517	3
0	4	3	47	41	1
1	4	3	516	515	2
2	4	3	400	389	2
3	4	3	516	523	3
4	4	3	141	145	1
5	4	3	283	291	2
6	4	3	104	106	1
7	4	3	74	78	5
8	4	3	42	45	3
-7	5	3	129	127	2
-6	5	3	56	60	1
-5	5	3	134	132	30
-4	5	3	258	252	7
-3	5	3	148	150	1
-2	5	3	412	423	4
-1	5	3	176	162	12
0	5	3	670	693	4
1	5	3	175	161	9
2	5	3	415	427	3
3	5	3	145	150	1
4	5	3	255	250	5
5	5	3	135	132	17
6	5	3	57	61	1
7	5	3	127	127	1
-7	6	3	65	62	2
-6	6	3	81	75	1
-5	6	3	219	219	1
-4	6	3	107	111	1
-3	6	3	192	200	1
-2	6	3	104	107	1
-1	6	3	339	338	2
0	6	3	194	192	1
1	6	3	338	337	2
2	6	3	104	107	1
3	6	3	191	197	1
4	6	3	107	111	1
5	6	3	215	216	1
6	6	3	83	75	1
7	6	3	63	63	1
-7	7	3	148	146	4
-6	7	3	205	203	5
-5	7	3	88	89	2
-4	7	3	244	243	6
-3	7	3	75	70	3
-2	7	3	114	123	1
-1	7	3	149	147	1
0	7	3	167	195	1

h	k	l	10Fo	10Fc	10s
1	7	3	149	147	1
2	7	3	111	124	1
3	7	3	74	71	5
4	7	3	240	246	2
5	7	3	91	89	1
6	7	3	201	202	2
7	7	3	147	146	3
-7	8	3	141	138	2
-6	8	3	89	86	2
-5	8	3	160	163	1
-4	8	3	216	221	2
-3	8	3	172	179	1
-2	8	3	189	197	3
-1	8	3	225	225	2
0	8	3	47	45	1
1	8	3	225	228	1
2	8	3	189	196	1
3	8	3	170	179	1
4	8	3	217	220	2
5	8	3	160	164	1
6	8	3	82	87	3
7	8	3	136	135	2
-6	9	3	176	174	2
-5	9	3	19	11	5
-4	9	3	131	139	2
-3	9	3	190	199	3
-2	9	3	251	261	3
-1	9	3	129	132	1
0	9	3	263	279	2
1	9	3	127	132	1
2	9	3	248	261	1
3	9	3	190	199	3
4	9	3	132	141	2
5	9	3	7	11	7
6	9	3	173	176	1
-6	10	3	71	68	2
-5	10	3	180	176	3
-4	10	3	80	79	2
-3	10	3	158	157	2
-2	10	3	315	328	3
-1	10	3	255	264	3
0	10	3	45	23	6
1	10	3	258	267	2
2	10	3	315	328	2
3	10	3	159	159	1
4	10	3	79	79	2
5	10	3	178	177	2
6	10	3	69	68	2
-5	11	3	68	67	2
-4	11	3	108	103	2
-3	11	3	84	91	2
-2	11	3	108	109	4
-1	11	3	61	62	1
0	11	3	149	148	1
1	11	3	63	62	1
2	11	3	105	109	1
3	11	3	85	90	1
4	11	3	105	104	1
5	11	3	66	66	2
-5	12	3	173	175	3
-4	12	3	98	94	2
-3	12	3	273	257	6
-2	12	3	52	43	6
-1	12	3	296	283	9
0	12	3	47	43	8
1	12	3	299	283	8
2	12	3	59	43	5
3	12	3	275	257	3
4	12	3	98	94	2
5	12	3	178	177	2
-4	13	3	33	29	4
-3	13	3	42	38	5
-2	13	3	101	103	1
-1	13	3	71	71	1
0	13	3	75	80	1
1	13	3	69	71	2
2	13	3	99	104	6
3	13	3	39	38	3
4	13	3	26	29	10
-3	14	3	168	161	4
-2	14	3	42	39	5
-1	14	3	172	159	3
0	14	3	18	15	7
1	14	3	172	160	2
2	14	3	46	40	4
3	14	3	169	160	6
0	15	3	27	25	5

h	k	l	10Fo	10Fc	10s
1	0	4	322	259	7
2	0	4	565	405	5
3	0	4	339	325	5
4	0	4	50	48	2
5	0	4	255	233	2
6	0	4	173	179	1
7	0	4	31	11	3
8	0	4	92	79	3
-8	1	4	17	17	16
-7	1	4	84	82	1
-6	1	4	120	126	1
-5	1	4	188	198	1
-4	1	4	36	42	1
-3	1	4	367	340	2
-2	1	4	514	520	3
-1	1	4	297	292	2
0	1	4	545	564	6
1	1	4	297	292	2
2	1	4	514	521	3
3	1	4	366	340	2
4	1	4	35	41	1
5	1	4	189	199	1
6	1	4	121	125	1
7	1	4	80	82	2
8	1	4	20	18	12
-8	2	4	207	183	3
-7	2	4	211	195	7
-6	2	4	99	88	13
-5	2	4	207	210	10
-4	2	4	162	137	3
-3	2	4	423	398	10
-2	2	4	432	372	65
-1	2	4	294	329	2
0	2	4	312	269	2
1	2	4	294	332	2
2	2	4	445	376	67
3	2	4	424	395	13
4	2	4	165	141	2
5	2	4	213	211	11
6	2	4	97	91	10
7	2	4	218	196	4
8	2	4	204	182	2
-8	3	4	77	76	2
-7	3	4	18	7	18
-6	3	4	132	137	1
-5	3	4	141	130	1
-4	3	4	351	361	2
-3	3	4	65	58	1
-2	3	4	531	533	3
-1	3	4	332	353	2
0	3	4	636	648	4
1	3	4	332	353	2
2	3	4	532	532	3
3	3	4	65	60	1
4	3	4	350	360	2
5	3	4	141	129	1
6	3	4	133	138	1
7	3	4	13	7	13
8	3	4	70	76	2
-7	4	4	94	95	10
-6	4	4	134	131	12
-5	4	4	256	251	11
-4	4	4	547	521	21
-3	4	4	229	213	17
-2	4	4	201	190	201
-1	4	4	534	525	14
0	4	4	61	9	13
1	4	4	539	528	9
2	4	4	202	189	201
3	4	4	225	215	21
4	4	4	545	522	20
5	4	4	265	254	10
6	4	4	134	132	13
7	4	4	97	92	3
-7	5	4	12	19	11
-6	5	4	52	56	1
-5	5	4	252	260	1
-4	5	4	242	248	1
-3	5	4	50	47	1
-2	5	4	245	239	1
-1	5	4	151	161	1
0	5	4	326	345	2
1	5	4	150	162	1
2	5	4	245	237	1
3	5	4	51	48	1
4	5	4	243	248	1
5	5	4	251	261	2

h	k	l	10Fo	10Fc	10s
6	5	4	54	54	1
7	5	4	0	19	1
-7	6	4	47	50	2
-6	6	4	151	156	5
-5	6	4	108	109	12
-4	6	4	307	296	12
-3	6	4	189	197	1
-2	6	4	46	58	2
-1	6	4	198	204	2
0	6	4	195	217	3
1	6	4	199	205	1
2	6	4	45	57	1
3	6	4	188	194	1
4	6	4	301	295	9
5	6	4	115	112	9
6	6	4	151	155	4
7	6	4	49	49	2
-7	7	4	62	68	4
-6	7	4	69	59	1
-5	7	4	124	133	1
-4	7	4	49	45	1
-3	7	4	162	163	1
-2	7	4	110	102	1
-1	7	4	24	34	2
0	7	4	122	124	1
1	7	4	22	33	1
2	7	4	113	105	1
3	7	4	162	164	1
4	7	4	47	46	1
5	7	4	126	134	1
6	7	4	65	56	1
7	7	4	62	68	2
-6	8	4	74	75	3
-5	8	4	131	133	1
-4	8	4	150	151	1
-3	8	4	144	145	5
-2	8	4	123	131	5
-1	8	4	273	275	4
0	8	4	322	341	2
1	8	4	270	277	2
2	8	4	119	128	1
3	8	4	146	146	2
4	8	4	149	150	2
5	8	4	135	134	1
6	8	4	76	75	4
-6	9	4	99	100	2
-5	9	4	64	66	5
-4	9	4	84	81	1
-3	9	4	104	107	1
-2	9	4	95	97	1
-1	9	4	165	170	1
0	9	4	173	172	1
1	9	4	162	167	1
2	9	4	98	100	1
3	9	4	108	109	1
4	9	4	79	82	1
5	9	4	69	67	2
6	9	4	99	98	1
-6	10	4	55	62	2
-5	10	4	91	95	1
-4	10	4	82	87	2
-3	10	4	122	129	2
-2	10	4	138	143	3
-1	10	4	69	70	2
0	10	4	115	117	1
1	10	4	72	72	3
2	10	4	137	143	3
3	10	4	122	129	1
4	10	4	82	87	1
5	10	4	87	95	1
6	10	4	60	61	2
-5	11	4	112	117	2
-4	11	4	118	115	2
-3	11	4	118	111	3
-2	11	4	76	70	2
-1	11	4	136	139	2
0	11	4	152	138	15
1	11	4	139	141	3
2	11	4	72	67	1
3	11	4	117	109	2
4	11	4	121	115	2
5	11	4	113	115	2
-4	12	4	32	28	4
-3	12	4	110	113	2
-2	12	4	68	69	3
-1	12	4	75	82	1
0	12	4	32	28	11

Table 6. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
1	12	4	77	82	2
2	12	4	68	70	2
3	12	4	114	114	2
4	12	4	20	28	8
-4	13	4	51	45	3
-3	13	4	71	74	2
-2	13	4	198	197	9
-1	13	4	155	145	1
0	13	4	153	141	11
1	13	4	151	144	2
2	13	4	204	195	9
3	13	4	78	73	2
4	13	4	40	45	3
-2	14	4	81	87	2
-1	14	4	46	48	3
0	14	4	61	60	2
1	14	4	48	48	3
2	14	4	88	87	2
1	0	5	298	297	3
2	0	5	108	114	1
3	0	5	25	23	1
4	0	5	23	26	1
5	0	5	164	174	1
6	0	5	79	73	1
7	0	5	12	22	8
8	0	5	17	13	16
-8	1	5	45	38	8
-7	1	5	184	181	4
-6	1	5	69	31	14
-5	1	5	163	163	11
-4	1	5	61	53	4
-3	1	5	190	94	8
-2	1	5	274	265	24
-1	1	5	572	535	40
0	1	5	390	372	5
1	1	5	554	541	17
2	1	5	279	264	22
3	1	5	195	95	8
4	1	5	58	51	5
5	1	5	164	163	5
6	1	5	72	32	10
7	1	5	185	181	4
8	1	5	58	38	4
-8	2	5	133	132	7
-7	2	5	112	114	1
-6	2	5	47	47	1
-5	2	5	186	196	2
-4	2	5	103	95	1
-3	2	5	272	269	2
-2	2	5	261	236	1
-1	2	5	301	292	2
0	2	5	210	201	1
1	2	5	300	292	2
2	2	5	260	237	1
3	2	5	274	269	1
4	2	5	103	95	2
5	2	5	186	195	1
6	2	5	47	47	1
7	2	5	112	114	1
8	2	5	131	132	2
-8	3	5	67	36	11
-7	3	5	112	118	13
-6	3	5	138	138	6
-5	3	5	454	430	36
-4	3	5	336	317	32
-3	3	5	341	333	32
-2	3	5	385	392	2
-1	3	5	580	592	40
0	3	5	684	678	5
1	3	5	594	592	40
2	3	5	384	391	3
3	3	5	366	334	34
4	3	5	364	318	33
5	3	5	498	430	34
6	3	5	138	139	1
7	3	5	123	119	12
8	3	5	78	36	13
-7	4	5	61	70	2
-6	4	5	70	72	1
-5	4	5	42	47	2
-4	4	5	142	147	1
-3	4	5	20	23	2
-2	4	5	447	446	2
-1	4	5	780	763	5
0	4	5	216	236	1
1	4	5	780	763	5
2	4	5	446	444	3

h	k	l	10Fo	10Fc	10s
3	4	5	23	24	2
4	4	5	143	147	1
5	4	5	41	47	1
6	4	5	69	73	1
7	4	5	67	70	2
-7	5	5	177	181	6
-6	5	5	80	78	3
-5	5	5	229	231	24
-4	5	5	91	77	15
-3	5	5	384	378	30
-2	5	5	254	232	16
-1	5	5	518	540	16
0	5	5	31	21	6
1	5	5	512	540	19
2	5	5	256	232	15
3	5	5	387	378	26
4	5	5	91	77	19
5	5	5	238	230	20
6	5	5	84	78	3
7	5	5	183	181	7
-7	6	5	62	65	3
-6	6	5	113	115	2
-5	6	5	124	130	1
-4	6	5	265	266	2
-3	6	5	33	30	1
-2	6	5	131	135	1
-1	6	5	233	234	1
0	6	5	272	285	1
1	6	5	233	235	1
2	6	5	133	138	1
3	6	5	33	30	1
4	6	5	264	265	1
5	6	5	123	131	1
6	6	5	114	116	1
7	6	5	65	65	2
-7	7	5	148	155	3
-6	7	5	33	32	4
-5	7	5	104	108	3
-4	7	5	174	175	1
-3	7	5	345	357	3
-2	7	5	105	96	2
-1	7	5	192	208	10
0	7	5	44	41	9
1	7	5	192	208	2
2	7	5	104	97	1
3	7	5	344	356	2
4	7	5	173	175	1
5	7	5	106	108	1
6	7	5	32	31	3
7	7	5	156	154	2
-6	8	5	131	131	2
-5	8	5	49	55	2
-4	8	5	293	303	4
-3	8	5	78	89	1
-2	8	5	257	258	3
-1	8	5	101	106	1
0	8	5	283	286	2
1	8	5	102	107	1
2	8	5	257	260	2
3	8	5	77	90	1
4	8	5	296	304	4
5	8	5	51	55	1
6	8	5	127	129	1
-6	9	5	27	34	6
-5	9	5	69	67	5
-4	9	5	64	61	1
-3	9	5	40	47	1
-2	9	5	147	153	9
-1	9	5	148	163	8
0	9	5	235	242	5
1	9	5	149	164	6
2	9	5	147	152	11
3	9	5	43	45	5
4	9	5	67	61	1
5	9	5	73	68	4
6	9	5	28	34	5
-6	10	5	181	173	4
-5	10	5	51	45	2
-4	10	5	165	159	2
-3	10	5	157	162	1
-2	10	5	108	105	1
-1	10	5	73	70	3
0	10	5	165	157	2
1	10	5	72	70	3
2	10	5	114	104	1
3	10	5	162	162	1
4	10	5	164	158	1

h	k	l	10Fo	10Fc	10s
5	10	5	47	46	2
6	10	5	184	174	3
-5	11	5	55	57	3
-4	11	5	110	107	2
-3	11	5	74	67	2
-2	11	5	80	83	2
-1	11	5	95	100	2
0	11	5	255	261	2
1	11	5	100	100	1
2	11	5	80	83	1
3	11	5	69	68	1
4	11	5	111	107	4
5	11	5	58	58	3
-4	12	5	184	176	3
-3	12	5	154	160	3
-2	12	5	111	110	5
-1	12	5	92	88	2
0	12	5	215	214	2
1	12	5	99	88	3
2	12	5	119	108	3
3	12	5	160	159	3
4	12	5	189	177	2
-4	13	5	7	18	6
-3	13	5	83	86	2
-2	13	5	129	137	2
-1	13	5	36	29	5
0	13	5	140	148	1
1	13	5	26	30	3
2	13	5	130	137	2
3	13	5	83	85	2
4	13	5	20	17	9
-2	14	5	163	163	2
-1	14	5	129	129	2
0	14	5	167	165	3
1	14	5	133	129	2
2	14	5	169	161	2
1	0	6	560	530	7
2	0	6	297	318	2
3	0	6	189	186	3
4	0	6	209	203	2
5	0	6	53	37	6
6	0	6	165	162	1
7	0	6	26	12	6
8	0	6	206	177	7
-8	1	6	84	77	2
-7	1	6	46	53	2
-6	1	6	53	54	1
-5	1	6	140	141	1
-4	1	6	117	126	1
-3	1	6	171	163	1
-2	1	6	116	114	1
-1	1	6	200	196	1
0	1	6	137	141	1
1	1	6	199	195	1
2	1	6	114	114	1
3	1	6	171	163	1
4	1	6	118	126	1
5	1	6	139	141	1
6	1	6	52	55	2
7	1	6	50	53	2
8	1	6	82	78	3
-8	2	6	233	221	10
-7	2	6	142	134	7
-6	2	6	279	273	6
-5	2	6	135	130	4
-4	2	6	550	489	29
-3	2	6	250	228	18
-2	2	6	426	405	19
-1	2	6	383	365	11
0	2	6	119	165	3
1	2	6	380	363	8
2	2	6	433	400	19
3	2	6	269	231	16
4	2	6	563	491	30
5	2	6	138	128	4
6	2	6	288	274	4
7	2	6	146	133	5
8	2	6	223	220	3
-8	3	6	108	115	2
-7	3	6	121	128	1
-6	3	6	13	15	6
-5	3	6	259	270	2
-4	3	6	79	77	1
-3	3	6	136	141	1
-2	3	6	29	32	1
-1	3	6	179	166	1
0	3	6	507	529	4

h	k	l	10Fo	10Fc	10s
1	3	6	177	164	1
2	3	6	26	32	1
3	3	6	133	140	1
4	3	6	79	77	1
5	3	6	260	270	2
6	3	6	17	15	4
7	3	6	120	128	2
8	3	6	113	116	2
-7	4	6	55	50	2
-6	4	6	52	28	17
-5	4	6	192	180	19
-4	4	6	212	203	14
-3	4	6	106	92	2
-2	4	6	412	408	27
-1	4	6	221	159	88
0	4	6	755	752	39
1	4	6	232	158	90
2	4	6	431	410	28
3	4	6	108	93	3
4	4	6	214	202	18
5	4	6	197	181	22
6	4	6	52	28	10
7	4	6	62	49	4
-7	5	6	79	86	2
-6	5	6	51	57	2
-5	5	6	148	149	1
-4	5	6	258	266	2
-3	5	6	257	259	1
-2	5	6	295	285	2
-1	5	6	185	165	1
0	5	6	25	34	1
1	5	6	182	162	1
2	5	6	295	285	2
3	5	6	255	258	1
4	5	6	259	267	2
5	5	6	147	147	1
6	5	6	54	57	3
7	5	6	77	86	1
-7	6	6	91	87	10
-6	6	6	122	118	6
-5	6	6	160	153	1
-4	6	6	123	124	3
-3	6	6	81	83	2
-2	6	6	306	303	6
-1	6	6	350	331	9
0	6	6	446	472	3
1	6	6	348	330	12
2	6	6	308	305	12
3	6	6	78	82	1
4	6	6	120	120	1
5	6	6	158	152	1
6	6	6	121	118	3
7	6	6	91	88	6
-7	7	6	40	39	4
-6	7	6	76	76	1
-5	7	6	103	109	5
-4	7	6	146	149	1
-3	7	6	39	42	2
-2	7	6	128	119	1
-1	7	6	201	207	1
0	7	6	163	151	1
1	7	6	200	208	1
2	7	6	127	118	1
3	7	6	39	46	2
4	7	6	142	148	1
5	7	6	108	110	1
6	7	6	78	76	2
7	7	6	42	38	3
-6	8	6	173	176	5
-5	8	6	71	71	6
-4	8	6	306	312	3
-3	8	6	120	121	11
-2	8	6	129	135	1
-1	8	6	233	237	4
0	8	6	279	296	3
1	8	6	233	237	4
2	8	6	128	136	1
3	8	6	117	122	7
4	8	6	307	313	2
5	8	6	70	70	4
6	8	6	169	176	2
-6	9	6	76	81	2
-5	9	6	163	168	2
-4	9	6	44	39	4
-3	9	6	164	155	3
-2	9	6	111	119	1
-1	9	6	264	263	3

h	k	l	10Fo	10Fc	10s
0	9	6	182	193	1
1	9	6	266	263	4
2	9	6	114	119	1
3	9	6	162	155	9
4	9	6	46	40	2
5	9	6	158	167	3
6	9	6	83	82	2
-6	10	6	114	121	4
-5	10	6	80	84	4
-4	10	6	69	71	3
-3	10	6	92	92	2
-2	10	6	37	40	4
-1	10	6	191	201	1
0	10	6	25	21	24
1	10	6	193	201	2
2	10	6	41	40	1
3	10	6	94	92	2
4	10	6	74	73	1
5	10	6	80	84	3
6	10	6	112	123	2
-5	11	6	91	90	2
-4	11	6	92	87	1
-3	11	6	148	140	4
-2	11	6	16	24	9
-1	11	6	215	204	19
0	11	6	46	40	2
1	11	6	222	205	16
2	11	6	24	25	5
3	11	6	146	139	6
4	11	6	91	87	2
5	11	6	94	92	2
-4	12	6	37	35	3
-3	12	6	50	42	3
-2	12	6	69	72	2
-1	12	6	22	15	5
0	12	6	136	140	1
1	12	6	13	15	8
2	12	6	74	73	2
3	12	6	40	42	5
4	12	6	39	36	4
-3	13	6	148	145	3
-2	13	6	77	68	13
-1	13	6	107	100	6
0	13	6	64	38	16
1	13	6	113	100	5
2	13	6	93	69	13
3	13	6	147	143	2
-2	14	6	11	17	11
-1	14	6	34	38	6
0	14	6	8	8	8
1	14	6	35	38	5
2	14	6	22	17	9
1	0	7	77	90	1
2	0	7	2	13	2
3	0	7	169	157	1
4	0	7	83	92	1
5	0	7	177	191	2
6	0	7	186	193	2
7	0	7	48	53	2
8	0	7	55	56	3
-8	1	7	138	139	5
-7	1	7	121	127	12
-6	1	7	76	68	16
-5	1	7	247	228	8
-4	1	7	272	268	6
-3	1	7	167	129	7
-2	1	7	88	93	11
-1	1	7	160	154	137
1	1	7	177	151	70
2	1	7	91	88	13
3	1	7	177	126	8
4	1	7	273	267	5
5	1	7	250	227	2
6	1	7	63	69	10
7	1	7	133	129	14
8	1	7	139	139	2
-8	2	7	65	74	3
-7	2	7	65	67	2
-6	2	7	61	61	1
-5	2	7	130	123	1
-4	2	7	171	171	1
-3	2	7	192	180	1
-2	2	7	182	189	1
-1	2	7	362	359	3
0	2	7	223	229	2
1	2	7	361	360	2
2	2	7	181	190	1

h	k	l	10Fo	10Fc	10s
3	2	7	193	180	1
4	2	7	169	170	1
5	2	7	130	124	1
6	2	7	63	61	3
7	2	7	70	68	2
8	2	7	67	74	3
-7	3	7	129	121	6
-6	3	7	122	123	3
-5	3	7	167	157	7
-4	3	7	357	326	28
-3	3	7	67	63	2
-2	3	7	453	457	18
-1	3	7	185	187	27
0	3	7	119	56	73
1	3	7	181	188	29
2	3	7	458	455	20
3	3	7	66	59	1
4	3	7	358	326	27
5	3	7	172	159	5
6	3	7	129	123	1
7	3	7	128	119	5
-7	4	7	42	42	2
-6	4	7	159	169	1
-5	4	7	53	59	1
-4	4	7	9	7	8
-3	4	7	103	110	1
-2	4	7	171	171	1
-1	4	7	528	528	3
0	4	7	133	134	1
1	4	7	527	528	3
2	4	7	168	169	1
3	4	7	103	111	1
4	4	7	15	8	3
5	4	7	58	61	1
6	4	7	157	169	2
7	4	7	45	43	3
-7	5	7	131	129	5
-6	5	7	125	125	9
-5	5	7	59	57	1
-4	5	7	414	403	21
-3	5	7	224	226	4
-2	5	7	221	196	1
-1	5	7	146	119	4
0	5	7	161	136	1
1	5	7	148	122	4
2	5	7	223	198	1
3	5	7	223	223	7
4	5	7	409	400	25
5	5	7	64	59	1
6	5	7	121	124	11
7	5	7	128	127	2
-7	6	7	146	149	2
-6	6	7	81	81	1
-5	6	7	155	157	4
-4	6	7	153	157	3
-3	6	7	112	122	2
-2	6	7	14	12	3
-1	6	7	194	181	1
0	6	7	64	35	1
1	6	7	194	181	1
2	6	7	12	10	4
3	6	7	115	124	1
4	6	7	157	158	1
5	6	7	154	157	1
6	6	7	76	79	1
7	6	7	148	150	2
-7	7	7	115	121	12
-6	7	7	113	110	11
-5	7	7	184	186	3
-4	7	7	71	66	10
-3	7	7	68	66	1
-2	7	7	85	82	85
-1	7	7	37	34	3
0	7	7	121	118	71
1	7	7	34	35	1
2	7	7	85	81	29
3	7	7	67	66	1
4	7	7	63	64	7
5	7	7	184	186	3
6	7	7	110	108	5
7	7	7	119	122	4
-6	8	7	65	68	2
-5	8	7	138	143	3
-4	8	7	63	66	7
-3	8	7	187	199	8
-2	8	7	71	71	1
-1	8	7	121	126	3

h	k	l	10Fo	10Fc	10s
0	8	7	62	64	10
1	8	7	122	125	4
2	8	7	67	71	1
3	8	7	185	200	3
4	8	7	65	64	1
5	8	7	142	143	2
6	8	7	66	68	2
-6	9	7	85	91	1
-5	9	7	115	115	2
-4	9	7	69	68	6
-3	9	7	197	203	2
-2	9	7	242	253	9
-1	9	7	231	221	9
0	9	7	25	26	24
1	9	7	225	222	7
2	9	7	240	252	12
3	9	7	196	203	2
4	9	7	71	69	3
5	9	7	112	116	2
6	9	7	93	92	2
-5	10	7	161	159	2
-4	10	7	139	135	5
-3	10	7	77	80	1
-2	10	7	104	107	2
-1	10	7	88	87	7
0	10	7	104	107	3
1	10	7	90	87	4
2	10	7	105	107	1
3	10	7	78	81	3
4	10	7	139	134	2
5	10	7	160	159	1
-5	11	7	28	32	5
-4	11	7	68	71	2
-3	11	7	50	51	5
-2	11	7	89	91	2
-1	11	7	158	158	2
0	11	7	30	25	2
1	11	7	153	158	3
2	11	7	88	90	5
3	11	7	45	51	3
4	11	7	67	70	2
5	11	7	40	32	3
-4	12	7	49	49	2
-3	12	7	135	125	4
-2	12	7	38	33	3
-1	12	7	93	93	1
0	12	7	128	110	25
1	12	7	95	91	1
2	12	7	26	31	5
3	12	7	135	124	3
4	12	7	45	48	4
-3	13	7	85	86	2
-2	13	7	154	161	2
-1	13	7	77	88	1
0	13	7	164	168	1
1	13	7	81	88	2
2	13	7	154	160	2
3	13	7	87	87	2
-2	14	7	81	83	3
-1	14	7	167	159	4
0	14	7	102	100	2
1	14	7	163	158	2
2	14	7	85	84	4
1	0	8	568	556	4
2	0	8	139	137	10
3	0	8	401	406	6
4	0	8	169	155	43
5	0	8	250	204	12
6	0	8	100	64	13
7	0	8	153	140	2
8	0	8	48	36	7
-8	1	8	41	31	7
-7	1	8	108	112	1
-6	1	8	113	115	2
-5	1	8	16	11	3
-4	1	8	61	58	1
-3	1	8	275	279	1
-2	1	8	31	26	1
-1	1	8	148	142	1
0	1	8	548	547	6
1	1	8	147	143	1
2	1	8	31	25	1
3	1	8	277	278	2
4	1	8	62	58	2
5	1	8	12	11	4
6	1	8	114	114	2
7	1	8	105	112	2

h	k	l	10Fo	10Fc	10s
8	1	8	31	31	4
-7	2	8	190	182	5
-6	2	8	92	93	9
-5	2	8	351	331	10
-4	2	8	217	208	5
-3	2	8	471	463	17
-2	2	8	287	271	31
-1	2	8	598	620	4
0	2	8	59	20	16
1	2	8	592	623	5
2	2	8	298	271	31
3	2	8	478	463	17
4	2	8	216	208	4
5	2	8	359	332	15
6	2	8	105	93	10
7	2	8	190	183	6
-7	3	8	95	95	1
-6	3	8	107	104	1
-5	3	8	92	88	1
-4	3	8	260	260	2
-3	3	8	77	77	1
-2	3	8	96	86	1
-1	3	8	113	105	1
0	3	8	82	93	1
1	3	8	113	105	1
2	3	8	93	84	1
3	3	8	79	78	1
4	3	8	259	262	2
5	3	8	89	88	1
6	3	8	111	105	1
7	3	8	97	95	3
-7	4	8	177	164	12
-6	4	8	114	114	2
-5	4	8	245	240	12
-4	4	8	279	258	25
-3	4	8	333	329	8
-2	4	8	114	79	72
-1	4	8	335	347	15
0	4	8	54	5	53
1	4	8	334	344	15
2	4	8	119	80	62
3	4	8	334	330	9
4	4	8	293	258	26
5	4	8	246	238	14
6	4	8	118	114	3
7	4	8	161	164	19
-7	5	8	15	22	11
-6	5	8	93	99	1
-5	5	8	89	92	1
-4	5	8	289	300	2
-3	5	8	50	53	1
-2	5	8	99	91	1
-1	5	8	99	106	1
0	5	8	250	266	1
1	5	8	99	106	1
2	5	8	95	88	1
3	5	8	47	53	1
4	5	8	293	300	2
5	5	8	89	92	1
6	5	8	96	100	1
7	5	8	21	23	7
-7	6	8	129	139	3
-6	6	8	42	36	3
-5	6	8	157	150	9
-4	6	8	159	162	2
-3	6	8	64	65	4
-2	6	8	146	144	6
-1	6	8	208	197	19
0	6	8	126	107	4
1	6	8	200	197	16
2	6	8	142	144	7
3	6	8	59	63	5
4	6	8	164	162	4
5	6	8	158	150	9
6	6	8	44	36	6
7	6	8	132	137	3
-7	7	8	120	120	2
-6	7	8	135	140	1
-5	7	8	82	80	2
-4	7	8	228	234	8
-3	7	8	35	36	3
-2	7	8	359	354	5
-1	7	8	46	46	6
0	7	8	321	330	3
1	7	8	40	47	1
2	7	8	357	357	3
3	7	8	32	36	1

h	k	l	10Fo	10Fc	10s
4	7	8	232	235	2
5	7	8	81	80	1
6	7	8	135	140	4
7	7	8	118	120	2
-6	8	8	79	75	1
-5	8	8	64	59	13
-4	8	8	131	126	6
-3	8	8	160	156	1
-2	8	8	50	36	1
-1	8	8	227	237	11
0	8	8	349	350	34
1	8	8	228	238	20
2	8	8	44	36	4
3	8	8	152	154	2
4	8	8	132	126	5
5	8	8	63	59	13
6	8	8	80	75	2
-6	9	8	113	117	4
-5	9	8	41	42	4
-4	9	8	246	244	13
-3	9	8	41	46	2
-2	9	8	312	304	5
-1	9	8	169	176	2
0	9	8	485	468	14
1	9	8	169	177	3
2	9	8	316	304	6
3	9	8	47	45	2
4	9	8	251	243	9
5	9	8	41	43	2
6	9	8	109	115	2
-5	10	8	61	57	2
-4	10	8	0	20	1
-3	10	8	55	53	6
-2	10	8	101	97	2
-1	10	8	48	47	2
0	10	8	205	211	2
1	10	8	44	45	3
2	10	8	96	97	4
3	10	8	53	51	3
4	10	8	30	20	6
5	10	8	53	57	2
-5	11	8	97	97	4
-4	11	8	132	133	3
-3	11	8	78	72	3
-2	11	8	107	105	3
-1	11	8	66	69	1
0	11	8	256	241	23
1	11	8	65	69	1
2	11	8	108	102	2
3	11	8	75	72	2
4	11	8	131	131	3
5	11	8	97	98	2
-4	12	8	49	46	6
-3	12	8	109	110	2
-2	12	8	36	31	4
-1	12	8	26	26	7
0	12	8	295	298	3
1	12	8	25	26	4
2	12	8	29	31	4
3	12	8	106	110	2
4	12	8	44	46	3
-3	13	8	50	49	3
-2	13	8	171	167	6
-1	13	8	67	56	8
0	13	8	62	61	3
1	13	8	77	57	6
2	13	8	170	165	2
3	13	8	47	49	3
-2	14	8	57	57	2
-1	14	8	43	44	3
0	14	8	40	41	3
1	14	8	43	44	3
2	14	8	54	58	3
1	0	9	164	170	1
2	0	9	288	286	2
3	0	9	218	215	1
4	0	9	228	243	2
5	0	9	228	229	3
6	0	9	56	56	2
7	0	9	19	22	12
-7	1	9	149	142	10
-6	1	9	166	162	5
-5	1	9	166	165	4
-4	1	9	379	367	25
-3	1	9	179	169	22
-2	1	9	338	345	12
-1	1	9	412	406	3

h	k	l	10Fo	10Fc	10s
0	1	9	339	327	65
1	1	9	422	406	6
2	1	9	343	345	14
3	1	9	178	167	14
4	1	9	414	368	23
5	1	9	166	163	1
6	1	9	178	164	14
7	1	9	159	143	14
-7	2	9	72	69	2
-6	2	9	86	88	1
-5	2	9	68	71	1
-4	2	9	98	100	1
-3	2	9	224	226	1
-2	2	9	272	266	1
-1	2	9	64	63	1
0	2	9	460	474	4
1	2	9	63	62	1
2	2	9	270	266	1
3	2	9	223	227	2
4	2	9	99	99	1
5	2	9	67	70	2
6	2	9	83	88	2
7	2	9	68	70	2
-7	3	9	71	58	9
-6	3	9	243	244	8
-5	3	9	281	277	7
-4	3	9	266	253	7
-3	3	9	89	91	3
-2	3	9	93	48	14
-1	3	9	169	151	6
0	3	9	476	502	4
1	3	9	166	148	6
2	3	9	100	49	12
3	3	9	90	90	2
4	3	9	266	256	6
5	3	9	287	277	8
6	3	9	255	246	11
7	3	9	63	57	5
-7	4	9	122	131	2
-6	4	9	58	62	2
-5	4	9	93	104	1
-4	4	9	137	141	1
-3	4	9	71	73	1
-2	4	9	282	281	2
-1	4	9	293	293	1
0	4	9	290	312	2
1	4	9	293	291	2
2	4	9	278	280	2
3	4	9	73	75	1
4	4	9	137	142	1
5	4	9	94	104	3
6	4	9	55	62	2
7	4	9	126	131	2
-7	5	9	53	21	14
-6	5	9	60	56	5
-5	5	9	64	24	19
-4	5	9	123	102	17
-3	5	9	129	130	17
-2	5	9	248	245	18
-1	5	9	141	120	8
0	5	9	109	128	1
1	5	9	140	122	9
2	5	9	256	246	20
3	5	9	129	129	17
4	5	9	111	99	22
5	5	9	49	22	22
6	5	9	55	56	3
7	5	9	41	21	8
-7	6	9	38	45	4
-6	6	9	85	91	3
-5	6	9	127	131	3
-4	6	9	132	141	6
-3	6	9	162	164	1
-2	6	9	244	227	1
-1	6	9	148	153	1
0	6	9	72	87	2
1	6	9	152	156	1
2	6	9	245	227	2
3	6	9	163	165	1
4	6	9	137	140	4
5	6	9	126	133	1
6	6	9	87	90	2
7	6	9	49	45	3
-6	7	9	116	117	11
-5	7	9	72	66	17
-4	7	9	204	200	7
-3	7	9	182	181	24

Table 6. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
-2	7	9	109	102	3
-1	7	9	137	129	16
0	7	9	21	26	2
1	7	9	132	127	11
2	7	9	104	102	3
3	7	9	171	181	27
4	7	9	195	198	4
5	7	9	70	65	13
6	7	9	119	117	10
-6	8	9	95	85	3
-5	8	9	176	181	3
-4	8	9	148	160	1
-3	8	9	153	158	5
-2	8	9	79	83	9
-1	8	9	235	238	2
0	8	9	211	219	2
1	8	9	237	237	2
2	8	9	88	85	4
3	8	9	159	161	1
4	8	9	151	161	2
5	8	9	180	181	6
6	8	9	90	84	2
-6	9	9	47	49	4
-5	9	9	82	79	7
-4	9	9	139	142	3
-3	9	9	70	72	15
-2	9	9	203	203	10
-1	9	9	278	280	27
0	9	9	46	24	45
1	9	9	271	281	3
2	9	9	206	202	12
3	9	9	75	72	37
4	9	9	137	141	2
5	9	9	75	78	3
6	9	9	45	48	3
-5	10	9	62	64	3
-4	10	9	75	76	1
-3	10	9	241	240	13
-2	10	9	137	136	3
-1	10	9	237	230	13
0	10	9	90	89	1
1	10	9	242	229	10
2	10	9	140	136	2
3	10	9	253	239	14
4	10	9	74	77	2
5	10	9	58	62	4
-5	11	9	54	49	5
-4	11	9	35	30	3
-3	11	9	45	47	2
-2	11	9	96	100	4
-1	11	9	45	40	2
0	11	9	183	185	2
1	11	9	39	40	2
2	11	9	101	101	3
3	11	9	51	46	3
4	11	9	30	30	4
5	11	9	51	49	6
-4	12	9	86	84	2
-3	12	9	122	124	2
-2	12	9	115	115	3
-1	12	9	162	150	10
0	12	9	101	90	6
1	12	9	169	152	10
2	12	9	115	113	3
3	12	9	123	121	4
4	12	9	84	84	2
-3	13	9	50	52	4
-2	13	9	96	97	2
-1	13	9	41	45	4
0	13	9	22	13	5
1	13	9	45	45	2
2	13	9	96	97	2
3	13	9	51	51	3
-1	14	9	34	31	3
0	14	9	25	21	5
1	14	9	38	34	3
0	0	10	865	787	13
1	0	10	190	166	3
2	0	10	193	194	24
3	0	10	162	147	9
4	0	10	395	399	11
5	0	10	146	120	12
6	0	10	69	68	2
7	0	10	252	236	4
-7	1	10	82	80	2
-6	1	10	92	93	1
-5	1	10	96	97	1

h	k	l	10Fo	10Fc	10s
-4	1	10	232	240	2
-3	1	10	452	448	3
-2	1	10	66	63	1
-1	1	10	160	154	1
0	1	10	428	429	4
1	1	10	158	154	1
2	1	10	68	63	1
3	1	10	451	448	3
4	1	10	231	240	2
5	1	10	95	97	1
6	1	10	95	94	3
7	1	10	75	80	7
-7	2	10	35	30	3
-6	2	10	69	81	3
-5	2	10	109	107	17
-4	2	10	384	369	18
-3	2	10	104	96	29
-2	2	10	482	469	23
-1	2	10	47	35	21
0	2	10	720	716	8
1	2	10	61	37	12
2	2	10	484	465	16
3	2	10	106	93	16
4	2	10	387	369	26
5	2	10	127	107	13
6	2	10	75	80	2
7	2	10	23	30	7
-7	3	10	96	98	1
-6	3	10	52	53	2
-5	3	10	118	112	2
-4	3	10	56	57	1
-3	3	10	177	181	1
-2	3	10	113	108	1
-1	3	10	184	186	1
0	3	10	179	169	1
1	3	10	181	185	1
2	3	10	114	108	1
3	3	10	173	180	1
4	3	10	58	58	1
5	3	10	110	113	1
6	3	10	54	53	2
7	3	10	96	99	4
-7	4	10	103	102	3
-6	4	10	137	139	1
-5	4	10	97	89	13
-4	4	10	325	306	9
-3	4	10	44	48	1
-2	4	10	252	267	2
-1	4	10	132	91	97
0	4	10	308	308	41
1	4	10	128	94	115
2	4	10	251	269	4
3	4	10	42	48	1
4	4	10	318	304	12
5	4	10	104	88	13
6	4	10	136	137	2
7	4	10	102	101	2
-7	5	10	94	93	1
-6	5	10	86	88	1
-5	5	10	176	186	3
-4	5	10	192	196	1
-3	5	10	298	312	2
-2	5	10	76	74	1
-1	5	10	226	226	2
0	5	10	129	126	1
1	5	10	226	223	1
2	5	10	79	75	1
3	5	10	301	311	2
4	5	10	196	197	2
5	5	10	178	184	3
6	5	10	82	88	1
7	5	10	98	93	3
-7	6	10	69	63	2
-6	6	10	174	160	15
-5	6	10	117	111	13
-4	6	10	186	178	7
-3	6	10	176	177	4
-2	6	10	181	174	20
-1	6	10	53	47	16
0	6	10	273	271	32
1	6	10	45	46	16
2	6	10	179	175	25
3	6	10	179	176	6
4	6	10	186	176	10
5	6	10	111	110	14
6	6	10	169	159	16
7	6	10	60	62	2

h	k	l	10Fo	10Fc	10s
-6	7	10	101	104	1
-5	7	10	152	151	4
-4	7	10	69	71	1
-3	7	10	161	170	2
-2	7	10	107	102	1
-1	7	10	251	254	11
0	7	10	127	121	2
1	7	10	257	255	9
2	7	10	101	101	1
3	7	10	161	170	2
4	7	10	71	71	1
5	7	10	152	150	2
6	7	10	100	103	2
-6	8	10	94	83	15
-5	8	10	115	120	2
-4	8	10	155	153	14
-3	8	10	108	102	25
-2	8	10	280	273	20
-1	8	10	97	97	12
0	8	10	161	148	160
1	8	10	97	98	8
2	8	10	274	273	23
3	8	10	105	101	25
4	8	10	159	155	17
5	8	10	114	121	2
6	8	10	84	82	12
-6	9	10	52	52	2
-5	9	10	80	81	2
-4	9	10	115	116	2
-3	9	10	176	182	8
-2	9	10	130	131	8
-1	9	10	410	409	6
0	9	10	212	218	2
1	9	10	414	410	4
2	9	10	130	132	7
3	9	10	185	183	6
4	9	10	117	115	3
5	9	10	79	82	1
6	9	10	57	53	2
-5	10	10	57	54	5
-4	10	10	50	36	11
-3	10	10	133	131	1
-2	10	10	140	141	4
-1	10	10	151	157	2
0	10	10	50	45	2
1	10	10	156	156	2
2	10	10	139	139	8
3	10	10	133	131	1
4	10	10	48	34	13
5	10	10	58	54	2
-4	11	10	58	59	3
-3	11	10	92	96	3
-2	11	10	208	207	2
-1	11	10	166	157	5
0	11	10	132	126	5
1	11	10	167	157	5
2	11	10	210	208	4
3	11	10	94	97	1
4	11	10	60	60	4
-4	12	10	24	5	7
-3	12	10	45	51	3
-2	12	10	83	87	2
-1	12	10	84	89	1
0	12	10	50	50	1
1	12	10	84	89	1
2	12	10	82	87	4
3	12	10	50	51	2
4	12	10	9	4	9
-3	13	10	169	167	2
-2	13	10	37	18	5
-1	13	10	120	110	3
0	13	10	51	49	3
1	13	10	117	109	2
2	13	10	45	18	3
3	13	10	171	166	2
-1	14	10	25	30	6
0	14	10	34	32	4
1	14	10	28	30	15
1	0	11	82	81	1
2	0	11	143	142	1
3	0	11	236	230	2
4	0	11	25	23	2
5	0	11	68	61	2
6	0	11	121	127	2
7	0	11	201	198	2
-7	1	11	126	124	3
-6	1	11	141	133	5

h	k	l	10Fo	10Fc	10s
-5	1	11	285	286	7
-4	1	11	90	82	17
-3	1	11	442	430	13
-2	1	11	179	156	27
-1	1	11	469	458	71
0	1	11	654	586	50
1	1	11	483	457	63
2	1	11	193	156	25
3	1	11	457	430	21
4	1	11	86	83	5
5	1	11	282	287	4
6	1	11	142	134	10
7	1	11	122	125	2
-7	2	11	33	39	4
-6	2	11	91	88	1
-5	2	11	179	180	2
-4	2	11	209	215	2
-3	2	11	95	101	1
-2	2	11	297	299	2
-1	2	11	142	141	1
0	2	11	54	42	1
1	2	11	141	142	1
2	2	11	296	300	2
3	2	11	94	101	1
4	2	11	211	215	2
5	2	11	178	180	1
6	2	11	93	89	2
7	2	11	38	39	6
-7	3	11	154	153	2
-6	3	11	90	89	7
-5	3	11	157	164	4
-4	3	11	325	303	20
-3	3	11	352	335	15
-2	3	11	142	133	29
-1	3	11	500	499	9
0	3	11	178	163	6
1	3	11	500	500	8
2	3	11	150	133	29
3	3	11	364	334	16
4	3	11	329	304	36
5	3	11	166	167	2
6	3	11	95	89	11
7	3	11	158	153	4
-7	4	11	42	45	3
-6	4	11	51	47	4
-5	4	11	118	122	1
-4	4	11	219	231	2
-3	4	11	110	114	1
-2	4	11	217	226	1
-1	4	11	293	286	2
0	4	11	577	584	6
1	4	11	290	286	2
2	4	11	213	224	2
3	4	11	107	114	1
4	4	11	221	230	2
5	4	11	121	122	3
6	4	11	54	49	3
7	4	11	54	45	3
-7	5	11	162	164	2
-6	5	11	94	91	2
-5	5	11	252	247	12
-4	5	11	104	108	1
-3	5	11	323	327	2
-2	5	11	163	156	7
-1	5	11	363	364	12
0	5	11	45	36	1
1	5	11	358	365	14
2	5	11	164	156	7
3	5	11	322	327	2
4	5	11	108	108	1
5	5	11	259	248	18
6	5	11	93	91	2
7	5	11	162	162	2
-6	6	11	168	171	2
-5	6	11	113	116	1
-4	6	11	261	263	10
-3	6	11	56	66	1
-2	6	11	241	239	4
-1	6	11	130	128	2
0	6	11	325	322	7
1	6	11	130	128	3
2	6	11	242	238	4
3	6	11	57	66	1
4	6	11	265	264	4
5	6	11	114	116	1
6	6	11	170	171	2
-6	7	11	128	126	4

h	k	l	10Fo	10Fc	10s
-5	7	11	156	146	4
-4	7	11	72	68	6
-3	7	11	58	45	8
-2	7	11	112	96	20
-1	7	11	245	249	6
0	7	11	61	31	61
1	7	11	248	251	5
2	7	11	106	97	22
3	7	11	63	41	12
4	7	11	72	68	6
5	7	11	154	146	3
6	7	11	130	126	3
-6	8	11	130	129	2
-5	8	11	30	33	6
-4	8	11	188	178	7
-3	8	11	148	156	1
-2	8	11	248	249	5
-1	8	11	34	32	2
0	8	11	374	380	3
1	8	11	31	32	1
2	8	11	253	251	4
3	8	11	149	156	1
4	8	11	190	179	5
5	8	11	38	33	2
6	8	11	128	128	2
-5	9	11	71	73	4
-4	9	11	36	25	20
-3	9	11	217	215	11
-2	9	11	191	197	10
-1	9	11	54	49	2
0	9	11	49	48	15
1	9	11	55	51	2
2	9	11	189	197	3
3	9	11	217	213	9
4	9	11	32	25	8
5	9	11	70	72	2
-5	10	11	49	43	4
-4	10	11	206	198	7
-3	10	11	81	83	4
-2	10	11	174	167	5
-1	10	11	94	91	3
0	10	11	215	198	15
1	10	11	97	91	2
2	10	11	174	166	6
3	10	11	83	83	2
4	10	11	208	196	5
5	10	11	56	43	3
-4	11	11	84	79	4
-3	11	11	17	10	14
-2	11	11	74	76	2
-1	11	11	75	73	6
0	11	11	35	26	35
1	11	11	72	73	12
2	11	11	72	77	4
3	11	11	26	11	7
4	11	11	81	80	4
-3	12	11	59	53	3
-2	12	11	179	169	3
-1	12	11	26	18	8
0	12	11	213	193	15
1	12	11	23	18	6
2	12	11	180	168	3
3	12	11	55	53	2
-2	13	11	88	96	3
-1	13	11	33	31	8
0	13	11	43	43	4
1	13	11	22	31	11
2	13	11	93	96	2
0	0	12	450	374	11
1	0	12	171	175	2
2	0	12	304	297	2
3	0	12	173	153	23
4	0	12	350	348	2
5	0	12	10	10	9
6	0	12	81	31	13
7	0	12	201	183	9
-7	1	12	55	64	15
-6	1	12	59	61	2
-5	1	12	126	129	1
-4	1	12	46	52	1
-3	1	12	240	248	2
-2	1	12	178	174	1
-1	1	12	412	396	4
0	1	12	194	174	2
1	1	12	410	396	4
2	1	12	177	174	2
3	1	12	239	248	2

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	1	12	48	52	1	4	7	12	73	73	2	-1	2	13	220	212	2	3	8	13	69	67	1	-5	3	14	50	56	2
5	1	12	126	129	2	5	7	12	88	89	1	0	2	13	230	241	2	4	8	13	34	27	8	-4	3	14	83	87	4
6	1	12	66	61	2	6	7	12	66	63	2	1	2	13	216	211	2	5	8	13	128	123	6	-3	3	14	123	129	1
7	1	12	62	64	2	-6	8	12	51	40	11	2	2	13	177	174	1	6	8	13	5	24	5	-2	3	14	148	151	1
-7	2	12	103	102	9	-5	8	12	146	143	5	3	2	13	142	147	1	-5	9	13	80	81	2	-1	3	14	134	138	6
-6	2	12	161	155	13	-4	8	12	132	130	2	4	2	13	147	154	1	-4	9	13	160	157	7	0	3	14	249	247	3
-5	2	12	230	224	16	-3	8	12	162	163	8	5	2	13	206	219	4	-3	9	13	47	25	7	1	3	14	135	138	6
-4	2	12	106	100	26	-2	8	12	142	140	16	6	2	13	32	40	5	-2	9	13	55	26	20	2	3	14	149	152	1
-3	2	12	178	170	14	-1	8	12	141	133	74	7	2	13	53	61	3	-1	9	13	86	80	15	3	3	14	124	129	1
-2	2	12	156	168	1	0	8	12	334	328	37	-7	3	13	29	19	4	0	9	13	39	50	2	4	3	14	84	86	1
-1	2	12	210	212	2	1	8	12	142	134	60	-6	3	13	26	42	4	1	9	13	79	79	19	5	3	14	53	56	2
0	2	12	283	291	12	2	8	12	150	139	20	-5	3	13	66	63	23	2	9	13	47	25	14	6	3	14	17	23	16
1	2	12	213	216	3	3	8	12	164	163	11	-4	3	13	175	178	7	3	9	13	51	24	6	7	3	14	71	71	3
2	2	12	155	169	1	4	8	12	128	129	3	-3	3	13	126	127	2	4	9	13	167	157	6	-6	4	14	39	31	9
3	2	12	182	167	13	5	8	12	144	144	4	-2	3	13	178	171	25	5	9	13	82	82	2	-5	4	14	190	182	12
4	2	12	114	100	19	6	8	12	43	41	3	-1	3	13	180	140	51	-5	10	13	58	59	3	-4	4	14	70	56	23
5	2	12	254	224	18	-5	9	12	88	86	2	0	3	13	972	835	55	-4	10	13	44	21	9	-3	4	14	423	405	18
6	2	12	168	155	9	-4	9	12	135	137	3	1	3	13	168	142	59	-3	10	13	187	178	7	-2	4	14	53	46	12
7	2	12	114	105	11	-3	9	12	106	110	1	2	3	13	180	173	24	-2	10	13	137	135	1	-1	4	14	514	490	22
-7	3	12	29	29	6	-2	9	12	115	115	2	3	3	13	123	126	4	-1	10	13	231	221	5	0	4	14	34	30	2
-6	3	12	95	98	2	-1	9	12	114	112	3	4	3	13	176	181	4	0	10	13	104	105	1	1	4	14	523	491	21
-5	3	12	48	50	4	0	9	12	0	6	1	5	3	13	106	63	16	1	10	13	231	222	2	2	4	14	58	47	13
-4	3	12	206	212	1	1	9	12	115	112	3	6	3	13	33	43	4	2	10	13	133	136	3	3	4	14	425	403	21
-3	3	12	227	231	1	2	9	12	124	117	1	7	3	13	27	20	7	3	10	13	187	178	5	4	4	14	86	55	34
-2	3	12	267	259	2	3	9	12	103	108	1	-7	4	13	37	36	3	4	10	13	33	21	4	5	4	14	207	185	12
-1	3	12	315	322	2	4	9	12	139	138	3	-6	4	13	57	53	2	5	10	13	64	60	4	6	4	14	52	32	6
0	3	12	58	68	5	5	9	12	81	87	2	-5	4	13	57	63	2	-4	11	13	45	35	6	-6	5	14	109	112	1
1	3	12	314	321	2	-5	10	12	51	50	3	-4	4	13	56	62	1	-3	11	13	143	145	4	-5	5	14	87	89	2
2	3	12	263	258	2	-4	10	12	65	65	2	-3	4	13	150	155	5	-2	11	13	40	28	40	-4	5	14	58	64	2
3	3	12	226	232	2	-3	10	12	49	31	29	-2	4	13	255	256	2	-1	11	13	101	107	2	-3	5	14	209	218	1
4	3	12	204	212	3	-2	10	12	129	129	15	-1	4	13	200	205	5	0	11	13	18	27	6	-2	5	14	281	276	4
5	3	12	45	49	2	-1	10	12	154	160	33	0	4	13	210	196	1	1	11	13	107	107	3	-1	5	14	190	196	6
6	3	12	94	99	2	0	10	12	205	199	21	1	4	13	197	203	9	2	11	13	50	28	31	0	5	14	286	298	20
7	3	12	27	29	7	1	10	12	150	159	26	2	4	13	251	256	2	3	11	13	145	145	3	1	5	14	190	195	4
-7	4	12	38	29	37	2	10	12	132	128	12	3	4	13	147	154	5	4	11	13	51	35	6	2	5	14	274	275	4
-6	4	12	145	147	6	3	10	12	44	30	19	4	4	13	57	62	1	-3	12	13	189	186	3	3	5	14	207	218	2
-5	4	12	44	26	16	4	10	12	70	64	2	5	4	13	58	62	2	-2	12	13	124	122	5	4	5	14	57	61	4
-4	4	12	90	60	24	5	10	12	53	50	3	6	4	13	55	53	3	-1	12	13	252	225	14	5	5	14	87	88	4
-3	4	12	226	216	16	-4	11	12	77	74	2	7	4	13	42	37	4	0	12	13	71	76	2	6	5	14	105	112	4
-2	4	12	229	222	31	-3	11	12	152	143	11	-6	5	13	159	155	12	1	12	13	244	225	11	-6	6	14	53	52	5
-1	4	12	266	263	9	-2	11	12	75	72	5	-5	5	13	64	57	5	2	12	13	126	122	4	-5	6	14	209	219	2
0	4	12	306	312	2	-1	11	12	199	189	5	-4	5	13	188	180	14	3	12	13	188	185	2	-4	6	14	124	128	1
1	4	12	269	264	10	0	11	12	205	204	3	-3	5	13	76	57	28	-2	13	13	139	146	3	-3	6	14	282	286	5
2	4	12	248	222	33	1	11	12	198	189	5	-2	5	13	518	508	25	-1	13	13	70	63	3	-2	6	14	241	239	11
3	4	12	234	218	14	2	11	12	78	71	2	-1	5	13	263	250	13	0	13	13	96	98	5	-1	6	14	364	357	21
4	4	12	91	63	38	3	11	12	156	142	7	0	5	13	647	607	44	1	13	13	64	63	3	0	6	14	86	68	44
5	4	12	57	28	9	4	11	12	73	75	3	1	5	13	264	250	15	2	13	13	143	146	2	1	6	14	372	358	21
6	4	12	145	148	8	-3	12	12	69	73	12	2	5	13	535	508	33	0	0	14	424	408	10	2	6	14	254	240	14
7	4	12	26	27	7	-2	12	12	61	61	4	3	5	13	72	57	26	1	0	14	72	29	8	3	6	14	291	287	6
-7	5	12	58	63	3	-1	12	12	63	63	2	4	5	13	180	180	11	2	0	14	39	17	6	4	6	14	124	127	1
-6	5	12	25	23	5	0	12	12	178	182	2	5	5	13	65	57	2	3	0	14	272	269	2	5	6	14	211	220	3
-5	5	12	63	61	1	1	12	12	67	63	3	6	5	13	154	154	17	4	0	14	93	98	4	6	6	14	62	52	5
-4	5	12	103	104	3	2	12	12	69	62	7	-6	6	13	71	65	2	5	0	14	315	310	4	-6	7	14	198	195	2
-3	5	12	128	138	1	3	12	12	83	73	17	-5	6	13	148	153	18	6	0	14	77	79	3	-5	7	14	114	110	5
-2	5	12	104	106	1	-2	13	12	141	141	2	-4	6	13	119	118	3	7	0	14	126	133	8	-4	7	14	234	233	14
-1	5	12	225	231	6	-1	13	12	144	148	2	-3	6	13	235	230	9	-7	1	14	99	105	2	-3	7	14	77	84	4
0	5	12	106	114	20	0	13	12	113	103	5	-2	6	13	98	99	3	-6	1	14	36	40	5	-2	7	14	185	184	3
1	5	12	226	230	6	1	13	12	151	149	3	-1	6	13	190	189	6	-5	1	14	103	105	2	-1	7	14	106	100	12
2	5	12	105	105	6	2	13	12	139	139	5	0	6	13	206	207	7	-4	1	14	183	190	2	0	7	14	227	231	2
3	5	12	129	137	1	1	0	13	121	105	1	1	6	13	193	189	8	-3	1	14	13	16	4	1	7	14	108	101	11
4	5	12	103	103	2	2	0	13	31	37	1	2	6	13	101	99	2	-2	1	14	141	143	1	2	7	14	188	183	4
5	5	12	62	63	2	3	0	13	242	234	2	3	6	13	231	229	8	-1	1	14	178	172	2	3	7	14	77	85	3
6	5	12	22	23	10	4	0	13	96	97	1	4	6	13	123	119	2	0	1	14	31	16	1	4	7	14	240	234	11
7	5	12	65	64	2	5	0	13	219	234	3	5	6	13	156	154	6	1	1	14	176	172	1	5	7	14	113	109	2
-6	6	12	86	85	2	6	0	13	168	167	2	6	6	13	69	65	6	2	1	14	143	143	1	6	7	14	197	195	3
-5	6	12	90	79	13	7	0	13	25	10	11	-6	7	13	94	75	17	3	1	14	16	16	4	-5	8	14	150	149	3
-4	6	12	195	202	3	-7	1	13	83	83	29	-5	7	13	95	89	6	4	1	14	183	190	2	-4	8	14	132	125	7
-3	6	12	166	162	18	-6	1	13	197	199	2	-4	7	13	164	143	13	5	1	14	100	105	1	-3	8	14	98	87	8
-2	6	12	161	175	4	-5	1	13	101	98	6	-3	7	13	173	163	18	6	1	14	41	40	6	-2	8	14	90	91	6
-1	6	12	201	192	19	-4	1	13	394	404	6	-2	7	13	232	230	11	7	1	14	104	105	3	-1	8	14	117	102	34
0	6	12	118	122	2	-3	1	13	278	275	8	-1	7	13	170	176	1	-7	2	14	97	100	2	0	8	14	246	242	5
1	6	12	204	193	19	-2	1	13	378	368	16	0	7	13	317	323	20	-6	2	14	72	66	10	1	8	14	112	105	34
2	6	12	167	176	5	-1	1	13	78	43	78	1	7	13	172	176	1	-5	2	14	112	113	5	2	8	14	89	90	6
3	6	12	167	160	17	0	1	13	191	148	4	2	7	13	236	229	11	-4	2	14	128	128	25	3	8	14	98	87	5
4	6	12	195	202	2	1	1	13	97	42	97	3	7	13	176	162	18	-3	2	14	149	153	10	4	8	14	127	125	6
5	6	12	92	78	10	2	1	13	379	364	12	4	7	13	160	143	14	-2	2	14	67	59	67	5	8	14	149	151	2
6	6	12	83	83	3	3	1	13	279	273	5	5	7	13	90	90	3	-1	2	14	416	396	19	-5	9	14	63	55	3
-6	7	12	69	64	2	4	1	13	401	405	12	6	7	13	85	75	15	0	2	14	108	104	3	-4	9	14	192	191	5
-5	7	12	84	89	1	5	1	13	110	99	14	-6	8	13	31	24	4	1	2	14	418	396	26	-3	9	14	73	68	2
-4	7	12	72	74	5	6	1	13	198	199	2	-5	8	13	126	122	5	2	2	14	82	59	55	-2	9	14	142	143	3
-3	7	12	156	157	5	7	1	13	79	82	3	-4	8	13	40	28	11	3	2	14	155	151	14	-1	9	14	140	149	4
-2	7	12	168	165	5	-7	2	13	52	60	2	-3	8	13	68	68	2	4	2	14	137	130	42	0	9	14	14	11	13
-1	7	12	163	165	8	-6	2	13	36	40	4	-2	8	13	84	83	2	5	2	14	110	113	1	1	9	14	145	149	2
0	7	12	300	285	11	-5	2	13	210	218	3	-1	8	13	350	346	8	6	2	14	75	66	3	2	9	14	138	142	1
1	7	12	167	167	6	-4	2	13	147	154	1	0	8	13	194	174	22	7	2	14	94	99	2	3	9	14	73	68	5
2	7	12	169	167	3	-3	2	13	141	146	1	1	8	13	357	347	6	-7	3	14	73	71	2	4	9	14	193	189	2
3	7	12	156	159	4	-2	2	13	179	175	1	2	8	13	81	82	2	-6	3	14	17	24	16	5	9	14	55	55	3

Table 6. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-4	10	14	106	102	6	3	4	15	100	101	2	1	0	16	117	124	2	-2	7	16	218	220	12	0	3	17	44	39	1
-3	10	14	82	80	1	4	4	15	139	145	4	2	0	16	379	386	4	-1	7	16	113	112	12	1	3	17	308	307	3
-2	10	14	103	103	9	5	4	15	125	125	2	3	0	16	14	13	4	0	7	16	93	95	4	2	3	17	126	130	1
-1	10	14	66	67	3	6	4	15	30	37	6	4	0	16	443	445	8	1	7	16	115	111	11	3	3	17	205	186	15
0	10	14	154	155	10	-6	5	15	73	71	2	5	0	16	105	107	6	2	7	16	222	220	8	4	3	17	159	161	14
1	10	14	71	68	5	-5	5	15	58	35	12	6	0	16	250	249	12	3	7	16	124	118	15	5	3	17	142	125	7
2	10	14	102	103	10	-4	5	15	82	69	18	-6	1	16	117	116	2	4	7	16	203	197	6	6	3	17	56	54	3
3	10	14	82	79	4	-3	5	15	60	37	60	-5	1	16	221	233	3	5	7	16	188	186	6	-6	4	17	91	92	2
4	10	14	105	102	4	-2	5	15	102	93	54	-4	1	16	91	98	2	-5	8	16	85	78	9	-5	4	17	0	4	1
-4	11	14	189	181	9	-1	5	15	359	326	33	-3	1	16	194	203	1	-4	8	16	166	154	11	-4	4	17	129	137	2
-3	11	14	64	68	2	0	5	15	383	352	22	-2	1	16	88	89	1	-3	8	16	78	72	2	-3	4	17	106	113	1
-2	11	14	202	184	7	1	5	15	365	325	32	-1	1	16	50	49	1	-2	8	16	152	135	18	-2	4	17	183	188	2
-1	11	14	52	17	13	2	5	15	115	92	47	0	1	16	26	20	1	-1	8	16	83	80	1	-1	4	17	218	227	2
0	11	14	95	85	9	3	5	15	68	39	38	1	1	16	50	48	1	0	8	16	47	47	1	0	4	17	160	158	3
1	11	14	44	17	15	4	5	15	87	71	21	2	1	16	89	89	1	1	8	16	82	80	1	1	4	17	221	227	2
2	11	14	198	183	7	5	5	15	67	33	9	3	1	16	195	202	2	2	8	16	161	137	19	2	4	17	184	189	2
3	11	14	70	68	3	6	5	15	71	71	4	4	1	16	93	98	1	3	8	16	73	72	5	3	4	17	107	112	2
4	11	14	186	182	4	-6	6	15	88	87	2	5	1	16	219	232	4	4	8	16	170	154	10	4	4	17	131	136	5
-3	12	14	109	111	3	-5	6	15	71	72	2	6	1	16	112	115	3	5	8	16	80	78	4	5	4	17	11	3	11
-2	12	14	94	101	14	-4	6	15	60	56	11	-6	2	16	163	162	2	-4	9	16	13	15	12	6	4	17	90	91	3
-1	12	14	117	115	3	-3	6	15	35	32	6	-5	2	16	53	51	2	-3	9	16	174	175	4	-6	5	17	54	57	5
0	12	14	104	102	28	-2	6	15	63	62	5	-4	2	16	146	149	7	-2	9	16	41	36	4	-5	5	17	137	134	8
1	12	14	118	115	4	-1	6	15	303	304	6	-3	2	16	234	245	2	-1	9	16	199	196	6	-4	5	17	107	111	2
2	12	14	104	102	13	0	6	15	169	167	1	-2	2	16	263	268	2	0	9	16	82	65	12	-3	5	17	142	141	5
3	12	14	112	111	9	1	6	15	302	304	5	-1	2	16	65	71	6	1	9	16	201	195	3	-2	5	17	142	145	39
-1	13	14	50	42	18	2	6	15	67	64	15	0	2	16	501	482	17	2	9	16	37	36	5	-1	5	17	93	56	49
0	13	14	270	262	6	3	6	15	30	34	11	1	2	16	73	71	4	3	9	16	178	174	4	0	5	17	414	371	35
1	13	14	44	42	8	4	6	15	64	58	11	2	2	16	257	267	2	4	9	16	28	15	6	1	5	17	100	59	44
1	0	15	310	315	3	5	6	15	70	70	2	3	2	16	239	245	5	-4	10	16	127	119	5	2	5	17	154	146	35
2	0	15	100	88	1	6	6	15	90	87	2	4	2	16	147	150	1	-3	10	16	36	22	3	3	5	17	148	142	6
3	0	15	10	9	9	-6	7	15	74	44	17	5	2	16	50	51	2	-2	10	16	82	70	28	4	5	17	108	109	2
4	0	15	113	115	1	-5	7	15	111	95	16	6	2	16	163	162	2	-1	10	16	53	54	4	5	5	17	145	135	4
5	0	15	54	53	2	-4	7	15	232	229	4	-6	3	16	142	145	2	0	10	16	74	70	2	6	5	17	70	56	6
6	0	15	151	151	3	-3	7	15	116	117	4	-5	3	16	50	49	3	1	10	16	56	54	3	-5	6	17	94	89	2
7	0	15	140	145	5	-2	7	15	139	135	6	-4	3	16	157	171	5	2	10	16	93	70	42	-4	6	17	58	53	2
-7	1	15	138	140	6	-1	7	15	81	81	11	-3	3	16	112	113	1	3	10	16	32	22	4	-3	6	17	63	65	2
-6	1	15	191	188	7	0	7	15	146	119	33	-2	3	16	179	176	2	4	10	16	120	119	5	-2	6	17	139	134	3
-5	1	15	330	319	12	1	7	15	84	83	10	-1	3	16	261	265	4	-3	11	16	257	249	7	-1	6	17	84	84	4
-4	1	15	101	107	9	2	7	15	141	137	6	0	3	16	173	181	1	-2	11	16	37	32	5	0	6	17	107	106	5
-3	1	15	272	277	3	3	7	15	116	114	3	1	3	16	263	263	10	-1	11	16	182	172	12	1	6	17	81	83	3
-2	1	15	182	185	1	4	7	15	235	230	5	2	3	16	173	176	2	0	11	16	46	35	4	2	6	17	141	134	3
-1	1	15	139	147	9	5	7	15	120	95	27	3	3	16	117	114	2	1	11	16	192	171	12	3	6	17	63	66	1
0	1	15	36	14	4	6	7	15	65	45	16	4	3	16	165	171	3	2	11	16	37	32	4	4	6	17	56	53	2
1	1	15	139	146	9	-5	8	15	82	74	17	5	3	16	46	48	4	3	11	16	256	249	7	5	6	17	90	88	2
2	1	15	178	185	1	-4	8	15	93	89	4	6	3	16	140	145	3	-2	12	16	90	82	42	-5	7	17	109	118	5
3	1	15	276	275	7	-3	8	15	175	163	11	-6	4	16	131	135	8	-1	12	16	16	12	9	-4	7	17	86	74	9
4	1	15	99	105	1	-2	8	15	37	14	10	-5	4	16	40	34	5	0	12	16	164	166	7	-3	7	17	188	188	3
5	1	15	321	319	17	-1	8	15	159	163	4	-4	4	16	149	147	3	1	12	16	12	12	12	-2	7	17	87	78	16
6	1	15	183	185	5	0	8	15	48	37	10	-3	4	16	126	124	11	2	12	16	87	83	25	-1	7	17	206	194	12
7	1	15	140	140	4	1	8	15	162	165	3	-2	4	16	213	203	45	1	0	17	30	22	29	0	7	17	112	95	6
-7	2	15	48	45	6	2	8	15	39	12	10	-1	4	16	144	121	25	2	0	17	354	361	3	1	7	17	214	196	11
-6	2	15	34	19	13	3	8	15	173	162	8	0	4	16	333	321	9	3	0	17	74	83	1	2	7	17	94	79	12
-5	2	15	34	38	2	4	8	15	98	89	3	1	4	16	147	121	25	4	0	17	71	77	1	3	7	17	189	189	5
-4	2	15	121	132	1	5	8	15	79	72	12	2	4	16	225	205	43	5	0	17	25	23	5	4	7	17	86	75	15
-3	2	15	169	176	1	-5	9	15	72	64	2	3	4	16	130	124	11	6	0	17	68	78	3	5	7	17	116	120	6
-2	2	15	313	314	4	-4	9	15	99	92	9	4	4	16	150	150	2	-6	1	17	84	83	2	-5	8	17	126	130	2
-1	2	15	154	146	2	-3	9	15	125	125	12	5	4	16	46	34	7	-5	1	17	170	168	13	-4	8	17	195	183	12
0	2	15	24	20	14	-2	9	15	30	28	3	6	4	16	146	136	6	-4	1	17	176	179	4	-3	8	17	28	4	11
1	2	15	151	146	1	-1	9	15	91	72	34	-6	5	16	15	9	14	-3	1	17	116	121	2	-2	8	17	190	193	5
2	2	15	310	314	5	0	9	15	35	24	15	-5	5	16	118	116	8	-2	1	17	157	156	4	-1	8	17	114	104	10
3	2	15	172	176	2	1	9	15	84	73	84	-4	5	16	108	118	9	-1	1	17	139	144	2	0	8	17	171	164	21
4	2	15	120	132	2	2	9	15	38	29	3	-3	5	16	145	150	3	0	1	17	22	31	3	1	8	17	107	106	8
5	2	15	39	37	3	3	9	15	131	125	23	-2	5	16	313	316	4	1	1	17	142	146	2	2	8	17	193	192	5
6	2	15	16	18	16	4	9	15	101	93	7	-1	5	16	168	172	5	2	1	17	152	154	16	3	8	17	23	5	7
7	2	15	55	45	4	5	9	15	71	64	5	0	5	16	122	128	6	3	1	17	124	123	2	4	8	17	190	181	10
-6	3	15	130	131	13	-4	10	15	112	97	10	1	5	16	169	174	4	4	1	17	174	179	9	5	8	17	132	130	5
-5	3	15	76	85	3	-3	10	15	86	81	4	2	5	16	307	316	5	5	1	17	163	167	2	-4	9	17	84	59	15
-4	3	15	209	198	5	-2	10	15	73	65	5	3	5	16	150	153	2	6	1	17	76	82	2	-3	9	17	76	64	4
-3	3	15	163	168	25	-1	10	15	49	34	6	4	5	16	111	118	10	-6	2	17	110	112	2	-2	9	17	71	66	8
-2	3	15	302	287	12	0	10	15	174	166	4	5	5	16	118	118	5	-5	2	17	111	113	2	-1	9	17	7	16	6
-1	3	15	191	167	7	1	10	15	50	33	8	6	5	16	15	9	15	-4	2	17	7	7	6	0	9	17	71	65	2
0	3	15	115	135	1	2	10	15	66	67	3	-6	6	16	96	88	7	-3	2	17	110	119	2	1	9	17	10	14	9
1	3	15	189	170	4	3	10	15	79	79	2	-5	6	16	102	82	16	-2	2	17	179	182	2	2	9	17	72	65	6
2	3	15	299	286	14	4	10	15	104	97	9	-4	6	16	168	157	12	-1	2	17	88	87	4	3	9	17	69	65	5
3	3	15	181	170	30	-3	11	15	128	139	21	-3	6	16	117	128	10	0	2	17	161	162	1	4	9	17	81	60	14
4	3	15	206	196	5	-2	11	15	42	32	8	-2	6	16	220	206	21	1	2	17	90	87	11	-3	10	17	46	29	8
5	3	15	85	87	2	-1	11	15	105	109	13	-1	6	16	51	19	10	2	2	17	179	183	1	-2	10	17	223	216	5
6	3	15	139	131	9	0	11	15	191	191	6	0	6	16	119	105	23	3	2	17	117	119	1	-1	10	17	89	86	5
-6	4	15	40	36	3	1	11	15	103	109	18	1	6	16	48	19	13	4	2	17	16	9	16	0	10	17	89	86	13
-5	4	15	124	126	2	2	11	15	31	33	7	2	6	16	247	205	27	5	2	17	113	113	3	1	10	17	96	85	6
-4	4	15	140	145	8	3	11	15	134	139	34	3	6	16	127	127	11	6	2	17	108	111	2	2	10	17	217	215	4
-3	4	15	99	101	1	-2	12	15	145	139	3	4	6	16	169	157	16	-6	3	17	58	53	2	3	10	17	47	29	8
-2	4	15	58	56	2	-1	12	15	92	98	2	5	6	16	101	83	12	-5	3	17	138	125	9	-2	11	17	73	63	17
-1	4	15	54	61	3	0	12	15	267	268	8	6	6	16	93	89	4	-4	3	17	171	163	12	-1	11	17	91	90	2
0	4	15	30	11	29	1	12	15	101	99	3	-5	7	16	184	185	10	-3	3	17	192	188	12	0	11	17	47	32	22
1	4	15	53	61	1	2	12	15	144	138	8	-4	7	16	205	197	4	-2	3	17	131	131	1	1	11	17	99	90	5
2	4	15	59	56	2	0	0	16	182	147	10	-3	7	16	138	118	26	-1	3	17	311	307	4	2	11	17	70	63	10

h	k	l	10Fo	10Fc	10s
-1	12	17	39	45	6
0	12	17	36	19	8
1	12	17	68	44	16
0	0	18	140	126	1
1	0	18	370	351	9
2	0	18	76	81	13
3	0	18	245	240	9
4	0	18	165	163	1
5	0	18	220	231	12
6	0	18	87	92	4
-6	1	18	55	52	3
-5	1	18	34	38	4
-4	1	18	60	59	4
-3	1	18	131	136	2
-2	1	18	156	155	3
-1	1	18	134	136	1
0	1	18	59	58	1
1	1	18	134	135	1
2	1	18	161	155	5
3	1	18	134	136	1
4	1	18	59	59	2
5	1	18	31	38	7
6	1	18	43	52	4
-6	2	18	107	105	2
-5	2	18	150	154	2
-4	2	18	137	129	2
-3	2	18	254	266	4
-2	2	18	243	240	19
-1	2	18	297	279	10
0	2	18	145	139	2
1	2	18	288	276	13
2	2	18	241	241	21
3	2	18	260	264	8
4	2	18	129	129	10
5	2	18	152	155	5
6	2	18	106	104	5
-6	3	18	57	53	4
-5	3	18	34	47	4
-4	3	18	156	161	2
-3	3	18	75	77	7
-2	3	18	56	47	14
-1	3	18	350	357	4
0	3	18	92	96	91
1	3	18	347	358	3
2	3	18	49	47	49
3	3	18	77	77	7
4	3	18	155	161	3
5	3	18	37	47	4
6	3	18	55	54	3
-6	4	18	109	111	3
-5	4	18	63	52	4
-4	4	18	92	86	2
-3	4	18	70	73	11
-2	4	18	70	65	3
-1	4	18	152	122	24
0	4	18	129	114	26
1	4	18	134	124	29
2	4	18	67	63	3
3	4	18	88	74	28
4	4	18	89	84	1
5	4	18	65	54	4
6	4	18	117	111	2
-5	5	18	96	99	3
-4	5	18	115	111	17
-3	5	18	78	78	4
-2	5	18	142	143	2
-1	5	18	72	71	7
0	5	18	219	225	2
1	5	18	70	71	7
2	5	18	147	145	3
3	5	18	75	79	3
4	5	18	116	113	10
5	5	18	94	98	3
-5	6	18	110	94	14
-4	6	18	82	66	5
-3	6	18	68	73	1
-2	6	18	119	102	19
-1	6	18	89	86	4
0	6	18	73	1	16
1	6	18	84	83	4
2	6	18	129	101	22
3	6	18	70	70	1
4	6	18	83	67	7
5	6	18	125	94	14
-5	7	18	51	43	3
-4	7	18	106	101	9
-3	7	18	76	73	4

h	k	l	10Fo	10Fc	10s
-2	7	18	141	138	5
-1	7	18	163	152	6
0	7	18	55	40	9
1	7	18	158	151	7
2	7	18	141	136	6
3	7	18	74	72	6
4	7	18	107	103	8
5	7	18	37	42	4
-4	8	18	78	81	2
-3	8	18	124	104	25
-2	8	18	34	33	4
-1	8	18	133	128	3
0	8	18	167	175	2
1	8	18	137	130	4
2	8	18	36	34	4
3	8	18	130	104	31
4	8	18	81	81	2
-4	9	18	189	180	9
-3	9	18	161	158	7
-2	9	18	60	55	4
-1	9	18	122	105	13
0	9	18	77	62	8
1	9	18	103	105	11
2	9	18	58	55	3
3	9	18	167	157	7
4	9	18	193	179	7
-3	10	18	179	160	22
-2	10	18	125	124	7
-1	10	18	131	125	17
0	10	18	93	100	3
1	10	18	147	125	16
2	10	18	140	125	7
3	10	18	177	158	24
-2	11	18	118	114	4
-1	11	18	41	36	7
0	11	18	150	148	18
1	11	18	50	38	3
2	11	18	115	114	7
1	0	19	43	41	1
2	0	19	26	34	1
3	0	19	41	42	1
4	0	19	38	38	2
5	0	19	0	10	1
6	0	19	0	25	1
-6	1	19	122	135	2
-5	1	19	28	27	15
-4	1	19	259	264	6
-3	1	19	110	106	2
-2	1	19	300	302	6
-1	1	19	165	172	3
0	1	19	410	410	4
1	1	19	165	172	10
2	1	19	300	302	3
3	1	19	107	106	5
4	1	19	257	263	4
5	1	19	29	26	11
6	1	19	128	134	3
-6	2	19	81	87	3
-5	2	19	37	39	4
-4	2	19	132	136	2
-3	2	19	143	151	17
-2	2	19	60	65	1
-1	2	19	118	122	1
0	2	19	49	47	1
1	2	19	118	121	2
2	2	19	61	65	3
3	2	19	151	151	2
4	2	19	135	136	2
5	2	19	39	38	5
6	2	19	76	87	4
-6	3	19	187	189	2
-5	3	19	53	48	7
-4	3	19	92	92	3
-3	3	19	117	116	4
-2	3	19	266	270	4
-1	3	19	71	43	61
0	3	19	258	273	3
1	3	19	56	43	56
2	3	19	270	272	6
3	3	19	120	116	4
4	3	19	86	90	4
5	3	19	53	48	3
6	3	19	195	189	3
-5	4	19	88	85	7
-4	4	19	77	79	2
-3	4	19	92	92	1
-2	4	19	112	118	1

h	k	l	10Fo	10Fc	10s
-1	4	19	246	252	7
0	4	19	44	43	44
1	4	19	247	252	7
2	4	19	113	118	3
3	4	19	93	93	2
4	4	19	79	79	4
5	4	19	87	85	7
-5	5	19	31	32	6
-4	5	19	156	153	3
-3	5	19	117	118	9
-2	5	19	74	72	1
-1	5	19	190	173	15
0	5	19	201	187	15
1	5	19	194	173	18
2	5	19	70	71	2
3	5	19	131	118	10
4	5	19	162	154	4
5	5	19	45	32	8
-5	6	19	84	88	2
-4	6	19	62	63	2
-3	6	19	66	51	10
-2	6	19	114	121	1
-1	6	19	68	55	15
0	6	19	132	134	7
1	6	19	69	56	17
2	6	19	117	121	6
3	6	19	61	52	10
4	6	19	62	64	3
5	6	19	85	88	6
-5	7	19	45	45	3
-4	7	19	118	109	12
-3	7	19	0	17	1
-2	7	19	203	179	20
-1	7	19	184	181	7
0	7	19	64	52	3
1	7	19	191	181	8
2	7	19	215	180	24
3	7	19	21	17	10
4	7	19	128	109	12
5	7	19	44	45	5
-4	8	19	66	45	9
-3	8	19	142	130	16
-2	8	19	121	120	6
-1	8	19	83	54	18
0	8	19	112	102	6
1	8	19	71	54	20
2	8	19	121	120	7
3	8	19	137	129	10
4	8	19	55	45	9
-3	9	19	78	60	10
-2	9	19	175	148	23
-1	9	19	109	103	4
0	9	19	112	71	17
1	9	19	114	103	5
2	9	19	185	148	34
3	9	19	77	60	8
-3	10	19	171	178	3
-2	10	19	85	83	5
-1	10	19	122	126	1
0	10	19	38	39	4
1	10	19	121	125	2
2	10	19	85	83	3
3	10	19	174	178	3
-1	11	19	52	56	3
0	11	19	176	177	2
1	11	19	60	55	2
0	0	20	161	173	2
1	0	20	15	16	3
2	0	20	70	70	1
3	0	20	21	19	4
4	0	20	40	48	13
5	0	20	104	113	3
6	0	20	10	11	10
-6	1	20	54	67	4
-5	1	20	78	79	2
-4	1	20	42	46	3
-3	1	20	109	113	2
-2	1	20	155	156	2
-1	1	20	39	35	4
0	1	20	41	22	2
1	1	20	37	35	13
2	1	20	154	156	1
3	1	20	113	113	5
4	1	20	45	46	5
5	1	20	75	79	2
6	1	20	67	67	4
-5	2	20	54	62	4

h	k	l	10Fo	10Fc	10s
-4	2	20	176	183	3
-3	2	20	210	216	2
-2	2	20	113	118	2
-1	2	20	167	170	5
0	2	20	103	95	32
1	2	20	169	172	5
2	2	20	109	116	4
3	2	20	214	216	2
4	2	20	176	183	5
5	2	20	61	63	4
-5	3	20	81	82	3
-4	3	20	61	61	2
-3	3	20	134	134	2
-2	3	20	95	98	2
-1	3	20	190	202	3
0	3	20	143	146	11
1	3	20	190	201	4
2	3	20	97	99	2
3	3	20	134	134	3
4	3	20	66	62	11
5	3	20	81	82	2
-5	4	20	139	139	4
-4	4	20	53	44	7
-3	4	20	32	25	3
-2	4	20	117	115	19
-1	4	20	101	96	5
0	4	20	425	406	30
1	4	20	93	94	5
2	4	20	124	115	33
3	4	20	40	27	5
4	4	20	60	43	7
5	4	20	142	139	2
-5	5	20	18	18	17
-4	5	20	79	74	4
-3	5	20	85	81	7
-2	5	20	63	56	5
-1	5	20	66	64	1
0	5	20	15	6	14
1	5	20	62	63	2
2	5	20	60	55	5
3	5	20	83	81	6
4	5	20	73	73	3
5	5	20	36	19	5
-5	6	20	65	58	4
-4	6	20	76	65	9
-3	6	20	92	91	3
-2	6	20	248	241	10
-1	6	20	154	138	14
0	6	20	145	138	10
1	6	20	155	140	16
2	6	20	243	240	12
3	6	20	101	92	2
4	6	20	78	66	6
5	6	20	79	59	3
-4	7	20	30	25	4
-3	7	20	75	58	17
-2	7	20	77	75	2
-1	7	20	181	168	11
0	7	20	91	6	27
1	7	20	182	168	13
2	7	20	74	75	4
3	7	20	73	59	18
4	7	20	18	23	17
-4	8	20	172	160	15
-3	8	20	127	119	12
-2	8	20	87	83	7
-1	8	20	186	174	7
0	8	20	0	7	1
1	8	20	190	173	7
2	8	20	90	83	9
3	8	20	136	118	12
4	8	20	191	159	14
-3	9	20	139	130	6
-2	9	20	116	123	2
-1	9	20	99	92	2
0	9	20	189	186	15
1	9	20	99	92	5
2	9	20	119	123	2
3	9	20	136	129	8
-2	10	20	69	60	10
-1	10	20	27	26	6
0	10	20	37	10	6
1	10	20	23	25	6
2	10	20	74	59	9
1	0	21	23	20	3
2	0	21	44	48	1
3	0	21	30	18	6

h	k	l	10Fo	10Fc	10s
4	0	21	135	132	2
5	0	21	35	45	4
-5	1	21	90	99	5
-4	1	21	120	122	2
-3	1	21	186	192	2
-2	1	21	121	128	1
-1	1	21	237	236	7
0	1	21	75	82	1
1	1	21	232	234	9
2	1	21	119	130	2
3	1	21	189	190	11
4	1	21	119	122	1
5	1	21	87	98	9
-5	2	21	60	64	3
-4	2	21	102	107	2
-3	2	21	50	49	12
-2	2	21	36	16	28
-1	2	21	93	93	1
0	2	21	171	150	10
1	2	21	91	94	1
2	2	21	38	17	3
3	2	21	51	50	6
4	2	21	106	107	7
5	2	21	68	64	4
-5	3	21	127	129	7
-4	3	21	125	137	5
-3	3	21	217	220	6
-2	3	21	30	10	9
-1	3	21	304	299	13
0	3	21	86	87	1
1	3	21	312	300	28
2	3	21	32	9	24
3	3	21	229	219	15
4	3	21	133	137	2
5	3	21	123	129	3
-5	4	21	20	13	20
-4	4	21	112	117	6
-3	4	21	75	73	2
-2	4	21	176	175	4
-1	4	21	126	127	7
0	4	21	228	226	13
1	4	21	129	127	7
2	4	21	180	176	7
3	4	21	73	73	2
4	4	21	114	116	13
5	4	21	21	13	10
-5	5	21	95	97	2
-4	5	21	43	37	3
-3	5	21	165	165	2
-2	5	21	152	150	7
-1	5	21	153	145	4
0	5	21	75	35	15
1	5	21	155	147	5
2	5	21	153	150	10
3	5	21	172	163	3
4	5	21	34	37	5
5	5	21	107	97	6
-4	6	21	80	69	7
-3	6	21	18	16	9
-2	6	21	137	133	3
-1	6	21	72	71	2
0	6	21	256	244	17
1	6	21	70	71	3
2	6	21	133	132	2
3	6	21	26	15	4
4	6	21	74	70	7
-4	7	21	63	56	22
-3	7	21	204	197	9
-2	7	21	117	117	6
-1	7	21	111	111	1
0	7	21	98	105	1
1	7	21	112	112	1
2	7	21	124	116	6
3	7	21	218	196	8
4	7	21	105	56	16
-3	8	21	105	101	6
-2	8	21	108	96	8
-1	8	21	102	101	5
0	8	21	94	60	31
1	8	21	103	100	17
2	8	21	100	95	11
3	8	21	100	101	4
-2	9	21	69	63	5
-1	9	21	83	63	10
0	9	21	94	97	1
1	9	21	80	63	8
2	9	21	72	63	4

h	k	l	10Fo	10Fc	10s
-1	10	21	49	31	8
0	10	21	64	64	2
1	10	21	45	32	14
0	0	22	196	195	7
1	0	22	92	85	2
2	0	22	106	106	1
3	0	22	15	2	8
4	0	22	198	206	3
5	0	22	120	128	3
-5	1	22	74	77	3
-4	1	22	94	98	2
-3	1	22	168	171	2
-2	1	22	74	77	1
-1	1	22	92	92	1
0	1	22	145	156	2
1	1	22	93	92	1
2	1	22	75	77	1
3	1	22	169	171	2
4	1	22	96	98	2
5	1	22	73	77	7
-5	2	22	94	97	13
-4	2	22	169	173	2
-3	2	22	129	131	2
-2	2	22	293	294	4
-1	2	22	96	95	1
0	2	22	213	214	3
1	2	22	92	96	2
2	2	22	296	295	7
3	2	22	137	131	4
4	2	22	168	171	2
5	2	22	98	97	3
-5	3	22	72	77	2
-4	3	22	108	117	6
-3	3	22	235	236	13
-2	3	22	76	69	6
-1	3	22	128	127	1
0	3	22	115	111	8
1	3	22	129	127	2
2	3	22	72	69	3
3	3	22	240	236	11
4	3	22	112	117	8
5	3	22	69	76	2
-5	4	22	73	76	3
-4	4	22	104	109	3
-3	4	22	57	54	4
-2	4	22	117	115	2
-1	4	22	119	104	8
0	4	22	157	162	2
1	4	22	116	104	7
2	4	22	119	114	1
3	4	22	64	55	19
4	4	22	119	108	10
5	4	22	77	77	4
-4	5	22	31	20	9
-3	5	22	67	63	6
-2	5	22	47	31	9
-1	5	22	236	228	15
0	5	22	146	132	7
1	5	22	241	227	14
2	5	22	51	31	15
3	5	22	66	63	7
4	5	22	36	20	7
-4	6	22	84	83	3
-3	6	22	56	49	2
-2	6	22	141	140	4
-1	6	22	94	70	21
0	6	22	111	104	1
1	6	22	96	71	18
2	6	22	154	140	6
3	6	22	61	49	3
4	6	22	89	83	2
-3	7	22	107	99	5
-2	7	22	69	19	9
-1	7	22	78	51	11

h	k	l	10Fo	10Fc	10s
0	7	22	29	26	5
1	7	22	77	53	14
2	7	22	49	19	18
3	7	22	99	97	5
-3	8	22	108	97	15
-2	8	22	131	129	7
-1	8	22	57	62	3
0	8	22	141	136	3
1	8	22	52	63	2
2	8	22	140	128	6
3	8	22	110	97	18
-2	9	22	55	57	5
-1	9	22	82	81	2
0	9	22	86	83	5
1	9	22	84	83	3
2	9	22	50	56	3
1	0	23	29	13	7
2	0	23	23	21	23
3	0	23	132	127	7
4	0	23	22	10	11
5	0	23	150	160	4
-5	1	23	68	75	3
-4	1	23	75	77	6
-3	1	23	112	117	2
-2	1	23	107	113	1
-1	1	23	98	99	3
0	1	23	73	70	23
1	1	23	97	101	1
2	1	23	110	114	2
3	1	23	112	118	2
4	1	23	80	79	5
5	1	23	69	76	6
-5	2	23	29	28	16
-4	2	23	40	43	3
-3	2	23	99	98	3
-2	2	23	97	104	4
-1	2	23	124	125	3
0	2	23	81	84	1
1	2	23	123	124	2
2	2	23	100	105	2
3	2	23	102	99	2
4	2	23	45	42	4
5	2	23	15	27	15
-4	3	23	109	114	3
-3	3	23	106	111	2
-2	3	23	199	196	4
-1	3	23	80	77	1
0	3	23	285	264	20
1	3	23	78	76	1
2	3	23	201	197	7
3	3	23	110	110	2
4	3	23	114	115	3
-4	4	23	118	124	3
-3	4	23	87	93	3
-2	4	23	84	72	6
-1	4	23	90	75	30
0	4	23	71	67	1
1	4	23	99	74	27
2	4	23	79	72	3
3	4	23	94	94	4
4	4	23	123	125	8
-4	5	23	91	90	6
-3	5	23	63	64	2
-2	5	23	137	138	9
-1	5	23	116	118	2
0	5	23	150	140	18
1	5	23	118	119	2
2	5	23	147	137	22
3	5	23	68	62	5
4	5	23	103	92	7
-3	6	23	59	10	16
-2	6	23	126	111	9
-1	6	23	202	189	14
0	6	23	67	20	20

h	k	l	10Fo	10Fc	10s
1	6	23	205	189	13
2	6	23	120	111	11
3	6	23	55	10	20
-3	7	23	78	74	11
-2	7	23	120	123	7
-1	7	23	110	110	7
0	7	23	42	20	9
1	7	23	109	109	5
2	7	23	131	122	7
3	7	23	87	74	10
-2	8	23	43	39	3
-1	8	23	75	53	10
0	8	23	30	23	4
1	8	23	66	52	13
2	8	23	42	38	3
-1	9	23	32	27	3
0	9	23	47	28	12
1	9	23	30	27	7
0	0	24	138	141	3
1	0	24	158	160	2
2	0	24	53	48	2
3	0	24	176	177	6
4	0	24	80	85	7
-4	1	24	18	25	17
-3	1	24	54	50	10
-2	1	24	91	97	13
-1	1	24	52	51	5
0	1	24	130	125	5
1	1	24	49	50	5
2	1	24	102	97	3
3	1	24	46	50	3
4	1	24	21	25	21
-4	2	24	55	54	3
-3	2	24	184	192	2
-2	2	24	30	29	5
-1	2	24	231	232	6
0	2	24	15	9	6
1	2	24	233	233	9
2	2	24	36	30	4
3	2	24	191	191	13
4	2	24	54	54	3
-4	3	24	14	21	13
-3	3	24	88	88	5
-2	3	24	74	74	7
-1	3	24	54	43	8
0	3	24	63	68	1
1	3	24	51	43	7
2	3	24	83	75	7
3	3	24	91	89	3
4	3	24	32	20	9
-4	4	24	94	101	2
-3	4	24	136	131	9
-2	4	24	132	128	4
-1	4	24	270	261	7
0	4	24	56	58	2
1	4	24	271	262	10
2	4	24	138	127	9
3	4	24	140	130	6
4	4	24	98	101	3
-3	5	24	66	48	12
-2	5	24	197	191	6
-1	5	24	91	88	5
0	5	24	104	102	7
1	5	24	90	88	3
2	5	24	195	191	5
3	5	24	61	48	8
-3	6	24	199	194	7
-2	6	24	66	69	2
-1	6	24	187	176	7
0	6	24	59	56	1
1	6	24	193	178	7
2	6	24	75	69	3
3	6	24	208	193	12
-2	7	24	178	177	3

h	k	l	10Fo	10Fc	10s
-1	7	24	73	67	8
0	7	24	193	174	14
1	7	24	72	67	6
2	7	24	176	177	5
-1	8	24	65	57	6
0	8	24	26	27	5
1	8	24	63	58	7
1	0	25	163	164	5
2	0	25	133	128	5
3	0	25	53	42	4
4	0	25	82	79	4
-4	1	25	113	118	3
-3	1	25	56	60	3
-2	1	25	255	262	4
-1	1	25	76	82	3
0	1	25	125	121	2
1	1	25	79	81	5
2	1	25	261	263	6
3	1	25	59	61	3
4	1	25	114	117	3
-4	2	25	30	9	11
-3	2	25	104	105	3
-2	2	25	113	39	24
-1	2	25	70	23	5
0	2	25	50	26	11
1	2	25	61	24	8
2	2	25	55	39	13
3	2	25	106	105	4
4	2	25	29	8	28
-3	3	25	36	35	5
-2	3	25	140	141	2
-1	3	25	72	73	3
0	3	25	103	95	2
1	3	25	69	74	3
2	3	25	139	140	18
3	3	25	47	36	17
-3	4	25	89	91	13
-2	4	25	92	82	9
-1	4	25	30	31	4
0	4	25	108	86	15
1	4	25	30	32	3
2	4	25	94	83	10
3	4	25	95	92	6
-3	5	25	80	76	2
-2	5	25	125	124	2
-1	5	25	77	72	2
0	5	25	119	115	1
1	5	25	80	72	3
2	5	25	138	123	3
3	5	25	79	76	2
-2	6	25	69	72	2
-1	6	25	169	167	2
0	6	25	43	47	2
1	6	25	168	168	2
2	6	25	73	71	2
-1	7	25	36	15	14
0	7	25	141	142	2
1	7	25	44	16	17
0	0	26	261	273	5
1	0	26	234	237	4
2	0	26	146	152	2
3	0	26	123	125	2
-3	1	26	106	93	5
-2	1	26	62	62	3
-1	1	26	116	92	9
0	1	26	40	11	4
1	1	26	103	92	12
2	1	26	60	62	3
3	1	26	99	93	8
-3	2	26	66	70	4
-2	2	26	189	199	3
-1	2	26	153	150	2
0	2	26	113	113	2
1	2	26	151	151	5

h	k	l	10Fo	10Fc	10s
2	2	26	190	200	3
3	2	26	66	72	2
-3	3	26	80	74	15
-2	3	26	39	31	4
-1	3	26	50	14	9
0	3	26	76	74	2
1	3	26	50	15	10
2	3	26	38	31	3
3	3	26	88	75	11
-3	4	26	100	102	3
-2	4	26	81	79	3
-1	4	26	43	50	2
0	4	26	22	23	5
1	4	26	49	50	2
2	4	26	82	78	3
3	4	26	105	101	6
-2	5	26	102	97	4
-1	5	26	137	119	13
0	5	26	37	29	6
1	5	26	136	119	16
2	5	26	104	97	7
-1	6	26	54	51	2
0	6	26	83	54	28
1	6	26	51	50	2
1	0	27	69	45	18
2	0	27	135	107	26
3	0	27	47	32	11
-3	1	27	154	161	6
-2	1	27	107	114	3
-1	1	27	228	226	3
0	1	27	94	99	2
1	1	27	227	228	4
2	1	27	112	114	2
3	1	27	153	161	3
-2	2	27	58	25	11
-1	2	27	36	32	13
0	2	27	59	5	19
1	2	27	38	32	6
2	2	27	44	25	21
-2	3	27	84	85	2
-1	3	27	64	67	3
0	3	27	3	14	3
1	3	27	63	66	7
2	3	27	89	85	5
-2	4	27	32	14	14
-1	4	27	54	53	2
0	4	27	179	163	11
1	4	27	50	53	4
2	4	27	20	14	19
-1	5	27	145	151	4
0	5	27	6	13	6
1	5	27	152	151	2
0	0	28	134	135	5
1	0	28	36	36	5
2	0	28	212	217	4
-2	1	28	36	38	5
-1	1	28	67	31	11
0	1	28	104	95	4
1	1	28	47	31	10
2	1	28	48	38	4
-2	2	28	83	92	3
-1	2	28	46	57	4
0	2	28	86	88	5
1	2	28	51	56	7
2	2	28	93	93	2
-1	3	28	33	17	5
0	3	28	62	70	4
1	3	28	32	17	31
0	4	28	60	71	6
0	1	29	123	124	3

Figure 1. View of 1 showing the atom labeling scheme. Thermal ellipsoids are scaled to the 50% probability level. Most hydrogen atoms have been removed for clarity.

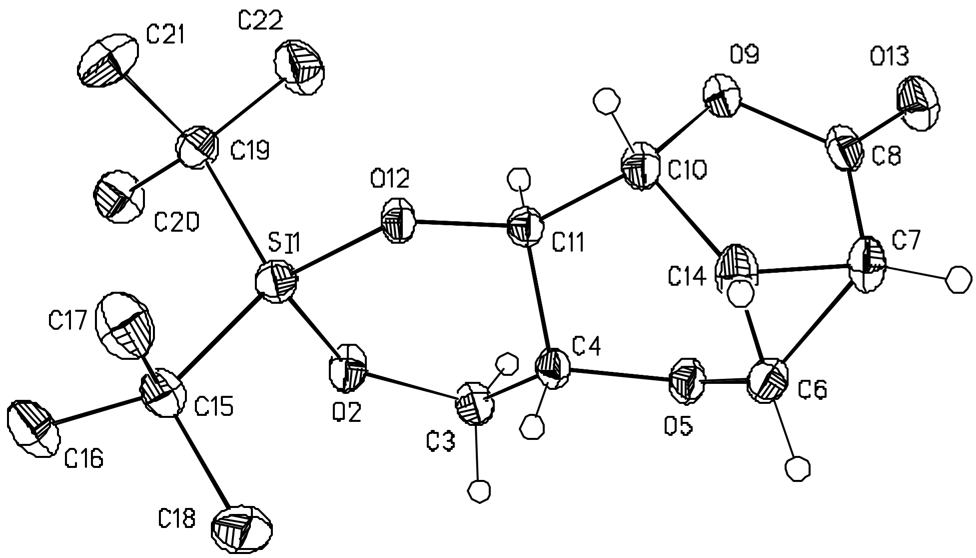
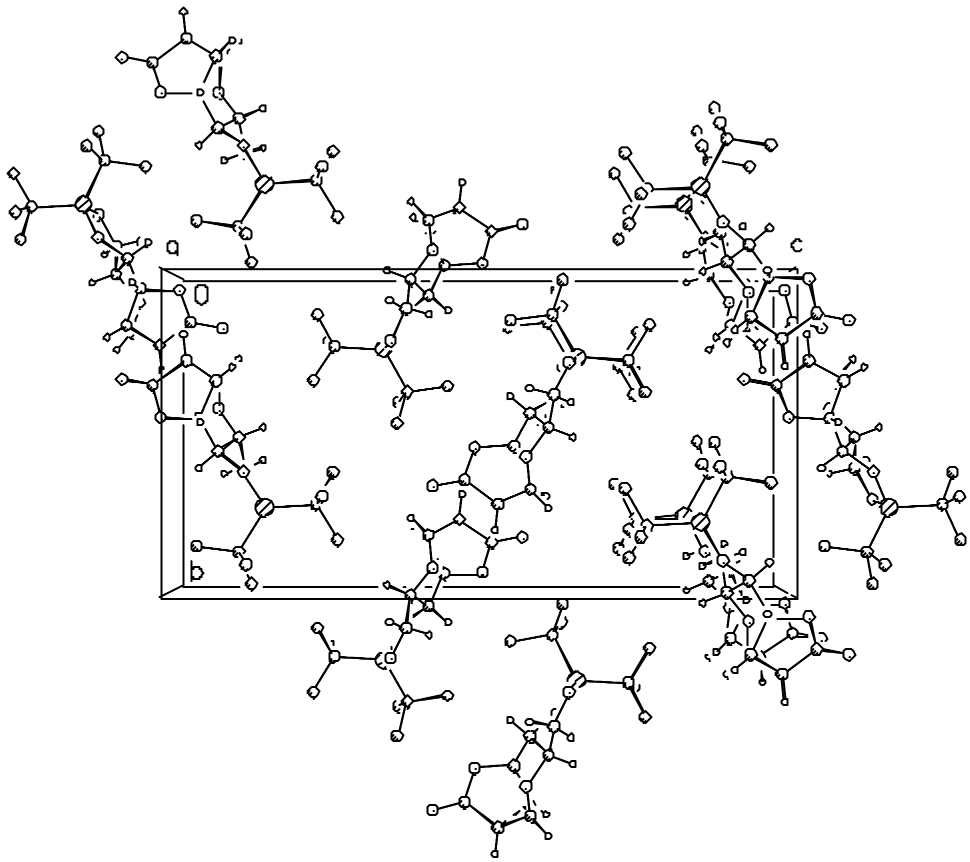


Figure 2. Unit cell packing diagram for 1. The view is approximately down the **a** axis.



References for X-ray Portion

1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

2) SIR92. (1993). A program for crystal structure solution. Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. J. Appl. Cryst. 26, 343-350.

3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

4) Flack, H. D. (1983). Acta Cryst. A39, 876-881.

5) $R_w(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$.
$S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

6) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

7) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.