Supporting Information for *J. Am. Chem. Soc.*, **1990**, 112(13), 5384-5385, DOI: 10.1021/ja00169a075

# JOHNSON
# 5384-5385

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# Facile Tungsten Alkylidene Synthesis: Alkylidene Transfer from a Phosphorane to a Tungsten Imido Complex


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Supplementary Material:

**General Considerations.** All manipulations of air- and/or water-sensitive compounds were performed using standard high-vacuum or Schlenk techniques. Argon was purified by passage through columns of BASF R3-11 catalyst (Chemalog) and 4 Å molecular sieves (Linde). Solid organometallic compounds were transferred and stored in a nitrogen-filled Vacuum Atmospheres drybox. NMR spectra were recorded with either a JEOL FX-90Q (89.60 MHz $^1H$; 22.53 MHz $^{13}C$) or a JEOL GX-400 (399.65 MHz $^1H$; 100.40 MHz $^{13}C$).

**Materials.** Toluene, benzene, diethyl ether and tetrahydrofuran were distilled or vacuum-transferred from sodium-benzophenone ketyl. *p*-Xylene was dried over $CaH_2$ and distilled under argon. Pentane was stirred over concentrated $H_2SO_4$, dried over $MgSO_4$ and $CaH_2$, and then transferred onto sodium-benzophenone ketyl solubilized with tetraglyme. Benzene-$d_6$, toluene-$d_8$, and THF-$d_8$ were dried over sodium-benzophenone ketyl. Chloroform-*d* and methylene chloride-$d_2$ were dried over $P_2O_5$, vacuum-transferred, and then degassed by repeated freeze-pump-thaw cycles. Isocyanates were purified by fractional distillation under argon. $W(NPh)Cl_4$ was synthesized according to the procedure of Nielson.[1] $(CF_3)_2CH_3COH$ was purchased from PCR, dissolved in $Et_2O$, and deprotonated with one equivalent of BuLi. White crystals of $(CF_3)_2CH_3COLi$ were obtained by recrystallization at low temperature from a $Et_2O$/pentane solution. Aryl ylides were synthesized by deprotonation of the phosphonium salt with an excess of NaH in refluxing THF until evolution of $H_2$ ceased. After filtering the solution, the ylide was recrystallized from THF at low temperature.

In the following experimental section, Ar = 2,6-$C_6H_3$-$Me_2$ and Ar' = *o*-$C_6H_4$-OMe as in the text.

**W(NAr)$Cl_4$($Et_2O$).** 2,6-Dimethylphenyl isocyanate (11.2 mL, 80.4 mmol) was added via syringe to a suspension of W(O)$Cl_4$ (25.02 g, 73.24 mmol) in 115 mL of toluene. After refluxing for 48 h, the toluene was removed in vacuo, and the resulting brick-red powder was dissolved in 400 mL of $Et_2O$. The solution was filtered and then slowly cooled to -50 °C to give 37.2 g of brown crystals in three crops (97.8%): $^1$H ($C_6D_6$) δ 6.75 (d, 2, J = 7.6, $H_m$), 5.89 (t, 1, J = 7.6, $H_p$), 4.34 (q, 4, J = 6.9, $Et_2O$), 3.29 (s, 6, Me), 1.07 (t, 6, J = 6.9, $Et_2O$); $^{13}$C ($C_6D_6$) δ 148.3 ($C_{ipso}$), 145.4 ($C_o$), 133.9 and 126.1 ($C_m$ and $C_p$), 65.9 ($Et_2O$), 17.6 (Me) and 13.0 ($Et_2O$). After removing the $Et_2O$ in vacuo (several days under vacuum), an elemental analysis was obtained for orange-brown W(NAr)$Cl_4$: Anal. Calcd for ($C_8H_9Cl_4NW$): C, 21.60; H, 2.04; N, 3.15. Found: C, 21.96; H, 2.15; N, 3.08.

**W(NAr)$Cl_2$[OCMe($CF_3$)$_2$]$_2$(THF).** Two equivalents of ($CF_3$)$_2$MeCOLi (17.14 g, 91.17 mmol) were dissolved in 90 mL of THF. The resulting solution was added slowly via cannula to a -78 °C solution of W(NAr)$Cl_4$($Et_2O$) (23.24 g, 44.79 mmol) in 60 mL of THF. After warming to room temperature, the solution was stirred for 19 h before removing the solvent in vacuo. The red powder was then dissolved in 150 mL of $Et_2O$, and the solution was filtered. Recrystallization at -50 °C afforded red crystals in 93.4% yield (33.8 g, 2 crops): $^1$H ($C_6D_6$) δ 6.80 (d, 2, J = 7.6, $H_m$), 6.35 (t, 1, J = 7.6, $H_p$), 4.25 (m, 4, THF), 2.93 (s, 6, Ar: Me), 1.54 (s, 6, OCMe($CF_3$)$_2$), 1.29 (m, 4, THF); $^{13}$C ($C_6D_6$) δ 148.7 ($C_{ipso}$), 144.9 ($C_o$), 131.5 and 127.8 ($C_m$ and $C_p$), 123.8 (q, $J_{CF}$ = 288, $CF_3$), 85.8 (septet, $J_{CF}$ = 30, *O*CMe($CF_3$)$_2$), 72.2 (THF), 25.1 (THF), 19.8 and 16.4 (Ar: Me and OCMe($CF_3$)$_2$). Anal. Calcd for ($C_{20}H_{23}Cl_2F_{12}NO_3W$): C, 29.73; H, 2.87; N, 1.73. Found: C, 29.72; H, 2.86; N, 1.76.

**W(CHAr')(NAr)[OCMe($CF_3$)$_2$]$_2$(THF) 1.** $^1$H NMR ($C_6D_6$) δ 10.81 (s, 1, *C*HAr'), 6.96 (m, 1, $H_{aryl}$), 6.95 (d, 2, J = 8.06, Ar: $H_m$), 6.75 (m, 1, $H_{aryl}$), 6.53 (d, 1, J = 7.32, Ar': H), 6.48 (m, 1, $H_{aryl}$), 6.26 (d, 1, J = 7.32, Ar': H), 3.93 (m, 4, THF), 3.59 (s, 3, OMe), 2.66 (s, 6, Ar: Me), 1.37 (m, 4, THF), 1.19 (s, 6, OCMe($CF_3$)$_2$). Difference NOE experiments: irrad. of δ 10.81 enhances δ 6.26, 2.66; irrad. of δ 3.93 enhances δ 3.59, 2.66, 1.37; irrad. of δ 3.59 enhances δ 6.53, 3.93; irrad. of δ 2.66 enhances δ 10.81, 6.95, 3.93; irrad. of δ 1.19 enhances δ 10.81. $^{13}$C NMR ($C_6D_6$) δ 240.2 ($J_{CH}$ = 151, $J_{CW}$ = 160, *C*HAr'), 158.0 (Ar': *C*OMe), 153.5 (Ar: $C_{ipso}$), 134.9 and 132.5 (Ar': $C_{ipso}$ and Ar: $C_o$), 128.0, 127.8, 125.6, 124.3, and 122.3 (all $C_{aryl}$), 107.8 (Ar': $C_m$), 124.8 (q, $J_{CF}$ = 291, $CF_3$), 124.6 (q, $J_{CF}$ = 290, $CF_3$), 81.0 (septet, $J_{CF}$ = 28, *O*CMe($CF_3$)$_2$), 70.3 (THF), 56.1 (OMe), 25.6 (THF), 18.9 and 18.1 (Ar: Me and OCMe($CF_3$)$_2$). Anal. Calcd for ($C_{28}H_{31}F_{12}NO_4W$): C, 39.22; H, 3.64; N, 1.63. Found: C, 39.33; H, 3.71; N, 1.65.

$^1$H NMR (-70 °C, tol-$d_8$) δ 10.78 (s, 1, C*H*Ar'), 6.99 (m, 3, $H_{aryl}$), 6.80 (m, 1, $H_{aryl}$), 6.48 (m, 2, $H_{aryl}$), 6.11 (d, 1, J = 7.32, $H_{aryl}$), 4.11 (br s, 4, THF), 3.40 (s, 3,

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OMe), 2.92 (s, 3, Ar: Me), 2.37 (s, 3, Ar: Me), 1.25 (s, 6, OCMe($CF_3$)$_2$), 1.22 (br s, 4, THF).

**W(CHAr')(NAr)[OCMe($CF_3$)$_2$]$_2$ 2.** A 150 mL toluene solution of the THF adduct **1** (7.92 g, 9.17 mmol) was heated to 50 °C as the solvent was removed in vacuo. The resulting red powder was dissolved in 30 mL of toluene, and the solution was filtered, layered with 120 mL of pentane, and cooled to -10 °C to give red crystals of **2** in 73% yield (5.2 g, 2 crops): $^1$H NMR ($C_6D_6$) δ 10.94 (s, 1, C*H*Ar'), 6.93 (m, 1, Ar': H), 6.90 (d, 2, J = 7.69, Ar: $H_m$), 6.73 (t, 1, J = 7.69, Ar: $H_p$), 6.49 (m, 2, Ar': H), 6.37 (d, 1, J = 6.96, Ar': H), 3.75 (s, 3, OMe), 2.69 (s, 6, Ar: Me), 1.11 (s, 6, OCMe($CF_3$)$_2$); $^{13}$C NMR ($C_6D_6$) δ 228.1 ($J_{CH}$ = 155, $J_{CW}$ = 172, *C*HAr'), 156.3 (Ar': *C*OMe), 153.0 (Ar: $C_{ipso}$), 135.6 and 132.4 (Ar': $C_{ipso}$ and Ar: $C_o$), 127.9, 126.8, 126.6, 123.6, and 122.6 (all $C_{aryl}$), 107.6 (Ar': $C_m$), 124.0 (q, $J_{CF}$ = 288, $CF_3$), 82.3 (septet, J = 29, O*C*Me($CF_3$)$_2$), 56.7 (OMe), 18.73 and 18.66 (Ar: Me and OCMe($CF_3$)$_2$). Anal. Calcd for ($C_{24}H_{23}F_{12}NO_3W$): C, 36.71; H, 2.95; N, 1.78. Found: C, 36.90; H, 3.03; N, 1.70.

**W(CHAr')(NAr)[OCMe($CF_3$)$_2$]$_2$($PMe_3$).** Complex **1** (2.01 g, 2.34 mmol) was dissolved in 50 mL of benzene. Three equivalents of $PMe_3$ (0.73 mL, 7.1 mmol) were added, and the red solution turned golden brown within a few minutes. After stirring for 12 h, the solvent was removed in vacuo, and the product was recrystallized from pentane at -50 °C to give 1.44 g of golden crystals (71.4%): (This complex was isolated as a 12:1 ratio of isomers. Spectroscopic data for the major isomer is reported here.) $^1$H NMR ($CD_2Cl_2$) δ 12.48 (d, 1, $J_{HP}$ = 7.08, C*H*Ar'), 7.32 (d, 1, J = 7.57, $H_{aryl}$), 7.22 (d, 2, J = 7.57, Ar: $H_m$), 7.18 (m, 1, $H_{aryl}$), 7.04 (m, 3, $H_{aryl}$), 4.05 (s, 3, OMe), 2.79 (s, 6, Ar: Me), 2.07 (s, 3, OCMe($CF_3$)$_2$), 1.45 (s, 3, OCMe($CF_3$)$_2$), 1.37 (d, 9, $J_{HP}$ = 9.52, $PMe_3$); $^{13}$C NMR ($CD_2Cl_2$) δ 259.5 ($J_{CH}$ = 147, $J_{CW}$ = 148, $J_{CP}$ = 15, *C*HAr'), 154.3 and 153.9 (Ar': *C*OMe and Ar: $C_{ipso}$), 136.4 and 132.4 (Ar': $C_{ipso}$ and Ar: $C_o$), 131.4, 130.3, 128.5, 126.8, and 121.1 (all $C_{aryl}$), 109.9 (Ar': $C_m$), 125.9 (q, $J_{CF}$ = 290, $CF_3$), 125.3 (q, $J_{CF}$ = 289, $CF_3$), 82.4 (septet, $J_{CF}$ = 28, O*C*Me($CF_3$)$_2$), 80.6 (septet, $J_{CF}$ = 28, O*C*Me($CF_3$)$_2$), 56.6 (OMe), 19.7, 19.4, and 18.2 (Ar: Me and OCMe($CF_3$)$_2$), 15.3 (d, $J_{CP}$ = 29, $PMe_3$); $^{31}$P NMR ($CD_2Cl_2$) δ 11.0 ($J_{WP}$ = 162). Anal. Calcd for ($C_{27}H_{32}F_{12}NO_3PW$): C, 37.65; H, 3.74; N, 1.63. Found: C, 37.89; H, 3.79; N, 1.56.

**W(CHPh)(NAr)[OCMe($CF_3$)$_2$]$_2$($PMe_3$).** A solution of $Ph_3P$=CHPh (2.25 g, 6.38 mmol) and W(NAr)$Cl_2$[OCMe($CF_3$)$_2$]$_2$(THF) (5.05 g, 6.25 mmol) in 50 mL of benzene was added to a 1% sodium amalgam (1.47 g Na, 64.1 mmol) and stirred for 3 h. After adding 1.98 mL of $PMe_3$ (3 equiv, 19.1 mmol) via syringe and stirring for an additional 16 h, the mixture was allowed to settle. The golden brown solution was separated from the residual sodium amalgam, which was then washed with 45 mL of benzene. The solvent was removed in vacuo, and the brown residue was dissolved in 90 mL of $Et_2O$. After filtering the solution, it was added via cannula to 0.66 g (6.6 mmol) of CuCl and stirred for 15 h. The $Et_2O$ was removed in vacuo and the solid was extracted with 230 mL of pentane to give a yellow-brown solution. After filtering and concentrating the solution, recrystallization at -50 °C afforded 2.51 g of yellow-brown crystals (48.3%): (This complex was isolated as an 18:1 ratio of isomers. Spectroscopic data for the major isomer is reported here.) $^1$H NMR ($C_6D_6$) δ 12.16 (d, 1, $J_{HP}$ = 9.59, C*H*Ph), 7.27 (t, 2, J = 7.57, $H_{aryl}$), 7.13 (m, 2, $H_{aryl}$), 6.91 (d, 2, J = 7.57, $H_{aryl}$), 6.78 (m, 1, $H_{aryl}$), 6.73 (t, 1, J = 7.57, $H_{aryl}$), 2.54 (s, 3, Ar: Me), 2.43 (s, 3, Ar: Me), 2.14 (s, 3, OCMe($CF_3$)$_2$), 1.40 (s, 3, OCMe($CF_3$)$_2$), 0.79 (d, 9, $J_{HP}$ = 9.28, $PMe_3$); $^{13}$C NMR ($C_6D_6$) δ 266.5 ($J_{CH}$ = 144, $J_{CW}$ = 154, $J_{CP}$ = 14, *C*HPh), 155.8 (Ar: $C_{ipso}$), 141.09 and 136.7 (Ph: $C_{ipso}$ and Ar: $C_o$), 134.4, 128.7, 128.1, 127.9, and 126.7 (all $C_{aryl}$), 125.7 (q, $J_{CF}$ = 289, $CF_3$), 125.1 (q, $J_{CF}$ = 289, $CF_3$), 82.8 (septet, $J_{CF}$ = 29, O*C*Me($CF_3$)$_2$), 80.4 (septet, $J_{CF}$ = 28, O*C*Me($CF_3$)$_2$), 19.2, 18.7, and 17.4 (Ar: Me and OCMe($CF_3$)$_2$), 14.2 (d, $J_{CP}$ = 29, $PMe_3$); $^{31}$P NMR ($CD_2Cl_2$) δ 12.7 ($J_{WP}$ = 159, $PMe_3$). Anal. Calcd for ($C_{26}H_{30}F_{12}NO_2PW$): C, 37.56; H, 3.64; N, 1.68. Found: C, 37.74; H, 3.69; N, 1.84.

**W(CHPh)(NAr)[OCMe($CF_3$)$_2$]$_2$($PPh_3$).** $^1$H NMR ($C_6D_6$) δ 12.30 (d, 1, $J_{HP}$ = 6.87, C*H*Ph), 7.5 - 6.5 (m, $H_{aryl}$), 2.63 (s, 3, Ar: Me), 2.16 (s, 3, OCMe($CF_3$)$_2$), 1.80 (s, 3, Ar: Me), 1.44 (s, 3, OCMe($CF_3$)$_2$); $^{31}$P NMR ($C_6D_6$) δ 37.4 ($J_{WP}$ = 142, $PPh_3$).

**W(NPh)$Cl_2$[OCMe($CF_3$)$_2$]$_2$(THF).** A solution of ($CF_3$)$_2$$CH_3$COLi (18.72 g, 99.55 mmol) in 120 mL of THF was added via cannula over a 15 minute period to a suspension of W(NPh)$Cl_4$ (20.74 g, 47.74 mmol) in 120 mL of THF cooled to 0 °C. After stirring the solution for 16 h at room temperature, the solvent was removed in vacuo, and the product was dissolved in 90 mL of $Et_2O$. Following filtration, the solution was cooled to -50 °C to afford 34.89 g of bright orange crystals (93.7%, 3 crops): $^1$H ($CD_2Cl_2$) δ 7.63 (dd, 2, $H_m$), 7.30 (d, 2, J = 7.57, $H_o$), 7.14 (t, 1, J = 7.57, $H_p$), 4.40 (m, 4, THF), 2.06 (m, 4, THF), 1.75 (s, 6, OCMe($CF_3$)$_2$); $^{13}$C ($CD_2Cl_2$) δ 150.7 ($C_{ipso}$), 132.3, 128.6, and 128.3 ($C_{aryl}$), 123.7 (q, $J_{CF}$ = 290, $CF_3$), 86.2 (septet, $J_{CF}$ = 30, O*C*Me($CF_3$)$_2$), 73.0 (THF), 25.9 (THF), 17.7 (OCMe($CF_3$)$_2$). Anal. Calcd for ($C_{18}H_{19}Cl_2F_{12}NO_3W$): C, 27.71; H, 2.46; N, 1.80. Found: C, 27.84; H, 2.47; N, 1.83.

**W(CHAr')(NPh)[OCMe($CF_3$)$_2$]$_2$(THF) 3.** A solution of $Ph_3P$=CHAr' (7.82 g, 20.5 mmol) and W(NPh)$Cl_2$[OCMe($CF_3$)$_2$]$_2$(THF) (15.49 g, 19.85 mmol) in 160 mL of benzene and 5 mL of THF was added to a 1% sodium amalgam (3.66 g Na, 8.02 equiv) and then stirred for 4.5 h. After the mixture settled, the solution was added via cannula to 2.07 g (20.9 mmol) of CuCl, and the residual sodium amalgam was washed with 60 mL of benzene. The combined benzene solutions were stirred with CuCl for 13 h before removing the solvent in vacuo and extracting the brown solid with 135 mL of pentane. THF (4 mL) was added to the red solution which was then filtered and slowly cooled to -50 °C. Burnt-orange crystals (10.5 g, 63.8%) were obtained: $^1$H NMR (THF-$d_8$) δ 10.46 (s, 1, C*H*Ar'), 7.38 (dd, 2, Ph: $H_m$), 7.23 (d, 2, J = 7.69, Ph: $H_o$), 7.11 (m, 3, $H_{aryl}$), 6.68 (t, 1, J = 7.69, $H_{aryl}$), 6.39 (d, 1, J = 7.69, Ar': H), 4.09 (s, 3, OMe), 3.61 (m, 4, THF), 1.78 (m, 4, THF), 1.14 (s, 6, OCMe($CF_3$)$_2$); $^{13}$C NMR (THF-$d_8$) δ 246.4 ($J_{CH}$ = 149, $J_{CW}$ = 161, *C*HAr'), 159.6 and 156.2 (Ar': *C*OMe and Ar: $C_{ipso}$), 133.5 (Ar': $C_{ipso}$), 129.0, 128.8, 126.5, 126.3 125.0, and 122.6 (all $C_{aryl}$), 108.4 (1, Ar': $C_m$), 125.6 (q, $J_{CF}$ = 288, $CF_3$), 80.9 (septet, $J_{CF}$

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= 28, O*C*Me($CF_3$)$_2$), 68.2 (THF), 57.1 (OMe), 26.4 (THF), 18.0 (OC*Me*($CF_3$)$_2$). Anal. Calcd for ($C_{26}H_{27}F_{12}NO_4W$): C, 37.66; H, 3.28; N, 1.69. Found: C, 37.93; H, 3.45; N, 2.16.

**W(N-2,6-$C_6H_3$-*i*-$Pr_2$)$Cl_4$.** 2,6-Diisopropylphenyl isocyanate (11.59 g, 57.00 mmol) was added via cannula to a suspension of W(O)$Cl_4$ (19.47 g, 57.00 mmol) in 100 mL of *p*-xylene. After refluxing for 12 h, the hot solution was added via cannula to 400 mL of pentane, inducing the precipitation of a red-brown powder. After cooling the solution to -50 °C, brick-red crystals (25.9 g, 90.5%) were isolated: $^1$H (THF-$d_8$) δ 7.63 (d, 2, J = 8.06, $H_m$), 6.74 (t, 1, J = 7.69, $H_p$), 4.62 (septet, 2, J = 6.59, C*H*$Me_2$), 1.37 (d, 12, J = 6.59, CH*$Me_2$*); $^{13}$C (THF-$d_8$) δ 156.3 ($C_{ipso}$), 146.1 ($C_o$), 135.0 and 122.7 ($C_m$ and $C_p$), 28.2 (*C*H($CH_3$)$_2$), 26.4 (CH($CH_3$)$_2$).

**W(N-2,6-$C_6H_3$-*i*-$Pr_2$)$Cl_4$(THF).** Brick-red W(N-2,6-$C_6H_3$-*i*-$Pr_2$)$Cl_4$ (3.02 g, 6.03 mmol) was dissolved in 10 mL of THF and 90 mL of $Et_2O$. After filtering the solution, recrystallization at -50 °C gave feathery green crystals (2.58 g, 74.7%): $^1$H ($CD_2Cl_2$) δ 7.59 (d, 2, J = 7.81, $H_m$), 6.71 (t, 1, J = 7.81, $H_p$), 4.74 (m, 4, THF), 4.58 (septet, 2, J = 6.59, C*H*$Me_2$), 2.17 (m, 4, THF), 1.40 (d, 12, J = 6.59, CH*$Me_2$*); $^{13}$C ($CD_2Cl_2$) δ 156.3 ($C_{ipso}$), 145.7 ($C_o$), 134.7 and 122.1 ($C_m$ and $C_p$), 74.1 (THF), 27.8 (*C*H($CH_3$)$_2$), 26.3 (CH(*C*$H_3$)$_2$), 26.1 (THF). Anal. Calcd for ($C_{16}H_{25}Cl_4NOW$): C, 33.54; H, 4.40; N, 2.44. Found: C, 33.72; H, 4.35; N, 2.57.

**W(N-2,6-$C_6H_3$-*i*-$Pr_2$)$Cl_2$[OCMe($CF_3$)$_2$]$_2$(THF).** Two equivalents of ($CF_3$)$_2$$CH_3$COLi (7.20 g, 38.3 mmol) were dissolved in 40 mL of THF. The resulting solution was added over a period of 10 minutes to a suspension of W(N-2,6-$C_6H_3$-*i*-$Pr_2$)$Cl_4$ (9.59 g, 19.1 mmol) in 40 mL of THF at 0 °C. After allowing the solution to warm to room temperature, it was stirred for 15 h before removing the solvent in vacuo. The red solid was dissolved in pentane, and the solution was filtered and slowly cooled to -50 °C. Red crystals (13.68 g) were isolated in 82.7% yield (2 crops): $^1$H ($C_6D_6$) δ 7.07 (d, 2, J = 8.06, $H_m$), 6.57 (t, 1, J = 8.06, $H_p$), 4.61 (septet, 2, J = 6.59, C*H*$Me_2$), 4.25 (m, 4, THF), 1.58 (s, 6, OCMe($CF_3$)$_2$), 1.29 (m, 4, THF), 1.28 (d, 12, J = 6.59, CH*$Me_2$*); $^{13}$C ($C_6D_6$) δ 154.1 ($C_o$), 146.6 ($C_{ipso}$), 132.1 and 123.5 ($C_m$ and $C_p$), 123.8 (q, $J_{CF}$ = 288, $CF_3$), 86.5 (septet, $J_{CF}$ = 30, O*C*Me($CF_3$)$_2$), 72.1 (THF), 27.6 (*C*H($CH_3$)$_2$), 25.1 (THF), 24.9 (CH(*C*$H_3$)$_2$), and 17.1 (OC*Me*($CF_3$)$_2$). Anal. Calcd for ($C_{24}H_{31}Cl_2F_{12}NO_3W$): C, 33.35; H, 3.62; N, 1.62. Found: C, 33.60; H, 3.65; N, 1.75.

**W(CHAr')(N-2,6-$C_6H_3$-*i*-$Pr_2$)[OCMe($CF_3$)$_2$]$_2$(THF) 4.** A solution of $Ph_3P$=CHAr' (7.12 g, 18.6 mmol) and W(N-2,6-$C_6H_3$-*i*-$Pr_2$)$Cl_2$[OCMe($CF_3$)$_2$]$_2$(THF) (15.16 g, 17.54 mmol) in 150 mL of benzene and 4 mL of THF was added via cannula to a 1% sodium amalgam (3.37 g Na, 8.35 equiv) and stirred for 8 h at room temperature. After the mixture settled, the orange-brown supernatant was added via cannula to CuCl (1.79 g, 18.1 mmol). Next, the residual sodium amalgam was washed with a total of 120 mL of benzene, and the combined benzene solutions were stirred with the CuCl for 12 h before removing the solvent in vacuo. Diethyl ether (330 mL) was used to extract the product from the brown solid. After filtering, the $Et_2O$ solution was cooled to -50 °C to yield 7.3 g of golden

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crystals (46%): $^1H$ NMR (THF-$d_8$) δ 10.60 (s, 1, C*H*Ar'), 7.17 (d, 2, J = 7.69, Ar: $H_m$), 7.13 (m, 2, $H_{aryl}$), 6.98 (t, 1, J = 7.69, Ar: $H_p$), 6.72 (m, 1, Ar': H), 6.41 (d, 1, J = 7.33, Ar': H), 4.03 (s, 3, OMe), 3.63 (m, 4, THF), 3.62 (m, 2, C*H*($CH_3$)$_2$), 1.78 (m, 4, THF), 1.34 (br s, 2, CH*($CH_3$)$_2$*), 1.18 (s, 6, OCMe($CF_3$)$_2$); $^{13}C$ NMR (THF-$d_8$) δ 248.1 ($J_{CH}$ = 148, $J_{CW}$ = 167, *C*HAr'), 159.8 (Ar': *C*OMe), 151.3 (Ar: $C_{ipso}$), 145.8 and 133.1 (Ar': $C_{ipso}$ and Ar: $C_o$), 129.3, 126.2, 125.2, 123.3, and 122.4 (all $C_{aryl}$), 108.7 (Ar': $C_m$), 125.6 (q, $J_{CF}$ = 290, $CF_3$), 125.4 (q, $J_{CF}$ = 291, $CF_3$), 80.8 (septet, $J_{CF}$ = 28.3, O*C*Me($CF_3$)$_2$), 68.1 (THF), 56.9 (OMe), 28.6 (*C*H($CH_3$)$_2$), 26.4 (THF), 24.4 (CH(*C*$H_3$)$_2$), 18.0 (OCMe($CF_3$)$_2$). Anal. Calcd for ($C_{32}H_{39}F_{12}NO_4W$): C, 42.08; H, 4.30; N, 1.53. Found: C, 42.22; H, 4.33; N, 1.82.

**X-ray Data Collection, Structure Determination and Refinement for W(CHAr')(NAr)[OCMe($CF_3$)$_2$]$_2$(THF) 1.** A yellow/gold crystal of approximate dimensions 0.32 x 0.34 x 0.40 mm was immersed in Paratone-N (lube-oil additive), mounted on a glass fiber and transferred to the Nicolet P3 diffractometer which is equipped with a modified LT-2 low temperature system. Determination of Laue symmetry, crystal class, unit cell parameters and the crystal's orientation matrix were carried out by previously described techniques similar to those of Churchill.[2] Low temperature (173 K) intensity data were collected via a $\theta$-2$\theta$ scan technique with MoK$\alpha$ radiation under the conditions given in Table 1.

All 6054 data were corrected for absorption and for Lorentz and polarization effects and placed on an approximately absolute scale. Any reflection with I(net) < 0 was assigned the value $|F_o| = 0$. The systematic extinctions observed were 0*k*0 for $k = 2n + 1$ and *h*0*l* for $l = 2n + 1$; the diffraction symmetry was 2/m. The centrosymmetric monoclinic space group $P2_1/c$ [$C^5_{2h}$; No. 14] is thus, uniquely defined.

All crystallographic calculations were carried out using either the UCI modified version of the UCLA Crystallographic Computing Package[3] or the SHELXTL PLUS program set.[4] The analytical scattering factors for neutral atoms were used throughout the analysis;[5a] both the real ($\Delta f'$) and imaginary ($i\Delta f''$) components of anomalous dispersion[5b] were included. The quantity minimized during least-squares analysis was $\Sigma w(|F_o| - |F_c|)^2$ where $w^{-1} = \sigma^2(|F_o| + 0.0005(|F_o|)^2$.

The structure was solved via an automatic Patterson routine (SHELXTL PLUS); and refined by full-matrix least-squares techniques. Hydrogen atoms were included using a riding model with d(C-H) = 0.96 Å and U(iso) = 0.08 Å$^2$. Refinement of positional and anisotropic thermal parameters led to convergence with $R_F$ = 3.8%, $R_{wF}$ = 4.4% and GOF = 1.39 for 415 variables refined against all 5269 unique data with $|F_o| > 0$; ($R_F$ = 3.1%, $R_{wF}$ = 4.1% for those 4576 data with $|F_o| > 6.0\sigma(|F_o|)$). A final difference-Fourier map yielded $\rho$(max) = 2.29 eÅ$^{-3}$ at a distance of 0.95 Å from tungsten.

Q. 5385-M7

Reactions of **1** and **2**:

**ROMP.** The THF adduct **1** polymerizes norbornene at a rate of 18 equiv/h at -40 °C (PDI = 1.5 (polydispersity index: $M_w/M_n$)) and cyclooctatetraene (COT) at room temperature to give shiny films of polyacetylene. THF-free **2** polymerizes norbornene at a rate of 17 equiv/h at -60 °C (PDI = 1.6). These rates are given for [W] = 0.012 M and [norbornene] = 0.63 M.[6] The molecular weights were obtained by GPC analysis vs. polystyrene standards, and the relatively broad polydispersities are typical of the nonliving nature of fluoro-alkoxide arylimido alkylidene catalysts.[6,7] Analysis by $^{13}C$ NMR spectroscopy indicated *cis*-polynorbornene was formed by the ROMP of norbornene initiated by both **1** and **2**.[8]

**Wittig-Type Reactions.** The Wittig-type reactions were carried out in $C_6D_6$ at room temperature unless specified otherwise for the following: EtC(O)H, PhC(O)H, PhC(O)Me, PhC(O)Ph, MeC(O)OEt (65 °C), and $MeC(O)NMe_2$ (65 °C). A mixture of trans and cis isomers was observed in all cases for the alkene products.

References and Footnotes:

(1) Nielson, A. J. In *Inorg. Syn.*; Schreeve, J. M., Ed.; John Wiley & Sons: New York, 1986; Vol. 24, pp 194-200.

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(3) UCLA Crystallographic Computing Package, University of California Los Angeles, 1981, C. Strouse; personal communication.

(4) Nicolet Instrument Corporation Madison, WI 1988.

(5) *International Tables for X-Ray Crystallography*, Kynoch Press: Birmingham, England, 1974; (a) pp 99-101; (b) pp 149-150.

(6) Schrock, R. R.; Feldman, J.; Cannizzo, L. F.; Grubbs, R. H. *Macromolecules* **1987**, *20*, 1169-1172.

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(8) Ivin, K. J.; Laverty, D. T.; Rooney, J. J. *Makromol. Chem.* **1977**, *178*, 1545-1559.

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Table 1. Experimental Data for the X-ray Diffraction Study

Formula: $C_{28}H_{31}NO_4F_{12}W$

Fw: 857.4

Temperature (K): 173

Crystal System: Monoclinic

Space Group: $P2_1/c$

$\underline{a}$ = 12.606(3) Å

$\underline{b}$ = 12.981(3) Å

$\underline{c}$ = 18.998(5) Å

$\beta$ = 91.85(2)°

$\underline{V}$ = 3108.0(13) $Å^3$

Z = 4

$D_{calcd,}$ $Mg/m^3$ = 1.830

Diffractometer: Nicolet P3

Radiation: MoK$\alpha$ ($\bar{\lambda}$ = 0.710730 Å)

Monochromator: Highly oriented graphite

Data Collected: $+h,+k,\pm l$

Scan Type: $\theta-2\theta$

Scan Range: 1.20° plus K$\alpha$-separation

Scan Speed: 3.0 deg $min^{-1}$ (in $\omega$)

$2\theta$ Range: 4.0 to 50.0°

$\mu$(MoK$\alpha$), $mm^{-1}$ = 3.90

Reflections Collected: 6054

Reflections with $|F_o| > 0$: 5269

No. of Variables: 415

$R_F$ = 3.8%, $R_{wF}$ = 4.4%

Goodness of Fit: 1.39

Q-5385-M9

Tables of crystal data, coordinates, bond distances and angles, and thermal parameters for the crystal structure of W(CHAr')(NAr)[OCMe$(CF_3)_2$]$_2$(THF) **1** (Ar = 2,6-$C_6H_3$-$Me_2$ and Ar' = *o*-$C_6H_4$-OMe).

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^4$)

| | x | y | z | U(eq) |
|---|---|---|---|---|
| W(1) | 2489.6(.1) | 1575.3(.1) | 1961.6(.1) | 182.9(.7) |
| C(1) | 4022(4) | 1477(3) | 1899(3) | 224(15) |
| C(2) | 4572(4) | 1899(4) | 1315(3) | 245(15) |
| C(3) | 5674(4) | 2045(4) | 1274(3) | 318(17) |
| C(4) | 6117(4) | 2482(4) | 688(3) | 344(18) |
| C(5) | 5469(5) | 2781(5) | 119(3) | 371(19) |
| C(6) | 4376(4) | 2641(4) | 132(3) | 307(17) |
| C(7) | 3955(4) | 2229(4) | 728(3) | 240(15) |
| C(8) | 2208(5) | 1998(5) | 180(3) | 340(18) |
| C(9) | 2165(4) | 829(4) | 3503(3) | 226(15) |
| C(10) | 2987(4) | 411(4) | 3936(3) | 268(16) |
| C(11) | 2758(4) | 105(4) | 4616(3) | 276(16) |
| C(12) | 1750(5) | 210(4) | 4869(3) | 329(17) |
| C(13) | 948(5) | 654(4) | 4445(3) | 307(17) |
| C(14) | 1136(4) | 961(4) | 3759(3) | 260(16) |
| C(15) | 4096(4) | 315(5) | 3678(3) | 347(18) |
| C(16) | 273(4) | 1447(4) | 3303(3) | 352(19) |
| C(17) | 2953(4) | 3866(4) | 2458(3) | 241(15) |
| C(18) | 2354(5) | 4082(5) | 3126(3) | 431(22) |
| C(19) | 2897(5) | 4820(4) | 1972(3) | 314(17) |
| C(20) | 4119(5) | 3643(5) | 2663(4) | 404(20) |
| C(21) | 2337(4) | -626(4) | 1242(3) | 296(17) |
| C(22) | 1532(5) | -1039(5) | 687(3) | 405(21) |
| C(23) | 2309(6) | -1325(4) | 1897(4) | 467(24) |
| C(24) | 3433(5) | -648(5) | 942(4) | 555(26) |
| C(25) | -23(4) | 1262(4) | 1390(3) | 300(17) |
| C(26) | -1041(4) | 1884(4) | 1445(3) | 352(18) |
| C(27) | -723(5) | 2919(4) | 1153(3) | 361(19) |
| C(28) | 388(4) | 3067(4) | 1469(3) | 321(17) |
| F(1) | 2377(4) | 3265(3) | 3551(2) | 641(17) |
| F(2) | 2774(3) | 4867(3) | 3512(2) | 531(13) |
| F(3) | 1335(3) | 4313(3) | 3012(2) | 617(15) |
| F(4) | 1938(3) | 5103(2) | 1790(2) | 475(12) |
| F(5) | 3409(3) | 5637(3) | 2255(2) | 505(13) |
| F(6) | 3390(3) | 4590(3) | 1371(2) | 508(13) |

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| | | | | |
|---|---|---|---|---|
| F(7) | 552(3) | -1120(3) | 910(2) | 555(14) |
| F(8) | 1473(4) | -406(3) | 133(2) | 632(16) |
| F(9) | 1799(3) | -1969(3) | 432(2) | 554(14) |
| F(10) | 3086(4) | -1080(3) | 2356(2) | 742(18) |
| F(11) | 2416(4) | -2309(3) | 1748(3) | 858(21) |
| F(12) | 1404(5) | -1231(4) | 2238(3) | 780(19) |
| N(1) | 2360(3) | 1134(3) | 2818(2) | 237(13) |
| O(1) | 2872(3) | 2084(3) | 812(2) | 267(11) |
| O(2) | 2402(3) | 3096(3) | 2102(2) | 231(10) |
| O(3) | 1972(3) | 345(3) | 1422(2) | 265(11) |
| O(4) | 823(3) | 2018(3) | 1546(2) | 235(10) |

* Equivalent isotropic U defined as one third of the trace of the orthogonalized $U_{ij}$ tensor

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Table 3. Interatomic Distances (Å) with Esd's

| | | | |
|---|---|---|---|
| W(1)-C(1) | 1.943(5) | W(1)-N(1) | 1.737(4) |
| W(1)-O(1) | 2.346(3) | W(1)-O(2) | 1.995(4) |
| W(1)-O(3) | 1.995(3) | W(1)-O(4) | 2.294(3) |
| | | | |
| C(1)-C(2) | 1.436(7) | C(2)-C(3) | 1.407(7) |
| C(2)-C(7) | 1.405(7) | C(3)-C(4) | 1.383(8) |
| C(4)-C(5) | 1.389(8) | C(5)-C(6) | 1.391(8) |
| C(6)-C(7) | 1.374(7) | C(7)-O(1) | 1.393(6) |
| C(8)-O(1) | 1.446(6) | | |
| | | | |
| C(9)-C(10) | 1.411(7) | C(9)-C(14) | 1.410(7) |
| C(9)-N(1) | 1.391(6) | C(10)-C(11) | 1.391(7) |
| C(10)-C(15) | 1.502(8) | C(11)-C(12) | 1.380(8) |
| C(12)-C(13) | 1.396(8) | C(13)-C(14) | 1.390(7) |
| C(14)-C(16) | 1.507(8) | | |
| | | | |
| C(17)-C(18) | 1.523(8) | C(17)-C(19) | 1.545(7) |
| C(17)-C(20) | 1.535(8) | C(17)-O(2) | 1.382(6) |
| C(18)-F(1) | 1.333(8) | C(18)-F(2) | 1.353(8) |
| C(18)-F(3) | 1.330(8) | C(19)-F(4) | 1.299(7) |
| C(19)-F(5) | 1.345(6) | C(19)-F(6) | 1.352(7) |
| C(21)-C(22) | 1.536(8) | C(21)-C(23) | 1.542(9) |
| C(21)-C(24) | 1.512(9) | C(21)-O(3) | 1.389(6) |
| C(22)-F(7) | 1.323(8) | C(22)-F(8) | 1.336(7) |
| C(22)-F(9) | 1.347(7) | C(23)-F(10) | 1.328(9) |
| C(23)-F(11) | 1.316(7) | C(23)-F(12) | 1.336(10) |
| | | | |
| C(25)-C(26) | 1.523(8) | C(25)-O(4) | 1.473(6) |
| C(26)-C(27) | 1.513(8) | C(27)-C(28) | 1.518(8) |
| C(28)-O(4) | 1.474(6) | | |

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Table 4. Interatomic Angles (Deg.) with Esd's

| | | | |
|---|---|---|---|
| C(1)-W(1)-N(1) | 99.2(2) | C(1)-W(1)-O(1) | 74.2(2) |
| N(1)-W(1)-O(1) | 173.0(2) | C(1)-W(1)-O(2) | 97.6(2) |
| N(1)-W(1)-O(2) | 101.2(2) | O(1)-W(1)-O(2) | 82.0(1) |
| C(1)-W(1)-O(3) | 103.0(2) | N(1)-W(1)-O(3) | 100.2(2) |
| O(1)-W(1)-O(3) | 79.7(1) | O(2)-W(1)-O(3) | 147.3(1) |
| C(1)-W(1)-O(4) | 153.7(2) | N(1)-W(1)-O(4) | 107.0(2) |
| O(1)-W(1)-O(4) | 79.8(1) | O(2)-W(1)-O(4) | 75.2(1) |
| O(3)-W(1)-O(4) | 75.1(1) | W(1)-N(1)-C(9) | 174.6(4) |
| W(1)-O(1)-C(7) | 112.1(3) | W(1)-O(1)-C(8) | 128.4(3) |
| W(1)-O(2)-C(17) | 138.8(3) | W(1)-O(3)-C(21) | 138.4(3) |
| W(1)-O(4)-C(25) | 123.5(3) | W(1)-O(4)-C(28) | 126.9(3) |
| W(1)-C(1)-C(2) | 121.9(4) | | |

| | | | |
|---|---|---|---|
| C(1)-C(2)-C(3) | 126.6(5) | C(1)-C(2)-C(7) | 117.4(5) |
| C(3)-C(2)-C(7) | 116.0(5) | C(2)-C(3)-C(4) | 121.6(5) |
| C(3)-C(4)-C(5) | 120.0(5) | C(4)-C(5)-C(6) | 120.5(5) |
| C(5)-C(6)-C(7) | 118.3(5) | C(2)-C(7)-C(6) | 123.6(5) |
| C(2)-C(7)-O(1) | 112.8(4) | C(6)-C(7)-O(1) | 123.6(4) |
| C(7)-O(1)-C(8) | 117.2(4) | | |

| | | | |
|---|---|---|---|
| C(10)-C(9)-C(14) | 120.8(4) | C(10)-C(9)-N(1) | 120.5(5) |
| C(14)-C(9)-N(1) | 118.7(4) | C(9)-C(10)-C(11) | 118.7(5) |
| C(9)-C(10)-C(15) | 121.0(5) | C(11)-C(10)-C(15) | 120.3(5) |
| C(10)-C(11)-C(12) | 121.1(5) | C(11)-C(12)-C(13) | 119.8(5) |
| C(12)-C(13)-C(14) | 121.1(5) | C(9)-C(14)-C(13) | 118.4(5) |
| C(9)-C(14)-C(16) | 120.5(5) | C(13)-C(14)-C(16) | 121.1(5) |

| | | | |
|---|---|---|---|
| C(18)-C(17)-C(19) | 109.7(5) | C(18)-C(17)-C(20) | 108.7(5) |
| C(19)-C(17)-C(20) | 109.1(4) | C(18)-C(17)-O(2) | 106.6(4) |
| C(19)-C(17)-O(2) | 105.9(4) | C(20)-C(17)-O(2) | 116.7(4) |
| C(17)-C(18)-F(1) | 110.9(5) | C(17)-C(18)-F(2) | 113.2(5) |
| F(1)-C(18)-F(2) | 105.7(5) | C(17)-C(18)-F(3) | 114.2(5) |
| F(1)-C(18)-F(3) | 106.2(5) | F(2)-C(18)-F(3) | 106.1(5) |

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| | | | |
|---|---|---|---|
| C(17)-C(19)-F(4) | 114.2(5) | C(17)-C(19)-F(5) | 112.3(4) |
| F(4)-C(19)-F(5) | 108.3(4) | C(17)-C(19)-F(6) | 108.4(4) |
| F(4)-C(19)-F(6) | 106.7(5) | F(5)-C(19)-F(6) | 106.5(5) |
| C(22)-C(21)-C(23) | 108.5(5) | C(22)-C(21)-C(24) | 109.0(5) |
| C(23)-C(21)-C(24) | 109.7(5) | C(22)-C(21)-O(3) | 105.6(4) |
| C(23)-C(21)-O(3) | 108.6(5) | C(24)-C(21)-O(3) | 115.1(5) |
| C(21)-C(22)-F(7) | 114.3(5) | C(21)-C(22)-F(8) | 110.2(5) |
| F(7)-C(22)-F(8) | 105.8(5) | C(21)-C(22)-F(9) | 113.1(5) |
| F(7)-C(22)-F(9) | 106.9(5) | F(8)-C(22)-F(9) | 106.0(5) |
| C(21)-C(23)-F(10) | 110.7(5) | C(21)-C(23)-F(11) | 113.1(6) |
| F(10)-C(23)-F(11) | 107.2(6) | C(21)-C(23)-F(12) | 112.3(5) |
| F(10)-C(23)-F(12) | 106.5(6) | F(11)-C(23)-F(12) | 106.8(6) |
| | | | |
| C(26)-C(25)-O(4) | 103.9(4) | C(25)-C(26)-C(27) | 102.2(4) |
| C(26)-C(27)-C(28) | 102.7(5) | C(27)-C(28)-O(4) | 104.9(4) |
| C(25)-O(4)-C(28) | 109.3(4) | | |

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Table 5. Anisotropic displacement coefficients ($Å^2x10^4$)

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| W(1) | 190(1) | 183(1) | 174(1) | -6(1) | -33(1) | 7(1) |
| C(1) | 259(27) | 235(26) | 179(24) | -70(20) | 13(20) | -9(20) |
| C(2) | 248(27) | 212(24) | 275(27) | 24(21) | -9(21) | 53(21) |
| C(3) | 240(28) | 349(30) | 367(31) | 41(26) | 31(24) | 45(23) |
| C(4) | 247(29) | 396(32) | 391(33) | 0(26) | 73(25) | 38(24) |
| C(5) | 353(33) | 349(32) | 419(34) | 17(27) | 101(27) | 65(26) |
| C(6) | 357(32) | 297(28) | 267(28) | -23(23) | 11(24) | 55(24) |
| C(7) | 246(27) | 246(25) | 227(26) | -15(21) | -4(21) | 6(21) |
| C(8) | 391(33) | 426(33) | 196(26) | 12(24) | -109(24) | -8(26) |
| C(9) | 309(28) | 194(24) | 172(24) | 9(20) | -20(21) | -28(21) |
| C(10) | 289(28) | 289(27) | 223(26) | -33(22) | -47(21) | -11(23) |
| C(11) | 399(31) | 236(26) | 191(25) | 41(21) | -20(22) | -16(22) |
| C(12) | 426(33) | 335(30) | 225(27) | 21(24) | -6(24) | -8(26) |
| C(13) | 348(31) | 272(28) | 304(29) | -6(22) | 62(24) | -64(23) |
| C(14) | 218(27) | 285(27) | 274(27) | -40(22) | -39(21) | -39(22) |
| C(15) | 287(29) | 441(33) | 308(29) | 29(27) | -57(23) | 43(26) |
| C(16) | 223(29) | 456(35) | 375(33) | 69(26) | 9(24) | 21(24) |
| C(17) | 262(28) | 243(26) | 215(26) | -31(21) | -33(21) | 1(21) |
| C(18) | 500(41) | 434(36) | 361(35) | -132(29) | 28(30) | -124(30) |
| C(19) | 379(31) | 193(26) | 363(32) | 18(24) | -71(25) | -93(24) |
| C(20) | 292(32) | 392(33) | 517(39) | -110(29) | -155(28) | 0(26) |
| C(21) | 324(30) | 192(25) | 366(31) | -85(23) | -79(24) | 8(22) |
| C(22) | 494(40) | 331(32) | 383(35) | -120(28) | -93(29) | 21(28) |
| C(23) | 741(51) | 81(25) | 562(44) | 35(25) | -254(39) | 10(27) |
| C(24) | 377(38) | 459(39) | 829(55) | -301(38) | 8(36) | 40(30) |
| C(25) | 186(27) | 319(28) | 388(32) | -49(24) | -117(23) | -42(22) |
| C(26) | 245(29) | 301(29) | 503(37) | 4(27) | -94(26) | 29(23) |
| C(27) | 316(31) | 286(29) | 474(36) | -1(27) | -114(26) | 11(24) |
| C(28) | 326(31) | 205(25) | 423(34) | 7(24) | -115(25) | 30(23) |
| F(1) | 1177(40) | 485(24) | 266(20) | -2(17) | 77(22) | -207(23) |
| F(2) | 725(27) | 434(21) | 434(21) | -226(18) | 8(19) | -107(19) |
| F(3) | 444(24) | 715(28) | 705(29) | -266(22) | 209(20) | -46(20) |
| F(4) | 478(22) | 299(18) | 635(24) | 77(17) | -179(18) | 12(16) |
| F(5) | 664(26) | 282(18) | 556(23) | -8(16) | -194(19) | -165(17) |
| F(6) | 641(25) | 506(22) | 380(20) | 54(17) | 79(18) | -158(19) |
| F(7) | 390(22) | 493(22) | 776(29) | -243(21) | -95(20) | -78(18) |

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| | | | | | | |
|---|---|---|---|---|---|---|
| F(8) | 1013(35) | 503(23) | 364(21) | -47(18) | -262(21) | -127(22) |
| F(9) | 659(26) | 381(20) | 614(25) | -314(19) | -79(20) | 30(19) |
| F(10) | 1133(40) | 435(23) | 624(28) | 43(21) | -508(27) | 108(24) |
| F(11) | 1464(50) | 154(18) | 920(35) | -50(20) | -517(33) | 125(23) |
| F(12) | 1044(40) | 714(30) | 589(29) | 235(24) | 144(27) | -194(28) |
| N(1) | 218(22) | 201(21) | 288(23) | -28(18) | -34(18) | 21(17) |
| O(1) | 251(19) | 347(20) | 199(18) | 12(16) | -48(15) | -1(16) |
| O(2) | 214(18) | 201(17) | 273(19) | -40(15) | -73(15) | -2(14) |
| O(3) | 271(19) | 219(18) | 301(19) | -41(16) | -48(15) | 38(15) |
| O(4) | 225(18) | 170(16) | 302(19) | 26(15) | -97(15) | 0(14) |

The anisotropic displacement exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$

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Table 6. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^4$)

| | x | y | z | U |
|---|---|---|---|---|
| H(1A) | 4425 | 1134 | 2267 | 800 |
| H(3A) | 6127 | 1834 | 1664 | 800 |
| H(4A) | 6870 | 2585 | 676 | 800 |
| H(5A) | 5778 | 3082 | -288 | 800 |
| H(6A) | 3926 | 2829 | -264 | 800 |
| H(8A) | 2582 | 2277 | -209 | 800 |
| H(8B) | 2049 | 1286 | 91 | 800 |
| H(8C) | 1560 | 2373 | 234 | 800 |
| H(11A) | 3313 | -182 | 4914 | 800 |
| H(12A) | 1600 | -22 | 5335 | 800 |
| H(13A) | 255 | 746 | 4630 | 800 |
| H(15A) | 4547 | 15 | 4040 | 800 |
| H(15B) | 4089 | -118 | 3268 | 800 |
| H(15C) | 4361 | 984 | 3558 | 800 |
| H(16A) | -373 | 1478 | 3556 | 800 |
| H(16B) | 481 | 2131 | 3174 | 800 |
| H(16C) | 163 | 1039 | 2886 | 800 |
| H(20A) | 4161 | 3060 | 2973 | 800 |
| H(20B) | 4496 | 3496 | 2243 | 800 |
| H(20C) | 4430 | 4233 | 2894 | 800 |
| H(24A) | 3438 | -215 | 533 | 800 |
| H(24B) | 3940 | -395 | 1288 | 800 |
| H(24C) | 3618 | -1339 | 813 | 800 |
| H(25A) | 39 | 975 | 927 | 800 |
| H(25B) | 6 | 714 | 1729 | 800 |
| H(26A) | -1252 | 1939 | 1924 | 800 |
| H(26B) | -1609 | 1580 | 1167 | 800 |
| H(27A) | -1192 | 3452 | 1303 | 800 |
| H(27B) | -720 | 2909 | 648 | 800 |
| H(28A) | 366 | 3399 | 1920 | 800 |
| H(28B) | 810 | 3476 | 1164 | 800 |

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# STRUCTURE DETERMINATION SUMMARY

## Crystal Data

| | |
|---|---|
| Empirical Formula | $C_{28}H_{31}NO_4F_{12}W$ |
| Color; Habit | Yellow/gold prisms |
| Crystal Size (mm) | 0.32 x 0.34 x 0.40 |
| Crystal System | Monoclinic |
| Space Group | $P2_1/c$ |
| Unit Cell Dimensions | $\underline{a}$ = 12.606(3) Å |
| | $\underline{b}$ = 12.981(3) Å |
| | $\underline{c}$ = 18.998(5) Å |
| | $\beta$ = 91.85(2)° |
| Volume | 3108.0(13) $Å^3$ |
| Z | 4 |
| Formula weight | 857.4 |
| Density(calc.) | 1.831 $Mg/m^3$ |
| Absorption Coefficient | 3.897 $mm^{-1}$ |
| F(000) | 1680 |

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Data Collection

| | |
|---|---|
| Diffractometer System | Nicolet R3m/V |
| Radiation | MoKα ($\lambda$ = 0.71069 Å) |
| Temperature (K) | 173 |
| Monochromator | Highly oriented graphite crystal |
| $2\theta$ Range | 4.0 to $50.0^{\circ}$ |
| Scan Type | $\theta-2\theta$ |
| Scan Speed | Constant; $3.00^{\circ}$/min. in $\omega$ |
| Scan Range ($\omega$) | $1.20^{\circ}$ plus Kα-separation |
| Background Measurement | Estimated from 96 step profile |
| Standard Reflections | 3 measured every 97 reflections |
| Index Ranges | $0 \leq h \leq 14$, $0 \leq k \leq 15$<br>$-22 \leq l \leq 22$ |
| Reflections Collected | 6054 |
| Observed Reflections | 5269 ($\lvert F_o \rvert > 0$) |
| Absorption Correction | Semi-empirical ($\psi$-scan method) |
| Min./Max. Transmission | 0.1250 / 0.1865 |

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## Solution and Refinement

| | |
|---|---|
| System Used | Nicolet SHELXTL PLUS (MicroVAX II) |
| Solution | Automatic Patterson |
| Refinement Method | Full-Matrix Least-Squares |
| Quantity Minimized | $\Sigma w(\lvert F_o\rvert-\lvert F_c\rvert)^2$ |
| Hydrogen Atoms | Riding model, fixed isotropic U |
| Weighting Scheme | $w^{-1} = \sigma^2(\lvert F_o\rvert) + 0.0005(\lvert F_o\rvert)^2$ |
| Final R Indices (obs. data) | $R_F = 3.8\%$, $R_{wF} = 4.4\%$ |
| R Indicies (all data) | $R_F = 3.8\%$, $R_{wF} = 4.4\%$ |
| Goodness-of-Fit | 1.39 |
| Number of Variables | 415 |
| Data-to-Parameter Ratio | 12.7:1 |
| Largest and Mean $\Delta/\sigma$ | < 0.001, < 0.001 |
| Largest Difference Peak | 2.29 eÅ$^{-3}$ |
| Largest Difference Hole | -1.47 eÅ$^{-3}$ |

Q. 5385-M20

# Tables of observed and calculated structure factors for the crystal structure of W(CHAr')(NAr)[OCMe($CF_3$)$_2$]$_2$(THF) **1** (Ar = 2,6-$C_6H_3$-$Me_2$ and Ar' = *o*-$C_6H_4$-OMe).

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 2 | 0 | 0 | 5287 | -5361 | 18 |
| 3 | 0 | 0 | 216 | -221 | 13 |
| 4 | 0 | 0 | 2669 | 2695 | 5 |
| 5 | 0 | 0 | 514 | 506 | 8 |
| 6 | 0 | 0 | 2900 | -2882 | 6 |
| 7 | 0 | 0 | 175 | 183 | 19 |
| 8 | 0 | 0 | 1571 | 1573 | 8 |
| 9 | 0 | 0 | 271 | 305 | 14 |
| 10 | 0 | 0 | 1486 | -1421 | 9 |
| 11 | 0 | 0 | 222 | -221 | 20 |
| 12 | 0 | 0 | 1221 | 1191 | 11 |
| 13 | 0 | 0 | 152 | 203 | 26 |
| 14 | 0 | 0 | 986 | -966 | 13 |
| 1 | 1 | 0 | 2944 | -2994 | 3 |
| 2 | 1 | 0 | 527 | 523 | 5 |
| 3 | 1 | 0 | 2561 | 2562 | 5 |
| 4 | 1 | 0 | 33 | 34 | 49 |
| 5 | 1 | 0 | 2965 | -2979 | 6 |
| 6 | 1 | 0 | 143 | -121 | 20 |
| 7 | 1 | 0 | 2109 | 2112 | 7 |
| 8 | 1 | 0 | 82 | 13 | 40 |
| 9 | 1 | 0 | 1391 | -1369 | 9 |
| 10 | 1 | 0 | 274 | -288 | 17 |
| 11 | 1 | 0 | 938 | 913 | 11 |
| 12 | 1 | 0 | 152 | 155 | 25 |
| 13 | 1 | 0 | 977 | -972 | 12 |
| 14 | 1 | 0 | 142 | -149 | 41 |
| 0 | 2 | 0 | 755 | -734 | 4 |
| 1 | 2 | 0 | 319 | 312 | 5 |
| 2 | 2 | 0 | 698 | -663 | 5 |
| 3 | 2 | 0 | 274 | 230 | 10 |
| 4 | 2 | 0 | 1450 | -1426 | 6 |
| 5 | 2 | 0 | 398 | -397 | 9 |
| 6 | 2 | 0 | 2078 | 2022 | 7 |
| 7 | 2 | 0 | 155 | 146 | 16 |
| 8 | 2 | 0 | 728 | -757 | 9 |
| 9 | 2 | 0 | 40 | -18 | 64 |
| 10 | 2 | 0 | 714 | 720 | 12 |
| 12 | 2 | 0 | 540 | -518 | 13 |
| 13 | 2 | 0 | 291 | -293 | 17 |
| 14 | 2 | 0 | 520 | 495 | 15 |
| 1 | 3 | 0 | 935 | -891 | 4 |
| 2 | 3 | 0 | 210 | -197 | 10 |
| 3 | 3 | 0 | 481 | 496 | 7 |
| 4 | 3 | 0 | 598 | 599 | 7 |
| 5 | 3 | 0 | 651 | -636 | 8 |
| 6 | 3 | 0 | 158 | 89 | 20 |
| 7 | 3 | 0 | 706 | 709 | 9 |
| 8 | 3 | 0 | 127 | 88 | 29 |
| 9 | 3 | 0 | 133 | -47 | 32 |
| 10 | 3 | 0 | 121 | -102 | 37 |
| 11 | 3 | 0 | 54 | -69 | 65 |
| 12 | 3 | 0 | 47 | -66 | 71 |
| 13 | 3 | 0 | 228 | -210 | 21 |
| 0 | 4 | 0 | 1292 | -1249 | 5 |
| 1 | 4 | 0 | 1068 | -1032 | 5 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 2 | 4 | 0 | 919 | 913 | 5 |
| 3 | 4 | 0 | 232 | -229 | 10 |
| 4 | 4 | 0 | 1616 | -1582 | 6 |
| 5 | 4 | 0 | 89 | -38 | 30 |
| 6 | 4 | 0 | 1258 | 1256 | 7 |
| 8 | 4 | 0 | 1574 | -1546 | 8 |
| 9 | 4 | 0 | 381 | -375 | 14 |
| 10 | 4 | 0 | 1132 | 1122 | 11 |
| 11 | 4 | 0 | 443 | 479 | 13 |
| 12 | 4 | 0 | 914 | -892 | 11 |
| 13 | 4 | 0 | 159 | -186 | 37 |
| 14 | 4 | 0 | 672 | 644 | 15 |
| 1 | 5 | 0 | 2144 | 2101 | 5 |
| 2 | 5 | 0 | 517 | -484 | 6 |
| 3 | 5 | 0 | 2240 | -2215 | 6 |
| 4 | 5 | 0 | 259 | -275 | 11 |
| 5 | 5 | 0 | 2228 | 2212 | 6 |
| 6 | 5 | 0 | 512 | 527 | 9 |
| 7 | 5 | 0 | 1834 | -1814 | 8 |
| 8 | 5 | 0 | 211 | -181 | 19 |
| 9 | 5 | 0 | 1753 | 1750 | 9 |
| 10 | 5 | 0 | 195 | 182 | 23 |
| 11 | 5 | 0 | 1327 | -1334 | 10 |
| 12 | 5 | 0 | 173 | -182 | 32 |
| 13 | 5 | 0 | 1133 | 1128 | 12 |
| 14 | 5 | 0 | 145 | 128 | 42 |
| 0 | 6 | 0 | 2071 | 2018 | 6 |
| 1 | 6 | 0 | 141 | 126 | 13 |
| 2 | 6 | 0 | 2177 | -2194 | 6 |
| 3 | 6 | 0 | 277 | -251 | 9 |
| 4 | 6 | 0 | 2323 | 2345 | 6 |
| 5 | 6 | 0 | 288 | 289 | 12 |
| 6 | 6 | 0 | 1742 | -1749 | 7 |
| 7 | 6 | 0 | 93 | 76 | 39 |
| 8 | 6 | 0 | 1251 | 1242 | 9 |
| 9 | 6 | 0 | 242 | -231 | 18 |
| 10 | 6 | 0 | 1067 | -1057 | 10 |
| 11 | 6 | 0 | 115 | 132 | 42 |
| 12 | 6 | 0 | 1043 | 1032 | 11 |
| 13 | 6 | 0 | 123 | -61 | 43 |
| 1 | 7 | 0 | 2038 | -2017 | 6 |
| 2 | 7 | 0 | 172 | 187 | 12 |
| 3 | 7 | 0 | 1451 | 1424 | 7 |
| 4 | 7 | 0 | 408 | -412 | 10 |
| 5 | 7 | 0 | 1410 | -1413 | 7 |
| 6 | 7 | 0 | 87 | -89 | 38 |
| 7 | 7 | 0 | 761 | 755 | 10 |
| 8 | 7 | 0 | 124 | -121 | 35 |
| 9 | 7 | 0 | 812 | -801 | 10 |
| 10 | 7 | 0 | 21 | 90 | 84 |
| 11 | 7 | 0 | 672 | 637 | 13 |
| 12 | 7 | 0 | 116 | 163 | 47 |
| 13 | 7 | 0 | 554 | -538 | 15 |
| 0 | 8 | 0 | 325 | -278 | 11 |
| 1 | 8 | 0 | 156 | -140 | 12 |
| 2 | 8 | 0 | 73 | 75 | 38 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 3 | 8 | 0 | 131 | 148 | 18 |
| 4 | 8 | 0 | 208 | 177 | 20 |
| 5 | 8 | 0 | 239 | 254 | 13 |
| 6 | 8 | 0 | 134 | 108 | 31 |
| 7 | 8 | 0 | 427 | 425 | 11 |
| 8 | 8 | 0 | 139 | -81 | 33 |
| 9 | 8 | 0 | 369 | -357 | 14 |
| 10 | 8 | 0 | 288 | 278 | 19 |
| 11 | 8 | 0 | 58 | -24 | 65 |
| 12 | 8 | 0 | 82 | -108 | 58 |
| 1 | 9 | 0 | 821 | -804 | 8 |
| 2 | 9 | 0 | 531 | 525 | 9 |
| 3 | 9 | 0 | 707 | 640 | 9 |
| 5 | 9 | 0 | 516 | -477 | 12 |
| 6 | 9 | 0 | 167 | 70 | 27 |
| 7 | 9 | 0 | 391 | 353 | 13 |
| 8 | 9 | 0 | 281 | -258 | 19 |
| 9 | 9 | 0 | 235 | -237 | 18 |
| 10 | 9 | 0 | 109 | -16 | 44 |
| 11 | 9 | 0 | 544 | 535 | 14 |
| 0 | 10 | 0 | 880 | -836 | 9 |
| 1 | 10 | 0 | 348 | 359 | 12 |
| 2 | 10 | 0 | 1188 | 1165 | 8 |
| 3 | 10 | 0 | 189 | -159 | 19 |
| 4 | 10 | 0 | 950 | -928 | 9 |
| 5 | 10 | 0 | 332 | -348 | 13 |
| 6 | 10 | 0 | 981 | 933 | 9 |
| 7 | 10 | 0 | 117 | 84 | 37 |
| 8 | 10 | 0 | 1216 | -1211 | 10 |
| 9 | 10 | 0 | 134 | -135 | 38 |
| 10 | 10 | 0 | 881 | 862 | 12 |
| 11 | 10 | 0 | 195 | 194 | 20 |
| 1 | 11 | 0 | 1141 | 1092 | 9 |
| 2 | 11 | 0 | 446 | 409 | 12 |
| 3 | 11 | 0 | 986 | -930 | 9 |
| 4 | 11 | 0 | 252 | -281 | 15 |
| 5 | 11 | 0 | 1201 | 1145 | 9 |
| 6 | 11 | 0 | 91 | 47 | 45 |
| 7 | 11 | 0 | 1072 | -1070 | 10 |
| 9 | 11 | 0 | 1009 | 981 | 11 |
| 10 | 11 | 0 | 20 | 130 | 81 |
| 0 | 12 | 0 | 576 | 529 | 11 |
| 1 | 12 | 0 | 113 | -90 | 38 |
| 2 | 12 | 0 | 1122 | -1061 | 9 |
| 3 | 12 | 0 | 180 | -104 | 23 |
| 4 | 12 | 0 | 938 | 961 | 10 |
| 6 | 12 | 0 | 877 | -853 | 11 |
| 8 | 12 | 0 | 960 | 912 | 12 |
| 1 | 13 | 0 | 556 | -607 | 12 |
| 2 | 13 | 0 | 160 | 24 | 29 |
| 3 | 13 | 0 | 570 | 602 | 12 |
| 5 | 13 | 0 | 473 | -456 | 14 |
| 6 | 13 | 0 | 86 | 49 | 53 |
| 7 | 13 | 0 | 368 | 258 | 17 |
| 8 | 13 | 0 | 187 | 102 | 43 |
| 0 | 14 | 0 | 336 | 300 | 19 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 1 | 14 | 0 | 51 | -28 | 67 |
| 2 | 14 | 0 | 261 | -206 | 21 |
| 4 | 14 | 0 | 310 | 273 | 21 |
| 5 | 14 | 0 | 142 | 62 | 38 |
| 6 | 14 | 0 | 349 | -355 | 16 |
| 1 | 15 | 0 | 861 | -840 | 12 |
| 2 | 15 | 0 | 71 | -22 | 61 |
| 3 | 15 | 0 | 632 | 634 | 15 |
| -13 | 1 | 1 | 763 | 722 | 13 |
| -11 | 1 | 1 | 754 | -752 | 12 |
| -10 | 1 | 1 | 392 | -371 | 15 |
| -9 | 1 | 1 | 728 | 718 | 10 |
| -8 | 1 | 1 | 385 | 394 | 13 |
| -7 | 1 | 1 | 1070 | -1070 | 8 |
| -6 | 1 | 1 | 93 | -7 | 31 |
| -5 | 1 | 1 | 1799 | 1804 | 6 |
| -4 | 1 | 1 | 126 | 150 | 19 |
| -3 | 1 | 1 | 1371 | -1393 | 5 |
| -2 | 1 | 1 | 114 | -114 | 13 |
| -1 | 1 | 1 | 1856 | 1918 | 3 |
| 1 | 1 | 1 | 1143 | -1085 | 3 |
| 2 | 1 | 1 | 1280 | -1272 | 4 |
| 3 | 1 | 1 | 521 | 484 | 7 |
| 4 | 1 | 1 | 823 | 832 | 6 |
| 5 | 1 | 1 | 1247 | -1256 | 6 |
| 6 | 1 | 1 | 645 | -647 | 8 |
| 7 | 1 | 1 | 1114 | 1138 | 8 |
| 8 | 1 | 1 | 582 | 565 | 10 |
| 9 | 1 | 1 | 795 | -801 | 10 |
| 10 | 1 | 1 | 572 | -560 | 13 |
| 11 | 1 | 1 | 549 | 546 | 12 |
| 12 | 1 | 1 | 392 | 415 | 15 |
| 13 | 1 | 1 | 541 | -518 | 17 |
| 14 | 1 | 1 | 263 | -214 | 24 |
| -14 | 2 | 1 | 944 | 905 | 12 |
| -13 | 2 | 1 | 186 | 227 | 23 |
| -12 | 2 | 1 | 1186 | -1159 | 11 |
| -11 | 2 | 1 | 514 | -516 | 13 |
| -10 | 2 | 1 | 891 | 843 | 11 |
| -9 | 2 | 1 | 93 | 81 | 41 |
| -8 | 2 | 1 | 1615 | -1621 | 8 |
| -7 | 2 | 1 | 585 | -575 | 9 |
| -6 | 2 | 1 | 1644 | 1659 | 7 |
| -5 | 2 | 1 | 444 | 454 | 8 |
| -4 | 2 | 1 | 2224 | -2264 | 5 |
| -3 | 2 | 1 | 1330 | -1367 | 5 |
| -2 | 2 | 1 | 444 | 386 | 6 |
| -1 | 2 | 1 | 136 | 32 | 11 |
| 0 | 2 | 1 | 1609 | -1553 | 41 |
| 1 | 2 | 1 | 109 | 21 | 12 |
| 2 | 2 | 1 | 1885 | 1794 | 4 |
| 3 | 2 | 1 | 1104 | 1082 | 5 |
| 4 | 2 | 1 | 1819 | -1768 | 5 |
| 5 | 2 | 1 | 1400 | -1389 | 6 |
| 6 | 2 | 1 | 1889 | 1883 | 7 |
| 7 | 2 | 1 | 1013 | 1016 | 8 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 8 | 2 | 1 | 1401 | -1408 | 8 |
| 9 | 2 | 1 | 675 | -684 | 11 |
| 10 | 2 | 1 | 1048 | 1062 | 10 |
| 11 | 2 | 1 | 130 | 135 | 37 |
| 12 | 2 | 1 | 988 | -993 | 12 |
| 13 | 2 | 1 | 312 | -326 | 16 |
| 14 | 2 | 1 | 931 | 888 | 13 |
| -14 | 3 | 1 | 197 | 206 | 23 |
| -13 | 3 | 1 | 1023 | -1001 | 11 |
| -12 | 3 | 1 | 377 | -357 | 14 |
| -11 | 3 | 1 | 1140 | 1100 | 10 |
| -10 | 3 | 1 | 385 | 369 | 17 |
| -9 | 3 | 1 | 1401 | -1405 | 9 |
| -8 | 3 | 1 | 327 | -305 | 13 |
| -7 | 3 | 1 | 1420 | 1449 | 8 |
| -6 | 3 | 1 | 780 | 800 | 8 |
| -5 | 3 | 1 | 1870 | -1914 | 6 |
| -4 | 3 | 1 | 1130 | -1161 | 6 |
| -3 | 3 | 1 | 2323 | 2363 | 5 |
| -2 | 3 | 1 | 1242 | 1261 | 5 |
| -1 | 3 | 1 | 2911 | -2999 | 4 |
| 0 | 3 | 1 | 2443 | -2465 | 44 |
| 1 | 3 | 1 | 3335 | 3348 | 4 |
| 2 | 3 | 1 | 1809 | 1774 | 4 |
| 3 | 3 | 1 | 2193 | -2122 | 5 |
| 4 | 3 | 1 | 376 | -377 | 8 |
| 5 | 3 | 1 | 1624 | 1602 | 6 |
| 6 | 3 | 1 | 635 | 659 | 8 |
| 7 | 3 | 1 | 1484 | -1484 | 7 |
| 8 | 3 | 1 | 457 | -448 | 12 |
| 9 | 3 | 1 | 1534 | 1545 | 9 |
| 10 | 3 | 1 | 181 | 119 | 24 |
| 11 | 3 | 1 | 1288 | -1282 | 10 |
| 12 | 3 | 1 | 555 | -554 | 14 |
| 13 | 3 | 1 | 889 | 866 | 12 |
| 14 | 3 | 1 | 410 | 365 | 19 |
| -14 | 4 | 1 | 729 | -672 | 15 |
| -13 | 4 | 1 | 147 | -110 | 38 |
| -12 | 4 | 1 | 959 | 916 | 11 |
| -11 | 4 | 1 | 339 | 337 | 16 |
| -10 | 4 | 1 | 925 | -913 | 10 |
| -9 | 4 | 1 | 332 | -316 | 15 |
| -8 | 4 | 1 | 1326 | 1335 | 8 |
| -7 | 4 | 1 | 931 | 939 | 8 |
| -6 | 4 | 1 | 1094 | -1095 | 7 |
| -5 | 4 | 1 | 1233 | -1222 | 7 |
| -4 | 4 | 1 | 542 | 529 | 7 |
| -3 | 4 | 1 | 472 | 465 | 7 |
| -2 | 4 | 1 | 995 | -972 | 5 |
| -1 | 4 | 1 | 1777 | -1752 | 5 |
| 0 | 4 | 1 | 1795 | 1766 | 26 |
| 1 | 4 | 1 | 1441 | 1409 | 5 |
| 2 | 4 | 1 | 1311 | -1277 | 5 |
| 3 | 4 | 1 | 233 | -215 | 9 |
| 4 | 4 | 1 | 1348 | 1308 | 6 |
| 5 | 4 | 1 | 93 | 75 | 29 |

Q.5385-M21

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 6 | 4 | 1 | 1524 | -1474 | 7 |
| 7 | 4 | 1 | 255 | -251 | 14 |
| 8 | 4 | 1 | 1012 | 997 | 9 |
| 9 | 4 | 1 | 323 | 348 | 14 |
| 10 | 4 | 1 | 1016 | -1012 | 10 |
| 11 | 4 | 1 | 333 | -317 | 16 |
| 12 | 4 | 1 | 555 | 552 | 13 |
| 13 | 4 | 1 | 308 | 338 | 23 |
| 14 | 4 | 1 | 525 | -508 | 16 |
| -13 | 5 | 1 | 241 | 188 | 29 |
| -11 | 5 | 1 | 212 | -163 | 28 |
| -9 | 5 | 1 | 264 | 254 | 16 |
| -8 | 5 | 1 | 254 | 267 | 16 |
| -7 | 5 | 1 | 351 | -336 | 12 |
| -6 | 5 | 1 | 486 | -507 | 9 |
| -5 | 5 | 1 | 157 | 131 | 18 |
| -4 | 5 | 1 | 111 | 130 | 17 |
| -3 | 5 | 1 | 365 | -334 | 8 |
| -2 | 5 | 1 | 953 | -956 | 6 |
| -1 | 5 | 1 | 413 | -396 | 7 |
| 0 | 5 | 1 | 329 | 334 | 6 |
| 1 | 5 | 1 | 181 | 158 | 10 |
| 2 | 5 | 1 | 342 | -357 | 8 |
| 3 | 5 | 1 | 368 | -318 | 8 |
| 5 | 5 | 1 | 353 | -321 | 11 |
| 6 | 5 | 1 | 247 | -279 | 12 |
| 7 | 5 | 1 | 325 | 294 | 13 |
| 8 | 5 | 1 | 187 | 203 | 16 |
| 9 | 5 | 1 | 145 | 11 | 29 |
| 10 | 5 | 1 | 433 | 431 | 13 |
| 11 | 5 | 1 | 334 | 368 | 15 |
| 13 | 5 | 1 | 265 | -221 | 23 |
| 14 | 5 | 1 | 116 | -90 | 48 |
| -13 | 6 | 1 | 137 | -156 | 42 |
| -12 | 6 | 1 | 326 | 336 | 18 |
| -11 | 6 | 1 | 51 | 116 | 66 |
| -10 | 6 | 1 | 791 | -798 | 11 |
| -9 | 6 | 1 | 54 | -8 | 61 |
| -8 | 6 | 1 | 814 | 839 | 9 |
| -7 | 6 | 1 | 87 | 66 | 39 |
| -6 | 6 | 1 | 466 | -486 | 10 |
| -5 | 6 | 1 | 471 | 467 | 9 |
| -4 | 6 | 1 | 1357 | 1364 | 6 |
| -3 | 6 | 1 | 480 | 450 | 8 |
| -2 | 6 | 1 | 552 | -576 | 7 |
| -1 | 6 | 1 | 165 | -130 | 14 |
| 0 | 6 | 1 | 267 | 275 | 7 |
| 1 | 6 | 1 | 604 | 570 | 7 |
| 2 | 6 | 1 | 864 | -856 | 6 |
| 3 | 6 | 1 | 124 | -97 | 19 |
| 4 | 6 | 1 | 909 | 872 | 7 |
| 5 | 6 | 1 | 105 | 13 | 28 |
| 6 | 6 | 1 | 626 | -619 | 9 |
| 7 | 6 | 1 | 292 | -264 | 14 |
| 8 | 6 | 1 | 1010 | 1023 | 9 |
| 9 | 6 | 1 | 341 | 337 | 18 |
| 10 | 6 | 1 | 522 | -507 | 13 |
| 11 | 6 | 1 | 365 | -371 | 18 |
| 12 | 6 | 1 | 519 | 516 | 15 |
| 13 | 6 | 1 | 316 | 322 | 17 |
| -13 | 7 | 1 | 802 | 805 | 13 |
| -12 | 7 | 1 | 174 | 180 | 24 |
| -11 | 7 | 1 | 946 | -963 | 11 |
| -10 | 7 | 1 | 144 | -41 | 34 |
| -9 | 7 | 1 | 1511 | 1511 | 9 |
| -8 | 7 | 1 | 410 | 401 | 13 |
| -7 | 7 | 1 | 1275 | -1269 | 9 |
| -6 | 7 | 1 | 474 | -449 | 11 |
| -5 | 7 | 1 | 945 | 933 | 8 |
| -4 | 7 | 1 | 378 | 369 | 10 |
| -3 | 7 | 1 | 1012 | -982 | 7 |
| -2 | 7 | 1 | 145 | -113 | 16 |
| -1 | 7 | 1 | 1304 | 1286 | 6 |
| 0 | 7 | 1 | 141 | 107 | 10 |
| 1 | 7 | 1 | 1307 | -1278 | 6 |
| 2 | 7 | 1 | 66 | 56 | 36 |
| 3 | 7 | 1 | 1333 | 1307 | 7 |
| 4 | 7 | 1 | 600 | 545 | 8 |
| 5 | 7 | 1 | 1156 | -1146 | 8 |
| 6 | 7 | 1 | 598 | -621 | 9 |
| 7 | 7 | 1 | 1085 | 1062 | 9 |
| 8 | 7 | 1 | 423 | 410 | 12 |
| 9 | 7 | 1 | 1173 | -1160 | 10 |
| 10 | 7 | 1 | 732 | -714 | 12 |
| 11 | 7 | 1 | 906 | 921 | 11 |
| 12 | 7 | 1 | 379 | 369 | 18 |
| 13 | 7 | 1 | 692 | -702 | 14 |
| -12 | 8 | 1 | 843 | -828 | 12 |
| -11 | 8 | 1 | 220 | -257 | 20 |
| -10 | 8 | 1 | 1219 | 1208 | 10 |
| -9 | 8 | 1 | 472 | 474 | 13 |
| -8 | 8 | 1 | 1311 | -1302 | 9 |
| -7 | 8 | 1 | 446 | -423 | 13 |
| -6 | 8 | 1 | 1545 | 1539 | 8 |
| -5 | 8 | 1 | 338 | 348 | 12 |
| -4 | 8 | 1 | 1963 | -1908 | 7 |
| -3 | 8 | 1 | 595 | -581 | 9 |
| -2 | 8 | 1 | 2008 | 1980 | 7 |
| -1 | 8 | 1 | 399 | 379 | 9 |
| 0 | 8 | 1 | 1959 | -1922 | 11 |
| 1 | 8 | 1 | 675 | -675 | 8 |
| 2 | 8 | 1 | 1606 | 1561 | 7 |
| 3 | 8 | 1 | 850 | 803 | 8 |
| 4 | 8 | 1 | 1457 | -1428 | 8 |
| 5 | 8 | 1 | 905 | -888 | 8 |
| 6 | 8 | 1 | 1145 | 1125 | 8 |
| 7 | 8 | 1 | 547 | 542 | 11 |
| 8 | 8 | 1 | 1081 | -1083 | 9 |
| 9 | 8 | 1 | 398 | -363 | 17 |
| 10 | 8 | 1 | 954 | 954 | 11 |
| 11 | 8 | 1 | 505 | 491 | 14 |
| 12 | 8 | 1 | 980 | -935 | 12 |
| -12 | 9 | 1 | 178 | -256 | 34 |
| -11 | 9 | 1 | 687 | 639 | 13 |
| -10 | 9 | 1 | 442 | 417 | 15 |
| -9 | 9 | 1 | 953 | -928 | 10 |
| -8 | 9 | 1 | 482 | -455 | 12 |
| -7 | 9 | 1 | 1037 | 1019 | 10 |
| -6 | 9 | 1 | 382 | 369 | 13 |
| -5 | 9 | 1 | 1398 | -1386 | 8 |
| -4 | 9 | 1 | 235 | -235 | 16 |
| -3 | 9 | 1 | 1811 | 1776 | 7 |
| -2 | 9 | 1 | 697 | 651 | 9 |
| -1 | 9 | 1 | 929 | -905 | 8 |
| 0 | 9 | 1 | 446 | -427 | 7 |
| 1 | 9 | 1 | 1124 | 1092 | 7 |
| 2 | 9 | 1 | 448 | 428 | 10 |
| 3 | 9 | 1 | 1111 | -1092 | 8 |
| 4 | 9 | 1 | 745 | -734 | 9 |
| 5 | 9 | 1 | 1212 | 1205 | 8 |
| 6 | 9 | 1 | 390 | 399 | 13 |
| 7 | 9 | 1 | 963 | -964 | 9 |
| 8 | 9 | 1 | 249 | -223 | 20 |
| 9 | 9 | 1 | 602 | 612 | 12 |
| 10 | 9 | 1 | 405 | 378 | 16 |
| 11 | 9 | 1 | 774 | -730 | 12 |
| 12 | 9 | 1 | 168 | -184 | 26 |
| -11 | 10 | 1 | 276 | 261 | 27 |
| -10 | 10 | 1 | 546 | -485 | 14 |
| -9 | 10 | 1 | 271 | -247 | 20 |
| -8 | 10 | 1 | 345 | 250 | 17 |
| -7 | 10 | 1 | 203 | 185 | 19 |
| -6 | 10 | 1 | 466 | -458 | 12 |
| -5 | 10 | 1 | 601 | -579 | 11 |
| -4 | 10 | 1 | 575 | 535 | 10 |
| -3 | 10 | 1 | 466 | 434 | 12 |
| -2 | 10 | 1 | 738 | -710 | 9 |
| -1 | 10 | 1 | 460 | -406 | 11 |
| 0 | 10 | 1 | 820 | 810 | 6 |
| 1 | 10 | 1 | 198 | 188 | 18 |
| 2 | 10 | 1 | 794 | -759 | 9 |
| 3 | 10 | 1 | 70 | -98 | 48 |
| 4 | 10 | 1 | 525 | 503 | 11 |
| 5 | 10 | 1 | 162 | -150 | 23 |
| 6 | 10 | 1 | 651 | -645 | 11 |
| 7 | 10 | 1 | 97 | -85 | 44 |
| 8 | 10 | 1 | 573 | 510 | 13 |
| 9 | 10 | 1 | 217 | 240 | 21 |
| 10 | 10 | 1 | 424 | -395 | 16 |
| 11 | 10 | 1 | 240 | -234 | 24 |
| -10 | 11 | 1 | 22 | -120 | 89 |
| -9 | 11 | 1 | 146 | -50 | 38 |
| -8 | 11 | 1 | 296 | -220 | 18 |
| -7 | 11 | 1 | 354 | 294 | 16 |
| -6 | 11 | 1 | 200 | -81 | 28 |
| -5 | 11 | 1 | 581 | -551 | 12 |
| -4 | 11 | 1 | 137 | 36 | 32 |
| -3 | 11 | 1 | 479 | 496 | 10 |
| -2 | 11 | 1 | 148 | 33 | 21 |
| -1 | 11 | 1 | 674 | -688 | 11 |
| 0 | 11 | 1 | 128 | -100 | 23 |
| 1 | 11 | 1 | 438 | 425 | 11 |
| 2 | 11 | 1 | 365 | 396 | 13 |
| 3 | 11 | 1 | 478 | -438 | 11 |
| 4 | 11 | 1 | 116 | -169 | 38 |
| 5 | 11 | 1 | 327 | 249 | 14 |
| 6 | 11 | 1 | 182 | 212 | 24 |
| 7 | 11 | 1 | 288 | -222 | 16 |
| 8 | 11 | 1 | 188 | -114 | 40 |
| 9 | 11 | 1 | 225 | 198 | 18 |
| 10 | 11 | 1 | 21 | -38 | 83 |
| -9 | 12 | 1 | 306 | -306 | 19 |
| -8 | 12 | 1 | 396 | 391 | 15 |
| -7 | 12 | 1 | 269 | 260 | 19 |
| -6 | 12 | 1 | 520 | -539 | 13 |
| -5 | 12 | 1 | 160 | -201 | 26 |
| -4 | 12 | 1 | 821 | 768 | 10 |
| -3 | 12 | 1 | 474 | 480 | 13 |
| -2 | 12 | 1 | 885 | -840 | 10 |
| -1 | 12 | 1 | 340 | -352 | 14 |
| 0 | 12 | 1 | 887 | 830 | 7 |
| 1 | 12 | 1 | 235 | 244 | 17 |
| 2 | 12 | 1 | 778 | -724 | 10 |
| 3 | 12 | 1 | 269 | 269 | 15 |
| 4 | 12 | 1 | 777 | 745 | 11 |
| 6 | 12 | 1 | 605 | -574 | 13 |
| 7 | 12 | 1 | 176 | -114 | 28 |
| 8 | 12 | 1 | 775 | 745 | 12 |
| -8 | 13 | 1 | 384 | 399 | 16 |
| -7 | 13 | 1 | 1013 | -998 | 11 |
| -6 | 13 | 1 | 222 | -245 | 20 |
| -5 | 13 | 1 | 1034 | 1042 | 10 |
| -4 | 13 | 1 | 369 | 365 | 17 |
| -3 | 13 | 1 | 830 | -822 | 11 |
| -2 | 13 | 1 | 497 | -520 | 12 |
| -1 | 13 | 1 | 896 | 886 | 11 |
| 0 | 13 | 1 | 132 | 143 | 21 |
| 1 | 13 | 1 | 1130 | -1141 | 10 |
| 2 | 13 | 1 | 319 | -335 | 17 |
| 3 | 13 | 1 | 1253 | 1276 | 10 |
| 4 | 13 | 1 | 283 | 312 | 15 |
| 5 | 13 | 1 | 1038 | -1009 | 11 |
| 6 | 13 | 1 | 463 | -454 | 14 |
| 7 | 13 | 1 | 991 | 956 | 11 |
| 8 | 13 | 1 | 386 | 408 | 17 |
| -6 | 14 | 1 | 938 | 911 | 12 |
| -5 | 14 | 1 | 20 | 80 | 80 |
| -4 | 14 | 1 | 862 | -872 | 12 |
| -3 | 14 | 1 | 236 | -212 | 23 |
| -2 | 14 | 1 | 946 | 975 | 11 |
| -1 | 14 | 1 | 297 | 301 | 17 |
| 0 | 14 | 1 | 944 | -958 | 9 |
| 1 | 14 | 1 | 410 | -414 | 15 |
| 2 | 14 | 1 | 958 | 958 | 11 |
| 3 | 14 | 1 | 415 | 421 | 14 |
| 4 | 14 | 1 | 818 | -823 | 11 |
| 5 | 14 | 1 | 447 | -450 | 15 |
| 6 | 14 | 1 | 755 | 729 | 12 |
| -3 | 15 | 1 | 564 | 550 | 14 |
| -2 | 15 | 1 | 206 | 253 | 22 |
| -1 | 15 | 1 | 765 | -774 | 12 |
| 0 | 15 | 1 | 111 | -124 | 35 |
| 1 | 15 | 1 | 591 | 571 | 14 |
| 2 | 15 | 1 | 61 | 182 | 70 |
| 3 | 15 | 1 | 520 | -565 | 14 |
| -14 | 0 | 2 | 713 | 709 | 15 |
| -13 | 0 | 2 | 592 | 574 | 14 |
| -12 | 0 | 2 | 1144 | -1145 | 11 |
| -11 | 0 | 2 | 596 | -581 | 13 |
| -10 | 0 | 2 | 988 | 944 | 10 |
| -9 | 0 | 2 | 555 | 539 | 11 |
| -8 | 0 | 2 | 2020 | -2060 | 8 |
| -7 | 0 | 2 | 279 | -228 | 13 |
| -6 | 0 | 2 | 2715 | 2750 | 6 |
| -5 | 0 | 2 | 1162 | 1170 | 6 |
| -4 | 0 | 2 | 2431 | -2507 | 5 |
| -3 | 0 | 2 | 2591 | -2693 | 5 |
| -2 | 0 | 2 | 2891 | 3045 | 4 |
| -1 | 0 | 2 | 2365 | 2529 | 3 |
| 0 | 0 | 2 | 3392 | -3458 | 131 |
| 1 | 0 | 2 | 2647 | -2621 | 3 |
| 2 | 0 | 2 | 3196 | 3246 | 4 |
| 3 | 0 | 2 | 1294 | 1291 | 5 |
| 4 | 0 | 2 | 2451 | -2472 | 5 |
| 5 | 0 | 2 | 1058 | -1058 | 7 |
| 6 | 0 | 2 | 1076 | 1146 | 8 |
| 7 | 0 | 2 | 613 | 600 | 9 |
| 8 | 0 | 2 | 1445 | -1474 | 8 |
| 9 | 0 | 2 | 1433 | -1472 | 9 |
| 10 | 0 | 2 | 1276 | 1298 | 10 |
| 11 | 0 | 2 | 1422 | 1454 | 10 |
| 12 | 0 | 2 | 906 | -895 | 12 |
| 13 | 0 | 2 | 692 | -731 | 13 |
| 14 | 0 | 2 | 839 | 818 | 13 |
| -14 | 1 | 2 | 449 | 394 | 19 |
| -13 | 1 | 2 | 1002 | -967 | 12 |
| -12 | 1 | 2 | 497 | -473 | 13 |
| -11 | 1 | 2 | 765 | 735 | 12 |
| -10 | 1 | 2 | 501 | 506 | 12 |
| -9 | 1 | 2 | 1129 | -1144 | 9 |
| -8 | 1 | 2 | 767 | -773 | 9 |
| -7 | 1 | 2 | 1088 | 1145 | 8 |
| -6 | 1 | 2 | 1039 | 1048 | 8 |
| -5 | 1 | 2 | 1587 | -1613 | 6 |
| -4 | 1 | 2 | 462 | -447 | 8 |
| -3 | 1 | 2 | 783 | 766 | 6 |
| -2 | 1 | 2 | 260 | -175 | 8 |
| -1 | 1 | 2 | 1558 | -1598 | 3 |
| 0 | 1 | 2 | 1799 | -1800 | 89 |
| 1 | 1 | 2 | 2594 | 2532 | 3 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 2 | 1 | 2 | 247 | 209 | 7 |
| 3 | 1 | 2 | 1753 | -1752 | 5 |
| 4 | 1 | 2 | 1161 | -1158 | 6 |
| 5 | 1 | 2 | 2027 | 2003 | 6 |
| 6 | 1 | 2 | 1729 | 1724 | 7 |
| 7 | 1 | 2 | 1361 | -1372 | 8 |
| 8 | 1 | 2 | 679 | -698 | 10 |
| 9 | 1 | 2 | 1167 | 1202 | 9 |
| 10 | 1 | 2 | 557 | 571 | 14 |
| 11 | 1 | 2 | 1162 | -1169 | 11 |
| 12 | 1 | 2 | 824 | -840 | 12 |
| 13 | 1 | 2 | 677 | 653 | 14 |
| 14 | 1 | 2 | 590 | 590 | 16 |
| -14 | 2 | 2 | 533 | -441 | 18 |
| -13 | 2 | 2 | 318 | -255 | 23 |
| -12 | 2 | 2 | 704 | 703 | 13 |
| -11 | 2 | 2 | 175 | 155 | 17 |
| -10 | 2 | 2 | 504 | -483 | 14 |
| -9 | 2 | 2 | 506 | -478 | 12 |
| -8 | 2 | 2 | 396 | 395 | 13 |
| -7 | 2 | 2 | 754 | 763 | 9 |
| -6 | 2 | 2 | 209 | -221 | 14 |
| -5 | 2 | 2 | 1492 | -1445 | 6 |
| -4 | 2 | 2 | 624 | 628 | 7 |
| -3 | 2 | 2 | 729 | 719 | 6 |
| -2 | 2 | 2 | 694 | -684 | 5 |
| -1 | 2 | 2 | 68 | 33 | 24 |
| 0 | 2 | 2 | 134 | 109 | 14 |
| 1 | 2 | 2 | 1946 | 1843 | 4 |
| 2 | 2 | 2 | 701 | -646 | 5 |
| 3 | 2 | 2 | 983 | -955 | 5 |
| 4 | 2 | 2 | 1019 | 999 | 6 |
| 5 | 2 | 2 | 1013 | 1006 | 7 |
| 6 | 2 | 2 | 1395 | -1382 | 7 |
| 7 | 2 | 2 | 929 | -926 | 8 |
| 8 | 2 | 2 | 1206 | 1211 | 8 |
| 9 | 2 | 2 | 409 | 384 | 13 |
| 10 | 2 | 2 | 701 | -693 | 12 |
| 11 | 2 | 2 | 295 | -280 | 20 |
| 12 | 2 | 2 | 430 | 442 | 15 |
| 13 | 2 | 2 | 321 | 319 | 18 |
| 14 | 2 | 2 | 307 | -276 | 24 |
| -14 | 3 | 2 | 80 | 90 | 59 |
| -13 | 3 | 2 | 103 | 64 | 49 |
| -11 | 3 | 2 | 120 | -35 | 38 |
| -10 | 3 | 2 | 178 | -123 | 28 |
| -9 | 3 | 2 | 288 | -304 | 16 |
| -8 | 3 | 2 | 434 | -431 | 11 |
| -7 | 3 | 2 | 473 | 477 | 10 |
| -6 | 3 | 2 | 466 | -413 | 9 |
| -5 | 3 | 2 | 993 | -983 | 7 |
| -4 | 3 | 2 | 214 | -240 | 12 |
| -3 | 3 | 2 | 407 | 399 | 8 |
| -2 | 3 | 2 | 181 | 128 | 13 |
| -1 | 3 | 2 | 448 | -443 | 6 |
| 0 | 3 | 2 | 2290 | 2273 | 68 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 1 | 3 | 2 | 1122 | 1089 | 4 |
| 2 | 3 | 2 | 465 | 447 | 6 |
| 3 | 3 | 2 | 540 | -531 | 6 |
| 4 | 3 | 2 | 1124 | -1083 | 6 |
| 5 | 3 | 2 | 264 | 236 | 12 |
| 6 | 3 | 2 | 465 | -442 | 10 |
| 7 | 3 | 2 | 531 | -531 | 9 |
| 9 | 3 | 2 | 310 | 281 | 14 |
| 10 | 3 | 2 | 270 | 288 | 18 |
| 11 | 3 | 2 | 331 | -349 | 17 |
| 12 | 3 | 2 | 339 | -363 | 18 |
| 14 | 3 | 2 | 89 | 96 | 57 |
| -14 | 4 | 2 | 536 | -542 | 16 |
| -13 | 4 | 2 | 265 | -222 | 25 |
| -12 | 4 | 2 | 759 | 803 | 12 |
| -11 | 4 | 2 | 515 | 526 | 12 |
| -10 | 4 | 2 | 584 | -605 | 13 |
| -9 | 4 | 2 | 516 | -557 | 12 |
| -8 | 4 | 2 | 626 | 665 | 10 |
| -7 | 4 | 2 | 1201 | 1243 | 8 |
| -6 | 4 | 2 | 941 | -935 | 8 |
| -5 | 4 | 2 | 817 | -844 | 7 |
| -4 | 4 | 2 | 696 | 682 | 7 |
| -3 | 4 | 2 | 328 | 338 | 8 |
| -2 | 4 | 2 | 1107 | -1111 | 5 |
| -1 | 4 | 2 | 1099 | -1119 | 5 |
| 0 | 4 | 2 | 3078 | 3055 | 77 |
| 1 | 4 | 2 | 168 | 168 | 10 |
| 2 | 4 | 2 | 2012 | -1942 | 5 |
| 3 | 4 | 2 | 477 | -454 | 7 |
| 4 | 4 | 2 | 1452 | 1414 | 6 |
| 5 | 4 | 2 | 1153 | 1123 | 7 |
| 6 | 4 | 2 | 1379 | -1352 | 7 |
| 7 | 4 | 2 | 452 | -437 | 10 |
| 8 | 4 | 2 | 1244 | 1275 | 8 |
| 9 | 4 | 2 | 779 | 762 | 11 |
| 10 | 4 | 2 | 826 | -834 | 11 |
| 11 | 4 | 2 | 885 | -914 | 11 |
| 12 | 4 | 2 | 382 | 420 | 17 |
| 13 | 4 | 2 | 541 | 563 | 14 |
| 14 | 4 | 2 | 525 | -524 | 16 |
| -14 | 5 | 2 | 448 | -436 | 17 |
| -13 | 5 | 2 | 959 | 969 | 12 |
| -12 | 5 | 2 | 709 | 734 | 13 |
| -11 | 5 | 2 | 1042 | -1036 | 11 |
| -10 | 5 | 2 | 675 | -671 | 12 |
| -9 | 5 | 2 | 1141 | 1122 | 9 |
| -8 | 5 | 2 | 1059 | 1074 | 9 |
| -7 | 5 | 2 | 1161 | -1172 | 8 |
| -6 | 5 | 2 | 854 | -899 | 8 |
| -5 | 5 | 2 | 1765 | 1759 | 7 |
| -4 | 5 | 2 | 1252 | 1283 | 6 |
| -3 | 5 | 2 | 1784 | -1784 | 6 |
| -2 | 5 | 2 | 1984 | -1988 | 5 |
| -1 | 5 | 2 | 1931 | 1955 | 5 |
| 0 | 5 | 2 | 1725 | 1669 | 42 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 1 | 5 | 2 | 1917 | -1877 | 5 |
| 2 | 5 | 2 | 986 | -956 | 6 |
| 3 | 5 | 2 | 1573 | 1515 | 6 |
| 4 | 5 | 2 | 1322 | 1271 | 6 |
| 5 | 5 | 2 | 2066 | -2041 | 6 |
| 6 | 5 | 2 | 1625 | -1591 | 7 |
| 7 | 5 | 2 | 1512 | 1537 | 8 |
| 8 | 5 | 2 | 1225 | 1207 | 9 |
| 9 | 5 | 2 | 751 | -762 | 10 |
| 10 | 5 | 2 | 869 | -867 | 11 |
| 11 | 5 | 2 | 882 | 924 | 11 |
| 12 | 5 | 2 | 729 | 744 | 12 |
| 13 | 5 | 2 | 807 | -792 | 12 |
| 14 | 5 | 2 | 567 | -583 | 15 |
| -13 | 6 | 2 | 426 | 453 | 16 |
| -12 | 6 | 2 | 858 | -871 | 12 |
| -11 | 6 | 2 | 534 | -518 | 13 |
| -10 | 6 | 2 | 924 | 926 | 11 |
| -9 | 6 | 2 | 720 | 729 | 11 |
| -8 | 6 | 2 | 1230 | -1254 | 9 |
| -7 | 6 | 2 | 855 | -888 | 9 |
| -6 | 6 | 2 | 1680 | 1691 | 7 |
| -5 | 6 | 2 | 654 | 679 | 8 |
| -4 | 6 | 2 | 1783 | -1777 | 6 |
| -3 | 6 | 2 | 878 | -902 | 7 |
| -2 | 6 | 2 | 1365 | 1408 | 6 |
| -1 | 6 | 2 | 1296 | 1299 | 6 |
| 0 | 6 | 2 | 1672 | -1661 | 31 |
| 1 | 6 | 2 | 1125 | -1107 | 6 |
| 2 | 6 | 2 | 682 | 678 | 6 |
| 3 | 6 | 2 | 1025 | 1024 | 6 |
| 4 | 6 | 2 | 1027 | -1051 | 7 |
| 5 | 6 | 2 | 1272 | -1260 | 7 |
| 6 | 6 | 2 | 1504 | 1483 | 8 |
| 7 | 6 | 2 | 977 | 954 | 8 |
| 8 | 6 | 2 | 858 | -870 | 10 |
| 9 | 6 | 2 | 672 | -657 | 11 |
| 10 | 6 | 2 | 819 | 840 | 11 |
| 11 | 6 | 2 | 579 | 561 | 12 |
| 12 | 6 | 2 | 712 | -704 | 12 |
| 13 | 6 | 2 | 589 | -589 | 16 |
| -13 | 7 | 2 | 396 | -407 | 17 |
| -12 | 7 | 2 | 314 | -311 | 19 |
| -11 | 7 | 2 | 656 | 641 | 13 |
| -10 | 7 | 2 | 501 | 523 | 12 |
| -9 | 7 | 2 | 855 | -852 | 11 |
| -8 | 7 | 2 | 384 | -404 | 12 |
| -7 | 7 | 2 | 990 | 1009 | 9 |
| -6 | 7 | 2 | 853 | 859 | 9 |
| -5 | 7 | 2 | 531 | -527 | 9 |
| -4 | 7 | 2 | 591 | -574 | 8 |
| -3 | 7 | 2 | 1135 | 1081 | 7 |
| -2 | 7 | 2 | 550 | 534 | 8 |
| -1 | 7 | 2 | 1597 | -1603 | 6 |
| 0 | 7 | 2 | 1437 | -1390 | 20 |
| 1 | 7 | 2 | 789 | 812 | 7 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 2 | 7 | 2 | 833 | 819 | 7 |
| 3 | 7 | 2 | 695 | -711 | 7 |
| 4 | 7 | 2 | 762 | -750 | 8 |
| 5 | 7 | 2 | 948 | 919 | 8 |
| 6 | 7 | 2 | 626 | 605 | 9 |
| 7 | 7 | 2 | 414 | -370 | 15 |
| 8 | 7 | 2 | 372 | -400 | 14 |
| 9 | 7 | 2 | 464 | 444 | 13 |
| 10 | 7 | 2 | 783 | 754 | 11 |
| 11 | 7 | 2 | 550 | -531 | 14 |
| 12 | 7 | 2 | 376 | -314 | 18 |
| 13 | 7 | 2 | 498 | 485 | 16 |
| -11 | 8 | 2 | 111 | 86 | 45 |
| -10 | 8 | 2 | 199 | -200 | 20 |
| -9 | 8 | 2 | 198 | -198 | 25 |
| -8 | 8 | 2 | 252 | 172 | 22 |
| -7 | 8 | 2 | 177 | -136 | 18 |
| -6 | 8 | 2 | 207 | -180 | 15 |
| -5 | 8 | 2 | 255 | -184 | 14 |
| -4 | 8 | 2 | 256 | -233 | 15 |
| -3 | 8 | 2 | 444 | 327 | 11 |
| -2 | 8 | 2 | 621 | 659 | 8 |
| -1 | 8 | 2 | 296 | -228 | 13 |
| 0 | 8 | 2 | 178 | -202 | 15 |
| 2 | 8 | 2 | 156 | -143 | 16 |
| 4 | 8 | 2 | 124 | 74 | 28 |
| 6 | 8 | 2 | 77 | -49 | 45 |
| 7 | 8 | 2 | 101 | -76 | 39 |
| 8 | 8 | 2 | 155 | 159 | 23 |
| 9 | 8 | 2 | 288 | 288 | 15 |
| 10 | 8 | 2 | 370 | -326 | 16 |
| 11 | 8 | 2 | 133 | -54 | 38 |
| 12 | 8 | 2 | 154 | 103 | 37 |
| -12 | 9 | 2 | 184 | -218 | 31 |
| -11 | 9 | 2 | 355 | 316 | 17 |
| -10 | 9 | 2 | 266 | 181 | 30 |
| -9 | 9 | 2 | 498 | -489 | 13 |
| -8 | 9 | 2 | 599 | -561 | 12 |
| -7 | 9 | 2 | 696 | 694 | 10 |
| -6 | 9 | 2 | 227 | 171 | 15 |
| -5 | 9 | 2 | 733 | -722 | 9 |
| -4 | 9 | 2 | 555 | -557 | 10 |
| -3 | 9 | 2 | 541 | 491 | 10 |
| -2 | 9 | 2 | 1141 | 1105 | 8 |
| -1 | 9 | 2 | 472 | -399 | 12 |
| 0 | 9 | 2 | 343 | -307 | 16 |
| 1 | 9 | 2 | 538 | 539 | 9 |
| 2 | 9 | 2 | 370 | 342 | 11 |
| 3 | 9 | 2 | 308 | -314 | 12 |
| 5 | 9 | 2 | 178 | 195 | 18 |
| 6 | 9 | 2 | 110 | 48 | 37 |
| 7 | 9 | 2 | 417 | -455 | 14 |
| 8 | 9 | 2 | 474 | -479 | 12 |
| 9 | 9 | 2 | 222 | 211 | 27 |
| 10 | 9 | 2 | 283 | 326 | 18 |
| 11 | 9 | 2 | 223 | -152 | 28 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 12 | 9 | 2 | 383 | -358 | 17 |
| -11 | 10 | 2 | 541 | 556 | 14 |
| -10 | 10 | 2 | 886 | -871 | 12 |
| -9 | 10 | 2 | 696 | -663 | 13 |
| -8 | 10 | 2 | 1032 | 1014 | 10 |
| -7 | 10 | 2 | 871 | 867 | 10 |
| -6 | 10 | 2 | 823 | -819 | 10 |
| -5 | 10 | 2 | 539 | -501 | 11 |
| -4 | 10 | 2 | 1035 | 1036 | 9 |
| -3 | 10 | 2 | 908 | 913 | 9 |
| -2 | 10 | 2 | 844 | -831 | 9 |
| -1 | 10 | 2 | 945 | -935 | 9 |
| 0 | 10 | 2 | 1031 | 1015 | 17 |
| 1 | 10 | 2 | 941 | 918 | 8 |
| 2 | 10 | 2 | 1089 | -1108 | 8 |
| 3 | 10 | 2 | 1022 | -1003 | 9 |
| 4 | 10 | 2 | 806 | 797 | 9 |
| 5 | 10 | 2 | 961 | 930 | 9 |
| 6 | 10 | 2 | 811 | -781 | 10 |
| 7 | 10 | 2 | 951 | -982 | 10 |
| 8 | 10 | 2 | 536 | 519 | 13 |
| 9 | 10 | 2 | 617 | 611 | 12 |
| 10 | 10 | 2 | 535 | -529 | 14 |
| 11 | 10 | 2 | 680 | -681 | 14 |
| -10 | 11 | 2 | 524 | -543 | 15 |
| -9 | 11 | 2 | 623 | 600 | 13 |
| -8 | 11 | 2 | 769 | 777 | 12 |
| -7 | 11 | 2 | 850 | -817 | 11 |
| -6 | 11 | 2 | 608 | -611 | 12 |
| -5 | 11 | 2 | 995 | 979 | 10 |
| -4 | 11 | 2 | 569 | 562 | 11 |
| -3 | 11 | 2 | 1148 | -1148 | 9 |
| -2 | 11 | 2 | 897 | -887 | 9 |
| -1 | 11 | 2 | 930 | 902 | 9 |
| 0 | 11 | 2 | 599 | 563 | 7 |
| 1 | 11 | 2 | 1145 | -1125 | 9 |
| 2 | 11 | 2 | 921 | -897 | 9 |
| 3 | 11 | 2 | 1027 | 1007 | 9 |
| 4 | 11 | 2 | 858 | 851 | 10 |
| 5 | 11 | 2 | 748 | -747 | 10 |
| 6 | 11 | 2 | 751 | -751 | 10 |
| 7 | 11 | 2 | 1013 | 1022 | 10 |
| 8 | 11 | 2 | 662 | 669 | 12 |
| 9 | 11 | 2 | 989 | -961 | 11 |
| 10 | 11 | 2 | 631 | -622 | 13 |
| -9 | 12 | 2 | 385 | 368 | 17 |
| -8 | 12 | 2 | 481 | -467 | 15 |
| -7 | 12 | 2 | 395 | -401 | 14 |
| -6 | 12 | 2 | 505 | 486 | 14 |
| -5 | 12 | 2 | 526 | 488 | 14 |
| -4 | 12 | 2 | 744 | -764 | 10 |
| -3 | 12 | 2 | 405 | -371 | 12 |
| -2 | 12 | 2 | 728 | 699 | 10 |
| -1 | 12 | 2 | 302 | 244 | 14 |
| 0 | 12 | 2 | 807 | -771 | 8 |
| 1 | 12 | 2 | 401 | -348 | 14 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$ 

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 2 | 12 | 2 | 974 | 951 | 10 |
| 3 | 12 | 2 | 641 | 626 | 11 |
| 4 | 12 | 2 | 697 | -676 | 11 |
| 5 | 12 | 2 | 555 | -582 | 12 |
| 6 | 12 | 2 | 642 | 643 | 11 |
| 7 | 12 | 2 | 504 | 484 | 14 |
| 8 | 12 | 2 | 681 | -612 | 13 |
| 9 | 12 | 2 | 420 | -415 | 15 |
| -8 | 13 | 2 | 183 | -153 | 28 |
| -7 | 13 | 2 | 345 | 346 | 19 |
| -6 | 13 | 2 | 192 | 70 | 30 |
| -5 | 13 | 2 | 259 | -263 | 19 |
| -4 | 13 | 2 | 322 | -288 | 16 |
| -3 | 13 | 2 | 386 | 384 | 15 |
| -2 | 13 | 2 | 292 | 283 | 15 |
| -1 | 13 | 2 | 275 | -292 | 17 |
| 0 | 13 | 2 | 192 | -26 | 42 |
| 1 | 13 | 2 | 417 | 436 | 13 |
| 2 | 13 | 2 | 197 | 209 | 25 |
| 3 | 13 | 2 | 461 | -388 | 13 |
| 4 | 13 | 2 | 119 | -79 | 40 |
| 5 | 13 | 2 | 308 | 246 | 16 |
| 6 | 13 | 2 | 154 | 117 | 42 |
| 7 | 13 | 2 | 314 | -266 | 16 |
| -6 | 14 | 2 | 163 | 126 | 37 |
| -5 | 14 | 2 | 149 | 0 | 37 |
| -4 | 14 | 2 | 170 | -83 | 30 |
| -3 | 14 | 2 | 188 | -185 | 21 |
| -2 | 14 | 2 | 20 | 29 | 79 |
| -1 | 14 | 2 | 268 | 226 | 18 |
| 0 | 14 | 2 | 227 | -234 | 19 |
| 1 | 14 | 2 | 281 | -238 | 18 |
| 2 | 14 | 2 | 241 | 248 | 24 |
| 3 | 14 | 2 | 313 | 315 | 18 |
| 4 | 14 | 2 | 84 | -72 | 57 |
| 5 | 14 | 2 | 237 | -269 | 23 |
| 6 | 14 | 2 | 160 | 136 | 38 |
| -3 | 15 | 2 | 408 | 379 | 17 |
| -2 | 15 | 2 | 458 | 482 | 15 |
| -1 | 15 | 2 | 493 | -409 | 16 |
| 0 | 15 | 2 | 415 | -379 | 16 |
| 1 | 15 | 2 | 506 | 494 | 14 |
| 2 | 15 | 2 | 429 | 382 | 15 |
| 3 | 15 | 2 | 459 | -466 | 15 |
| -14 | 1 | 3 | 374 | 348 | 22 |
| -13 | 1 | 3 | 511 | -483 | 15 |
| -12 | 1 | 3 | 588 | -580 | 14 |
| -11 | 1 | 3 | 356 | 341 | 16 |
| -10 | 1 | 3 | 563 | 581 | 12 |
| -9 | 1 | 3 | 599 | -616 | 11 |
| -8 | 1 | 3 | 921 | -943 | 9 |
| -7 | 1 | 3 | 442 | 434 | 10 |
| -6 | 1 | 3 | 1313 | 1369 | 7 |
| -5 | 1 | 3 | 529 | -520 | 8 |
| -4 | 1 | 3 | 1238 | -1278 | 6 |
| -3 | 1 | 3 | 1388 | 1417 | 5 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -2 | 1 | 3 | 1453 | 1482 | 5 |
| -1 | 1 | 3 | 549 | 576 | 5 |
| 0 | 1 | 3 | 1679 | -1649 | 85 |
| 1 | 1 | 3 | 857 | -827 | 4 |
| 2 | 1 | 3 | 1199 | 1168 | 5 |
| 3 | 1 | 3 | 866 | -829 | 6 |
| 4 | 1 | 3 | 1652 | -1620 | 6 |
| 5 | 1 | 3 | 749 | 763 | 7 |
| 6 | 1 | 3 | 1452 | 1443 | 7 |
| 7 | 1 | 3 | 823 | -849 | 9 |
| 8 | 1 | 3 | 1106 | -1103 | 9 |
| 9 | 1 | 3 | 601 | 620 | 11 |
| 10 | 1 | 3 | 739 | 763 | 11 |
| 11 | 1 | 3 | 573 | -563 | 13 |
| 12 | 1 | 3 | 657 | -665 | 13 |
| 13 | 1 | 3 | 296 | 289 | 19 |
| 14 | 1 | 3 | 540 | 533 | 15 |
| -14 | 2 | 3 | 502 | -479 | 17 |
| -13 | 2 | 3 | 858 | -815 | 13 |
| -12 | 2 | 3 | 799 | 803 | 12 |
| -11 | 2 | 3 | 1003 | 1006 | 11 |
| -10 | 2 | 3 | 873 | -865 | 11 |
| -9 | 2 | 3 | 1097 | -1112 | 9 |
| -8 | 2 | 3 | 695 | 683 | 10 |
| -7 | 2 | 3 | 683 | 725 | 9 |
| -6 | 2 | 3 | 658 | -652 | 8 |
| -5 | 2 | 3 | 865 | -895 | 7 |
| -4 | 2 | 3 | 1528 | 1545 | 6 |
| -3 | 2 | 3 | 1754 | 1781 | 5 |
| -2 | 2 | 3 | 1186 | -1212 | 5 |
| -1 | 2 | 3 | 1579 | -1592 | 4 |
| 0 | 2 | 3 | 566 | 535 | 28 |
| 1 | 2 | 3 | 2188 | 2100 | 4 |
| 2 | 2 | 3 | 881 | -813 | 5 |
| 3 | 2 | 3 | 1500 | -1440 | 5 |
| 4 | 2 | 3 | 708 | 682 | 7 |
| 5 | 2 | 3 | 1715 | 1693 | 6 |
| 6 | 2 | 3 | 920 | -903 | 8 |
| 7 | 2 | 3 | 2206 | -2207 | 7 |
| 8 | 2 | 3 | 780 | 790 | 10 |
| 9 | 2 | 3 | 948 | 956 | 10 |
| 10 | 2 | 3 | 1372 | -1447 | 10 |
| 11 | 2 | 3 | 1213 | -1257 | 10 |
| 12 | 2 | 3 | 610 | 607 | 13 |
| 13 | 2 | 3 | 860 | 872 | 12 |
| 14 | 2 | 3 | 532 | -535 | 16 |
| -14 | 3 | 3 | 697 | -682 | 14 |
| -13 | 3 | 3 | 734 | 725 | 13 |
| -12 | 3 | 3 | 1104 | 1102 | 11 |
| -11 | 3 | 3 | 639 | -644 | 13 |
| -10 | 3 | 3 | 876 | -865 | 11 |
| -9 | 3 | 3 | 1152 | 1177 | 9 |
| -8 | 3 | 3 | 1214 | 1264 | 9 |
| -7 | 3 | 3 | 984 | -995 | 8 |
| -6 | 3 | 3 | 1808 | -1860 | 7 |
| -5 | 3 | 3 | 858 | 861 | 7 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -4 | 3 | 3 | 1079 | 1104 | 6 |
| -3 | 3 | 3 | 1487 | -1506 | 5 |
| -2 | 3 | 3 | 1629 | -1657 | 5 |
| -1 | 3 | 3 | 838 | 861 | 5 |
| 0 | 3 | 3 | 2909 | 2910 | 108 |
| 1 | 3 | 3 | 2450 | -2339 | 4 |
| 2 | 3 | 3 | 1838 | -1768 | 5 |
| 3 | 3 | 3 | 1360 | 1295 | 5 |
| 4 | 3 | 3 | 1469 | 1457 | 6 |
| 5 | 3 | 3 | 896 | -893 | 7 |
| 6 | 3 | 3 | 1862 | -1845 | 7 |
| 7 | 3 | 3 | 998 | 1028 | 8 |
| 8 | 3 | 3 | 1433 | 1452 | 8 |
| 9 | 3 | 3 | 519 | -527 | 12 |
| 10 | 3 | 3 | 1291 | -1310 | 10 |
| 11 | 3 | 3 | 562 | 589 | 13 |
| 12 | 3 | 3 | 1063 | 1056 | 11 |
| 13 | 3 | 3 | 427 | -400 | 16 |
| 14 | 3 | 3 | 792 | -772 | 14 |
| -14 | 4 | 3 | 416 | 399 | 18 |
| -13 | 4 | 3 | 640 | 648 | 15 |
| -12 | 4 | 3 | 490 | -491 | 16 |
| -11 | 4 | 3 | 838 | -837 | 11 |
| -10 | 4 | 3 | 164 | 151 | 24 |
| -9 | 4 | 3 | 753 | 779 | 11 |
| -8 | 4 | 3 | 748 | -752 | 9 |
| -7 | 4 | 3 | 1246 | -1256 | 8 |
| -6 | 4 | 3 | 820 | 845 | 8 |
| -5 | 4 | 3 | 1425 | 1404 | 7 |
| -4 | 4 | 3 | 527 | -540 | 8 |
| -3 | 4 | 3 | 874 | -836 | 6 |
| -2 | 4 | 3 | 131 | 77 | 17 |
| -1 | 4 | 3 | 425 | 416 | 7 |
| 0 | 4 | 3 | 598 | -579 | 29 |
| 1 | 4 | 3 | 1902 | -1820 | 5 |
| 2 | 4 | 3 | 1453 | 1377 | 5 |
| 3 | 4 | 3 | 1882 | 1803 | 5 |
| 4 | 4 | 3 | 1016 | -967 | 6 |
| 5 | 4 | 3 | 1279 | -1268 | 7 |
| 6 | 4 | 3 | 683 | 643 | 8 |
| 7 | 4 | 3 | 1055 | 1040 | 8 |
| 8 | 4 | 3 | 292 | -288 | 14 |
| 9 | 4 | 3 | 564 | -575 | 12 |
| 10 | 4 | 3 | 338 | 371 | 13 |
| 11 | 4 | 3 | 857 | 858 | 11 |
| 12 | 4 | 3 | 204 | -179 | 21 |
| 13 | 4 | 3 | 675 | -673 | 13 |
| 14 | 4 | 3 | 322 | 305 | 21 |
| -14 | 5 | 3 | 269 | 248 | 24 |
| -13 | 5 | 3 | 92 | -63 | 54 |
| -12 | 5 | 3 | 278 | -235 | 21 |
| -11 | 5 | 3 | 133 | -38 | 35 |
| -10 | 5 | 3 | 111 | 85 | 41 |
| -9 | 5 | 3 | 374 | -369 | 14 |
| -8 | 5 | 3 | 116 | -186 | 36 |
| -7 | 5 | 3 | 58 | 93 | 51 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -6 | 5 | 3 | 753 | 700 | 9 |
| -5 | 5 | 3 | 263 | 266 | 12 |
| -4 | 5 | 3 | 676 | -680 | 7 |
| -3 | 5 | 3 | 134 | -149 | 17 |
| -2 | 5 | 3 | 193 | 182 | 12 |
| -1 | 5 | 3 | 677 | 663 | 6 |
| 0 | 5 | 3 | 598 | -559 | 16 |
| 1 | 5 | 3 | 174 | 155 | 9 |
| 2 | 5 | 3 | 474 | 444 | 7 |
| 3 | 5 | 3 | 408 | 373 | 8 |
| 4 | 5 | 3 | 204 | -220 | 11 |
| 5 | 5 | 3 | 591 | 561 | 8 |
| 6 | 5 | 3 | 883 | 860 | 8 |
| 7 | 5 | 3 | 217 | -265 | 16 |
| 8 | 5 | 3 | 330 | -325 | 14 |
| 9 | 5 | 3 | 176 | 176 | 31 |
| 10 | 5 | 3 | 476 | 500 | 13 |
| 11 | 5 | 3 | 473 | -490 | 15 |
| 12 | 5 | 3 | 184 | -146 | 33 |
| 13 | 5 | 3 | 97 | 122 | 52 |
| 14 | 5 | 3 | 55 | 126 | 74 |
| -13 | 6 | 3 | 201 | 198 | 30 |
| -12 | 6 | 3 | 264 | -221 | 25 |
| -11 | 6 | 3 | 263 | -281 | 18 |
| -10 | 6 | 3 | 402 | 400 | 13 |
| -9 | 6 | 3 | 590 | 573 | 12 |
| -8 | 6 | 3 | 282 | -275 | 18 |
| -7 | 6 | 3 | 690 | -707 | 9 |
| -6 | 6 | 3 | 872 | 864 | 8 |
| -5 | 6 | 3 | 672 | 705 | 8 |
| -4 | 6 | 3 | 492 | -494 | 8 |
| -3 | 6 | 3 | 450 | -474 | 9 |
| -2 | 6 | 3 | 663 | -669 | 7 |
| -1 | 6 | 3 | 230 | 233 | 10 |
| 0 | 6 | 3 | 400 | -398 | 8 |
| 1 | 6 | 3 | 175 | -225 | 12 |
| 2 | 6 | 3 | 1299 | 1223 | 6 |
| 3 | 6 | 3 | 888 | 870 | 7 |
| 4 | 6 | 3 | 713 | -704 | 8 |
| 5 | 6 | 3 | 836 | -831 | 8 |
| 6 | 6 | 3 | 792 | 782 | 8 |
| 7 | 6 | 3 | 647 | 668 | 9 |
| 8 | 6 | 3 | 281 | -290 | 16 |
| 9 | 6 | 3 | 313 | -348 | 15 |
| 10 | 6 | 3 | 91 | -105 | 48 |
| 11 | 6 | 3 | 454 | 427 | 14 |
| 12 | 6 | 3 | 20 | 50 | 81 |
| 13 | 6 | 3 | 410 | -383 | 18 |
| -13 | 7 | 3 | 480 | -467 | 16 |
| -12 | 7 | 3 | 606 | -581 | 14 |
| -11 | 7 | 3 | 614 | 613 | 14 |
| -10 | 7 | 3 | 719 | 693 | 12 |
| -9 | 7 | 3 | 494 | -502 | 13 |
| -8 | 7 | 3 | 847 | -862 | 10 |
| -7 | 7 | 3 | 818 | 805 | 10 |
| -6 | 7 | 3 | 937 | 916 | 9 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 7 | 3 | 840 | -835 | 8 |
| -4 | 7 | 3 | 1364 | -1353 | 7 |
| -3 | 7 | 3 | 635 | 644 | 8 |
| -2 | 7 | 3 | 1450 | 1481 | 6 |
| -1 | 7 | 3 | 1624 | -1593 | 6 |
| 0 | 7 | 3 | 1297 | -1327 | 36 |
| 1 | 7 | 3 | 1683 | 1601 | 6 |
| 2 | 7 | 3 | 1924 | 1881 | 6 |
| 3 | 7 | 3 | 1075 | -1040 | 7 |
| 4 | 7 | 3 | 1211 | -1176 | 7 |
| 5 | 7 | 3 | 445 | 411 | 11 |
| 6 | 7 | 3 | 999 | 991 | 8 |
| 7 | 7 | 3 | 669 | -670 | 10 |
| 8 | 7 | 3 | 1301 | -1290 | 9 |
| 9 | 7 | 3 | 756 | 763 | 11 |
| 10 | 7 | 3 | 869 | 831 | 11 |
| 11 | 7 | 3 | 309 | -308 | 16 |
| 12 | 7 | 3 | 875 | -872 | 12 |
| 13 | 7 | 3 | 378 | 374 | 18 |
| -12 | 8 | 3 | 482 | 461 | 16 |
| -11 | 8 | 3 | 745 | 726 | 12 |
| -10 | 8 | 3 | 611 | -574 | 13 |
| -9 | 8 | 3 | 873 | -890 | 11 |
| -8 | 8 | 3 | 950 | 939 | 10 |
| -7 | 8 | 3 | 1274 | 1285 | 9 |
| -6 | 8 | 3 | 1035 | -1013 | 9 |
| -5 | 8 | 3 | 1538 | -1553 | 8 |
| -4 | 8 | 3 | 1328 | 1317 | 8 |
| -3 | 8 | 3 | 1955 | 1960 | 7 |
| -2 | 8 | 3 | 1329 | -1319 | 7 |
| -1 | 8 | 3 | 2184 | -2241 | 7 |
| 0 | 8 | 3 | 1152 | 1122 | 24 |
| 1 | 8 | 3 | 1839 | 1830 | 7 |
| 2 | 8 | 3 | 970 | -926 | 7 |
| 3 | 8 | 3 | 1710 | -1665 | 7 |
| 4 | 8 | 3 | 346 | 306 | 11 |
| 5 | 8 | 3 | 1365 | 1339 | 8 |
| 6 | 8 | 3 | 761 | -729 | 9 |
| 7 | 8 | 3 | 1273 | -1256 | 9 |
| 8 | 8 | 3 | 770 | 790 | 11 |
| 9 | 8 | 3 | 1207 | 1180 | 10 |
| 10 | 8 | 3 | 387 | -406 | 15 |
| 11 | 8 | 3 | 836 | -821 | 12 |
| 12 | 8 | 3 | 426 | 438 | 16 |
| -12 | 9 | 3 | 549 | 543 | 15 |
| -11 | 9 | 3 | 486 | -485 | 15 |
| -10 | 9 | 3 | 815 | -802 | 12 |
| -9 | 9 | 3 | 464 | 455 | 14 |
| -8 | 9 | 3 | 1188 | 1176 | 10 |
| -7 | 9 | 3 | 786 | -774 | 10 |
| -6 | 9 | 3 | 1016 | -1042 | 9 |
| -5 | 9 | 3 | 974 | 963 | 9 |
| -4 | 9 | 3 | 1134 | 1113 | 8 |
| -3 | 9 | 3 | 860 | -887 | 8 |
| -2 | 9 | 3 | 1214 | -1191 | 8 |
| -1 | 9 | 3 | 835 | 841 | 8 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$ 

| 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 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 9 | 3 | 1024 | 1019 | 29 | -7 | 12 | 3 | 678 | -683 | 12 | -10 | 0 | 4 | 415 | -403 | 13 | -12 | 2 | 4 | 300 | -324 | 17 | -12 | 4 | 4 | 284 | -278 | 19 |
| 1 | 9 | 3 | 522 | -498 | 9 | -6 | 12 | 3 | 318 | 287 | 18 | -9 | 0 | 4 | 1292 | -1319 | 9 | -11 | 2 | 4 | 601 | -595 | 13 | -11 | 4 | 4 | 687 | -686 | 12 |
| 2 | 9 | 3 | 1428 | -1385 | 7 | -5 | 12 | 3 | 649 | 648 | 12 | -8 | 0 | 4 | 940 | 920 | 9 | -10 | 2 | 4 | 242 | 244 | 19 | -10 | 4 | 4 | 129 | 97 | 35 |
| 3 | 9 | 3 | 350 | 317 | 10 | -4 | 12 | 3 | 299 | -298 | 16 | -7 | 0 | 4 | 2299 | 2357 | 7 | -9 | 2 | 4 | 743 | 782 | 11 | -9 | 4 | 4 | 1046 | 1057 | 10 |
| 4 | 9 | 3 | 1074 | 1015 | 8 | -3 | 12 | 3 | 556 | -522 | 12 | -6 | 0 | 4 | 135 | -99 | 23 | -8 | 2 | 4 | 205 | -176 | 17 | -8 | 4 | 4 | 120 | -63 | 33 |
| 5 | 9 | 3 | 674 | -644 | 10 | -2 | 12 | 3 | 469 | 445 | 12 | -5 | 0 | 4 | 2162 | -2210 | 6 | -7 | 2 | 4 | 950 | -1009 | 8 | -7 | 4 | 4 | 1339 | -1345 | 8 |
| 6 | 9 | 3 | 1186 | -1165 | 9 | -1 | 12 | 3 | 738 | 717 | 10 | -4 | 0 | 4 | 192 | -192 | 11 | -6 | 2 | 4 | 232 | 198 | 14 | -6 | 4 | 4 | 119 | 101 | 27 |
| 7 | 9 | 3 | 370 | 375 | 16 | 0 | 12 | 3 | 574 | -570 | 17 | -3 | 0 | 4 | 1720 | 1739 | 5 | -5 | 2 | 4 | 554 | 570 | 8 | -5 | 4 | 4 | 1247 | 1234 | 7 |
| 8 | 9 | 3 | 779 | 731 | 10 | 1 | 12 | 3 | 372 | -330 | 13 | -2 | 0 | 4 | 798 | -819 | 5 | -4 | 2 | 4 | 514 | -512 | 7 | -4 | 4 | 4 | 283 | -288 | 9 |
| 9 | 9 | 3 | 364 | -366 | 15 | 2 | 12 | 3 | 720 | 689 | 10 | -1 | 0 | 4 | 3256 | -3525 | 4 | -3 | 2 | 4 | 564 | -569 | 7 | -3 | 4 | 4 | 1573 | -1555 | 6 |
| 10 | 9 | 3 | 478 | -455 | 14 | 3 | 12 | 3 | 301 | 253 | 15 | 0 | 0 | 4 | 552 | -569 | 24 | -2 | 2 | 4 | 870 | 900 | 5 | -2 | 4 | 4 | 697 | 701 | 6 |
| 11 | 9 | 3 | 239 | 226 | 23 | 4 | 12 | 3 | 602 | -601 | 11 | 1 | 0 | 4 | 2136 | 2027 | 4 | -1 | 2 | 4 | 1436 | 1482 | 5 | -1 | 4 | 4 | 1499 | 1519 | 5 |
| -11 | 10 | 3 | 372 | -349 | 17 | 5 | 12 | 3 | 417 | -387 | 13 | 2 | 0 | 4 | 1728 | -1685 | 5 | 0 | 2 | 4 | 239 | -218 | 28 | 0 | 4 | 4 | 891 | -860 | 46 |
| -10 | 10 | 3 | 126 | 161 | 43 | 6 | 12 | 3 | 416 | 379 | 14 | 3 | 0 | 4 | 3511 | -3501 | 5 | 1 | 2 | 4 | 223 | 157 | 9 | 1 | 4 | 4 | 389 | -336 | 7 |
| -9 | 10 | 3 | 645 | 620 | 13 | 7 | 12 | 3 | 744 | 709 | 11 | 4 | 0 | 4 | 342 | 282 | 10 | 2 | 2 | 4 | 621 | 582 | 6 | 2 | 4 | 4 | 1569 | 1482 | 5 |
| -8 | 10 | 3 | 295 | -267 | 17 | 8 | 12 | 3 | 288 | -307 | 18 | 5 | 0 | 4 | 2308 | 2297 | 6 | 3 | 2 | 4 | 722 | 672 | 6 | 3 | 4 | 4 | 861 | 835 | 6 |
| -7 | 10 | 3 | 705 | -676 | 12 | 9 | 12 | 3 | 648 | -617 | 13 | 6 | 0 | 4 | 365 | 340 | 11 | 4 | 2 | 4 | 661 | -658 | 7 | 4 | 4 | 4 | 275 | -258 | 11 |
| -6 | 10 | 3 | 132 | 83 | 34 | -7 | 13 | 3 | 373 | 361 | 17 | 7 | 0 | 4 | 1362 | -1434 | 8 | 5 | 2 | 4 | 1822 | -1727 | 6 | 5 | 4 | 4 | 774 | -765 | 7 |
| -5 | 10 | 3 | 606 | 542 | 11 | -6 | 13 | 3 | 873 | 886 | 12 | 8 | 0 | 4 | 128 | -32 | 30 | 7 | 2 | 4 | 1333 | 1314 | 8 | 6 | 4 | 4 | 819 | 815 | 8 |
| -4 | 10 | 3 | 225 | -238 | 19 | -5 | 13 | 3 | 644 | -638 | 12 | 9 | 0 | 4 | 1215 | 1241 | 9 | 8 | 2 | 4 | 123 | 66 | 32 | 7 | 4 | 4 | 1283 | 1289 | 8 |
| -3 | 10 | 3 | 866 | -820 | 9 | -4 | 13 | 3 | 866 | -863 | 11 | 10 | 0 | 4 | 598 | -643 | 12 | 9 | 2 | 4 | 1260 | -1268 | 9 | 8 | 4 | 4 | 129 | -96 | 34 |
| -2 | 10 | 3 | 408 | 401 | 12 | -3 | 13 | 3 | 571 | 565 | 12 | 11 | 0 | 4 | 1390 | -1432 | 10 | 10 | 2 | 4 | 172 | -165 | 22 | 9 | 4 | 4 | 818 | -830 | 10 |
| -1 | 10 | 3 | 944 | 928 | 9 | -2 | 13 | 3 | 986 | 1010 | 10 | 12 | 0 | 4 | 280 | 294 | 18 | 11 | 2 | 4 | 865 | 881 | 11 | 10 | 4 | 4 | 93 | -111 | 46 |
| 0 | 10 | 3 | 660 | -618 | 20 | -1 | 13 | 3 | 495 | -502 | 14 | 13 | 0 | 4 | 1263 | 1271 | 11 | 12 | 2 | 4 | 222 | 238 | 26 | 11 | 4 | 4 | 958 | 997 | 11 |
| 1 | 10 | 3 | 496 | -470 | 10 | 0 | 13 | 3 | 1125 | -1141 | 8 | 14 | 0 | 4 | 160 | -135 | 39 | 13 | 2 | 4 | 429 | -414 | 21 | 12 | 4 | 4 | 147 | -112 | 28 |
| 2 | 10 | 3 | 827 | 787 | 9 | 1 | 13 | 3 | 682 | 689 | 11 | -14 | 1 | 4 | 781 | -748 | 14 | 14 | 2 | 4 | 73 | -14 | 63 | 13 | 4 | 4 | 737 | -743 | 14 |
| 3 | 10 | 3 | 416 | 371 | 12 | 2 | 13 | 3 | 1139 | 1161 | 10 | -13 | 1 | 4 | 185 | 194 | 26 | -14 | 3 | 4 | 132 | -84 | 44 | 14 | 4 | 4 | 109 | 93 | 51 |
| 4 | 10 | 3 | 465 | -433 | 11 | 3 | 13 | 3 | 600 | -585 | 13 | -12 | 1 | 4 | 1068 | 1054 | 11 | -13 | 3 | 4 | 166 | 122 | 35 | -14 | 5 | 4 | 951 | 906 | 13 |
| 5 | 10 | 3 | 722 | -704 | 10 | 4 | 13 | 3 | 1005 | -1021 | 11 | -11 | 1 | 4 | 300 | -343 | 16 | -12 | 3 | 4 | 94 | 34 | 51 | -13 | 5 | 4 | 307 | -355 | 19 |
| 6 | 10 | 3 | 294 | 295 | 14 | 5 | 13 | 3 | 525 | 543 | 14 | -10 | 1 | 4 | 1037 | -1037 | 10 | -11 | 3 | 4 | 181 | 59 | 32 | -12 | 5 | 4 | 948 | -915 | 12 |
| 7 | 10 | 3 | 353 | 364 | 15 | 6 | 13 | 3 | 949 | 931 | 11 | -9 | 1 | 4 | 221 | 221 | 16 | -10 | 3 | 4 | 259 | -272 | 17 | -11 | 5 | 4 | 364 | 332 | 18 |
| 8 | 10 | 3 | 214 | -218 | 20 | 7 | 13 | 3 | 503 | -450 | 14 | -8 | 1 | 4 | 1139 | 1148 | 8 | -9 | 3 | 4 | 89 | -130 | 45 | -10 | 5 | 4 | 1159 | 1163 | 10 |
| 9 | 10 | 3 | 481 | -458 | 14 | -6 | 14 | 3 | 589 | -599 | 14 | -7 | 1 | 4 | 949 | -961 | 8 | -8 | 3 | 4 | 234 | 238 | 19 | -9 | 5 | 4 | 178 | -109 | 22 |
| 11 | 10 | 3 | 426 | 433 | 14 | -5 | 14 | 3 | 849 | -880 | 12 | -6 | 1 | 4 | 1164 | -1233 | 7 | -7 | 3 | 4 | 79 | -1 | 39 | -8 | 5 | 4 | 1531 | -1538 | 8 |
| -10 | 11 | 3 | 132 | 8 | 42 | -4 | 14 | 3 | 615 | 642 | 13 | -5 | 1 | 4 | 621 | 623 | 8 | -6 | 3 | 4 | 298 | -310 | 12 | -7 | 5 | 4 | 265 | 264 | 13 |
| -9 | 11 | 3 | 278 | 270 | 21 | -3 | 14 | 3 | 872 | 878 | 12 | -4 | 1 | 4 | 1256 | 1306 | 6 | -5 | 3 | 4 | 524 | 551 | 8 | -6 | 5 | 4 | 1883 | 1862 | 7 |
| -8 | 11 | 3 | 198 | -29 | 25 | -2 | 14 | 3 | 510 | -481 | 14 | -3 | 1 | 4 | 579 | -596 | 6 | -4 | 3 | 4 | 284 | 257 | 10 | -5 | 5 | 4 | 448 | -422 | 9 |
| -7 | 11 | 3 | 121 | -139 | 36 | -1 | 14 | 3 | 909 | -966 | 11 | -2 | 1 | 4 | 1456 | -1490 | 5 | -3 | 3 | 4 | 433 | 405 | 7 | -4 | 5 | 4 | 1880 | -1879 | 6 |
| -6 | 11 | 3 | 254 | -175 | 19 | 0 | 14 | 3 | 530 | 516 | 11 | -1 | 1 | 4 | 923 | 946 | 5 | -2 | 3 | 4 | 91 | 27 | 23 | -3 | 5 | 4 | 330 | 358 | 9 |
| -5 | 11 | 3 | 426 | 429 | 13 | 1 | 14 | 3 | 910 | 937 | 11 | 0 | 1 | 4 | 1495 | 1470 | 60 | -1 | 3 | 4 | 978 | -984 | 5 | -2 | 5 | 4 | 2281 | 2308 | 6 |
| -4 | 11 | 3 | 289 | 199 | 17 | 2 | 14 | 3 | 474 | -480 | 14 | 1 | 1 | 4 | 294 | 285 | 8 | 0 | 3 | 4 | 688 | 665 | 36 | -1 | 5 | 4 | 541 | -544 | 7 |
| -3 | 11 | 3 | 409 | -428 | 12 | 3 | 14 | 3 | 977 | -999 | 11 | 2 | 1 | 4 | 1287 | -1237 | 5 | 1 | 3 | 4 | 328 | 315 | 7 | 0 | 5 | 4 | 2419 | -2356 | 92 |
| -2 | 11 | 3 | 241 | -72 | 13 | 4 | 14 | 3 | 464 | 467 | 14 | 3 | 1 | 4 | 175 | 141 | 12 | 2 | 3 | 4 | 233 | -220 | 8 | 1 | 5 | 4 | 1321 | 1209 | 6 |
| -1 | 11 | 3 | 155 | 179 | 32 | 5 | 14 | 3 | 809 | 811 | 12 | 4 | 1 | 4 | 1771 | 1720 | 6 | 3 | 3 | 4 | 617 | 598 | 6 | 2 | 5 | 4 | 1714 | 1631 | 6 |
| 0 | 11 | 3 | 335 | 338 | 15 | 6 | 14 | 3 | 323 | -381 | 16 | 5 | 1 | 4 | 921 | -894 | 7 | 4 | 3 | 4 | 214 | 237 | 10 | 3 | 5 | 4 | 257 | -257 | 10 |
| 1 | 11 | 3 | 196 | -45 | 15 | -3 | 15 | 3 | 424 | -417 | 16 | 6 | 1 | 4 | 1729 | -1714 | 7 | 5 | 3 | 4 | 665 | -640 | 8 | 4 | 5 | 4 | 1637 | -1581 | 6 |
| 2 | 11 | 3 | 410 | -408 | 12 | -2 | 15 | 3 | 660 | -657 | 13 | 7 | 1 | 4 | 513 | 511 | 11 | 6 | 3 | 4 | 582 | -606 | 9 | 5 | 5 | 4 | 236 | -182 | 14 |
| 3 | 11 | 3 | 189 | -46 | 20 | -1 | 15 | 3 | 414 | 422 | 16 | 8 | 1 | 4 | 1231 | 1204 | 9 | 7 | 3 | 4 | 182 | 189 | 17 | 6 | 5 | 4 | 1975 | 1921 | 7 |
| 4 | 11 | 3 | 432 | 412 | 12 | 0 | 15 | 3 | 516 | 499 | 13 | 9 | 1 | 4 | 220 | -212 | 18 | 8 | 3 | 4 | 34 | 9 | 37 | 7 | 5 | 4 | 153 | -177 | 24 |
| 5 | 11 | 3 | 240 | 199 | 15 | 1 | 15 | 3 | 432 | -450 | 15 | 10 | 1 | 4 | 1401 | -1419 | 10 | 9 | 3 | 4 | 491 | -493 | 12 | 8 | 5 | 4 | 1626 | -1612 | 8 |
| 6 | 11 | 3 | 220 | -179 | 22 | 2 | 15 | 3 | 566 | -572 | 15 | 11 | 1 | 4 | 483 | 510 | 16 | 10 | 3 | 4 | 168 | 120 | 22 | 9 | 5 | 4 | 179 | 154 | 24 |
| 7 | 11 | 3 | 209 | -60 | 22 | 3 | 15 | 3 | 285 | 314 | 17 | 12 | 1 | 4 | 1230 | 1254 | 11 | 11 | 3 | 4 | 172 | 162 | 24 | 10 | 5 | 4 | 1295 | 1283 | 10 |
| 8 | 11 | 3 | 171 | 125 | 33 | -14 | 0 | 4 | 332 | -339 | 18 | 13 | 1 | 4 | 157 | -155 | 38 | 12 | 3 | 4 | 248 | 227 | 26 | 11 | 5 | 4 | 90 | -17 | 48 |
| 9 | 11 | 3 | 111 | -64 | 47 | -13 | 0 | 4 | 1048 | -1018 | 12 | 14 | 1 | 4 | 890 | -888 | 14 | 14 | 3 | 4 | 201 | -215 | 24 | 12 | 5 | 4 | 1052 | -1080 | 11 |
| -9 | 12 | 3 | 343 | 282 | 22 | -12 | 0 | 4 | 313 | 316 | 19 | -14 | 2 | 4 | 109 | 151 | 50 | -14 | 4 | 4 | 87 | 131 | 60 | 13 | 5 | 4 | 71 | 66 | 62 |
| -8 | 12 | 3 | 309 | -323 | 17 | -11 | 0 | 4 | 1097 | 1098 | 11 | -13 | 2 | 4 | 503 | 473 | 16 | -13 | 4 | 4 | 682 | 665 | 14 | -13 | 6 | 4 | 765 | -757 | 14 |

J.5385-MQS

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -12 | 6 | 4 | 403 | 412 | 16 |
| -11 | 6 | 4 | 1019 | 994 | 11 |
| -10 | 6 | 4 | 341 | -336 | 16 |
| -9 | 6 | 4 | 1316 | -1318 | 10 |
| -8 | 6 | 4 | 445 | 433 | 12 |
| -7 | 6 | 4 | 1218 | 1225 | 8 |
| -6 | 6 | 4 | 436 | -437 | 11 |
| -5 | 6 | 4 | 1484 | -1474 | 7 |
| -4 | 6 | 4 | 614 | 634 | 8 |
| -3 | 6 | 4 | 1683 | 1713 | 6 |
| -2 | 6 | 4 | 861 | -847 | 7 |
| -1 | 6 | 4 | 1977 | -2029 | 6 |
| 0 | 6 | 4 | 45 | -19 | 43 |
| 1 | 6 | 4 | 2538 | 2429 | 6 |
| 2 | 6 | 4 | 227 | -203 | 11 |
| 3 | 6 | 4 | 2251 | -2114 | 6 |
| 4 | 6 | 4 | 125 | -23 | 20 |
| 5 | 6 | 4 | 2051 | 1983 | 7 |
| 6 | 6 | 4 | 207 | -223 | 23 |
| 7 | 6 | 4 | 1596 | -1574 | 8 |
| 8 | 6 | 4 | 464 | 485 | 12 |
| 9 | 6 | 4 | 1227 | 1227 | 9 |
| 10 | 6 | 4 | 98 | -134 | 47 |
| 11 | 6 | 4 | 1234 | -1220 | 11 |
| 12 | 6 | 4 | 156 | 79 | 36 |
| 13 | 6 | 4 | 843 | 823 | 13 |
| -13 | 7 | 4 | 265 | 271 | 23 |
| -12 | 7 | 4 | 642 | 616 | 14 |
| -11 | 7 | 4 | 138 | -169 | 22 |
| -10 | 7 | 4 | 613 | -573 | 12 |
| -9 | 7 | 4 | 356 | 368 | 13 |
| -8 | 7 | 4 | 813 | 793 | 10 |
| -7 | 7 | 4 | 522 | -539 | 11 |
| -6 | 7 | 4 | 1270 | -1259 | 8 |
| -5 | 7 | 4 | 159 | 144 | 18 |
| -4 | 7 | 4 | 1080 | 1061 | 7 |
| -3 | 7 | 4 | 277 | -314 | 12 |
| -2 | 7 | 4 | 1284 | -1303 | 7 |
| -1 | 7 | 4 | 364 | -354 | 10 |
| 0 | 7 | 4 | 2005 | 1949 | 61 |
| 1 | 7 | 4 | 159 | 156 | 16 |
| 2 | 7 | 4 | 1887 | -1782 | 6 |
| 3 | 7 | 4 | 132 | 156 | 19 |
| 4 | 7 | 4 | 1206 | 1132 | 7 |
| 6 | 7 | 4 | 1029 | -1008 | 8 |
| 7 | 7 | 4 | 357 | 351 | 13 |
| 8 | 7 | 4 | 1116 | 1109 | 9 |
| 9 | 7 | 4 | 87 | -85 | 48 |
| 10 | 7 | 4 | 743 | -731 | 12 |
| 11 | 7 | 4 | 95 | 30 | 50 |
| 12 | 7 | 4 | 599 | 601 | 14 |
| 13 | 7 | 4 | 21 | -69 | 83 |
| -12 | 8 | 4 | 117 | -72 | 46 |
| -11 | 8 | 4 | 242 | -227 | 20 |
| -10 | 8 | 4 | 134 | 20 | 36 |
| -9 | 8 | 4 | 242 | 219 | 21 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -8 | 8 | 4 | 272 | -273 | 16 |
| -7 | 8 | 4 | 167 | -42 | 23 |
| -6 | 8 | 4 | 134 | -177 | 31 |
| -5 | 8 | 4 | 214 | 180 | 21 |
| -4 | 8 | 4 | 405 | 402 | 11 |
| -3 | 8 | 4 | 275 | 144 | 11 |
| -2 | 8 | 4 | 163 | -134 | 28 |
| -1 | 8 | 4 | 356 | -512 | 14 |
| 0 | 8 | 4 | 487 | 486 | 8 |
| 1 | 8 | 4 | 143 | 77 | 17 |
| 3 | 8 | 4 | 217 | -228 | 15 |
| 4 | 8 | 4 | 421 | -395 | 11 |
| 5 | 8 | 4 | 565 | -552 | 10 |
| 6 | 8 | 4 | 294 | -315 | 13 |
| 7 | 8 | 4 | 197 | 167 | 19 |
| 9 | 8 | 4 | 110 | -102 | 41 |
| 10 | 8 | 4 | 119 | -28 | 40 |
| 11 | 8 | 4 | 268 | 234 | 18 |
| -12 | 9 | 4 | 365 | 350 | 20 |
| -11 | 9 | 4 | 128 | -163 | 31 |
| -10 | 9 | 4 | 528 | -505 | 15 |
| -9 | 9 | 4 | 225 | 168 | 30 |
| -8 | 9 | 4 | 590 | 584 | 12 |
| -7 | 9 | 4 | 65 | 35 | 55 |
| -6 | 9 | 4 | 558 | -571 | 11 |
| -5 | 9 | 4 | 166 | 140 | 22 |
| -4 | 9 | 4 | 744 | 720 | 9 |
| -3 | 9 | 4 | 122 | 94 | 30 |
| -2 | 9 | 4 | 919 | -893 | 9 |
| -1 | 9 | 4 | 124 | -112 | 28 |
| 0 | 9 | 4 | 583 | 556 | 97 |
| 1 | 9 | 4 | 311 | -309 | 11 |
| 2 | 9 | 4 | 908 | -876 | 8 |
| 3 | 9 | 4 | 210 | 207 | 17 |
| 4 | 9 | 4 | 805 | 754 | 9 |
| 5 | 9 | 4 | 399 | -415 | 11 |
| 6 | 9 | 4 | 572 | -549 | 10 |
| 7 | 9 | 4 | 139 | 169 | 32 |
| 8 | 9 | 4 | 524 | 545 | 12 |
| 9 | 9 | 4 | 169 | -93 | 43 |
| 10 | 9 | 4 | 365 | -372 | 16 |
| -11 | 10 | 4 | 815 | -798 | 13 |
| -10 | 10 | 4 | 275 | 275 | 20 |
| -9 | 10 | 4 | 911 | 872 | 12 |
| -8 | 10 | 4 | 152 | -178 | 30 |
| -7 | 10 | 4 | 1204 | -1189 | 10 |
| -6 | 10 | 4 | 519 | 531 | 12 |
| -5 | 10 | 4 | 1224 | 1236 | 9 |
| -4 | 10 | 4 | 128 | -179 | 26 |
| -3 | 10 | 4 | 1193 | -1195 | 9 |
| -2 | 10 | 4 | 220 | -236 | 17 |
| -1 | 10 | 4 | 1461 | 1410 | 8 |
| 0 | 10 | 4 | 415 | -386 | 28 |
| 1 | 10 | 4 | 1774 | -1721 | 8 |
| 2 | 10 | 4 | 170 | -130 | 15 |
| 3 | 10 | 4 | 1526 | 1472 | 8 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 4 | 10 | 4 | 65 | 123 | 52 |
| 5 | 10 | 4 | 1080 | -995 | 9 |
| 6 | 10 | 4 | 302 | 296 | 14 |
| 7 | 10 | 4 | 1166 | 1135 | 10 |
| 8 | 10 | 4 | 110 | -135 | 42 |
| 9 | 10 | 4 | 920 | -918 | 11 |
| 10 | 10 | 4 | 224 | 201 | 22 |
| 11 | 10 | 4 | 696 | 677 | 13 |
| -10 | 11 | 4 | 826 | 814 | 13 |
| -9 | 11 | 4 | 292 | -304 | 17 |
| -8 | 11 | 4 | 1066 | -1057 | 11 |
| -7 | 11 | 4 | 239 | 286 | 19 |
| -6 | 11 | 4 | 1327 | 1353 | 10 |
| -5 | 11 | 4 | 208 | -215 | 20 |
| -4 | 11 | 4 | 1306 | -1273 | 9 |
| -3 | 11 | 4 | 188 | 164 | 19 |
| -2 | 11 | 4 | 1362 | 1343 | 9 |
| -1 | 11 | 4 | 216 | -205 | 17 |
| 0 | 11 | 4 | 1156 | -1107 | 22 |
| 1 | 11 | 4 | 499 | 486 | 11 |
| 2 | 11 | 4 | 1400 | 1342 | 9 |
| 3 | 11 | 4 | 201 | -190 | 21 |
| 4 | 11 | 4 | 1367 | -1299 | 9 |
| 5 | 11 | 4 | 191 | 189 | 28 |
| 6 | 11 | 4 | 1115 | 1121 | 10 |
| 7 | 11 | 4 | 217 | -188 | 24 |
| 8 | 11 | 4 | 1059 | -1056 | 10 |
| 9 | 11 | 4 | 120 | 95 | 42 |
| 10 | 11 | 4 | 854 | 831 | 12 |
| -9 | 12 | 4 | 704 | -668 | 14 |
| -8 | 12 | 4 | 143 | -116 | 38 |
| -7 | 12 | 4 | 767 | 762 | 12 |
| -6 | 12 | 4 | 210 | -205 | 21 |
| -5 | 12 | 4 | 823 | -853 | 11 |
| -4 | 12 | 4 | 233 | 229 | 20 |
| -3 | 12 | 4 | 1064 | 1099 | 10 |
| -2 | 12 | 4 | 124 | 95 | 35 |
| -1 | 12 | 4 | 990 | -942 | 10 |
| 0 | 12 | 4 | 265 | 267 | 14 |
| 1 | 12 | 4 | 1011 | 974 | 10 |
| 2 | 12 | 4 | 214 | -42 | 26 |
| 3 | 12 | 4 | 694 | -674 | 11 |
| 4 | 12 | 4 | 164 | 120 | 18 |
| 5 | 12 | 4 | 765 | 729 | 10 |
| 6 | 12 | 4 | 90 | -143 | 31 |
| 7 | 12 | 4 | 795 | -776 | 11 |
| 8 | 12 | 4 | 56 | 107 | 68 |
| 9 | 12 | 4 | 660 | 611 | 13 |
| -7 | 13 | 4 | 188 | 187 | 33 |
| -6 | 13 | 4 | 310 | -273 | 20 |
| -5 | 13 | 4 | 123 | -132 | 41 |
| -4 | 13 | 4 | 386 | 418 | 15 |
| -3 | 13 | 4 | 124 | 14 | 39 |
| -2 | 13 | 4 | 436 | -412 | 15 |
| 0 | 13 | 4 | 410 | 385 | 11 |
| 2 | 13 | 4 | 383 | -363 | 16 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 3 | 13 | 4 | 130 | 110 | 43 |
| 4 | 13 | 4 | 330 | 318 | 17 |
| 5 | 13 | 4 | 96 | -37 | 50 |
| 6 | 13 | 4 | 283 | -234 | 19 |
| 7 | 13 | 4 | 130 | 74 | 41 |
| -5 | 14 | 4 | 297 | -287 | 21 |
| -3 | 14 | 4 | 217 | 222 | 24 |
| -2 | 14 | 4 | 106 | -117 | 46 |
| -1 | 14 | 4 | 370 | -379 | 18 |
| 1 | 14 | 4 | 211 | 250 | 25 |
| 2 | 14 | 4 | 40 | 146 | 79 |
| 3 | 14 | 4 | 297 | -240 | 20 |
| 5 | 14 | 4 | 341 | 328 | 21 |
| -2 | 15 | 4 | 680 | -680 | 15 |
| 0 | 15 | 4 | 600 | 575 | 10 |
| 1 | 15 | 4 | 210 | -227 | 30 |
| 2 | 15 | 4 | 661 | -646 | 13 |
| -14 | 1 | 5 | 550 | -472 | 17 |
| -13 | 1 | 5 | 75 | 32 | 59 |
| -12 | 1 | 5 | 720 | 686 | 12 |
| -11 | 1 | 5 | 310 | -316 | 16 |
| -10 | 1 | 5 | 840 | -825 | 11 |
| -9 | 1 | 5 | 235 | 201 | 18 |
| -8 | 1 | 5 | 1335 | 1347 | 8 |
| -7 | 1 | 5 | 538 | 544 | 10 |
| -6 | 1 | 5 | 1528 | -1536 | 7 |
| -5 | 1 | 5 | 684 | -651 | 8 |
| -4 | 1 | 5 | 910 | 929 | 6 |
| -3 | 1 | 5 | 675 | -704 | 6 |
| -2 | 1 | 5 | 748 | -763 | 6 |
| -1 | 1 | 5 | 707 | 748 | 5 |
| 0 | 1 | 5 | 1203 | 1188 | 52 |
| 1 | 1 | 5 | 617 | -609 | 6 |
| 2 | 1 | 5 | 1578 | -1515 | 5 |
| 3 | 1 | 5 | 325 | -306 | 8 |
| 4 | 1 | 5 | 136 | 38 | 19 |
| 6 | 1 | 5 | 889 | -868 | 8 |
| 7 | 1 | 5 | 56 | 97 | 50 |
| 8 | 1 | 5 | 1041 | 1029 | 9 |
| 9 | 1 | 5 | 129 | 75 | 34 |
| 10 | 1 | 5 | 517 | -495 | 12 |
| 11 | 1 | 5 | 249 | -244 | 32 |
| 12 | 1 | 5 | 573 | 552 | 14 |
| 13 | 1 | 5 | 190 | 174 | 36 |
| 14 | 1 | 5 | 550 | -551 | 16 |
| -14 | 2 | 5 | 138 | -123 | 32 |
| -13 | 2 | 5 | 924 | 899 | 13 |
| -12 | 2 | 5 | 51 | -32 | 68 |
| -11 | 2 | 5 | 1142 | -1117 | 11 |
| -10 | 2 | 5 | 253 | 273 | 18 |
| -9 | 2 | 5 | 1293 | 1291 | 9 |
| -8 | 2 | 5 | 144 | -185 | 30 |
| -7 | 2 | 5 | 1218 | -1216 | 8 |
| -6 | 2 | 5 | 173 | 189 | 14 |
| -5 | 2 | 5 | 1711 | 1768 | 7 |
| -4 | 2 | 5 | 39 | -95 | 47 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -3 | 2 | 5 | 1611 | -1662 | 6 |
| -2 | 2 | 5 | 38 | 11 | 42 |
| -1 | 2 | 5 | 2513 | 2620 | 5 |
| 0 | 2 | 5 | 1345 | 1338 | 70 |
| 1 | 2 | 5 | 2014 | -1933 | 5 |
| 2 | 2 | 5 | 531 | 503 | 6 |
| 3 | 2 | 5 | 1037 | 966 | 6 |
| 4 | 2 | 5 | 217 | -212 | 11 |
| 5 | 2 | 5 | 1678 | -1653 | 7 |
| 6 | 2 | 5 | 159 | -162 | 16 |
| 7 | 2 | 5 | 2148 | 2147 | 8 |
| 8 | 2 | 5 | 102 | 80 | 38 |
| 9 | 2 | 5 | 1338 | -1338 | 9 |
| 11 | 2 | 5 | 1291 | 1302 | 10 |
| 12 | 2 | 5 | 166 | 204 | 30 |
| 13 | 2 | 5 | 916 | -928 | 12 |
| -14 | 3 | 5 | 918 | 877 | 13 |
| -13 | 3 | 5 | 150 | 150 | 39 |
| -12 | 3 | 5 | 1124 | -1098 | 11 |
| -11 | 3 | 5 | 152 | -157 | 22 |
| -10 | 3 | 5 | 939 | 960 | 10 |
| -9 | 3 | 5 | 132 | 203 | 34 |
| -8 | 3 | 5 | 1489 | -1492 | 9 |
| -7 | 3 | 5 | 98 | 121 | 34 |
| -6 | 3 | 5 | 1398 | 1435 | 7 |
| -5 | 3 | 5 | 131 | 65 | 20 |
| -4 | 3 | 5 | 1242 | -1334 | 6 |
| -2 | 3 | 5 | 2404 | 2501 | 5 |
| 0 | 3 | 5 | 2460 | -2427 | 126 |
| 1 | 3 | 5 | 305 | -300 | 8 |
| 2 | 3 | 5 | 3259 | 3166 | 5 |
| 3 | 3 | 5 | 534 | 504 | 7 |
| 4 | 3 | 5 | 2422 | -2401 | 6 |
| 5 | 3 | 5 | 769 | -738 | 8 |
| 6 | 3 | 5 | 2106 | 2079 | 7 |
| 7 | 3 | 5 | 641 | 649 | 9 |
| 8 | 3 | 5 | 1462 | -1470 | 9 |
| 9 | 3 | 5 | 168 | -166 | 23 |
| 10 | 3 | 5 | 1274 | 1320 | 10 |
| 11 | 3 | 5 | 224 | 235 | 26 |
| 12 | 3 | 5 | 1233 | -1214 | 11 |
| 13 | 3 | 5 | 172 | -141 | 29 |
| 14 | 3 | 5 | 891 | 884 | 13 |
| -14 | 4 | 5 | 99 | 88 | 54 |
| -13 | 4 | 5 | 771 | -759 | 12 |
| -12 | 4 | 5 | 298 | -325 | 19 |
| -11 | 4 | 5 | 591 | 572 | 13 |
| -10 | 4 | 5 | 271 | 286 | 18 |
| -9 | 4 | 5 | 1045 | -1053 | 9 |
| -8 | 4 | 5 | 132 | -158 | 31 |
| -7 | 4 | 5 | 1223 | 1249 | 8 |
| -6 | 4 | 5 | 119 | 103 | 28 |
| -5 | 4 | 5 | 1016 | -1058 | 8 |
| -4 | 4 | 5 | 618 | 642 | 8 |
| -3 | 4 | 5 | 1345 | 1361 | 6 |
| -2 | 4 | 5 | 330 | -338 | 8 |

Q-5385-M26



Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -1 | 4 | 5 | 568 | -579 | 7 |
| 0 | 4 | 5 | 448 | -442 | 11 |
| 1 | 4 | 5 | 935 | 899 | 6 |
| 2 | 4 | 5 | 149 | -99 | 20 |
| 3 | 4 | 5 | 1587 | -1526 | 6 |
| 4 | 4 | 5 | 271 | -241 | 10 |
| 5 | 4 | 5 | 1699 | 1661 | 7 |
| 6 | 4 | 5 | 180 | 193 | 16 |
| 7 | 4 | 5 | 1089 | -1060 | 8 |
| 9 | 4 | 5 | 704 | 677 | 12 |
| 10 | 4 | 5 | 198 | 218 | 21 |
| 11 | 4 | 5 | 1094 | -1101 | 11 |
| 12 | 4 | 5 | 332 | -337 | 17 |
| 13 | 4 | 5 | 706 | 691 | 13 |
| 14 | 4 | 5 | 225 | 218 | 27 |
| -12 | 5 | 5 | 558 | 541 | 15 |
| -11 | 5 | 5 | 140 | 113 | 27 |
| -10 | 5 | 5 | 300 | -321 | 15 |
| -9 | 5 | 5 | 156 | -184 | 23 |
| -8 | 5 | 5 | 520 | 515 | 11 |
| -7 | 5 | 5 | 268 | -288 | 14 |
| -6 | 5 | 5 | 304 | -319 | 14 |
| -4 | 5 | 5 | 384 | 346 | 9 |
| -3 | 5 | 5 | 74 | -25 | 32 |
| -2 | 5 | 5 | 336 | -336 | 9 |
| -1 | 5 | 5 | 992 | 979 | 6 |
| 0 | 5 | 5 | 141 | -76 | 15 |
| 1 | 5 | 5 | 136 | -117 | 17 |
| 2 | 5 | 5 | 164 | 127 | 13 |
| 3 | 5 | 5 | 838 | 790 | 6 |
| 4 | 5 | 5 | 535 | 545 | 8 |
| 5 | 5 | 5 | 113 | 87 | 28 |
| 6 | 5 | 5 | 343 | -341 | 11 |
| 7 | 5 | 5 | 508 | -516 | 11 |
| 8 | 5 | 5 | 202 | 116 | 22 |
| 10 | 5 | 5 | 478 | -491 | 13 |
| 11 | 5 | 5 | 396 | -435 | 16 |
| 12 | 5 | 5 | 161 | 177 | 31 |
| 13 | 5 | 5 | 249 | 180 | 33 |
| -13 | 6 | 5 | 340 | -322 | 21 |
| -12 | 6 | 5 | 74 | 77 | 60 |
| -11 | 6 | 5 | 497 | 480 | 14 |
| -10 | 6 | 5 | 245 | 253 | 18 |
| -9 | 6 | 5 | 261 | -207 | 21 |
| -8 | 6 | 5 | 531 | -508 | 12 |
| -7 | 6 | 5 | 344 | 331 | 13 |
| -6 | 6 | 5 | 177 | -156 | 20 |
| -5 | 6 | 5 | 541 | -533 | 9 |
| -4 | 6 | 5 | 125 | -162 | 17 |
| -3 | 6 | 5 | 379 | -347 | 9 |
| -1 | 6 | 5 | 550 | -625 | 9 |
| 0 | 6 | 5 | 618 | -593 | 26 |
| 1 | 6 | 5 | 831 | 759 | 7 |
| 2 | 6 | 5 | 588 | 561 | 7 |
| 3 | 6 | 5 | 1528 | -1461 | 7 |
| 4 | 6 | 5 | 169 | -190 | 13 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 5 | 6 | 5 | 1105 | 1067 | 8 |
| 6 | 6 | 5 | 77 | -92 | 41 |
| 7 | 6 | 5 | 903 | -873 | 9 |
| 9 | 6 | 5 | 516 | 514 | 13 |
| 10 | 6 | 5 | 211 | -223 | 19 |
| 11 | 6 | 5 | 307 | -271 | 19 |
| 13 | 6 | 5 | 292 | 312 | 20 |
| -13 | 7 | 5 | 70 | -66 | 66 |
| -12 | 7 | 5 | 801 | 771 | 13 |
| -11 | 7 | 5 | 181 | -88 | 32 |
| -10 | 7 | 5 | 1061 | -1056 | 11 |
| -9 | 7 | 5 | 108 | 73 | 40 |
| -8 | 7 | 5 | 830 | 838 | 10 |
| -7 | 7 | 5 | 132 | 108 | 32 |
| -6 | 7 | 5 | 1442 | -1413 | 9 |
| -5 | 7 | 5 | 107 | 108 | 33 |
| -4 | 7 | 5 | 1433 | 1435 | 8 |
| -3 | 7 | 5 | 117 | -95 | 26 |
| -2 | 7 | 5 | 1266 | -1254 | 7 |
| -1 | 7 | 5 | 552 | -565 | 8 |
| 0 | 7 | 5 | 1574 | 1533 | 61 |
| 1 | 7 | 5 | 848 | -808 | 7 |
| 2 | 7 | 5 | 1584 | -1494 | 7 |
| 3 | 7 | 5 | 513 | 496 | 8 |
| 4 | 7 | 5 | 1218 | 1165 | 7 |
| 5 | 7 | 5 | 133 | 137 | 28 |
| 6 | 7 | 5 | 1360 | -1337 | 8 |
| 7 | 7 | 5 | 151 | -41 | 29 |
| 8 | 7 | 5 | 1388 | 1385 | 9 |
| 9 | 7 | 5 | 212 | 237 | 18 |
| 10 | 7 | 5 | 943 | -929 | 11 |
| 11 | 7 | 5 | 138 | -148 | 39 |
| 12 | 7 | 5 | 863 | 875 | 12 |
| -11 | 8 | 5 | 1072 | -1051 | 12 |
| -10 | 8 | 5 | 93 | 13 | 47 |
| -9 | 8 | 5 | 908 | 912 | 11 |
| -8 | 8 | 5 | 172 | 200 | 20 |
| -7 | 8 | 5 | 1533 | -1522 | 9 |
| -6 | 8 | 5 | 81 | -95 | 34 |
| -5 | 8 | 5 | 1952 | 1932 | 8 |
| -4 | 8 | 5 | 325 | 305 | 12 |
| -3 | 8 | 5 | 1729 | -1736 | 8 |
| -2 | 8 | 5 | 542 | -523 | 9 |
| -1 | 8 | 5 | 1726 | 1732 | 7 |
| 0 | 8 | 5 | 88 | 17 | 25 |
| 1 | 8 | 5 | 1869 | -1760 | 7 |
| 2 | 8 | 5 | 344 | 331 | 11 |
| 3 | 8 | 5 | 1779 | 1693 | 7 |
| 4 | 8 | 5 | 199 | 169 | 16 |
| 5 | 8 | 5 | 1294 | -1253 | 8 |
| 6 | 8 | 5 | 384 | -387 | 13 |
| 7 | 8 | 5 | 1499 | 1505 | 8 |
| 8 | 8 | 5 | 284 | 273 | 20 |
| 9 | 8 | 5 | 1125 | -1121 | 10 |
| 10 | 8 | 5 | 60 | -62 | 63 |
| 11 | 8 | 5 | 907 | 885 | 12 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 12 | 8 | 5 | 240 | 267 | 22 |
| -10 | 9 | 5 | 860 | 828 | 13 |
| -9 | 9 | 5 | 316 | 285 | 19 |
| -8 | 9 | 5 | 747 | -717 | 11 |
| -7 | 9 | 5 | 246 | -244 | 16 |
| -6 | 9 | 5 | 1181 | 1178 | 9 |
| -5 | 9 | 5 | 51 | 58 | 57 |
| -4 | 9 | 5 | 1419 | -1394 | 8 |
| -3 | 9 | 5 | 169 | -173 | 19 |
| -2 | 9 | 5 | 1108 | 1122 | 8 |
| -1 | 9 | 5 | 423 | 434 | 10 |
| 0 | 9 | 5 | 1733 | -1688 | 50 |
| 1 | 9 | 5 | 458 | -457 | 10 |
| 2 | 9 | 5 | 1463 | 1405 | 8 |
| 3 | 9 | 5 | 500 | 461 | 10 |
| 4 | 9 | 5 | 1169 | -1114 | 8 |
| 5 | 9 | 5 | 282 | -261 | 15 |
| 6 | 9 | 5 | 1191 | 1144 | 9 |
| 7 | 9 | 5 | 221 | -212 | 19 |
| 8 | 9 | 5 | 1092 | -1061 | 10 |
| 10 | 9 | 5 | 860 | 839 | 12 |
| 11 | 9 | 5 | 141 | 129 | 41 |
| -11 | 10 | 5 | 402 | 386 | 16 |
| -10 | 10 | 5 | 52 | 40 | 71 |
| -9 | 10 | 5 | 489 | -471 | 14 |
| -7 | 10 | 5 | 684 | 671 | 12 |
| -6 | 10 | 5 | 225 | 232 | 19 |
| -5 | 10 | 5 | 421 | -403 | 14 |
| -4 | 10 | 5 | 207 | -207 | 19 |
| -3 | 10 | 5 | 801 | 781 | 9 |
| -2 | 10 | 5 | 222 | 144 | 22 |
| -1 | 10 | 5 | 969 | -952 | 9 |
| 0 | 10 | 5 | 133 | 75 | 24 |
| 1 | 10 | 5 | 1262 | 1170 | 8 |
| 2 | 10 | 5 | 325 | 302 | 13 |
| 3 | 10 | 5 | 846 | -809 | 9 |
| 5 | 10 | 5 | 677 | 635 | 10 |
| 6 | 10 | 5 | 134 | 131 | 27 |
| 7 | 10 | 5 | 609 | -605 | 11 |
| 8 | 10 | 5 | 175 | -186 | 25 |
| 9 | 10 | 5 | 645 | 610 | 13 |
| 10 | 10 | 5 | 198 | 198 | 27 |
| -9 | 11 | 5 | 125 | 12 | 42 |
| -8 | 11 | 5 | 130 | 23 | 39 |
| -6 | 11 | 5 | 220 | 255 | 21 |
| -5 | 11 | 5 | 131 | 163 | 42 |
| -4 | 11 | 5 | 197 | -213 | 17 |
| -2 | 11 | 5 | 448 | 472 | 12 |
| -1 | 11 | 5 | 244 | 255 | 17 |
| 0 | 11 | 5 | 393 | -358 | 10 |
| 1 | 11 | 5 | 353 | -347 | 12 |
| 2 | 11 | 5 | 345 | 299 | 13 |
| 3 | 11 | 5 | 270 | 269 | 16 |
| 4 | 11 | 5 | 244 | -174 | 16 |
| 5 | 11 | 5 | 166 | -193 | 23 |
| 6 | 11 | 5 | 156 | 79 | 33 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 7 | 11 | 5 | 143 | 15 | 35 |
| 8 | 11 | 5 | 270 | -242 | 20 |
| -8 | 12 | 5 | 93 | -17 | 52 |
| -7 | 12 | 5 | 551 | 539 | 14 |
| -5 | 12 | 5 | 716 | -719 | 12 |
| -4 | 12 | 5 | 279 | -267 | 21 |
| -3 | 12 | 5 | 706 | 692 | 12 |
| -2 | 12 | 5 | 135 | 123 | 34 |
| -1 | 12 | 5 | 930 | -907 | 10 |
| 0 | 12 | 5 | 243 | 247 | 17 |
| 1 | 12 | 5 | 1018 | 1002 | 10 |
| 3 | 12 | 5 | 989 | -976 | 10 |
| 4 | 12 | 5 | 250 | -260 | 19 |
| 5 | 12 | 5 | 598 | 577 | 12 |
| 6 | 12 | 5 | 113 | 3 | 42 |
| 7 | 12 | 5 | 761 | -759 | 12 |
| 8 | 12 | 5 | 180 | -182 | 23 |
| -6 | 13 | 5 | 1108 | -1126 | 11 |
| -5 | 13 | 5 | 99 | 15 | 48 |
| -4 | 13 | 5 | 1080 | 1087 | 11 |
| -3 | 13 | 5 | 48 | 89 | 70 |
| -2 | 13 | 5 | 1080 | -1120 | 11 |
| -1 | 13 | 5 | 133 | -158 | 37 |
| 0 | 13 | 5 | 1072 | 1066 | 21 |
| 1 | 13 | 5 | 304 | 299 | 16 |
| 2 | 13 | 5 | 1073 | -1043 | 10 |
| 3 | 13 | 5 | 225 | -240 | 23 |
| 4 | 13 | 5 | 1169 | 1146 | 10 |
| 5 | 13 | 5 | 181 | 164 | 28 |
| 6 | 13 | 5 | 1051 | -1001 | 11 |
| 7 | 13 | 5 | 173 | -167 | 26 |
| -5 | 14 | 5 | 954 | 966 | 12 |
| -3 | 14 | 5 | 958 | -955 | 12 |
| -2 | 14 | 5 | 143 | 37 | 36 |
| -1 | 14 | 5 | 938 | 958 | 11 |
| 0 | 14 | 5 | 98 | -24 | 35 |
| 1 | 14 | 5 | 957 | -940 | 11 |
| 2 | 14 | 5 | 223 | -200 | 22 |
| 3 | 14 | 5 | 966 | 980 | 11 |
| 4 | 14 | 5 | 139 | 187 | 40 |
| 5 | 14 | 5 | 872 | -830 | 12 |
| 0 | 15 | 5 | 634 | -645 | 10 |
| -14 | 0 | 6 | 372 | -344 | 15 |
| -13 | 0 | 6 | 917 | 848 | 12 |
| -12 | 0 | 6 | 439 | 426 | 14 |
| -11 | 0 | 6 | 1041 | -986 | 11 |
| -10 | 0 | 6 | 523 | -510 | 13 |
| -9 | 0 | 6 | 1538 | 1525 | 9 |
| -8 | 0 | 6 | 937 | 952 | 9 |
| -7 | 0 | 6 | 1900 | -1939 | 8 |
| -6 | 0 | 6 | 1238 | -1204 | 8 |
| -5 | 0 | 6 | 2515 | 2561 | 6 |
| -4 | 0 | 6 | 1277 | 1284 | 6 |
| -3 | 0 | 6 | 3435 | -3580 | 6 |
| -2 | 0 | 6 | 1228 | -1273 | 6 |
| -1 | 0 | 6 | 3770 | 4058 | 5 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 0 | 0 | 6 | 2315 | 2309 | 81 |
| 1 | 0 | 6 | 2673 | -2618 | 5 |
| 2 | 0 | 6 | 1554 | -1485 | 6 |
| 3 | 0 | 6 | 1197 | 1171 | 6 |
| 4 | 0 | 6 | 2168 | 2137 | 6 |
| 5 | 0 | 6 | 837 | -856 | 8 |
| 6 | 0 | 6 | 924 | -923 | 8 |
| 7 | 0 | 6 | 1438 | 1528 | 8 |
| 8 | 0 | 6 | 716 | 707 | 11 |
| 9 | 0 | 6 | 697 | -711 | 12 |
| 10 | 0 | 6 | 841 | -846 | 11 |
| 11 | 0 | 6 | 1242 | 1272 | 11 |
| 12 | 0 | 6 | 632 | 647 | 13 |
| 13 | 0 | 6 | 994 | -1003 | 13 |
| 14 | 0 | 6 | 577 | -559 | 16 |
| -14 | 1 | 6 | 857 | 766 | 15 |
| -13 | 1 | 6 | 321 | 287 | 20 |
| -12 | 1 | 6 | 882 | -837 | 12 |
| -11 | 1 | 6 | 383 | -370 | 14 |
| -10 | 1 | 6 | 1097 | 1081 | 10 |
| -9 | 1 | 6 | 648 | 656 | 11 |
| -8 | 1 | 6 | 1535 | -1562 | 9 |
| -7 | 1 | 6 | 328 | -311 | 13 |
| -6 | 1 | 6 | 2244 | 2306 | 7 |
| -5 | 1 | 6 | 608 | 598 | 8 |
| -4 | 1 | 6 | 1773 | -1852 | 6 |
| -3 | 1 | 6 | 627 | -606 | 7 |
| -2 | 1 | 6 | 2473 | 2562 | 5 |
| -1 | 1 | 6 | 1817 | 1898 | 5 |
| 0 | 1 | 6 | 956 | -914 | 42 |
| 1 | 1 | 6 | 633 | -610 | 6 |
| 2 | 1 | 6 | 1748 | 1662 | 5 |
| 3 | 1 | 6 | 152 | 85 | 11 |
| 4 | 1 | 6 | 2254 | -2201 | 6 |
| 5 | 1 | 6 | 1005 | -975 | 7 |
| 6 | 1 | 6 | 1298 | 1308 | 8 |
| 7 | 1 | 6 | 504 | 535 | 11 |
| 8 | 1 | 6 | 1369 | -1367 | 9 |
| 9 | 1 | 6 | 652 | -635 | 12 |
| 10 | 1 | 6 | 934 | 936 | 10 |
| 11 | 1 | 6 | 869 | 875 | 12 |
| 12 | 1 | 6 | 678 | -688 | 14 |
| 13 | 1 | 6 | 485 | -477 | 14 |
| 14 | 1 | 6 | 748 | 745 | 14 |
| -14 | 2 | 6 | 114 | 132 | 35 |
| -13 | 2 | 6 | 460 | -447 | 16 |
| -12 | 2 | 6 | 274 | -280 | 23 |
| -11 | 2 | 6 | 646 | 646 | 13 |
| -10 | 2 | 6 | 295 | 333 | 14 |
| -9 | 2 | 6 | 977 | -980 | 10 |
| -7 | 2 | 6 | 993 | 1000 | 9 |
| -6 | 2 | 6 | 324 | 330 | 11 |
| -5 | 2 | 6 | 523 | -500 | 9 |
| -4 | 2 | 6 | 175 | -163 | 17 |
| -3 | 2 | 6 | 908 | 912 | 6 |
| -2 | 2 | 6 | 826 | -849 | 6 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -1 | 2 | 6 | 1459 | -1512 | 5 |
| 0 | 2 | 6 | 251 | -259 | 9 |
| 1 | 2 | 6 | 1563 | 1480 | 5 |
| 2 | 2 | 6 | 222 | 232 | 10 |
| 3 | 2 | 6 | 1456 | -1425 | 6 |
| 4 | 2 | 6 | 1083 | -1042 | 7 |
| 5 | 2 | 6 | 1264 | 1212 | 7 |
| 6 | 2 | 6 | 1016 | 1001 | 8 |
| 7 | 2 | 6 | 602 | -600 | 10 |
| 8 | 2 | 6 | 588 | -594 | 10 |
| 9 | 2 | 6 | 161 | 159 | 25 |
| 10 | 2 | 6 | 642 | 666 | 13 |
| 11 | 2 | 6 | 580 | -600 | 13 |
| 12 | 2 | 6 | 270 | -287 | 20 |
| 13 | 2 | 6 | 375 | 375 | 18 |
| 14 | 2 | 6 | 233 | 233 | 27 |
| -14 | 3 | 6 | 125 | 20 | 46 |
| -13 | 3 | 6 | 108 | 93 | 49 |
| -12 | 3 | 6 | 140 | -118 | 37 |
| -11 | 3 | 6 | 110 | -142 | 44 |
| -10 | 3 | 6 | 137 | 152 | 35 |
| -9 | 3 | 6 | 430 | 427 | 13 |
| -8 | 3 | 6 | 79 | 54 | 46 |
| -7 | 3 | 6 | 114 | 110 | 32 |
| -6 | 3 | 6 | 637 | 662 | 9 |
| -5 | 3 | 6 | 78 | 84 | 35 |
| -4 | 3 | 6 | 382 | -406 | 9 |
| -3 | 3 | 6 | 423 | -453 | 8 |
| -2 | 3 | 6 | 215 | -223 | 11 |
| -1 | 3 | 6 | 961 | 990 | 6 |
| 0 | 3 | 6 | 403 | 383 | 27 |
| 1 | 3 | 6 | 885 | -853 | 6 |
| 2 | 3 | 6 | 39 | 111 | 43 |
| 3 | 3 | 6 | 463 | 446 | 8 |
| 4 | 3 | 6 | 727 | -727 | 7 |
| 5 | 3 | 6 | 16 | 53 | 64 |
| 6 | 3 | 6 | 609 | 583 | 9 |
| 7 | 3 | 6 | 93 | -12 | 37 |
| 8 | 3 | 6 | 125 | 32 | 32 |
| 9 | 3 | 6 | 94 | -107 | 43 |
| 11 | 3 | 6 | 129 | 81 | 37 |
| 12 | 3 | 6 | 99 | -65 | 50 |
| 14 | 3 | 6 | 241 | 253 | 25 |
| -14 | 4 | 6 | 353 | 314 | 21 |
| -13 | 4 | 6 | 734 | -711 | 14 |
| -12 | 4 | 6 | 272 | -296 | 19 |
| -11 | 4 | 6 | 726 | 711 | 12 |
| -10 | 4 | 6 | 282 | 211 | 19 |
| -9 | 4 | 6 | 956 | -993 | 10 |
| -8 | 4 | 6 | 700 | -719 | 10 |
| -7 | 4 | 6 | 1066 | 1100 | 9 |
| -6 | 4 | 6 | 626 | 625 | 9 |
| -5 | 4 | 6 | 1008 | -1046 | 7 |
| -4 | 4 | 6 | 579 | -585 | 8 |
| -3 | 4 | 6 | 760 | 821 | 7 |
| -2 | 4 | 6 | 93 | 51 | 26 |
| -1 | 4 | 6 | 1289 | -1303 | 6 |
| 0 | 4 | 6 | 551 | 523 | 15 |
| 1 | 4 | 6 | 1598 | 1542 | 6 |
| 2 | 4 | 6 | 312 | 296 | 9 |
| 3 | 4 | 6 | 1579 | -1545 | 6 |
| 4 | 4 | 6 | 611 | -600 | 7 |
| 5 | 4 | 6 | 564 | 520 | 9 |
| 6 | 4 | 6 | 587 | 552 | 9 |
| 7 | 4 | 6 | 867 | -843 | 9 |
| 8 | 4 | 6 | 1034 | -1061 | 9 |
| 9 | 4 | 6 | 878 | 869 | 10 |
| 10 | 4 | 6 | 332 | 352 | 14 |
| 11 | 4 | 6 | 592 | -568 | 13 |
| 12 | 4 | 6 | 386 | -351 | 18 |
| 13 | 4 | 6 | 511 | 538 | 14 |
| -13 | 5 | 6 | 502 | -476 | 16 |
| -12 | 5 | 6 | 1036 | 1013 | 11 |
| -11 | 5 | 6 | 352 | 355 | 18 |
| -10 | 5 | 6 | 1168 | -1168 | 10 |
| -9 | 5 | 6 | 547 | -549 | 12 |
| -8 | 5 | 6 | 1116 | 1101 | 9 |
| -7 | 5 | 6 | 345 | 351 | 12 |
| -6 | 5 | 6 | 1208 | -1242 | 8 |
| -5 | 5 | 6 | 1004 | -1010 | 8 |
| -4 | 5 | 6 | 1322 | 1375 | 7 |
| -3 | 5 | 6 | 746 | 741 | 8 |
| -2 | 5 | 6 | 2301 | -2378 | 6 |
| -1 | 5 | 6 | 553 | -612 | 8 |
| 0 | 5 | 6 | 2029 | 1996 | 90 |
| 1 | 5 | 6 | 1112 | 1071 | 6 |
| 2 | 5 | 6 | 1604 | -1564 | 6 |
| 3 | 5 | 6 | 1070 | -1010 | 7 |
| 4 | 5 | 6 | 1492 | 1413 | 7 |
| 5 | 5 | 6 | 1030 | 999 | 8 |
| 6 | 5 | 6 | 1442 | -1382 | 8 |
| 7 | 5 | 6 | 1111 | -1105 | 8 |
| 8 | 5 | 6 | 1469 | 1459 | 9 |
| 9 | 5 | 6 | 846 | 808 | 10 |
| 10 | 5 | 6 | 1227 | -1246 | 11 |
| 11 | 5 | 6 | 462 | -459 | 14 |
| 12 | 5 | 6 | 882 | 878 | 13 |
| 13 | 5 | 6 | 373 | 384 | 19 |
| -13 | 6 | 6 | 815 | 796 | 14 |
| -12 | 6 | 6 | 231 | 244 | 18 |
| -11 | 6 | 6 | 960 | -926 | 11 |
| -10 | 6 | 6 | 268 | -262 | 21 |
| -9 | 6 | 6 | 992 | 982 | 10 |
| -8 | 6 | 6 | 473 | 449 | 13 |
| -7 | 6 | 6 | 1572 | -1628 | 8 |
| -6 | 6 | 6 | 413 | -415 | 12 |
| -5 | 6 | 6 | 1581 | 1617 | 8 |
| -4 | 6 | 6 | 373 | 417 | 10 |
| -3 | 6 | 6 | 1507 | -1564 | 7 |
| -2 | 6 | 6 | 828 | -853 | 7 |
| -1 | 6 | 6 | 2215 | 2283 | 6 |
| 0 | 6 | 6 | 1803 | 1762 | 81 |
| 1 | 6 | 6 | 2022 | -1914 | 6 |
| 2 | 6 | 6 | 1358 | -1247 | 6 |
| 3 | 6 | 6 | 2212 | 2136 | 6 |
| 4 | 6 | 6 | 882 | 833 | 8 |
| 5 | 6 | 6 | 1717 | -1667 | 7 |
| 6 | 6 | 6 | 742 | -742 | 9 |
| 7 | 6 | 6 | 1579 | 1543 | 8 |
| 8 | 6 | 6 | 566 | 566 | 11 |
| 9 | 6 | 6 | 1378 | -1365 | 10 |
| 10 | 6 | 6 | 495 | -477 | 14 |
| 11 | 6 | 6 | 982 | 974 | 11 |
| 12 | 6 | 6 | 598 | 578 | 13 |
| 13 | 6 | 6 | 879 | -882 | 13 |
| -12 | 7 | 6 | 607 | -594 | 15 |
| -11 | 7 | 6 | 174 | -20 | 31 |
| -10 | 7 | 6 | 660 | 627 | 13 |
| -9 | 7 | 6 | 277 | 289 | 17 |
| -8 | 7 | 6 | 1128 | -1132 | 10 |
| -7 | 7 | 6 | 494 | -507 | 12 |
| -6 | 7 | 6 | 1223 | 1254 | 9 |
| -5 | 7 | 6 | 578 | 588 | 11 |
| -4 | 7 | 6 | 1444 | -1460 | 8 |
| -3 | 7 | 6 | 1004 | -976 | 8 |
| -2 | 7 | 6 | 1204 | 1196 | 8 |
| -1 | 7 | 6 | 586 | 633 | 10 |
| 0 | 7 | 6 | 925 | -902 | 45 |
| 1 | 7 | 6 | 492 | -472 | 9 |
| 2 | 7 | 6 | 1762 | 1681 | 7 |
| 3 | 7 | 6 | 563 | 556 | 9 |
| 4 | 7 | 6 | 1519 | -1464 | 7 |
| 5 | 7 | 6 | 750 | -730 | 9 |
| 6 | 7 | 6 | 931 | 908 | 9 |
| 7 | 7 | 6 | 335 | 338 | 13 |
| 8 | 7 | 6 | 907 | -879 | 10 |
| 9 | 7 | 6 | 378 | -361 | 14 |
| 10 | 7 | 6 | 664 | 659 | 12 |
| 11 | 7 | 6 | 574 | 560 | 14 |
| 12 | 7 | 6 | 722 | -709 | 14 |
| -12 | 8 | 6 | 99 | 38 | 53 |
| -11 | 8 | 6 | 303 | 281 | 20 |
| -9 | 8 | 6 | 107 | 46 | 42 |
| -8 | 8 | 6 | 19 | -92 | 74 |
| -7 | 8 | 6 | 214 | 192 | 21 |
| -5 | 8 | 6 | 214 | -149 | 23 |
| -4 | 8 | 6 | 151 | 180 | 24 |
| -3 | 8 | 6 | 437 | 436 | 10 |
| -2 | 8 | 6 | 47 | -22 | 52 |
| -1 | 8 | 6 | 390 | -325 | 12 |
| 0 | 8 | 6 | 188 | -172 | 20 |
| 2 | 8 | 6 | 262 | -250 | 11 |
| 3 | 8 | 6 | 241 | -214 | 14 |
| 4 | 8 | 6 | 126 | 127 | 29 |
| 5 | 8 | 6 | 247 | 214 | 20 |
| 6 | 8 | 6 | 392 | 365 | 11 |
| 7 | 8 | 6 | 91 | -109 | 45 |
| 8 | 8 | 6 | 87 | -19 | 46 |
| 9 | 8 | 6 | 111 | 141 | 39 |
| 11 | 8 | 6 | 136 | -6 | 41 |
| -11 | 9 | 6 | 196 | -123 | 27 |
| -10 | 9 | 6 | 325 | 326 | 18 |
| -9 | 9 | 6 | 299 | 309 | 16 |
| -8 | 9 | 6 | 130 | -132 | 38 |
| -7 | 9 | 6 | 365 | -385 | 14 |
| -6 | 9 | 6 | 610 | 615 | 11 |
| -5 | 9 | 6 | 382 | 363 | 14 |
| -4 | 9 | 6 | 421 | -406 | 13 |
| -3 | 9 | 6 | 340 | -344 | 12 |
| -2 | 9 | 6 | 168 | 71 | 23 |
| -1 | 9 | 6 | 368 | 329 | 13 |
| 0 | 9 | 6 | 843 | -806 | 75 |
| 1 | 9 | 6 | 95 | -56 | 37 |
| 2 | 9 | 6 | 518 | 499 | 9 |
| 3 | 9 | 6 | 126 | 142 | 31 |
| 4 | 9 | 6 | 437 | -414 | 11 |
| 5 | 9 | 6 | 64 | -21 | 51 |
| 6 | 9 | 6 | 816 | 795 | 10 |
| 7 | 9 | 6 | 189 | 149 | 27 |
| 8 | 9 | 6 | 460 | -462 | 13 |
| 9 | 9 | 6 | 127 | -40 | 39 |
| 10 | 9 | 6 | 541 | 527 | 14 |
| 11 | 9 | 6 | 110 | 93 | 46 |
| -10 | 10 | 6 | 409 | 391 | 18 |
| -9 | 10 | 6 | 858 | -811 | 12 |
| -8 | 10 | 6 | 435 | -437 | 14 |
| -7 | 10 | 6 | 711 | 704 | 12 |
| -6 | 10 | 6 | 337 | 352 | 14 |
| -5 | 10 | 6 | 1160 | -1144 | 10 |
| -4 | 10 | 6 | 619 | -597 | 11 |
| -3 | 10 | 6 | 1061 | 1061 | 10 |
| -2 | 10 | 6 | 744 | 744 | 9 |
| -1 | 10 | 6 | 952 | -927 | 9 |
| 0 | 10 | 6 | 606 | -601 | 20 |
| 1 | 10 | 6 | 951 | 889 | 9 |
| 2 | 10 | 6 | 408 | 413 | 11 |
| 3 | 10 | 6 | 1167 | -1099 | 9 |
| 4 | 10 | 6 | 579 | -541 | 10 |
| 5 | 10 | 6 | 1182 | 1142 | 9 |
| 6 | 10 | 6 | 417 | 418 | 12 |
| 7 | 10 | 6 | 1087 | -1057 | 10 |
| 8 | 10 | 6 | 406 | -376 | 14 |
| 9 | 10 | 6 | 1002 | 984 | 11 |
| 10 | 10 | 6 | 445 | 456 | 15 |
| -9 | 11 | 6 | 406 | -368 | 16 |
| -8 | 11 | 6 | 792 | 807 | 12 |
| -7 | 11 | 6 | 420 | 413 | 14 |
| -6 | 11 | 6 | 968 | -1004 | 10 |
| -5 | 11 | 6 | 243 | -210 | 22 |
| -4 | 11 | 6 | 1271 | 1274 | 10 |
| -3 | 11 | 6 | 460 | 451 | 12 |
| -2 | 11 | 6 | 911 | -880 | 10 |
| -1 | 11 | 6 | 536 | -522 | 12 |
| 0 | 11 | 6 | 1495 | 1490 | 56 |
| 1 | 11 | 6 | 713 | 697 | 9 |
| 2 | 11 | 6 | 1573 | -1495 | 9 |
| 3 | 11 | 6 | 852 | -844 | 9 |
| 4 | 11 | 6 | 1140 | 1094 | 9 |
| 5 | 11 | 6 | 742 | 721 | 10 |
| 6 | 11 | 6 | 1049 | -1057 | 10 |
| 7 | 11 | 6 | 664 | -675 | 12 |
| 8 | 11 | 6 | 848 | 853 | 12 |
| 9 | 11 | 6 | 558 | 551 | 13 |
| -8 | 12 | 6 | 203 | 141 | 37 |
| -7 | 12 | 6 | 563 | -553 | 13 |
| -6 | 12 | 6 | 332 | -316 | 18 |
| -5 | 12 | 6 | 727 | 748 | 11 |
| -4 | 12 | 6 | 473 | 488 | 14 |
| -3 | 12 | 6 | 824 | -842 | 11 |
| -2 | 12 | 6 | 589 | -598 | 14 |
| -1 | 12 | 6 | 725 | 735 | 11 |
| 0 | 12 | 6 | 592 | 576 | 12 |
| 1 | 12 | 6 | 869 | -864 | 10 |
| 2 | 12 | 6 | 701 | -683 | 11 |
| 3 | 12 | 6 | 874 | 854 | 10 |
| 4 | 12 | 6 | 542 | 530 | 13 |
| 5 | 12 | 6 | 809 | -794 | 11 |
| 6 | 12 | 6 | 520 | -535 | 14 |
| 7 | 12 | 6 | 730 | 721 | 12 |
| 8 | 12 | 6 | 399 | 420 | 17 |
| -7 | 13 | 6 | 231 | -210 | 27 |
| -6 | 13 | 6 | 252 | 218 | 34 |
| -5 | 13 | 6 | 304 | 304 | 21 |
| -4 | 13 | 6 | 278 | -257 | 18 |
| -3 | 13 | 6 | 285 | -305 | 19 |
| -2 | 13 | 6 | 177 | 139 | 23 |
| -1 | 13 | 6 | 262 | 276 | 20 |
| 0 | 13 | 6 | 464 | -508 | 10 |
| 1 | 13 | 6 | 374 | -378 | 14 |
| 2 | 13 | 6 | 308 | 322 | 18 |
| 4 | 13 | 6 | 113 | -116 | 47 |
| 5 | 13 | 6 | 138 | -169 | 40 |
| 6 | 13 | 6 | 379 | 398 | 15 |
| -5 | 14 | 6 | 150 | 237 | 31 |
| -4 | 14 | 6 | 148 | 95 | 37 |
| -3 | 14 | 6 | 188 | -229 | 29 |
| -2 | 14 | 6 | 170 | -185 | 29 |
| -1 | 14 | 6 | 258 | 271 | 20 |
| 0 | 14 | 6 | 136 | 187 | 24 |
| 1 | 14 | 6 | 157 | -201 | 37 |
| 3 | 14 | 6 | 229 | 269 | 22 |
| 4 | 14 | 6 | 264 | 307 | 23 |
| -14 | 1 | 7 | 443 | 418 | 17 |
| -13 | 1 | 7 | 566 | 540 | 14 |
| -12 | 1 | 7 | 364 | -336 | 18 |
| -11 | 1 | 7 | 259 | -216 | 18 |
| -10 | 1 | 7 | 610 | 596 | 13 |
| -9 | 1 | 7 | 601 | 583 | 11 |
| -8 | 1 | 7 | 484 | -511 | 12 |
| -7 | 1 | 7 | 764 | -766 | 9 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -6 | 1 | 7 | 549 | 555 | 9 |
| -5 | 1 | 7 | 593 | 628 | 8 |
| -4 | 1 | 7 | 160 | -103 | 15 |
| -3 | 1 | 7 | 651 | -684 | 7 |
| -2 | 1 | 7 | 184 | 198 | 10 |
| -1 | 1 | 7 | 677 | 691 | 6 |
| 0 | 1 | 7 | 913 | -914 | 33 |
| 1 | 1 | 7 | 506 | -479 | 8 |
| 2 | 1 | 7 | 463 | 479 | 7 |
| 3 | 1 | 7 | 672 | 658 | 7 |
| 4 | 1 | 7 | 131 | 61 | 24 |
| 5 | 1 | 7 | 784 | -770 | 8 |
| 6 | 1 | 7 | 427 | 426 | 11 |
| 7 | 1 | 7 | 695 | 694 | 10 |
| 8 | 1 | 7 | 508 | -541 | 12 |
| 9 | 1 | 7 | 574 | -555 | 13 |
| 10 | 1 | 7 | 592 | 622 | 14 |
| 11 | 1 | 7 | 838 | 862 | 14 |
| 12 | 1 | 7 | 448 | -451 | 17 |
| 13 | 1 | 7 | 451 | -460 | 17 |
| 14 | 1 | 7 | 314 | 343 | 22 |
| -14 | 2 | 7 | 662 | 617 | 15 |
| -13 | 2 | 7 | 710 | -683 | 14 |
| -12 | 2 | 7 | 817 | -797 | 12 |
| -11 | 2 | 7 | 714 | 720 | 12 |
| -10 | 2 | 7 | 554 | 530 | 12 |
| -9 | 2 | 7 | 742 | -747 | 11 |
| -8 | 2 | 7 | 977 | -994 | 9 |
| -7 | 2 | 7 | 1275 | 1310 | 8 |
| -6 | 2 | 7 | 1251 | 1306 | 8 |
| -5 | 2 | 7 | 868 | -871 | 8 |
| -4 | 2 | 7 | 1159 | -1229 | 7 |
| -3 | 2 | 7 | 345 | 316 | 9 |
| -2 | 2 | 7 | 1572 | 1660 | 6 |
| -1 | 2 | 7 | 1183 | -1202 | 6 |
| 0 | 2 | 7 | 1814 | -1810 | 87 |
| 1 | 2 | 7 | 1040 | 976 | 6 |
| 2 | 2 | 7 | 638 | 604 | 7 |
| 3 | 2 | 7 | 1518 | -1437 | 6 |
| 4 | 2 | 7 | 1374 | -1328 | 6 |
| 5 | 2 | 7 | 982 | 945 | 7 |
| 6 | 2 | 7 | 1426 | 1355 | 8 |
| 7 | 2 | 7 | 988 | -986 | 9 |
| 8 | 2 | 7 | 734 | -703 | 10 |
| 9 | 2 | 7 | 1038 | 1043 | 10 |
| 10 | 2 | 7 | 982 | 1010 | 11 |
| 11 | 2 | 7 | 510 | -504 | 14 |
| 12 | 2 | 7 | 688 | -689 | 14 |
| 13 | 2 | 7 | 623 | 654 | 14 |
| -14 | 3 | 7 | 691 | -633 | 14 |
| -13 | 3 | 7 | 782 | -767 | 13 |
| -12 | 3 | 7 | 569 | 548 | 15 |
| -11 | 3 | 7 | 642 | 623 | 12 |
| -10 | 3 | 7 | 906 | -911 | 11 |
| -9 | 3 | 7 | 1139 | -1151 | 10 |
| -8 | 3 | 7 | 812 | 831 | 10 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -7 | 3 | 7 | 1369 | 1403 | 8 |
| -6 | 3 | 7 | 1262 | -1292 | 8 |
| -5 | 3 | 7 | 1419 | -1501 | 7 |
| -4 | 3 | 7 | 1600 | 1659 | 7 |
| -3 | 3 | 7 | 1623 | 1705 | 6 |
| -2 | 3 | 7 | 1459 | -1482 | 6 |
| -1 | 3 | 7 | 1804 | -1911 | 6 |
| 0 | 3 | 7 | 1782 | 1747 | 97 |
| 1 | 3 | 7 | 2183 | 2084 | 5 |
| 2 | 3 | 7 | 1631 | -1591 | 6 |
| 3 | 3 | 7 | 1686 | -1624 | 6 |
| 4 | 3 | 7 | 726 | 697 | 7 |
| 5 | 3 | 7 | 1449 | 1406 | 7 |
| 6 | 3 | 7 | 756 | -719 | 9 |
| 7 | 3 | 7 | 880 | -874 | 9 |
| 8 | 3 | 7 | 922 | 915 | 9 |
| 9 | 3 | 7 | 434 | 408 | 13 |
| 10 | 3 | 7 | 676 | -690 | 11 |
| 11 | 3 | 7 | 814 | -827 | 12 |
| 12 | 3 | 7 | 461 | 482 | 17 |
| 13 | 3 | 7 | 695 | 681 | 15 |
| -13 | 4 | 7 | 575 | 537 | 15 |
| -12 | 4 | 7 | 679 | 656 | 13 |
| -11 | 4 | 7 | 580 | -559 | 12 |
| -10 | 4 | 7 | 654 | -650 | 12 |
| -9 | 4 | 7 | 375 | 406 | 13 |
| -8 | 4 | 7 | 1307 | 1309 | 9 |
| -7 | 4 | 7 | 723 | -708 | 10 |
| -6 | 4 | 7 | 1069 | -1044 | 8 |
| -5 | 4 | 7 | 824 | 866 | 8 |
| -4 | 4 | 7 | 976 | 995 | 7 |
| -3 | 4 | 7 | 742 | -755 | 7 |
| -2 | 4 | 7 | 1058 | -1026 | 6 |
| -1 | 4 | 7 | 680 | 681 | 7 |
| 0 | 4 | 7 | 1011 | 975 | 54 |
| 1 | 4 | 7 | 323 | -263 | 10 |
| 2 | 4 | 7 | 670 | -634 | 7 |
| 3 | 4 | 7 | 950 | 926 | 7 |
| 4 | 4 | 7 | 322 | 320 | 11 |
| 5 | 4 | 7 | 1208 | -1191 | 7 |
| 6 | 4 | 7 | 998 | -950 | 8 |
| 7 | 4 | 7 | 742 | 728 | 9 |
| 8 | 4 | 7 | 546 | 516 | 11 |
| 9 | 4 | 7 | 451 | -472 | 15 |
| 10 | 4 | 7 | 509 | -520 | 12 |
| 11 | 4 | 7 | 242 | 174 | 24 |
| 12 | 4 | 7 | 454 | 445 | 15 |
| 13 | 4 | 7 | 384 | -369 | 19 |
| -13 | 5 | 7 | 179 | 147 | 29 |
| -12 | 5 | 7 | 174 | -207 | 23 |
| -11 | 5 | 7 | 350 | -338 | 17 |
| -10 | 5 | 7 | 231 | 208 | 25 |
| -9 | 5 | 7 | 516 | 500 | 12 |
| -8 | 5 | 7 | 251 | -208 | 19 |
| -7 | 5 | 7 | 351 | -365 | 13 |
| -6 | 5 | 7 | 62 | -44 | 46 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 5 | 7 | 89 | -54 | 34 |
| -4 | 5 | 7 | 367 | -349 | 10 |
| -3 | 5 | 7 | 721 | -694 | 8 |
| -2 | 5 | 7 | 291 | 267 | 9 |
| -1 | 5 | 7 | 938 | 956 | 7 |
| 0 | 5 | 7 | 501 | 480 | 23 |
| 1 | 5 | 7 | 319 | -304 | 9 |
| 2 | 5 | 7 | 421 | -392 | 9 |
| 3 | 5 | 7 | 189 | -183 | 11 |
| 4 | 5 | 7 | 258 | -243 | 11 |
| 5 | 5 | 7 | 554 | -537 | 9 |
| 6 | 5 | 7 | 60 | -69 | 49 |
| 7 | 5 | 7 | 240 | 267 | 14 |
| 8 | 5 | 7 | 129 | -99 | 34 |
| 9 | 5 | 7 | 267 | -254 | 25 |
| 10 | 5 | 7 | 122 | 50 | 39 |
| 11 | 5 | 7 | 348 | 319 | 14 |
| 12 | 5 | 7 | 197 | -210 | 24 |
| 13 | 5 | 7 | 140 | -198 | 35 |
| -13 | 6 | 7 | 262 | 241 | 22 |
| -12 | 6 | 7 | 119 | 134 | 45 |
| -11 | 6 | 7 | 245 | -261 | 21 |
| -10 | 6 | 7 | 377 | -377 | 15 |
| -9 | 6 | 7 | 146 | 1 | 36 |
| -8 | 6 | 7 | 118 | -145 | 38 |
| -7 | 6 | 7 | 41 | 44 | 66 |
| -6 | 6 | 7 | 172 | -135 | 22 |
| -5 | 6 | 7 | 737 | 750 | 9 |
| -4 | 6 | 7 | 213 | 247 | 16 |
| -3 | 6 | 7 | 502 | -526 | 9 |
| -2 | 6 | 7 | 342 | -370 | 10 |
| -1 | 6 | 7 | 240 | -218 | 16 |
| 0 | 6 | 7 | 1058 | 1058 | 64 |
| 1 | 6 | 7 | 329 | -315 | 10 |
| 2 | 6 | 7 | 644 | -621 | 8 |
| 3 | 6 | 7 | 831 | 793 | 8 |
| 4 | 6 | 7 | 555 | 556 | 9 |
| 5 | 6 | 7 | 853 | -839 | 8 |
| 6 | 6 | 7 | 356 | -369 | 12 |
| 7 | 6 | 7 | 884 | 891 | 9 |
| 8 | 6 | 7 | 400 | 424 | 14 |
| 9 | 6 | 7 | 288 | -324 | 16 |
| 10 | 6 | 7 | 75 | -110 | 56 |
| 12 | 6 | 7 | 169 | 57 | 51 |
| -12 | 7 | 7 | 813 | -802 | 12 |
| -11 | 7 | 7 | 473 | -437 | 14 |
| -10 | 7 | 7 | 803 | 781 | 11 |
| -9 | 7 | 7 | 677 | 654 | 13 |
| -8 | 7 | 7 | 552 | -560 | 12 |
| -7 | 7 | 7 | 661 | -672 | 11 |
| -6 | 7 | 7 | 887 | 898 | 9 |
| -5 | 7 | 7 | 930 | 925 | 9 |
| -4 | 7 | 7 | 598 | -598 | 9 |
| -3 | 7 | 7 | 772 | -757 | 9 |
| -2 | 7 | 7 | 647 | 686 | 9 |
| -1 | 7 | 7 | 898 | 898 | 8 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 0 | 7 | 7 | 938 | -933 | 54 |
| 1 | 7 | 7 | 1106 | -1023 | 7 |
| 2 | 7 | 7 | 1115 | 1070 | 7 |
| 3 | 7 | 7 | 1020 | 997 | 8 |
| 4 | 7 | 7 | 836 | -831 | 9 |
| 5 | 7 | 7 | 1052 | -1025 | 8 |
| 6 | 7 | 7 | 1044 | 1020 | 9 |
| 7 | 7 | 7 | 1282 | 1252 | 9 |
| 8 | 7 | 7 | 825 | -839 | 10 |
| 9 | 7 | 7 | 995 | -1001 | 11 |
| 10 | 7 | 7 | 558 | 548 | 14 |
| 11 | 7 | 7 | 689 | 673 | 13 |
| 12 | 7 | 7 | 641 | -621 | 15 |
| -12 | 8 | 7 | 508 | -494 | 15 |
| -11 | 8 | 7 | 911 | 860 | 12 |
| -10 | 8 | 7 | 789 | 769 | 12 |
| -9 | 8 | 7 | 982 | -959 | 11 |
| -8 | 8 | 7 | 897 | -890 | 10 |
| -7 | 8 | 7 | 788 | 753 | 10 |
| -6 | 8 | 7 | 949 | 935 | 9 |
| -5 | 8 | 7 | 1081 | -1129 | 9 |
| -4 | 8 | 7 | 1121 | -1144 | 9 |
| -3 | 8 | 7 | 979 | 982 | 8 |
| -2 | 8 | 7 | 1051 | 1056 | 8 |
| -1 | 8 | 7 | 999 | -1017 | 8 |
| 0 | 8 | 7 | 1377 | -1346 | 62 |
| 1 | 8 | 7 | 1247 | 1191 | 8 |
| 2 | 8 | 7 | 1427 | 1372 | 8 |
| 3 | 8 | 7 | 553 | -518 | 10 |
| 4 | 8 | 7 | 1237 | -1178 | 8 |
| 5 | 8 | 7 | 594 | 568 | 11 |
| 6 | 8 | 7 | 1209 | 1166 | 9 |
| 7 | 8 | 7 | 896 | -871 | 10 |
| 8 | 8 | 7 | 1094 | -1075 | 10 |
| 9 | 8 | 7 | 783 | 796 | 12 |
| 10 | 8 | 7 | 857 | 863 | 12 |
| 11 | 8 | 7 | 894 | -887 | 12 |
| -11 | 9 | 7 | 514 | 505 | 16 |
| -10 | 9 | 7 | 591 | -600 | 14 |
| -9 | 9 | 7 | 636 | 578 | 13 |
| -8 | 9 | 7 | 793 | 808 | 11 |
| -7 | 9 | 7 | 720 | 708 | 12 |
| -6 | 9 | 7 | 846 | -865 | 11 |
| -5 | 9 | 7 | 736 | -764 | 10 |
| -4 | 9 | 7 | 927 | 939 | 9 |
| -3 | 9 | 7 | 911 | 915 | 9 |
| -2 | 9 | 7 | 1012 | -1008 | 9 |
| -1 | 9 | 7 | 1021 | -1009 | 9 |
| 0 | 9 | 7 | 520 | 524 | 24 |
| 1 | 9 | 7 | 1059 | 995 | 8 |
| 2 | 9 | 7 | 758 | -732 | 9 |
| 3 | 9 | 7 | 566 | -534 | 10 |
| 4 | 9 | 7 | 1132 | 1117 | 9 |
| 5 | 9 | 7 | 814 | 759 | 10 |
| 6 | 9 | 7 | 774 | -721 | 10 |
| 7 | 9 | 7 | 744 | -704 | 10 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 8 | 9 | 7 | 809 | 792 | 11 |
| 9 | 9 | 7 | 721 | 700 | 12 |
| 10 | 9 | 7 | 570 | -599 | 14 |
| 11 | 9 | 7 | 632 | -612 | 14 |
| -10 | 10 | 7 | 260 | -254 | 21 |
| -9 | 10 | 7 | 451 | 466 | 15 |
| -8 | 10 | 7 | 268 | 308 | 19 |
| -7 | 10 | 7 | 298 | -300 | 17 |
| -6 | 10 | 7 | 445 | -498 | 14 |
| -5 | 10 | 7 | 396 | 377 | 13 |
| -4 | 10 | 7 | 650 | 617 | 13 |
| -3 | 10 | 7 | 582 | -546 | 12 |
| -2 | 10 | 7 | 300 | -296 | 16 |
| -1 | 10 | 7 | 483 | 486 | 12 |
| 0 | 10 | 7 | 405 | 409 | 19 |
| 1 | 10 | 7 | 746 | -737 | 9 |
| 2 | 10 | 7 | 775 | -745 | 10 |
| 3 | 10 | 7 | 657 | 630 | 10 |
| 4 | 10 | 7 | 493 | 468 | 11 |
| 5 | 10 | 7 | 383 | -378 | 13 |
| 6 | 10 | 7 | 517 | -541 | 12 |
| 7 | 10 | 7 | 269 | 258 | 20 |
| 8 | 10 | 7 | 631 | 617 | 12 |
| 9 | 10 | 7 | 230 | -218 | 23 |
| 10 | 10 | 7 | 370 | -374 | 16 |
| -9 | 11 | 7 | 144 | -137 | 39 |
| -8 | 11 | 7 | 141 | 154 | 39 |
| -7 | 11 | 7 | 200 | 203 | 29 |
| -6 | 11 | 7 | 338 | -353 | 15 |
| -5 | 11 | 7 | 203 | -183 | 24 |
| -4 | 11 | 7 | 139 | 174 | 35 |
| -3 | 11 | 7 | 37 | 120 | 70 |
| -2 | 11 | 7 | 148 | -151 | 25 |
| -1 | 11 | 7 | 580 | -574 | 12 |
| 0 | 11 | 7 | 290 | 336 | 60 |
| 1 | 11 | 7 | 68 | 15 | 53 |
| 2 | 11 | 7 | 320 | -93 | 15 |
| 3 | 11 | 7 | 174 | -49 | 19 |
| 4 | 11 | 7 | 95 | 4 | 45 |
| 5 | 11 | 7 | 137 | 111 | 35 |
| 6 | 11 | 7 | 263 | -261 | 17 |
| 8 | 11 | 7 | 77 | 37 | 56 |
| 9 | 11 | 7 | 141 | 190 | 41 |
| -8 | 12 | 7 | 483 | 472 | 17 |
| -7 | 12 | 7 | 501 | -510 | 15 |
| -6 | 12 | 7 | 456 | -449 | 15 |
| -5 | 12 | 7 | 679 | 699 | 12 |
| -4 | 12 | 7 | 391 | 371 | 16 |
| -3 | 12 | 7 | 673 | -687 | 12 |
| -2 | 12 | 7 | 524 | -523 | 13 |
| -1 | 12 | 7 | 842 | 861 | 11 |
| 0 | 12 | 7 | 494 | 489 | 18 |
| 1 | 12 | 7 | 910 | -891 | 11 |
| 2 | 12 | 7 | 281 | -238 | 15 |
| 3 | 12 | 7 | 668 | 674 | 11 |
| 4 | 12 | 7 | 488 | 460 | 13 |

J-5385-M29



Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 5 | 12 | 7 | 534 | -547 | 12 |
| 6 | 12 | 7 | 598 | -575 | 13 |
| 7 | 12 | 7 | 501 | 486 | 14 |
| 8 | 12 | 7 | 499 | 504 | 13 |
| -6 | 13 | 7 | 772 | 785 | 13 |
| -5 | 13 | 7 | 604 | 601 | 14 |
| -4 | 13 | 7 | 662 | -676 | 12 |
| -3 | 13 | 7 | 454 | -463 | 14 |
| -2 | 13 | 7 | 691 | 653 | 13 |
| -1 | 13 | 7 | 759 | 780 | 13 |
| 0 | 13 | 7 | 948 | -938 | 21 |
| 1 | 13 | 7 | 716 | -732 | 11 |
| 2 | 13 | 7 | 820 | 804 | 12 |
| 3 | 13 | 7 | 923 | 922 | 11 |
| 4 | 13 | 7 | 868 | -859 | 12 |
| 5 | 13 | 7 | 1013 | -997 | 11 |
| 6 | 13 | 7 | 791 | 764 | 12 |
| -4 | 14 | 7 | 486 | -486 | 15 |
| -3 | 14 | 7 | 663 | 676 | 13 |
| -2 | 14 | 7 | 582 | 586 | 13 |
| -1 | 14 | 7 | 698 | -708 | 13 |
| 0 | 14 | 7 | 594 | -633 | 17 |
| 1 | 14 | 7 | 781 | 773 | 12 |
| 2 | 14 | 7 | 781 | 791 | 12 |
| 3 | 14 | 7 | 608 | -579 | 12 |
| 4 | 14 | 7 | 771 | -795 | 12 |
| -14 | 0 | 8 | 909 | 842 | 13 |
| -13 | 0 | 8 | 562 | -532 | 15 |
| -12 | 0 | 8 | 1008 | -963 | 11 |
| -11 | 0 | 8 | 652 | 649 | 12 |
| -10 | 0 | 8 | 1068 | 1045 | 11 |
| -9 | 0 | 8 | 454 | -439 | 13 |
| -8 | 0 | 8 | 1947 | -1962 | 9 |
| -7 | 0 | 8 | 975 | 999 | 9 |
| -6 | 0 | 8 | 1948 | 1971 | 7 |
| -5 | 0 | 8 | 1334 | -1350 | 7 |
| -4 | 0 | 8 | 2350 | -2431 | 7 |
| -3 | 0 | 8 | 1295 | 1361 | 7 |
| -2 | 0 | 8 | 2689 | 2819 | 6 |
| -1 | 0 | 8 | 1880 | -1915 | 6 |
| 0 | 0 | 8 | 1337 | -1380 | 55 |
| 1 | 0 | 8 | 1139 | 1127 | 6 |
| 2 | 0 | 8 | 1739 | 1715 | 6 |
| 3 | 0 | 8 | 1151 | -1107 | 7 |
| 4 | 0 | 8 | 1218 | -1222 | 8 |
| 5 | 0 | 8 | 623 | 615 | 9 |
| 6 | 0 | 8 | 1578 | 1576 | 8 |
| 7 | 0 | 8 | 598 | -581 | 11 |
| 8 | 0 | 8 | 1668 | -1678 | 9 |
| 9 | 0 | 8 | 1134 | 1185 | 10 |
| 10 | 0 | 8 | 1212 | 1244 | 11 |
| 11 | 0 | 8 | 346 | -360 | 18 |
| 12 | 0 | 8 | 1004 | -997 | 13 |
| 13 | 0 | 8 | 341 | 328 | 18 |
| -14 | 1 | 8 | 411 | -407 | 16 |
| -13 | 1 | 8 | 782 | -730 | 14 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -12 | 1 | 8 | 434 | 419 | 15 |
| -11 | 1 | 8 | 898 | 893 | 11 |
| -10 | 1 | 8 | 460 | -446 | 14 |
| -9 | 1 | 8 | 1288 | -1267 | 9 |
| -8 | 1 | 8 | 603 | 642 | 11 |
| -7 | 1 | 8 | 1384 | 1416 | 8 |
| -6 | 1 | 8 | 592 | -603 | 9 |
| -5 | 1 | 8 | 1157 | -1210 | 7 |
| -4 | 1 | 8 | 899 | 920 | 7 |
| -3 | 1 | 8 | 1175 | 1217 | 7 |
| -2 | 1 | 8 | 1397 | -1430 | 6 |
| -1 | 1 | 8 | 1625 | -1667 | 6 |
| 0 | 1 | 8 | 555 | 522 | 15 |
| 1 | 1 | 8 | 1342 | 1303 | 6 |
| 2 | 1 | 8 | 1593 | -1554 | 6 |
| 3 | 1 | 8 | 1443 | -1400 | 6 |
| 4 | 1 | 8 | 1554 | 1500 | 7 |
| 5 | 1 | 8 | 1785 | 1750 | 7 |
| 6 | 1 | 8 | 861 | -860 | 9 |
| 7 | 1 | 8 | 1330 | -1333 | 9 |
| 8 | 1 | 8 | 804 | 804 | 11 |
| 9 | 1 | 8 | 942 | 892 | 11 |
| 10 | 1 | 8 | 340 | -350 | 20 |
| 11 | 1 | 8 | 1019 | -1010 | 12 |
| 12 | 1 | 8 | 266 | 291 | 20 |
| 13 | 1 | 8 | 906 | 879 | 14 |
| -14 | 2 | 8 | 399 | -386 | 17 |
| -13 | 2 | 8 | 211 | 188 | 28 |
| -12 | 2 | 8 | 382 | 374 | 18 |
| -11 | 2 | 8 | 232 | -246 | 18 |
| -10 | 2 | 8 | 139 | -112 | 35 |
| -9 | 2 | 8 | 67 | 95 | 55 |
| -8 | 2 | 8 | 668 | 657 | 10 |
| -7 | 2 | 8 | 372 | -394 | 11 |
| -6 | 2 | 8 | 507 | -499 | 10 |
| -5 | 2 | 8 | 384 | 387 | 11 |
| -4 | 2 | 8 | 198 | 206 | 13 |
| -3 | 2 | 8 | 76 | -143 | 34 |
| -2 | 2 | 8 | 1334 | -1315 | 6 |
| -1 | 2 | 8 | 15 | 26 | 58 |
| 0 | 2 | 8 | 1221 | 1214 | 49 |
| 1 | 2 | 8 | 406 | -382 | 8 |
| 2 | 2 | 8 | 1657 | -1583 | 6 |
| 3 | 2 | 8 | 871 | 828 | 7 |
| 4 | 2 | 8 | 882 | 849 | 7 |
| 5 | 2 | 8 | 141 | 124 | 21 |
| 6 | 2 | 8 | 389 | -390 | 10 |
| 7 | 2 | 8 | 305 | 324 | 13 |
| 8 | 2 | 8 | 812 | 801 | 11 |
| 9 | 2 | 8 | 482 | -496 | 13 |
| 10 | 2 | 8 | 495 | -498 | 14 |
| 12 | 2 | 8 | 530 | 538 | 15 |
| 13 | 2 | 8 | 73 | -113 | 64 |
| -13 | 3 | 8 | 231 | -183 | 32 |
| -12 | 3 | 8 | 126 | 117 | 43 |
| -11 | 3 | 8 | 298 | 325 | 18 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -10 | 3 | 8 | 205 | -94 | 36 |
| -9 | 3 | 8 | 360 | -385 | 14 |
| -8 | 3 | 8 | 39 | 44 | 65 |
| -7 | 3 | 8 | 394 | 418 | 13 |
| -6 | 3 | 8 | 407 | -401 | 11 |
| -5 | 3 | 8 | 206 | -201 | 15 |
| -4 | 3 | 8 | 369 | 354 | 10 |
| -2 | 3 | 8 | 169 | 139 | 14 |
| -1 | 3 | 8 | 404 | -431 | 8 |
| 0 | 3 | 8 | 731 | -709 | 38 |
| 1 | 3 | 8 | 591 | 575 | 8 |
| 2 | 3 | 8 | 674 | 642 | 7 |
| 3 | 3 | 8 | 969 | -923 | 6 |
| 4 | 3 | 8 | 149 | 145 | 18 |
| 5 | 3 | 8 | 342 | 337 | 10 |
| 6 | 3 | 8 | 293 | -295 | 12 |
| 7 | 3 | 8 | 277 | -285 | 15 |
| 9 | 3 | 8 | 479 | 504 | 13 |
| 10 | 3 | 8 | 132 | 102 | 30 |
| 11 | 3 | 8 | 153 | -139 | 35 |
| 12 | 3 | 8 | 140 | -69 | 38 |
| 13 | 3 | 8 | 150 | 213 | 42 |
| -13 | 4 | 8 | 285 | 249 | 23 |
| -12 | 4 | 8 | 672 | 660 | 14 |
| -11 | 4 | 8 | 471 | -431 | 14 |
| -10 | 4 | 8 | 875 | -871 | 11 |
| -9 | 4 | 8 | 517 | 515 | 12 |
| -8 | 4 | 8 | 603 | 624 | 11 |
| -7 | 4 | 8 | 249 | -242 | 18 |
| -6 | 4 | 8 | 787 | -813 | 9 |
| -5 | 4 | 8 | 519 | 484 | 9 |
| -4 | 4 | 8 | 1045 | 1057 | 8 |
| -3 | 4 | 8 | 495 | -479 | 9 |
| -2 | 4 | 8 | 430 | -409 | 9 |
| -1 | 4 | 8 | 858 | 899 | 7 |
| 0 | 4 | 8 | 1199 | 1184 | 69 |
| 1 | 4 | 8 | 978 | -931 | 7 |
| 2 | 4 | 8 | 1506 | -1442 | 6 |
| 3 | 4 | 8 | 143 | -82 | 18 |
| 4 | 4 | 8 | 1091 | 1047 | 7 |
| 5 | 4 | 8 | 240 | -214 | 13 |
| 6 | 4 | 8 | 1421 | -1382 | 8 |
| 7 | 4 | 8 | 175 | 16 | 26 |
| 8 | 4 | 8 | 1090 | 1064 | 9 |
| 9 | 4 | 8 | 220 | -230 | 20 |
| 10 | 4 | 8 | 1259 | -1257 | 10 |
| 11 | 4 | 8 | 185 | 176 | 25 |
| 12 | 4 | 8 | 854 | 845 | 13 |
| 13 | 4 | 8 | 160 | -163 | 38 |
| -13 | 5 | 8 | 930 | 879 | 13 |
| -12 | 5 | 8 | 356 | -369 | 15 |
| -11 | 5 | 8 | 883 | -853 | 12 |
| -10 | 5 | 8 | 643 | 642 | 12 |
| -9 | 5 | 8 | 747 | 749 | 11 |
| -8 | 5 | 8 | 437 | -423 | 12 |
| -7 | 5 | 8 | 969 | -972 | 9 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -6 | 5 | 8 | 756 | 752 | 9 |
| -5 | 5 | 8 | 1362 | 1384 | 8 |
| -4 | 5 | 8 | 814 | -811 | 8 |
| -3 | 5 | 8 | 1772 | -1770 | 7 |
| -2 | 5 | 8 | 527 | 552 | 9 |
| -1 | 5 | 8 | 1974 | 2006 | 6 |
| 0 | 5 | 8 | 817 | -811 | 39 |
| 1 | 5 | 8 | 1645 | -1558 | 7 |
| 2 | 5 | 8 | 1153 | 1116 | 7 |
| 3 | 5 | 8 | 1553 | 1492 | 7 |
| 4 | 5 | 8 | 680 | -643 | 8 |
| 5 | 5 | 8 | 1569 | -1528 | 7 |
| 6 | 5 | 8 | 153 | 123 | 18 |
| 7 | 5 | 8 | 1488 | 1482 | 8 |
| 8 | 5 | 8 | 538 | -526 | 11 |
| 9 | 5 | 8 | 1292 | -1302 | 10 |
| 10 | 5 | 8 | 574 | 559 | 13 |
| 11 | 5 | 8 | 933 | 922 | 12 |
| 12 | 5 | 8 | 390 | -418 | 16 |
| 13 | 5 | 8 | 866 | -848 | 13 |
| -12 | 6 | 8 | 765 | -750 | 13 |
| -11 | 6 | 8 | 450 | 445 | 15 |
| -10 | 6 | 8 | 930 | 895 | 12 |
| -9 | 6 | 8 | 735 | -749 | 11 |
| -8 | 6 | 8 | 1152 | -1166 | 10 |
| -7 | 6 | 8 | 895 | 895 | 9 |
| -6 | 6 | 8 | 1395 | 1400 | 8 |
| -5 | 6 | 8 | 919 | -898 | 9 |
| -4 | 6 | 8 | 1513 | -1530 | 8 |
| -3 | 6 | 8 | 883 | 898 | 8 |
| -2 | 6 | 8 | 1598 | 1624 | 7 |
| -1 | 6 | 8 | 693 | -711 | 8 |
| 0 | 6 | 8 | 1495 | -1492 | 74 |
| 1 | 6 | 8 | 1034 | 994 | 7 |
| 2 | 6 | 8 | 1759 | 1689 | 7 |
| 3 | 6 | 8 | 1154 | -1157 | 7 |
| 4 | 6 | 8 | 1692 | -1624 | 7 |
| 5 | 6 | 8 | 972 | 957 | 8 |
| 6 | 6 | 8 | 1082 | 1031 | 9 |
| 7 | 6 | 8 | 944 | -914 | 10 |
| 8 | 6 | 8 | 913 | -909 | 10 |
| 9 | 6 | 8 | 518 | 531 | 12 |
| 10 | 6 | 8 | 976 | 937 | 11 |
| 11 | 6 | 8 | 351 | -388 | 14 |
| 12 | 6 | 8 | 814 | -794 | 13 |
| -12 | 7 | 8 | 390 | 357 | 17 |
| -11 | 7 | 8 | 437 | 442 | 15 |
| -10 | 7 | 8 | 491 | -461 | 16 |
| -9 | 7 | 8 | 762 | -722 | 12 |
| -8 | 7 | 8 | 358 | 310 | 16 |
| -7 | 7 | 8 | 1169 | 1162 | 9 |
| -6 | 7 | 8 | 338 | -324 | 14 |
| -5 | 7 | 8 | 791 | -778 | 10 |
| -4 | 7 | 8 | 552 | 570 | 10 |
| -3 | 7 | 8 | 549 | 557 | 10 |
| -2 | 7 | 8 | 785 | -799 | 8 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -1 | 7 | 8 | 726 | -747 | 9 |
| 0 | 7 | 8 | 792 | 813 | 26 |
| 1 | 7 | 8 | 1100 | 1054 | 8 |
| 2 | 7 | 8 | 506 | -467 | 10 |
| 3 | 7 | 8 | 915 | -901 | 8 |
| 4 | 7 | 8 | 675 | 655 | 9 |
| 5 | 7 | 8 | 959 | 912 | 9 |
| 6 | 7 | 8 | 578 | -572 | 10 |
| 7 | 7 | 8 | 862 | -842 | 9 |
| 8 | 7 | 8 | 438 | 441 | 12 |
| 9 | 7 | 8 | 693 | 660 | 12 |
| 10 | 7 | 8 | 336 | -363 | 17 |
| 11 | 7 | 8 | 668 | -664 | 13 |
| 12 | 7 | 8 | 288 | 289 | 18 |
| -11 | 8 | 8 | 71 | -43 | 64 |
| -10 | 8 | 8 | 166 | 159 | 28 |
| -9 | 8 | 8 | 141 | 37 | 35 |
| -8 | 8 | 8 | 246 | -183 | 23 |
| -7 | 8 | 8 | 45 | -28 | 66 |
| -6 | 8 | 8 | 113 | 146 | 38 |
| -5 | 8 | 8 | 122 | -143 | 34 |
| -4 | 8 | 8 | 122 | -138 | 32 |
| -3 | 8 | 8 | 250 | -217 | 16 |
| -2 | 8 | 8 | 274 | -271 | 15 |
| -1 | 8 | 8 | 115 | 98 | 30 |
| 1 | 8 | 8 | 214 | 122 | 11 |
| 2 | 8 | 8 | 421 | 404 | 10 |
| 3 | 8 | 8 | 345 | 326 | 12 |
| 4 | 8 | 8 | 185 | 149 | 20 |
| 5 | 8 | 8 | 245 | -253 | 14 |
| 6 | 8 | 8 | 162 | -97 | 31 |
| 7 | 8 | 8 | 520 | 518 | 12 |
| 8 | 8 | 8 | 380 | 363 | 13 |
| 10 | 8 | 8 | 172 | -151 | 25 |
| 11 | 8 | 8 | 134 | 165 | 43 |
| -11 | 9 | 8 | 318 | 310 | 19 |
| -10 | 9 | 8 | 213 | -217 | 21 |
| -9 | 9 | 8 | 636 | -619 | 13 |
| -8 | 9 | 8 | 217 | 212 | 26 |
| -7 | 9 | 8 | 428 | 422 | 14 |
| -6 | 9 | 8 | 230 | -273 | 17 |
| -5 | 9 | 8 | 694 | -718 | 10 |
| -4 | 9 | 8 | 173 | 136 | 27 |
| -3 | 9 | 8 | 670 | 679 | 11 |
| -2 | 9 | 8 | 266 | -217 | 16 |
| -1 | 9 | 8 | 216 | -239 | 17 |
| 0 | 9 | 8 | 310 | 319 | 10 |
| 1 | 9 | 8 | 444 | 388 | 11 |
| 2 | 9 | 8 | 88 | 52 | 40 |
| 3 | 9 | 8 | 386 | -375 | 11 |
| 4 | 9 | 8 | 223 | 214 | 15 |
| 5 | 9 | 8 | 362 | 348 | 13 |
| 6 | 9 | 8 | 340 | -339 | 14 |
| 7 | 9 | 8 | 449 | -445 | 14 |
| 8 | 9 | 8 | 294 | 317 | 15 |
| 9 | 9 | 8 | 653 | 625 | 12 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 10 | 9 | 8 | 247 | -246 | 24 |
| -10 | 10 | 8 | 627 | -596 | 14 |
| -9 | 10 | 8 | 505 | 490 | 14 |
| -8 | 10 | 8 | 697 | 677 | 12 |
| -7 | 10 | 8 | 347 | -357 | 16 |
| -6 | 10 | 8 | 827 | -832 | 11 |
| -5 | 10 | 8 | 364 | 380 | 15 |
| -4 | 10 | 8 | 884 | 863 | 10 |
| -3 | 10 | 8 | 263 | -270 | 15 |
| -2 | 10 | 8 | 663 | -646 | 10 |
| -1 | 10 | 8 | 276 | 309 | 16 |
| 0 | 10 | 8 | 1115 | 1107 | 32 |
| 1 | 10 | 8 | 367 | -349 | 12 |
| 2 | 10 | 8 | 1030 | -972 | 9 |
| 3 | 10 | 8 | 395 | 392 | 12 |
| 4 | 10 | 8 | 1102 | 1031 | 9 |
| 5 | 10 | 8 | 550 | -527 | 12 |
| 6 | 10 | 8 | 1433 | -1424 | 9 |
| 7 | 10 | 8 | 312 | 287 | 19 |
| 8 | 10 | 8 | 1128 | 1111 | 11 |
| 9 | 10 | 8 | 250 | -266 | 24 |
| -9 | 11 | 8 | 681 | 643 | 14 |
| -8 | 11 | 8 | 480 | -470 | 14 |
| -7 | 11 | 8 | 653 | -644 | 13 |
| -6 | 11 | 8 | 648 | 656 | 13 |
| -5 | 11 | 8 | 810 | 815 | 11 |
| -4 | 11 | 8 | 616 | -672 | 12 |
| -3 | 11 | 8 | 1007 | -1019 | 10 |
| -2 | 11 | 8 | 539 | 539 | 12 |
| -1 | 11 | 8 | 1087 | 1071 | 10 |
| 0 | 11 | 8 | 632 | -615 | 18 |
| 1 | 11 | 8 | 1611 | -1559 | 9 |
| 2 | 11 | 8 | 227 | 160 | 20 |
| 3 | 11 | 8 | 1257 | 1218 | 10 |
| 4 | 11 | 8 | 434 | -425 | 13 |
| 5 | 11 | 8 | 1065 | -1060 | 10 |
| 6 | 11 | 8 | 460 | 440 | 13 |
| 7 | 11 | 8 | 1091 | 1079 | 11 |
| 8 | 11 | 8 | 358 | -325 | 18 |
| -8 | 12 | 8 | 453 | -423 | 15 |
| -7 | 12 | 8 | 269 | 274 | 18 |
| -6 | 12 | 8 | 603 | 612 | 14 |
| -5 | 12 | 8 | 437 | -454 | 16 |
| -4 | 12 | 8 | 720 | -755 | 13 |
| -3 | 12 | 8 | 388 | 446 | 15 |
| -2 | 12 | 8 | 661 | 668 | 11 |
| -1 | 12 | 8 | 531 | -560 | 12 |
| 0 | 12 | 8 | 1086 | -1101 | 15 |
| 1 | 12 | 8 | 573 | 569 | 12 |
| 2 | 12 | 8 | 890 | 863 | 10 |
| 3 | 12 | 8 | 490 | -494 | 14 |
| 4 | 12 | 8 | 708 | -708 | 12 |
| 5 | 12 | 8 | 349 | 345 | 15 |
| 6 | 12 | 8 | 792 | 782 | 12 |
| 7 | 12 | 8 | 322 | -338 | 17 |
| -6 | 13 | 8 | 123 | -100 | 44 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 13 | 8 | 188 | -222 | 26 |
| -4 | 13 | 8 | 107 | 59 | 45 |
| -3 | 13 | 8 | 414 | 479 | 15 |
| -2 | 13 | 8 | 211 | -183 | 25 |
| -1 | 13 | 8 | 152 | -170 | 35 |
| 0 | 13 | 8 | 320 | 344 | 17 |
| 1 | 13 | 8 | 68 | 128 | 61 |
| 2 | 13 | 8 | 231 | -292 | 17 |
| 3 | 13 | 8 | 433 | -453 | 15 |
| 4 | 13 | 8 | 159 | 215 | 27 |
| 5 | 13 | 8 | 290 | 271 | 22 |
| -3 | 14 | 8 | 162 | 200 | 35 |
| -2 | 14 | 8 | 409 | 430 | 16 |
| -1 | 14 | 8 | 209 | -245 | 28 |
| 0 | 14 | 8 | 453 | -479 | 13 |
| 1 | 14 | 8 | 222 | 217 | 29 |
| 2 | 14 | 8 | 200 | 229 | 21 |
| 3 | 14 | 8 | 135 | -178 | 32 |
| -13 | 1 | 9 | 645 | -604 | 14 |
| -11 | 1 | 9 | 726 | 700 | 12 |
| -10 | 1 | 9 | 65 | -105 | 38 |
| -9 | 1 | 9 | 768 | -755 | 11 |
| -8 | 1 | 9 | 134 | 77 | 33 |
| -7 | 1 | 9 | 846 | 830 | 9 |
| -6 | 1 | 9 | 135 | -125 | 24 |
| -5 | 1 | 9 | 974 | -983 | 8 |
| -4 | 1 | 9 | 750 | -736 | 8 |
| -3 | 1 | 9 | 650 | 658 | 8 |
| -2 | 1 | 9 | 915 | 926 | 7 |
| -1 | 1 | 9 | 493 | -494 | 8 |
| 0 | 1 | 9 | 117 | 107 | 20 |
| 1 | 1 | 9 | 1152 | 1114 | 7 |
| 2 | 1 | 9 | 543 | -537 | 8 |
| 3 | 1 | 9 | 1241 | -1217 | 7 |
| 4 | 1 | 9 | 685 | 672 | 8 |
| 5 | 1 | 9 | 1309 | 1288 | 8 |
| 6 | 1 | 9 | 82 | 42 | 42 |
| 7 | 1 | 9 | 852 | -858 | 10 |
| 8 | 1 | 9 | 107 | 58 | 51 |
| 9 | 1 | 9 | 921 | 925 | 11 |
| 10 | 1 | 9 | 91 | -2 | 48 |
| 11 | 1 | 9 | 869 | -846 | 13 |
| 12 | 1 | 9 | 74 | -87 | 60 |
| 13 | 1 | 9 | 505 | 527 | 18 |
| -13 | 2 | 9 | 196 | 153 | 31 |
| -12 | 2 | 9 | 1060 | 1015 | 12 |
| -11 | 2 | 9 | 132 | -115 | 38 |
| -10 | 2 | 9 | 1080 | -1049 | 11 |
| -9 | 2 | 9 | 131 | -110 | 34 |
| -8 | 2 | 9 | 1250 | 1218 | 9 |
| -7 | 2 | 9 | 150 | 163 | 23 |
| -6 | 2 | 9 | 1336 | -1333 | 8 |
| -5 | 2 | 9 | 73 | 93 | 40 |
| -4 | 2 | 9 | 1687 | 1711 | 7 |
| -3 | 2 | 9 | 449 | 420 | 8 |
| -2 | 2 | 9 | 2242 | -2290 | 6 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -1 | 2 | 9 | 756 | -736 | 7 |
| 0 | 2 | 9 | 1721 | 1713 | 78 |
| 1 | 2 | 9 | 238 | -257 | 12 |
| 2 | 2 | 9 | 2177 | -2108 | 6 |
| 3 | 2 | 9 | 302 | 274 | 11 |
| 4 | 2 | 9 | 1907 | 1852 | 7 |
| 5 | 2 | 9 | 204 | -175 | 17 |
| 6 | 2 | 9 | 1718 | -1676 | 8 |
| 7 | 2 | 9 | 73 | 148 | 33 |
| 8 | 2 | 9 | 1298 | 1262 | 9 |
| 9 | 2 | 9 | 360 | -369 | 15 |
| 10 | 2 | 9 | 1076 | -1071 | 11 |
| 11 | 2 | 9 | 116 | -72 | 43 |
| 12 | 2 | 9 | 854 | 847 | 13 |
| -13 | 3 | 9 | 1001 | 934 | 12 |
| -11 | 3 | 9 | 857 | -833 | 12 |
| -10 | 3 | 9 | 269 | 225 | 23 |
| -9 | 3 | 9 | 1175 | 1167 | 10 |
| -8 | 3 | 9 | 263 | 307 | 15 |
| -7 | 3 | 9 | 1811 | -1851 | 8 |
| -6 | 3 | 9 | 102 | 40 | 35 |
| -5 | 3 | 9 | 1900 | 1906 | 7 |
| -4 | 3 | 9 | 408 | -421 | 10 |
| -3 | 3 | 9 | 2242 | -2278 | 7 |
| -2 | 3 | 9 | 116 | 84 | 21 |
| -1 | 3 | 9 | 2718 | 2782 | 6 |
| 0 | 3 | 9 | 92 | 56 | 20 |
| 1 | 3 | 9 | 2445 | -2325 | 6 |
| 2 | 3 | 9 | 335 | -329 | 9 |
| 3 | 3 | 9 | 1495 | 1444 | 6 |
| 4 | 3 | 9 | 127 | 159 | 17 |
| 5 | 3 | 9 | 1966 | -1903 | 7 |
| 6 | 3 | 9 | 259 | -336 | 11 |
| 7 | 3 | 9 | 1473 | 1450 | 9 |
| 8 | 3 | 9 | 318 | -330 | 14 |
| 9 | 3 | 9 | 1165 | -1155 | 10 |
| 11 | 3 | 9 | 1069 | 1067 | 11 |
| 13 | 3 | 9 | 860 | -841 | 13 |
| -13 | 4 | 9 | 132 | 17 | 43 |
| -12 | 4 | 9 | 630 | -573 | 14 |
| -11 | 4 | 9 | 150 | 124 | 35 |
| -10 | 4 | 9 | 758 | 742 | 12 |
| -8 | 4 | 9 | 1120 | -1101 | 10 |
| -7 | 4 | 9 | 205 | -202 | 16 |
| -6 | 4 | 9 | 1103 | 1099 | 9 |
| -5 | 4 | 9 | 389 | -394 | 12 |
| -4 | 4 | 9 | 1137 | -1150 | 8 |
| -3 | 4 | 9 | 385 | 392 | 10 |
| -2 | 4 | 9 | 1372 | 1381 | 7 |
| -1 | 4 | 9 | 452 | -468 | 9 |
| 0 | 4 | 9 | 1793 | -1751 | 89 |
| 1 | 4 | 9 | 217 | 214 | 16 |
| 2 | 4 | 9 | 1764 | 1705 | 7 |
| 3 | 4 | 9 | 205 | -181 | 19 |
| 4 | 4 | 9 | 1540 | -1491 | 7 |
| 5 | 4 | 9 | 155 | -172 | 19 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 6 | 4 | 9 | 1203 | 1153 | 8 |
| 7 | 4 | 9 | 110 | 55 | 35 |
| 8 | 4 | 9 | 863 | -849 | 11 |
| 9 | 4 | 9 | 304 | 300 | 18 |
| 10 | 4 | 9 | 851 | 844 | 11 |
| 11 | 4 | 9 | 203 | 176 | 34 |
| 12 | 4 | 9 | 673 | -680 | 14 |
| 13 | 4 | 9 | 152 | 129 | 39 |
| -13 | 5 | 9 | 244 | -241 | 22 |
| -12 | 5 | 9 | 91 | -87 | 53 |
| -11 | 5 | 9 | 119 | 109 | 43 |
| -10 | 5 | 9 | 261 | -273 | 17 |
| -9 | 5 | 9 | 307 | -295 | 17 |
| -8 | 5 | 9 | 122 | 86 | 36 |
| -7 | 5 | 9 | 643 | 641 | 11 |
| -6 | 5 | 9 | 330 | 337 | 12 |
| -5 | 5 | 9 | 279 | -236 | 13 |
| -4 | 5 | 9 | 157 | -138 | 19 |
| -3 | 5 | 9 | 434 | 448 | 10 |
| -2 | 5 | 9 | 232 | 229 | 14 |
| -1 | 5 | 9 | 483 | -506 | 9 |
| 0 | 5 | 9 | 521 | -509 | 27 |
| 1 | 5 | 9 | 303 | 308 | 10 |
| 2 | 5 | 9 | 231 | -206 | 14 |
| 3 | 5 | 9 | 616 | -594 | 9 |
| 4 | 5 | 9 | 315 | 317 | 10 |
| 5 | 5 | 9 | 566 | 527 | 10 |
| 6 | 5 | 9 | 104 | -75 | 36 |
| 7 | 5 | 9 | 523 | -518 | 12 |
| 8 | 5 | 9 | 199 | 192 | 19 |
| 9 | 5 | 9 | 519 | 532 | 12 |
| 10 | 5 | 9 | 99 | 122 | 46 |
| 11 | 5 | 9 | 197 | -233 | 26 |
| -12 | 6 | 9 | 309 | -323 | 19 |
| -10 | 6 | 9 | 266 | 216 | 19 |
| -8 | 6 | 9 | 525 | -507 | 12 |
| -7 | 6 | 9 | 110 | 127 | 39 |
| -6 | 6 | 9 | 640 | 646 | 11 |
| -5 | 6 | 9 | 200 | -187 | 16 |
| -4 | 6 | 9 | 302 | -319 | 13 |
| -3 | 6 | 9 | 306 | 321 | 13 |
| -2 | 6 | 9 | 792 | 768 | 8 |
| -1 | 6 | 9 | 234 | 242 | 13 |
| 0 | 6 | 9 | 540 | -538 | 49 |
| 1 | 6 | 9 | 191 | 187 | 13 |
| 2 | 6 | 9 | 530 | 501 | 9 |
| 3 | 6 | 9 | 158 | 139 | 16 |
| 4 | 6 | 9 | 642 | -641 | 9 |
| 5 | 6 | 9 | 82 | 35 | 41 |
| 6 | 6 | 9 | 787 | 741 | 9 |
| 7 | 6 | 9 | 136 | -13 | 31 |
| 8 | 6 | 9 | 234 | -151 | 27 |
| 9 | 6 | 9 | 203 | -199 | 20 |
| 10 | 6 | 9 | 283 | 258 | 20 |
| 11 | 6 | 9 | 98 | 26 | 49 |
| 12 | 6 | 9 | 393 | -369 | 18 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -12 | 7 | 9 | 319 | 311 | 23 |
| -11 | 7 | 9 | 819 | 777 | 13 |
| -10 | 7 | 9 | 293 | -294 | 19 |
| -9 | 7 | 9 | 1082 | -1053 | 11 |
| -8 | 7 | 9 | 223 | 225 | 19 |
| -7 | 7 | 9 | 1244 | 1203 | 10 |
| -6 | 7 | 9 | 203 | -178 | 20 |
| -5 | 7 | 9 | 1250 | -1259 | 9 |
| -4 | 7 | 9 | 261 | 276 | 16 |
| -3 | 7 | 9 | 1277 | 1267 | 8 |
| -2 | 7 | 9 | 401 | -385 | 11 |
| -1 | 7 | 9 | 1388 | -1395 | 8 |
| 0 | 7 | 9 | 591 | 585 | 24 |
| 1 | 7 | 9 | 1693 | 1573 | 8 |
| 2 | 7 | 9 | 219 | 203 | 15 |
| 3 | 7 | 9 | 1283 | -1230 | 8 |
| 4 | 7 | 9 | 232 | -224 | 14 |
| 5 | 7 | 9 | 1440 | 1359 | 8 |
| 6 | 7 | 9 | 51 | 56 | 59 |
| 7 | 7 | 9 | 1312 | -1276 | 9 |
| 8 | 7 | 9 | 178 | -268 | 25 |
| 9 | 7 | 9 | 970 | 957 | 11 |
| 10 | 7 | 9 | 101 | 127 | 48 |
| 11 | 7 | 9 | 827 | -807 | 12 |
| -11 | 8 | 9 | 256 | -267 | 19 |
| -10 | 8 | 9 | 990 | -942 | 11 |
| -9 | 8 | 9 | 439 | 401 | 15 |
| -8 | 8 | 9 | 1257 | 1202 | 10 |
| -7 | 8 | 9 | 491 | -493 | 13 |
| -6 | 8 | 9 | 1415 | -1359 | 9 |
| -5 | 8 | 9 | 279 | 255 | 16 |
| -4 | 8 | 9 | 1541 | 1517 | 8 |
| -3 | 8 | 9 | 136 | -116 | 22 |
| -2 | 8 | 9 | 1677 | -1683 | 8 |
| -1 | 8 | 9 | 138 | 135 | 18 |
| 0 | 8 | 9 | 1769 | 1710 | 79 |
| 1 | 8 | 9 | 219 | 217 | 16 |
| 2 | 8 | 9 | 1494 | -1368 | 8 |
| 3 | 8 | 9 | 189 | -164 | 19 |
| 4 | 8 | 9 | 1225 | 1182 | 9 |
| 5 | 8 | 9 | 142 | -138 | 32 |
| 6 | 8 | 9 | 1452 | -1398 | 9 |
| 7 | 8 | 9 | 166 | 57 | 30 |
| 8 | 8 | 9 | 1373 | 1366 | 9 |
| 9 | 8 | 9 | 100 | 40 | 47 |
| 10 | 8 | 9 | 1306 | -1294 | 11 |
| 11 | 8 | 9 | 132 | -97 | 44 |
| -10 | 9 | 9 | 177 | 140 | 27 |
| -9 | 9 | 9 | 831 | 823 | 12 |
| -8 | 9 | 9 | 357 | -362 | 17 |
| -7 | 9 | 9 | 970 | -973 | 11 |
| -6 | 9 | 9 | 343 | 349 | 14 |
| -5 | 9 | 9 | 978 | 990 | 10 |
| -3 | 9 | 9 | 1070 | -1027 | 9 |
| -1 | 9 | 9 | 1097 | 1084 | 9 |
| 0 | 9 | 9 | 333 | -347 | 28 |

Q.5385-M31



Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| 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 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 9 | 9 | 1393 | -1328 | 8 | -1 | 13 | 9 | 836 | -858 | 12 | 7 | 1 | 10 | 1615 | 1588 | 9 | -11 | 4 | 10 | 96 | -102 | 48 | -4 | 6 | 10 | 1287 | 1332 | 8 |
| 2 | 9 | 9 | 154 | 180 | 28 | 0 | 13 | 9 | 201 | 157 | 50 | 8 | 1 | 10 | 342 | 335 | 16 | -10 | 4 | 10 | 904 | 909 | 11 | -3 | 6 | 10 | 414 | 378 | 12 |
| 3 | 9 | 9 | 1542 | 1447 | 8 | 1 | 13 | 9 | 1121 | 1113 | 11 | 9 | 1 | 10 | 1450 | -1456 | 10 | -9 | 4 | 10 | 323 | 315 | 16 | -2 | 6 | 10 | 1308 | -1325 | 8 |
| 4 | 9 | 9 | 248 | -270 | 17 | 2 | 13 | 9 | 235 | -236 | 18 | 10 | 1 | 10 | 105 | -104 | 45 | -8 | 4 | 10 | 1137 | -1137 | 10 | -1 | 6 | 10 | 633 | -651 | 9 |
| 5 | 9 | 9 | 1125 | -1029 | 9 | 3 | 13 | 9 | 939 | -924 | 11 | 11 | 1 | 10 | 830 | 833 | 12 | -7 | 4 | 10 | 165 | -134 | 20 | 0 | 6 | 10 | 1343 | 1326 | 70 |
| 6 | 9 | 9 | 234 | 288 | 17 | 4 | 13 | 9 | 145 | -86 | 36 | 12 | 1 | 10 | 260 | 268 | 19 | -6 | 4 | 10 | 1350 | 1368 | 9 | 1 | 6 | 10 | 543 | 539 | 10 |
| 7 | 9 | 9 | 1016 | 1009 | 10 | 5 | 13 | 9 | 938 | 903 | 11 | 13 | 1 | 10 | 868 | -885 | 14 | -5 | 4 | 10 | 143 | 142 | 19 | 2 | 6 | 10 | 1928 | -1821 | 7 |
| 9 | 9 | 9 | 936 | -930 | 11 | -2 | 14 | 9 | 717 | -722 | 14 | -12 | 2 | 10 | 378 | -398 | 16 | -4 | 4 | 10 | 1102 | -1147 | 8 | 3 | 6 | 10 | 482 | -448 | 11 |
| 10 | 9 | 9 | 103 | 127 | 49 | 0 | 14 | 9 | 894 | 908 | 21 | -11 | 2 | 10 | 192 | -199 | 23 | -3 | 4 | 10 | 146 | -124 | 23 | 4 | 6 | 10 | 1437 | 1351 | 8 |
| -9 | 10 | 9 | 150 | 123 | 51 | 1 | 14 | 9 | 181 | -158 | 27 | -10 | 2 | 10 | 514 | 490 | 12 | -2 | 4 | 10 | 1248 | 1246 | 7 | 5 | 6 | 10 | 331 | 323 | 13 |
| -8 | 10 | 9 | 478 | -464 | 14 | 2 | 14 | 9 | 750 | -755 | 12 | -9 | 2 | 10 | 120 | -13 | 36 | 0 | 4 | 10 | 13[illegible] | -1309 | 69 | 6 | 6 | 10 | 1272 | -1233 | 9 |
| -7 | 10 | 9 | 106 | 66 | 31 | -13 | 0 | 10 | 113 | -49 | 49 | -8 | 2 | 10 | 609 | -611 | 11 | 1 | 4 | 10 | 143 | -107 | 20 | 7 | 6 | 10 | 433 | -411 | 12 |
| -6 | 10 | 9 | 504 | 512 | 12 | -12 | 0 | 10 | 930 | 902 | 12 | -7 | 2 | 10 | 149 | -177 | 19 | 2 | 4 | 10 | 1310 | 1269 | 7 | 8 | 6 | 10 | 1162 | 1169 | 10 |
| -5 | 10 | 9 | 103 | -130 | 42 | -10 | 0 | 10 | 1360 | -1310 | 11 | -6 | 2 | 10 | 721 | 700 | 10 | 3 | 4 | 10 | 151 | 47 | 26 | 9 | 6 | 10 | 170 | 134 | 29 |
| -4 | 10 | 9 | 747 | -723 | 11 | -9 | 0 | 10 | 132 | 87 | 35 | -4 | 2 | 10 | 705 | -695 | 8 | 4 | 4 | 10 | 1020 | -990 | 8 | 10 | 6 | 10 | 935 | -905 | 11 |
| -2 | 10 | 9 | 522 | 545 | 13 | -8 | 0 | 10 | 1238 | 1204 | 9 | -3 | 2 | 10 | 291 | -314 | 10 | 5 | 4 | 10 | 380 | -352 | 11 | 11 | 6 | 10 | 376 | -372 | 16 |
| -1 | 10 | 9 | 407 | -408 | 15 | -7 | 0 | 10 | 693 | 718 | 9 | -2 | 2 | 10 | 775 | 754 | 8 | 6 | 4 | 10 | 1196 | 1172 | 8 | -11 | 7 | 10 | 466 | -429 | 16 |
| 0 | 10 | 9 | 522 | -520 | 15 | -6 | 0 | 10 | 1525 | -1513 | 8 | -1 | 2 | 10 | 765 | 793 | 7 | 7 | 4 | 10 | 753 | 764 | 10 | -10 | 7 | 10 | 138 | -157 | 38 |
| 2 | 10 | 9 | 714 | 684 | 11 | -5 | 0 | 10 | 803 | -770 | 9 | 0 | 2 | 10 | 727 | -712 | 24 | 8 | 4 | 10 | 947 | -913 | 10 | -9 | 7 | 10 | 380 | 381 | 16 |
| 3 | 10 | 9 | 164 | 127 | 23 | -4 | 0 | 10 | 1697 | 1748 | 7 | 1 | 2 | 10 | 58 | 3 | 41 | 9 | 4 | 10 | 280 | -307 | 16 | -8 | 7 | 10 | 146 | 145 | 33 |
| 4 | 10 | 9 | 741 | -710 | 10 | -3 | 0 | 10 | 115 | 83 | 20 | 2 | 2 | 10 | 1180 | 1123 | 7 | 10 | 4 | 10 | 775 | 781 | 13 | -7 | 7 | 10 | 538 | -533 | 12 |
| 5 | 10 | 9 | 258 | -285 | 16 | -2 | 0 | 10 | 1828 | -1844 | 7 | 3 | 2 | 10 | 82 | -38 | 32 | 11 | 4 | 10 | 355 | 385 | 16 | -6 | 7 | 10 | 234 | -232 | 20 |
| 6 | 10 | 9 | 458 | 468 | 12 | -1 | 0 | 10 | 689 | -664 | 7 | 4 | 2 | 10 | 1405 | -1359 | 7 | 12 | 4 | 10 | 621 | -629 | 15 | -5 | 7 | 10 | 855 | 830 | 10 |
| 7 | 10 | 9 | 172 | 163 | 24 | 0 | 0 | 10 | 1629 | 1610 | 54 | 5 | 2 | 10 | 196 | -178 | 14 | -12 | 5 | 10 | 276 | -254 | 25 | -4 | 7 | 10 | 356 | 353 | 13 |
| 8 | 10 | 9 | 511 | -474 | 15 | 1 | 0 | 10 | 447 | 442 | 8 | 6 | 2 | 10 | 999 | 964 | 9 | -11 | 5 | 10 | 985 | 947 | 12 | -3 | 7 | 10 | 939 | -966 | 9 |
| 9 | 10 | 9 | 75 | -34 | 60 | 2 | 0 | 10 | 1896 | -1834 | 6 | 7 | 2 | 10 | 352 | 334 | 16 | -10 | 5 | 10 | 229 | 272 | 20 | -2 | 7 | 10 | 241 | -250 | 15 |
| -8 | 11 | 9 | 164 | -202 | 33 | 3 | 0 | 10 | 773 | -747 | 9 | 8 | 2 | 10 | 505 | -477 | 12 | -9 | 5 | 10 | 1198 | -1177 | 11 | -1 | 7 | 10 | 849 | 872 | 9 |
| -7 | 11 | 9 | 157 | -192 | 29 | 4 | 0 | 10 | 1714 | 1656 | 8 | 9 | 2 | 10 | 268 | -292 | 17 | -8 | 5 | 10 | 132 | 113 | 34 | 0 | 7 | 10 | 261 | 268 | 11 |
| -6 | 11 | 9 | 87 | 70 | 51 | 5 | 0 | 10 | 1033 | 1001 | 9 | 10 | 2 | 10 | 461 | 467 | 15 | -7 | 5 | 10 | 1432 | 1437 | 9 | 1 | 7 | 10 | 640 | -671 | 10 |
| -5 | 11 | 9 | 189 | 193 | 31 | 6 | 0 | 10 | 1727 | -1727 | 9 | 11 | 2 | 10 | 259 | 246 | 23 | -6 | 5 | 10 | 184 | 151 | 20 | 2 | 7 | 10 | 292 | -276 | 14 |
| -4 | 11 | 9 | 115 | -29 | 40 | 7 | 0 | 10 | 767 | -763 | 11 | 12 | 2 | 10 | 383 | -367 | 18 | -5 | 5 | 10 | 1373 | -1391 | 9 | 3 | 7 | 10 | 909 | 895 | 9 |
| -2 | 11 | 9 | 121 | -133 | 25 | 8 | 0 | 10 | 1892 | 1884 | 9 | 13 | 2 | 10 | 205 | -78 | 39 | -4 | 5 | 10 | 244 | -274 | 14 | 4 | 7 | 10 | 284 | 249 | 15 |
| -1 | 11 | 9 | 168 | 188 | 27 | 10 | 0 | 10 | 1754 | -1795 | 10 | -13 | 3 | 10 | 161 | 123 | 38 | -3 | 5 | 10 | 1727 | 1771 | 8 | 5 | 7 | 10 | 859 | -830 | 9 |
| 1 | 11 | 9 | 585 | -611 | 12 | 11 | 0 | 10 | 537 | -563 | 15 | -11 | 3 | 10 | 330 | -262 | 20 | -2 | 5 | 10 | 500 | 486 | 10 | 6 | 7 | 10 | 181 | -154 | 19 |
| 2 | 11 | 9 | 186 | 155 | 25 | 12 | 0 | 10 | 1034 | 1024 | 13 | -10 | 3 | 10 | 165 | -182 | 40 | -1 | 5 | 10 | 1667 | -1705 | 7 | 7 | 7 | 10 | 1011 | 978 | 10 |
| 3 | 11 | 9 | 309 | 289 | 18 | 13 | 0 | 10 | 421 | 436 | 23 | -9 | 3 | 10 | 660 | 644 | 11 | 0 | 5 | 10 | 291 | -288 | 18 | 8 | 7 | 10 | 153 | 159 | 23 |
| 4 | 11 | 9 | 97 | 145 | 46 | -13 | 1 | 10 | 813 | 776 | 13 | -8 | 3 | 10 | 119 | 107 | 37 | 1 | 5 | 10 | 1987 | 1843 | 7 | 9 | 7 | 10 | 806 | -807 | 11 |
| 5 | 11 | 9 | 225 | -131 | 28 | -12 | 1 | 10 | 245 | 127 | 35 | -7 | 3 | 10 | 238 | -202 | 15 | 2 | 5 | 10 | 524 | 497 | 10 | 10 | 7 | 10 | 233 | -240 | 26 |
| 7 | 11 | 9 | 111 | 112 | 45 | -11 | 1 | 10 | 1005 | -964 | 11 | -6 | 3 | 10 | 427 | -435 | 11 | 3 | 5 | 10 | 1424 | -1355 | 7 | 11 | 7 | 10 | 538 | 520 | 15 |
| -7 | 12 | 9 | 198 | 127 | 32 | -10 | 1 | 10 | 161 | 173 | 21 | -5 | 3 | 10 | 152 | 178 | 18 | 4 | 5 | 10 | 569 | -547 | 9 | -11 | 8 | 10 | 143 | 80 | 39 |
| -6 | 12 | 9 | 748 | 790 | 12 | -9 | 1 | 10 | 786 | 779 | 11 | -4 | 3 | 10 | 183 | 179 | 17 | 5 | 5 | 10 | 1403 | 1348 | 8 | -10 | 8 | 10 | 66 | 21 | 62 |
| -5 | 12 | 9 | 249 | -236 | 28 | -8 | 1 | 10 | 574 | 562 | 11 | -3 | 3 | 10 | 479 | -494 | 9 | 6 | 5 | 10 | 665 | 624 | 9 | -9 | 8 | 10 | 19 | 14 | 76 |
| -4 | 12 | 9 | 649 | -669 | 12 | -7 | 1 | 10 | 1278 | -1294 | 9 | -2 | 3 | 10 | 87 | -121 | 26 | 7 | 5 | 10 | 1334 | -1292 | 9 | -7 | 8 | 10 | 278 | -291 | 18 |
| -3 | 12 | 9 | 237 | 247 | 20 | -6 | 1 | 10 | 363 | -387 | 11 | -1 | 3 | 10 | 124 | -104 | 18 | 8 | 5 | 10 | 369 | -385 | 12 | -6 | 8 | 10 | 234 | -252 | 21 |
| -2 | 12 | 9 | 485 | 498 | 16 | -5 | 1 | 10 | 1120 | 1101 | 8 | 0 | 3 | 10 | 622 | 577 | 35 | 9 | 5 | 10 | 1085 | 1079 | 10 | -4 | 8 | 10 | 95 | 66 | 40 |
| -1 | 12 | 9 | 226 | -234 | 22 | -4 | 1 | 10 | 423 | -426 | 9 | 1 | 3 | 10 | 67 | -142 | 39 | 10 | 5 | 10 | 302 | 336 | 16 | -2 | 8 | 10 | 198 | 191 | 20 |
| 0 | 12 | 9 | 884 | -881 | 34 | -3 | 1 | 10 | 1500 | -1550 | 7 | 2 | 3 | 10 | 329 | -325 | 12 | 11 | 5 | 10 | 1023 | -1039 | 12 | -1 | 8 | 10 | 128 | -149 | 30 |
| 1 | 12 | 9 | 396 | 404 | 14 | -2 | 1 | 10 | 840 | -838 | 7 | 4 | 3 | 10 | 65 | 3 | 41 | 12 | 5 | 10 | 303 | -279 | 17 | 1 | 8 | 10 | 538 | 535 | 10 |
| 2 | 12 | 9 | 611 | 606 | 12 | -1 | 1 | 10 | 1515 | 1534 | 7 | 5 | 3 | 10 | 376 | -389 | 10 | -12 | 6 | 10 | 901 | 819 | 13 | 2 | 8 | 10 | 374 | 377 | 11 |
| 4 | 12 | 9 | 547 | -518 | 12 | 0 | 1 | 10 | 400 | 416 | 25 | 7 | 3 | 10 | 379 | 350 | 13 | -11 | 6 | 10 | 169 | 143 | 28 | 3 | 8 | 10 | 486 | -436 | 11 |
| 5 | 12 | 9 | 20 | 41 | 80 | 1 | 1 | 10 | 1983 | -1900 | 7 | 9 | 3 | 10 | 125 | 13 | 38 | -10 | 6 | 10 | 821 | -780 | 12 | 4 | 8 | 10 | 420 | -426 | 12 |
| 6 | 12 | 9 | 831 | 842 | 12 | 2 | 1 | 10 | 623 | -589 | 9 | 10 | 3 | 10 | 165 | -193 | 29 | -9 | 6 | 10 | 174 | -129 | 29 | 5 | 8 | 10 | 164 | 128 | 24 |
| -5 | 13 | 9 | 858 | -848 | 12 | 3 | 1 | 10 | 2201 | 2100 | 7 | 11 | 3 | 10 | 136 | 91 | 27 | -8 | 6 | 10 | 1096 | 1076 | 11 | 6 | 8 | 10 | 218 | 205 | 16 |
| -4 | 13 | 9 | 357 | 375 | 18 | 4 | 1 | 10 | 209 | 202 | 14 | 12 | 3 | 10 | 196 | 215 | 24 | -7 | 6 | 10 | 199 | 247 | 19 | 7 | 8 | 10 | 266 | -273 | 15 |
| -3 | 13 | 9 | 852 | 852 | 12 | 5 | 1 | 10 | 1368 | -1320 | 8 | -13 | 4 | 10 | 213 | 174 | 29 | -6 | 6 | 10 | 1289 | -1274 | 9 | 8 | 8 | 10 | 393 | -425 | 14 |
| -2 | 13 | 9 | 225 | -212 | 23 | 6 | 1 | 10 | 180 | -130 | 20 | -12 | 4 | 10 | 773 | -765 | 12 | -5 | 6 | 10 | 186 | -112 | 29 | -10 | 9 | 10 | 147 | -168 | 39 |

J.5385-M32

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -9 | 9 | 10 | 315 | 286 | 20 |
| -8 | 9 | 10 | 107 | 99 | 44 |
| -7 | 9 | 10 | 441 | -413 | 15 |
| -6 | 9 | 10 | 266 | -273 | 19 |
| -5 | 9 | 10 | 735 | 759 | 11 |
| -4 | 9 | 10 | 159 | 185 | 20 |
| -3 | 9 | 10 | 572 | -545 | 11 |
| -2 | 9 | 10 | 164 | -185 | 22 |
| -1 | 9 | 10 | 303 | 315 | 15 |
| 0 | 9 | 10 | 275 | 279 | 22 |
| 1 | 9 | 10 | 543 | -557 | 11 |
| 2 | 9 | 10 | 104 | 59 | 38 |
| 3 | 9 | 10 | 339 | 296 | 13 |
| 4 | 9 | 10 | 128 | -141 | 34 |
| 5 | 9 | 10 | 663 | -662 | 10 |
| 6 | 9 | 10 | 379 | -396 | 14 |
| 7 | 9 | 10 | 588 | 600 | 12 |
| 8 | 9 | 10 | 135 | 179 | 38 |
| 9 | 9 | 10 | 558 | -540 | 14 |
| 10 | 9 | 10 | 187 | -132 | 34 |
| -9 | 10 | 10 | 221 | 226 | 24 |
| -8 | 10 | 10 | 812 | -783 | 13 |
| -7 | 10 | 10 | 312 | -338 | 17 |
| -6 | 10 | 10 | 889 | 904 | 11 |
| -5 | 10 | 10 | 347 | 351 | 18 |
| -4 | 10 | 10 | 980 | -1018 | 11 |
| -3 | 10 | 10 | 361 | -346 | 16 |
| -2 | 10 | 10 | 1020 | 992 | 10 |
| -1 | 10 | 10 | 51 | 60 | 59 |
| 0 | 10 | 10 | 1403 | -1364 | 61 |
| 1 | 10 | 10 | 144 | -149 | 22 |
| 2 | 10 | 10 | 1359 | 1258 | 9 |
| 3 | 10 | 10 | 485 | 471 | 12 |
| 4 | 10 | 10 | 938 | -906 | 10 |
| 5 | 10 | 10 | 167 | -221 | 27 |
| 6 | 10 | 10 | 978 | 958 | 11 |
| 7 | 10 | 10 | 93 | 164 | 50 |
| 8 | 10 | 10 | 806 | -771 | 11 |
| 9 | 10 | 10 | 206 | -196 | 40 |
| -8 | 11 | 10 | 180 | -216 | 29 |
| -7 | 11 | 10 | 1066 | 1025 | 11 |
| -6 | 11 | 10 | 228 | 215 | 22 |
| -5 | 11 | 10 | 1196 | -1235 | 11 |
| -4 | 11 | 10 | 322 | -326 | 19 |
| -3 | 11 | 10 | 897 | 905 | 11 |
| -2 | 11 | 10 | 177 | 226 | 21 |
| -1 | 11 | 10 | 1078 | -1069 | 10 |
| 0 | 11 | 10 | 334 | -353 | 12 |
| 1 | 11 | 10 | 1229 | 1159 | 10 |
| 2 | 11 | 10 | 193 | 229 | 17 |
| 3 | 11 | 10 | 900 | -865 | 10 |
| 4 | 11 | 10 | 210 | -227 | 20 |
| 5 | 11 | 10 | 997 | 980 | 10 |
| 6 | 11 | 10 | 260 | 281 | 19 |
| 7 | 11 | 10 | 801 | -802 | 11 |
| -6 | 12 | 10 | 648 | -620 | 14 |
| -4 | 12 | 10 | 665 | 672 | 13 |
| -3 | 12 | 10 | 311 | 295 | 21 |
| -2 | 12 | 10 | 774 | -809 | 12 |
| -1 | 12 | 10 | 229 | -172 | 21 |
| 0 | 12 | 10 | 787 | 786 | 24 |
| 1 | 12 | 10 | 192 | 201 | 33 |
| 2 | 12 | 10 | 508 | -499 | 13 |
| 3 | 12 | 10 | 320 | -289 | 20 |
| 4 | 12 | 10 | 645 | 611 | 12 |
| 5 | 12 | 10 | 91 | 121 | 53 |
| 6 | 12 | 10 | 580 | -586 | 13 |
| -4 | 13 | 10 | 21 | 152 | 84 |
| -3 | 13 | 10 | 131 | -124 | 42 |
| -2 | 13 | 10 | 51 | 16 | 68 |
| -1 | 13 | 10 | 308 | 331 | 22 |
| 0 | 13 | 10 | 132 | 96 | 39 |
| 1 | 13 | 10 | 260 | -256 | 20 |
| 2 | 13 | 10 | 165 | -69 | 33 |
| 3 | 13 | 10 | 173 | 169 | 28 |
| 4 | 13 | 10 | 131 | 35 | 41 |
| -13 | 1 | 11 | 459 | 423 | 20 |
| -12 | 1 | 11 | 372 | 315 | 19 |
| -11 | 1 | 11 | 675 | -660 | 13 |
| -10 | 1 | 11 | 538 | -513 | 13 |
| -9 | 1 | 11 | 632 | 634 | 12 |
| -8 | 1 | 11 | 642 | 633 | 11 |
| -7 | 1 | 11 | 886 | -891 | 10 |
| -6 | 1 | 11 | 619 | -638 | 10 |
| -5 | 1 | 11 | 671 | 655 | 9 |
| -4 | 1 | 11 | 249 | 215 | 13 |
| -3 | 1 | 11 | 606 | -627 | 8 |
| -2 | 1 | 11 | 584 | -580 | 9 |
| -1 | 1 | 11 | 1030 | 1024 | 8 |
| 0 | 1 | 11 | 770 | 744 | 40 |
| 1 | 1 | 11 | 1281 | -1246 | 8 |
| 2 | 1 | 11 | 466 | -444 | 11 |
| 3 | 1 | 11 | 1410 | 1367 | 7 |
| 4 | 1 | 11 | 357 | 329 | 11 |
| 5 | 1 | 11 | 1036 | -1031 | 9 |
| 6 | 1 | 11 | 690 | -644 | 11 |
| 7 | 1 | 11 | 578 | 549 | 12 |
| 8 | 1 | 11 | 616 | 606 | 11 |
| 9 | 1 | 11 | 543 | -532 | 14 |
| 10 | 1 | 11 | 646 | -667 | 13 |
| 11 | 1 | 11 | 294 | 274 | 23 |
| 12 | 1 | 11 | 394 | 446 | 20 |
| -13 | 2 | 11 | 486 | 422 | 18 |
| -12 | 2 | 11 | 827 | -771 | 13 |
| -11 | 2 | 11 | 390 | -374 | 15 |
| -10 | 2 | 11 | 1037 | 977 | 11 |
| -9 | 2 | 11 | 623 | 638 | 12 |
| -8 | 2 | 11 | 978 | -976 | 10 |
| -7 | 2 | 11 | 1025 | -1044 | 9 |
| -6 | 2 | 11 | 957 | 988 | 9 |
| -5 | 2 | 11 | 647 | 640 | 9 |
| -4 | 2 | 11 | 1472 | -1527 | 8 |
| -3 | 2 | 11 | 1053 | -1065 | 8 |
| -2 | 2 | 11 | 1636 | 1694 | 7 |
| -1 | 2 | 11 | 1576 | 1615 | 7 |
| 0 | 2 | 11 | 1370 | -1355 | 52 |
| 1 | 2 | 11 | 1050 | -993 | 8 |
| 2 | 2 | 11 | 1538 | 1456 | 7 |
| 3 | 2 | 11 | 928 | 878 | 8 |
| 4 | 2 | 11 | 1318 | -1280 | 8 |
| 5 | 2 | 11 | 810 | -760 | 9 |
| 6 | 2 | 11 | 1320 | 1305 | 9 |
| 7 | 2 | 11 | 859 | 834 | 10 |
| 8 | 2 | 11 | 988 | -974 | 10 |
| 9 | 2 | 11 | 608 | -605 | 13 |
| 10 | 2 | 11 | 763 | 753 | 12 |
| 11 | 2 | 11 | 636 | 602 | 14 |
| 12 | 2 | 11 | 698 | -668 | 14 |
| -13 | 3 | 11 | 713 | -678 | 14 |
| -12 | 3 | 11 | 314 | -285 | 21 |
| -11 | 3 | 11 | 919 | 882 | 11 |
| -10 | 3 | 11 | 342 | 340 | 17 |
| -9 | 3 | 11 | 833 | -814 | 11 |
| -8 | 3 | 11 | 448 | -446 | 13 |
| -7 | 3 | 11 | 1330 | 1339 | 9 |
| -6 | 3 | 11 | 794 | 790 | 9 |
| -5 | 3 | 11 | 1371 | -1409 | 9 |
| -4 | 3 | 11 | 1058 | -1051 | 8 |
| -3 | 3 | 11 | 1322 | 1395 | 8 |
| -2 | 3 | 11 | 1207 | 1242 | 8 |
| -1 | 3 | 11 | 1448 | -1491 | 7 |
| 0 | 3 | 11 | 856 | -850 | 42 |
| 1 | 3 | 11 | 1320 | 1246 | 7 |
| 2 | 3 | 11 | 1512 | 1447 | 7 |
| 3 | 3 | 11 | 1336 | -1308 | 7 |
| 4 | 3 | 11 | 1488 | -1427 | 8 |
| 5 | 3 | 11 | 1239 | 1230 | 8 |
| 6 | 3 | 11 | 1220 | 1212 | 8 |
| 7 | 3 | 11 | 994 | -977 | 9 |
| 8 | 3 | 11 | 922 | -929 | 10 |
| 9 | 3 | 11 | 1176 | 1217 | 10 |
| 10 | 3 | 11 | 717 | 726 | 12 |
| 11 | 3 | 11 | 703 | -692 | 13 |
| 12 | 3 | 11 | 511 | -487 | 14 |
| -12 | 4 | 11 | 412 | 422 | 19 |
| -11 | 4 | 11 | 143 | 201 | 29 |
| -10 | 4 | 11 | 637 | -633 | 13 |
| -9 | 4 | 11 | 192 | -145 | 24 |
| -8 | 4 | 11 | 682 | 684 | 11 |
| -7 | 4 | 11 | 227 | 236 | 16 |
| -6 | 4 | 11 | 838 | -843 | 10 |
| -5 | 4 | 11 | 185 | -189 | 17 |
| -4 | 4 | 11 | 1011 | 1034 | 8 |
| -3 | 4 | 11 | 373 | 385 | 11 |
| -2 | 4 | 11 | 1111 | -1133 | 8 |
| -1 | 4 | 11 | 731 | -753 | 8 |
| 0 | 4 | 11 | 1023 | 989 | 54 |
| 1 | 4 | 11 | 843 | 820 | 8 |
| 2 | 4 | 11 | 1237 | -1181 | 8 |
| 3 | 4 | 11 | 1025 | -982 | 8 |
| 4 | 4 | 11 | 1124 | 1097 | 8 |
| 5 | 4 | 11 | 757 | 743 | 9 |
| 6 | 4 | 11 | 825 | -796 | 10 |
| 7 | 4 | 11 | 406 | -412 | 13 |
| 8 | 4 | 11 | 1110 | 1114 | 10 |
| 9 | 4 | 11 | 649 | 641 | 11 |
| 10 | 4 | 11 | 887 | -876 | 11 |
| 11 | 4 | 11 | 582 | -579 | 13 |
| 12 | 4 | 11 | 585 | 593 | 14 |
| -12 | 5 | 11 | 147 | 149 | 31 |
| -11 | 5 | 11 | 258 | -287 | 19 |
| -9 | 5 | 11 | 164 | 159 | 23 |
| -8 | 5 | 11 | 357 | 327 | 14 |
| -7 | 5 | 11 | 111 | 116 | 38 |
| -5 | 5 | 11 | 100 | 104 | 39 |
| -4 | 5 | 11 | 123 | 60 | 28 |
| -3 | 5 | 11 | 109 | 71 | 31 |
| -2 | 5 | 11 | 82 | 100 | 36 |
| -1 | 5 | 11 | 287 | 286 | 12 |
| 0 | 5 | 11 | 282 | -288 | 12 |
| 1 | 5 | 11 | 530 | -511 | 10 |
| 2 | 5 | 11 | 339 | -345 | 12 |
| 3 | 5 | 11 | 813 | 774 | 8 |
| 4 | 5 | 11 | 320 | 307 | 13 |
| 5 | 5 | 11 | 313 | -294 | 12 |
| 6 | 5 | 11 | 188 | -178 | 19 |
| 7 | 5 | 11 | 310 | 292 | 13 |
| 8 | 5 | 11 | 387 | 376 | 14 |
| 9 | 5 | 11 | 432 | -443 | 13 |
| 10 | 5 | 11 | 90 | -103 | 52 |
| -11 | 6 | 11 | 145 | 112 | 39 |
| -10 | 6 | 11 | 196 | -181 | 19 |
| -9 | 6 | 11 | 283 | -236 | 21 |
| -8 | 6 | 11 | 447 | 446 | 13 |
| -7 | 6 | 11 | 210 | 224 | 24 |
| -6 | 6 | 11 | 452 | -465 | 14 |
| -5 | 6 | 11 | 218 | -241 | 17 |
| -4 | 6 | 11 | 288 | 286 | 14 |
| -3 | 6 | 11 | 341 | 332 | 12 |
| -2 | 6 | 11 | 597 | -623 | 9 |
| -1 | 6 | 11 | 298 | -303 | 14 |
| 0 | 6 | 11 | 939 | 943 | 44 |
| 1 | 6 | 11 | 516 | 482 | 10 |
| 2 | 6 | 11 | 497 | -492 | 10 |
| 3 | 6 | 11 | 636 | -609 | 9 |
| 4 | 6 | 11 | 239 | 231 | 16 |
| 5 | 6 | 11 | 72 | -108 | 48 |
| 6 | 6 | 11 | 774 | -789 | 10 |
| 7 | 6 | 11 | 211 | -206 | 19 |
| 8 | 6 | 11 | 253 | 255 | 16 |
| 9 | 6 | 11 | 232 | 242 | 19 |
| 10 | 6 | 11 | 276 | -272 | 23 |
| 11 | 6 | 11 | 147 | -182 | 29 |
| -11 | 7 | 11 | 643 | -609 | 15 |
| -10 | 7 | 11 | 472 | -451 | 16 |
| -9 | 7 | 11 | 607 | 596 | 13 |
| -8 | 7 | 11 | 419 | 428 | 15 |
| -7 | 7 | 11 | 972 | -959 | 11 |
| -6 | 7 | 11 | 752 | -755 | 11 |
| -5 | 7 | 11 | 931 | 950 | 10 |
| -4 | 7 | 11 | 512 | 524 | 11 |
| -3 | 7 | 11 | 1159 | -1173 | 9 |
| -2 | 7 | 11 | 471 | -420 | 11 |
| -1 | 7 | 11 | 1204 | 1243 | 9 |
| 0 | 7 | 11 | 296 | 305 | 15 |
| 1 | 7 | 11 | 1670 | -1583 | 8 |
| 2 | 7 | 11 | 460 | -445 | 11 |
| 3 | 7 | 11 | 856 | 827 | 9 |
| 4 | 7 | 11 | 730 | 713 | 10 |
| 5 | 7 | 11 | 1004 | -996 | 9 |
| 6 | 7 | 11 | 782 | -773 | 10 |
| 7 | 7 | 11 | 1069 | 1035 | 10 |
| 8 | 7 | 11 | 456 | 451 | 14 |
| 9 | 7 | 11 | 661 | -653 | 12 |
| 10 | 7 | 11 | 559 | -538 | 14 |
| -10 | 8 | 11 | 730 | 695 | 14 |
| -9 | 8 | 11 | 520 | 515 | 15 |
| -8 | 8 | 11 | 886 | -853 | 11 |
| -7 | 8 | 11 | 553 | -520 | 12 |
| -6 | 8 | 11 | 1252 | 1270 | 10 |
| -5 | 8 | 11 | 573 | 569 | 12 |
| -4 | 8 | 11 | 1018 | -998 | 9 |
| -3 | 8 | 11 | 607 | -596 | 11 |
| -2 | 8 | 11 | 920 | 929 | 9 |
| -1 | 8 | 11 | 579 | 587 | 11 |
| 0 | 8 | 11 | 1303 | -1269 | 69 |
| 1 | 8 | 11 | 263 | -241 | 14 |
| 2 | 8 | 11 | 1370 | 1295 | 9 |
| 3 | 8 | 11 | 508 | 464 | 11 |
| 4 | 8 | 11 | 1270 | -1202 | 9 |
| 5 | 8 | 11 | 784 | -742 | 10 |
| 6 | 8 | 11 | 1129 | 1123 | 9 |
| 7 | 8 | 11 | 817 | 811 | 11 |
| 8 | 8 | 11 | 829 | -827 | 11 |
| 9 | 8 | 11 | 609 | -580 | 12 |
| 10 | 8 | 11 | 802 | 769 | 12 |
| -10 | 9 | 11 | 424 | 406 | 16 |
| -9 | 9 | 11 | 777 | -715 | 12 |
| -8 | 9 | 11 | 480 | -442 | 15 |
| -7 | 9 | 11 | 733 | 725 | 12 |
| -6 | 9 | 11 | 255 | 248 | 20 |
| -5 | 9 | 11 | 855 | -847 | 11 |
| -4 | 9 | 11 | 222 | -190 | 18 |
| -3 | 9 | 11 | 878 | 874 | 10 |
| -2 | 9 | 11 | 523 | 512 | 12 |
| -1 | 9 | 11 | 882 | -891 | 10 |
| 0 | 9 | 11 | 732 | -702 | 27 |
| 1 | 9 | 11 | 1221 | 1155 | 9 |
| 2 | 9 | 11 | 454 | 416 | 12 |
| 3 | 9 | 11 | 1036 | -981 | 9 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 4 | 9 | 11 | 429 | -392 | 12 |
| 5 | 9 | 11 | 813 | 800 | 10 |
| 6 | 9 | 11 | 316 | 292 | 15 |
| 7 | 9 | 11 | 841 | -840 | 11 |
| 8 | 9 | 11 | 328 | -327 | 17 |
| 9 | 9 | 11 | 618 | 597 | 13 |
| -9 | 10 | 11 | 258 | -182 | 34 |
| -8 | 10 | 11 | 320 | 304 | 20 |
| -7 | 10 | 11 | 263 | 300 | 18 |
| -6 | 10 | 11 | 477 | -473 | 14 |
| -5 | 10 | 11 | 306 | -325 | 18 |
| -4 | 10 | 11 | 431 | 424 | 15 |
| -3 | 10 | 11 | 322 | 368 | 15 |
| -2 | 10 | 11 | 447 | -485 | 14 |
| -1 | 10 | 11 | 370 | -403 | 14 |
| 0 | 10 | 11 | 336 | 371 | 12 |
| 1 | 10 | 11 | 310 | 341 | 15 |
| 3 | 10 | 11 | 274 | -317 | 15 |
| 4 | 10 | 11 | 353 | 341 | 18 |
| 5 | 10 | 11 | 382 | 418 | 14 |
| 6 | 10 | 11 | 301 | -312 | 15 |
| 7 | 10 | 11 | 345 | -345 | 15 |
| 8 | 10 | 11 | 354 | 323 | 18 |
| -7 | 11 | 11 | 177 | 182 | 33 |
| -6 | 11 | 11 | 140 | 32 | 38 |
| -5 | 11 | 11 | 96 | -93 | 49 |
| -3 | 11 | 11 | 135 | 153 | 37 |
| -2 | 11 | 11 | 138 | 129 | 33 |
| -1 | 11 | 11 | 82 | -39 | 50 |
| 0 | 11 | 11 | 75 | -128 | 43 |
| 1 | 11 | 11 | 300 | 232 | 21 |
| 2 | 11 | 11 | 224 | 186 | 22 |
| 3 | 11 | 11 | 137 | -124 | 30 |
| 5 | 11 | 11 | 150 | 134 | 38 |
| 6 | 11 | 11 | 88 | 67 | 53 |
| 7 | 11 | 11 | 90 | -10 | 53 |
| -6 | 12 | 11 | 456 | -438 | 16 |
| -5 | 12 | 11 | 276 | -324 | 23 |
| -4 | 12 | 11 | 593 | 569 | 14 |
| -3 | 12 | 11 | 323 | 281 | 17 |
| -2 | 12 | 11 | 570 | -582 | 13 |
| -1 | 12 | 11 | 287 | -207 | 25 |
| 0 | 12 | 11 | 336 | 330 | 25 |
| 1 | 12 | 11 | 152 | 194 | 22 |
| 2 | 12 | 11 | 551 | -554 | 13 |
| 3 | 12 | 11 | 230 | -244 | 18 |
| 4 | 12 | 11 | 514 | 497 | 14 |
| 5 | 12 | 11 | 377 | 379 | 16 |
| -3 | 13 | 11 | 808 | -805 | 13 |
| -2 | 13 | 11 | 516 | -531 | 15 |
| -1 | 13 | 11 | 686 | 669 | 13 |
| 0 | 13 | 11 | 607 | 609 | 10 |
| 1 | 13 | 11 | 720 | -692 | 12 |
| 2 | 13 | 11 | 547 | -550 | 14 |
| 3 | 13 | 11 | 744 | 719 | 12 |
| -12 | 0 | 12 | 774 | -731 | 13 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -11 | 0 | 12 | 651 | -640 | 14 |
| -10 | 0 | 12 | 961 | 917 | 11 |
| -9 | 0 | 12 | 527 | 499 | 13 |
| -8 | 0 | 12 | 1090 | -1067 | 10 |
| -7 | 0 | 12 | 1528 | -1524 | 9 |
| -6 | 0 | 12 | 1279 | 1290 | 9 |
| -5 | 0 | 12 | 1677 | 1663 | 8 |
| -4 | 0 | 12 | 1240 | -1307 | 9 |
| -3 | 0 | 12 | 1291 | -1314 | 8 |
| -2 | 0 | 12 | 1168 | 1206 | 8 |
| -1 | 0 | 12 | 1505 | 1554 | 7 |
| 0 | 0 | 12 | 1376 | -1303 | 52 |
| 1 | 0 | 12 | 1644 | -1563 | 8 |
| 2 | 0 | 12 | 1179 | 1153 | 8 |
| 3 | 0 | 12 | 1979 | 1953 | 7 |
| 4 | 0 | 12 | 535 | -518 | 12 |
| 5 | 0 | 12 | 1924 | -1870 | 9 |
| 6 | 0 | 12 | 860 | 851 | 10 |
| 7 | 0 | 12 | 1834 | 1837 | 9 |
| 8 | 0 | 12 | 1035 | -1035 | 12 |
| 9 | 0 | 12 | 1343 | -1383 | 11 |
| 10 | 0 | 12 | 613 | 609 | 14 |
| 11 | 0 | 12 | 907 | 901 | 13 |
| 12 | 0 | 12 | 678 | -680 | 14 |
| -12 | 1 | 12 | 552 | -515 | 14 |
| -11 | 1 | 12 | 681 | 647 | 14 |
| -10 | 1 | 12 | 762 | 719 | 12 |
| -9 | 1 | 12 | 1017 | -983 | 11 |
| -8 | 1 | 12 | 610 | -557 | 13 |
| -7 | 1 | 12 | 803 | 818 | 10 |
| -6 | 1 | 12 | 1009 | 1007 | 10 |
| -5 | 1 | 12 | 929 | -946 | 9 |
| -4 | 1 | 12 | 1085 | -1085 | 8 |
| -3 | 1 | 12 | 1188 | 1213 | 8 |
| -2 | 1 | 12 | 1408 | 1421 | 8 |
| -1 | 1 | 12 | 672 | -681 | 8 |
| 0 | 1 | 12 | 1231 | -1237 | 52 |
| 1 | 1 | 12 | 1211 | 1152 | 8 |
| 2 | 1 | 12 | 1480 | 1425 | 8 |
| 3 | 1 | 12 | 860 | -838 | 8 |
| 4 | 1 | 12 | 1308 | -1255 | 8 |
| 5 | 1 | 12 | 814 | 795 | 10 |
| 6 | 1 | 12 | 1098 | 1076 | 10 |
| 7 | 1 | 12 | 928 | -912 | 11 |
| 8 | 1 | 12 | 1060 | -1045 | 11 |
| 9 | 1 | 12 | 807 | 805 | 12 |
| 10 | 1 | 12 | 1016 | 984 | 12 |
| 11 | 1 | 12 | 425 | -464 | 16 |
| 12 | 1 | 12 | 887 | -853 | 14 |
| -12 | 2 | 12 | 338 | 315 | 20 |
| -11 | 2 | 12 | 366 | 323 | 19 |
| -10 | 2 | 12 | 560 | -534 | 13 |
| -9 | 2 | 12 | 349 | -334 | 15 |
| -8 | 2 | 12 | 318 | 285 | 17 |
| -7 | 2 | 12 | 319 | 283 | 15 |
| -6 | 2 | 12 | 303 | -297 | 13 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 2 | 12 | 117 | -60 | 33 |
| -4 | 2 | 12 | 555 | 577 | 9 |
| -3 | 2 | 12 | 377 | 351 | 10 |
| -2 | 2 | 12 | 134 | -158 | 15 |
| -1 | 2 | 12 | 581 | -577 | 8 |
| 0 | 2 | 12 | 178 | 159 | 13 |
| 1 | 2 | 12 | 997 | 942 | 9 |
| 2 | 2 | 12 | 594 | -579 | 11 |
| 3 | 2 | 12 | 1142 | -1122 | 8 |
| 4 | 2 | 12 | 284 | 273 | 14 |
| 5 | 2 | 12 | 577 | 548 | 9 |
| 6 | 2 | 12 | 86 | -17 | 45 |
| 7 | 2 | 12 | 562 | -569 | 12 |
| 9 | 2 | 12 | 457 | 469 | 14 |
| 10 | 2 | 12 | 240 | -253 | 23 |
| 11 | 2 | 12 | 345 | -347 | 19 |
| 12 | 2 | 12 | 348 | 313 | 22 |
| -12 | 3 | 12 | 238 | -195 | 29 |
| -11 | 3 | 12 | 176 | 212 | 36 |
| -10 | 3 | 12 | 40 | -17 | 77 |
| -9 | 3 | 12 | 19 | 89 | 77 |
| -8 | 3 | 12 | 310 | -319 | 16 |
| -7 | 3 | 12 | 234 | 235 | 19 |
| -6 | 3 | 12 | 508 | 498 | 11 |
| -5 | 3 | 12 | 94 | -33 | 38 |
| -4 | 3 | 12 | 130 | -142 | 21 |
| -3 | 3 | 12 | 288 | -302 | 12 |
| -1 | 3 | 12 | 408 | -412 | 10 |
| 0 | 3 | 12 | 360 | -364 | 10 |
| 1 | 3 | 12 | 677 | 632 | 9 |
| 2 | 3 | 12 | 429 | 413 | 11 |
| 4 | 3 | 12 | 132 | 116 | 21 |
| 5 | 3 | 12 | 159 | 140 | 18 |
| 6 | 3 | 12 | 262 | 265 | 16 |
| 7 | 3 | 12 | 104 | -74 | 40 |
| 8 | 3 | 12 | 171 | -168 | 20 |
| 10 | 3 | 12 | 86 | 30 | 52 |
| 12 | 3 | 12 | 193 | -159 | 43 |
| -12 | 4 | 12 | 490 | 445 | 15 |
| -11 | 4 | 12 | 552 | 528 | 15 |
| -10 | 4 | 12 | 477 | -451 | 14 |
| -9 | 4 | 12 | 402 | -371 | 15 |
| -8 | 4 | 12 | 835 | 834 | 11 |
| -7 | 4 | 12 | 625 | 617 | 11 |
| -6 | 4 | 12 | 948 | -956 | 9 |
| -5 | 4 | 12 | 828 | -816 | 9 |
| -4 | 4 | 12 | 606 | 632 | 10 |
| -3 | 4 | 12 | 494 | 525 | 10 |
| -2 | 4 | 12 | 685 | -688 | 9 |
| -1 | 4 | 12 | 815 | -818 | 8 |
| 0 | 4 | 12 | 819 | 807 | 44 |
| 1 | 4 | 12 | 946 | 866 | 9 |
| 2 | 4 | 12 | 835 | -807 | 9 |
| 3 | 4 | 12 | 1126 | -1080 | 8 |
| 4 | 4 | 12 | 561 | 535 | 10 |
| 5 | 4 | 12 | 1202 | 1174 | 9 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 6 | 4 | 12 | 304 | -306 | 13 |
| 7 | 4 | 12 | 900 | -892 | 10 |
| 8 | 4 | 12 | 542 | 555 | 12 |
| 9 | 4 | 12 | 770 | 781 | 11 |
| 10 | 4 | 12 | 448 | -424 | 15 |
| 11 | 4 | 12 | 576 | -573 | 15 |
| -12 | 5 | 12 | 568 | 535 | 15 |
| -11 | 5 | 12 | 844 | -812 | 14 |
| -10 | 5 | 12 | 749 | -699 | 12 |
| -9 | 5 | 12 | 544 | 527 | 13 |
| -8 | 5 | 12 | 903 | 858 | 11 |
| -7 | 5 | 12 | 872 | -857 | 11 |
| -6 | 5 | 12 | 849 | -855 | 10 |
| -5 | 5 | 12 | 1237 | 1248 | 9 |
| -4 | 5 | 12 | 860 | 845 | 9 |
| -3 | 5 | 12 | 1187 | -1180 | 8 |
| -2 | 5 | 12 | 1601 | -1617 | 8 |
| -1 | 5 | 12 | 698 | 709 | 9 |
| 0 | 5 | 12 | 1639 | 1611 | 82 |
| 1 | 5 | 12 | 841 | -804 | 9 |
| 2 | 5 | 12 | 1605 | -1526 | 8 |
| 3 | 5 | 12 | 855 | 830 | 9 |
| 4 | 5 | 12 | 1145 | 1098 | 9 |
| 5 | 5 | 12 | 828 | -802 | 10 |
| 6 | 5 | 12 | 1191 | -1165 | 9 |
| 7 | 5 | 12 | 876 | 855 | 10 |
| 8 | 5 | 12 | 1168 | 1157 | 10 |
| 9 | 5 | 12 | 775 | -800 | 11 |
| 10 | 5 | 12 | 805 | -770 | 12 |
| 11 | 5 | 12 | 510 | 519 | 14 |
| -11 | 6 | 12 | 652 | -630 | 14 |
| -10 | 6 | 12 | 676 | 647 | 13 |
| -9 | 6 | 12 | 910 | 876 | 11 |
| -8 | 6 | 12 | 490 | -497 | 14 |
| -7 | 6 | 12 | 1070 | -1064 | 11 |
| -6 | 6 | 12 | 731 | 715 | 11 |
| -5 | 6 | 12 | 899 | 915 | 10 |
| -4 | 6 | 12 | 929 | -939 | 9 |
| -3 | 6 | 12 | 1273 | -1298 | 9 |
| -2 | 6 | 12 | 920 | 906 | 9 |
| -1 | 6 | 12 | 1621 | 1670 | 8 |
| 0 | 6 | 12 | 1116 | -1070 | 43 |
| 1 | 6 | 12 | 1361 | -1275 | 8 |
| 2 | 6 | 12 | 1012 | 978 | 9 |
| 3 | 6 | 12 | 1253 | 1203 | 9 |
| 4 | 6 | 12 | 1010 | -967 | 9 |
| 5 | 6 | 12 | 1051 | -1016 | 9 |
| 6 | 6 | 12 | 965 | 940 | 10 |
| 7 | 6 | 12 | 993 | 971 | 10 |
| 8 | 6 | 12 | 681 | -665 | 11 |
| 9 | 6 | 12 | 761 | -766 | 11 |
| 10 | 6 | 12 | 571 | 566 | 14 |
| 11 | 6 | 12 | 768 | 727 | 13 |
| -11 | 7 | 12 | 331 | 349 | 20 |
| -10 | 7 | 12 | 339 | 334 | 17 |
| -9 | 7 | 12 | 301 | -285 | 17 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -8 | 7 | 12 | 717 | -705 | 12 |
| -7 | 7 | 12 | 446 | 436 | 15 |
| -6 | 7 | 12 | 885 | 889 | 11 |
| -5 | 7 | 12 | 517 | -534 | 12 |
| -4 | 7 | 12 | 812 | -781 | 10 |
| -3 | 7 | 12 | 323 | 331 | 13 |
| -2 | 7 | 12 | 871 | 876 | 10 |
| -1 | 7 | 12 | 466 | -472 | 12 |
| 0 | 7 | 12 | 466 | -435 | 23 |
| 1 | 7 | 12 | 744 | 707 | 10 |
| 2 | 7 | 12 | 459 | 435 | 12 |
| 3 | 7 | 12 | 846 | -824 | 9 |
| 4 | 7 | 12 | 965 | -918 | 10 |
| 5 | 7 | 12 | 375 | 367 | 14 |
| 6 | 7 | 12 | 723 | 749 | 11 |
| 7 | 7 | 12 | 376 | -377 | 15 |
| 8 | 7 | 12 | 761 | -763 | 11 |
| 9 | 7 | 12 | 408 | 413 | 16 |
| 10 | 7 | 12 | 518 | 521 | 15 |
| -10 | 8 | 12 | 143 | -108 | 40 |
| -7 | 8 | 12 | 121 | 83 | 40 |
| -6 | 8 | 12 | 96 | 21 | 46 |
| -5 | 8 | 12 | 177 | 168 | 28 |
| -4 | 8 | 12 | 119 | 106 | 36 |
| -3 | 8 | 12 | 128 | 19 | 31 |
| -2 | 8 | 12 | 321 | -301 | 18 |
| 0 | 8 | 12 | 492 | 453 | 26 |
| 1 | 8 | 12 | 105 | -104 | 39 |
| 3 | 8 | 12 | 289 | -290 | 14 |
| 6 | 8 | 12 | 197 | -237 | 19 |
| 7 | 8 | 12 | 86 | -126 | 52 |
| 8 | 8 | 12 | 132 | -82 | 39 |
| 9 | 8 | 12 | 68 | 105 | 62 |
| -9 | 9 | 12 | 87 | -88 | 55 |
| -8 | 9 | 12 | 437 | -432 | 16 |
| -7 | 9 | 12 | 129 | 163 | 41 |
| -6 | 9 | 12 | 508 | 533 | 14 |
| -5 | 9 | 12 | 249 | -197 | 29 |
| -4 | 9 | 12 | 347 | -365 | 15 |
| -3 | 9 | 12 | 391 | 370 | 14 |
| -2 | 9 | 12 | 294 | 291 | 18 |
| -1 | 9 | 12 | 435 | -454 | 13 |
| 0 | 9 | 12 | 379 | -392 | 16 |
| 1 | 9 | 12 | 704 | 680 | 11 |
| 2 | 9 | 12 | 204 | 176 | 19 |
| 3 | 9 | 12 | 542 | -524 | 11 |
| 4 | 9 | 12 | 336 | -359 | 14 |
| 5 | 9 | 12 | 475 | 491 | 13 |
| 6 | 9 | 12 | 699 | 705 | 11 |
| 7 | 9 | 12 | 458 | -488 | 14 |
| 8 | 9 | 12 | 419 | -395 | 15 |
| 9 | 9 | 12 | 144 | 163 | 31 |
| -8 | 10 | 12 | 386 | 365 | 19 |
| -7 | 10 | 12 | 681 | 687 | 13 |
| -6 | 10 | 12 | 514 | -504 | 14 |
| -5 | 10 | 12 | 822 | -851 | 12 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$



| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -4 | 10 | 12 | 620 | 625 | 14 |
| -3 | 10 | 12 | 606 | 620 | 13 |
| -2 | 10 | 12 | 763 | -761 | 12 |
| -1 | 10 | 12 | 818 | -851 | 11 |
| 0 | 10 | 12 | 649 | 655 | 8 |
| 1 | 10 | 12 | 983 | 946 | 10 |
| 2 | 10 | 12 | 702 | -654 | 11 |
| 3 | 10 | 12 | 508 | -466 | 13 |
| 4 | 10 | 12 | 534 | 533 | 12 |
| 5 | 10 | 12 | 778 | 778 | 11 |
| 6 | 10 | 12 | 542 | -534 | 13 |
| 7 | 10 | 12 | 844 | -827 | 12 |
| -7 | 11 | 12 | 611 | -612 | 14 |
| -6 | 11 | 12 | 792 | -773 | 14 |
| -5 | 11 | 12 | 554 | 553 | 13 |
| -4 | 11 | 12 | 810 | 830 | 12 |
| -3 | 11 | 12 | 502 | -525 | 14 |
| -2 | 11 | 12 | 704 | -728 | 12 |
| -1 | 11 | 12 | 697 | 729 | 13 |
| 0 | 11 | 12 | 1026 | 1020 | 26 |
| 1 | 11 | 12 | 598 | -559 | 12 |
| 2 | 11 | 12 | 832 | -798 | 11 |
| 3 | 11 | 12 | 526 | 522 | 13 |
| 4 | 11 | 12 | 787 | 800 | 11 |
| 5 | 11 | 12 | 440 | -438 | 16 |
| 6 | 11 | 12 | 788 | -768 | 13 |
| -5 | 12 | 12 | 681 | 702 | 14 |
| -4 | 12 | 12 | 385 | -403 | 17 |
| -3 | 12 | 12 | 627 | -629 | 13 |
| -2 | 12 | 12 | 411 | 446 | 15 |
| -1 | 12 | 12 | 751 | 764 | 12 |
| 0 | 12 | 12 | 418 | -431 | 20 |
| 1 | 12 | 12 | 804 | -823 | 12 |
| 2 | 12 | 12 | 486 | 500 | 14 |
| 3 | 12 | 12 | 543 | 545 | 13 |
| 4 | 12 | 12 | 436 | -448 | 14 |
| -1 | 13 | 12 | 298 | -346 | 19 |
| 0 | 13 | 12 | 218 | -238 | 34 |
| 1 | 13 | 12 | 302 | 321 | 18 |
| -12 | 1 | 13 | 481 | -450 | 17 |
| -11 | 1 | 13 | 229 | 257 | 18 |
| -10 | 1 | 13 | 733 | 688 | 12 |
| -9 | 1 | 13 | 203 | -263 | 19 |
| -8 | 1 | 13 | 629 | -616 | 11 |
| -7 | 1 | 13 | 671 | 662 | 11 |
| -6 | 1 | 13 | 605 | 613 | 11 |
| -5 | 1 | 13 | 698 | -695 | 10 |
| -4 | 1 | 13 | 426 | -438 | 12 |
| -3 | 1 | 13 | 392 | 391 | 12 |
| -2 | 1 | 13 | 579 | 564 | 10 |
| -1 | 1 | 13 | 95 | -25 | 33 |
| 0 | 1 | 13 | 565 | -553 | 22 |
| 1 | 1 | 13 | 307 | 276 | 12 |
| 2 | 1 | 13 | 988 | 924 | 9 |
| 3 | 1 | 13 | 223 | -217 | 22 |
| 4 | 1 | 13 | 1292 | -1250 | 9 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 5 | 1 | 13 | 129 | 34 | 33 |
| 6 | 1 | 13 | 904 | 876 | 10 |
| 7 | 1 | 13 | 101 | -65 | 42 |
| 8 | 1 | 13 | 961 | -947 | 11 |
| [illegible] | 1 | 13 | 274 | -232 | 26 |
| [illegible] | [illegible] | 13 | 809 | 825 | 14 |
| [illegible] | 1 | 13 | 123 | 102 | 46 |
| -12 | 2 | 13 | 423 | 404 | 16 |
| -11 | 2 | 13 | 983 | 897 | 12 |
| -10 | 2 | 13 | 350 | -348 | 17 |
| -9 | 2 | 13 | 1012 | -988 | 11 |
| -8 | 2 | 13 | 261 | 225 | 19 |
| -7 | 2 | 13 | 1092 | 1086 | 10 |
| -6 | 2 | 13 | 562 | -553 | 11 |
| -5 | 2 | 13 | 1232 | -1235 | 9 |
| -4 | 2 | 13 | 467 | 483 | 11 |
| -3 | 2 | 13 | 1291 | 1299 | 8 |
| -2 | 2 | 13 | 472 | -467 | 10 |
| -1 | 2 | 13 | 1497 | -1522 | 8 |
| 0 | 2 | 13 | 686 | 663 | 25 |
| 1 | 2 | 13 | 1509 | 1454 | 8 |
| 2 | 2 | 13 | 192 | -114 | 20 |
| 3 | 2 | 13 | 1345 | -1290 | 8 |
| 4 | 2 | 13 | 385 | 374 | 12 |
| 5 | 2 | 13 | 1247 | 1177 | 8 |
| 6 | 2 | 13 | 423 | -451 | 12 |
| 7 | 2 | 13 | 1146 | -1099 | 10 |
| 8 | 2 | 13 | 320 | 331 | 17 |
| 9 | 2 | 13 | 1299 | 1320 | 11 |
| 10 | 2 | 13 | 188 | -108 | 33 |
| 11 | 2 | 13 | 892 | -859 | 13 |
| -12 | 3 | 13 | 673 | 629 | 14 |
| -11 | 3 | 13 | 352 | -349 | 16 |
| -10 | 3 | 13 | 1071 | -1006 | 11 |
| -9 | 3 | 13 | 387 | 354 | 15 |
| -8 | 3 | 13 | 1060 | 1037 | 11 |
| -7 | 3 | 13 | 183 | -161 | 20 |
| -6 | 3 | 13 | 1521 | -1536 | 9 |
| -5 | 3 | 13 | 212 | 214 | 18 |
| -4 | 3 | 13 | 1713 | 1746 | 8 |
| -3 | 3 | 13 | 419 | -443 | 11 |
| -2 | 3 | 13 | 1764 | -1782 | 8 |
| -1 | 3 | 13 | 312 | 296 | 12 |
| 0 | 3 | 13 | 1697 | 1655 | 78 |
| 1 | 3 | 13 | 593 | -529 | 11 |
| 2 | 3 | 13 | 1702 | -1602 | 8 |
| 3 | 3 | 13 | 286 | 276 | 14 |
| 4 | 3 | 13 | 1694 | 1617 | 8 |
| 5 | 3 | 13 | 176 | 152 | 17 |
| 6 | 3 | 13 | 957 | -926 | 9 |
| 7 | 3 | 13 | 359 | 390 | 13 |
| 8 | 3 | 13 | 1105 | 1088 | 10 |
| 9 | 3 | 13 | 462 | -456 | 14 |
| 10 | 3 | 13 | 973 | -966 | 12 |
| 11 | 3 | 13 | 307 | 311 | 19 |
| -11 | 4 | 13 | 668 | -639 | 14 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -10 | 4 | 13 | 352 | 345 | 15 |
| -9 | 4 | 13 | 714 | 694 | 12 |
| -8 | 4 | 13 | 219 | -200 | 20 |
| -7 | 4 | 13 | 1005 | -996 | 10 |
| -6 | 4 | 13 | 186 | 200 | 19 |
| -5 | 4 | 13 | 1120 | 1100 | 9 |
| -4 | 4 | 13 | 101 | -33 | 24 |
| -3 | 4 | 13 | 973 | -984 | 9 |
| -2 | 4 | 13 | 110 | -90 | 19 |
| -1 | 4 | 13 | 1054 | 1099 | 9 |
| 0 | 4 | 13 | 66 | -90 | 33 |
| 1 | 4 | 13 | 643 | -584 | 10 |
| 2 | 4 | 13 | 318 | 321 | 15 |
| 3 | 4 | 13 | 1005 | 952 | 9 |
| 4 | 4 | 13 | 467 | -474 | 12 |
| 5 | 4 | 13 | 917 | -892 | 10 |
| 6 | 4 | 13 | 218 | 215 | 17 |
| 7 | 4 | 13 | 773 | 757 | 11 |
| 8 | 4 | 13 | 135 | -125 | 37 |
| 9 | 4 | 13 | 871 | -883 | 11 |
| 10 | 4 | 13 | 153 | 186 | 22 |
| 11 | 4 | 13 | 546 | 516 | 15 |
| -11 | 5 | 13 | 41 | 48 | 80 |
| -10 | 5 | 13 | 439 | 455 | 15 |
| -8 | 5 | 13 | 179 | -203 | 23 |
| -7 | 5 | 13 | 193 | -214 | 24 |
| -6 | 5 | 13 | 110 | -156 | 40 |
| -5 | 5 | 13 | 91 | -86 | 42 |
| -4 | 5 | 13 | 58 | -16 | 53 |
| -3 | 5 | 13 | 93 | 4 | 36 |
| -2 | 5 | 13 | 88 | -17 | 37 |
| -1 | 5 | 13 | 302 | 317 | 13 |
| 0 | 5 | 13 | 89 | 48 | 27 |
| 1 | 5 | 13 | 335 | -326 | 14 |
| 2 | 5 | 13 | 177 | -223 | 22 |
| 3 | 5 | 13 | 321 | 297 | 17 |
| 4 | 5 | 13 | 165 | -125 | 21 |
| 5 | 5 | 13 | 240 | -264 | 16 |
| 6 | 5 | 13 | 137 | 78 | 24 |
| 7 | 5 | 13 | 76 | 70 | 52 |
| 9 | 5 | 13 | 100 | -96 | 49 |
| 10 | 5 | 13 | 287 | 241 | 23 |
| 11 | 5 | 13 | 21 | 29 | 84 |
| -11 | 6 | 13 | 125 | -113 | 45 |
| -9 | 6 | 13 | 250 | 251 | 21 |
| -8 | 6 | 13 | 93 | -102 | 49 |
| -7 | 6 | 13 | 319 | -312 | 14 |
| -5 | 6 | 13 | 537 | 558 | 12 |
| -4 | 6 | 13 | 386 | -383 | 12 |
| -3 | 6 | 13 | 859 | -856 | 10 |
| -2 | 6 | 13 | 384 | 414 | 12 |
| -1 | 6 | 13 | 743 | 780 | 10 |
| 0 | 6 | 13 | 402 | -383 | 9 |
| 1 | 6 | 13 | 1124 | -1066 | 9 |
| 2 | 6 | 13 | 717 | 690 | 10 |
| 3 | 6 | 13 | 326 | 362 | 13 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 4 | 6 | 13 | 597 | -595 | 11 |
| 5 | 6 | 13 | 462 | -410 | 13 |
| 6 | 6 | 13 | 246 | 251 | 19 |
| 7 | 6 | 13 | 457 | 466 | 14 |
| 8 | 6 | 13 | 245 | -248 | 20 |
| 9 | 6 | 13 | 147 | -188 | 37 |
| 10 | 6 | 13 | 101 | 128 | 51 |
| -10 | 7 | 13 | 454 | 459 | 15 |
| -9 | 7 | 13 | 115 | -196 | 46 |
| -8 | 7 | 13 | 757 | -717 | 13 |
| -7 | 7 | 13 | 420 | 403 | 16 |
| -6 | 7 | 13 | 982 | 1025 | 11 |
| -5 | 7 | 13 | 232 | -210 | 23 |
| -4 | 7 | 13 | 804 | -788 | 11 |
| -3 | 7 | 13 | 302 | 307 | 16 |
| -2 | 7 | 13 | 905 | 906 | 10 |
| -1 | 7 | 13 | 551 | -564 | 11 |
| 0 | 7 | 13 | 917 | -888 | 54 |
| 1 | 7 | 13 | 441 | 416 | 13 |
| 2 | 7 | 13 | 795 | 742 | 10 |
| 3 | 7 | 13 | 535 | -514 | 12 |
| 4 | 7 | 13 | 939 | -879 | 9 |
| 5 | 7 | 13 | 398 | 351 | 14 |
| 6 | 7 | 13 | 1086 | 1083 | 10 |
| 7 | 7 | 13 | 135 | -168 | 34 |
| 8 | 7 | 13 | 904 | -917 | 12 |
| 9 | 7 | 13 | 322 | 321 | 20 |
| -9 | 8 | 13 | 930 | -872 | 13 |
| -8 | 8 | 13 | 370 | 349 | 17 |
| -7 | 8 | 13 | 944 | 923 | 11 |
| -6 | 8 | 13 | 324 | -315 | 19 |
| -5 | 8 | 13 | 814 | -849 | 11 |
| -4 | 8 | 13 | 364 | 362 | 14 |
| -3 | 8 | 13 | 813 | 783 | 11 |
| -2 | 8 | 13 | 288 | -297 | 16 |
| -1 | 8 | 13 | 962 | -970 | 10 |
| 0 | 8 | 13 | 119 | 105 | 27 |
| 1 | 8 | 13 | 1288 | 1197 | 9 |
| 2 | 8 | 13 | 396 | -374 | 13 |
| 3 | 8 | 13 | 1188 | -1129 | 9 |
| 4 | 8 | 13 | 131 | 173 | 37 |
| 5 | 8 | 13 | 1147 | 1142 | 9 |
| 6 | 8 | 13 | 263 | -263 | 22 |
| 7 | 8 | 13 | 1162 | -1159 | 10 |
| 8 | 8 | 13 | 319 | 337 | 16 |
| 9 | 8 | 13 | 922 | 892 | 11 |
| -8 | 9 | 13 | 806 | 759 | 13 |
| -7 | 9 | 13 | 207 | -189 | 26 |
| -6 | 9 | 13 | 849 | -849 | 12 |
| -5 | 9 | 13 | 352 | 374 | 15 |
| -4 | 9 | 13 | 756 | 824 | 12 |
| -3 | 9 | 13 | 178 | -153 | 22 |
| -2 | 9 | 13 | 968 | -1012 | 10 |
| -1 | 9 | 13 | 201 | 178 | 33 |
| 0 | 9 | 13 | 1298 | 1317 | 49 |
| 1 | 9 | 13 | 73 | -84 | 54 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 2 | 9 | 13 | 1062 | -1062 | 10 |
| 3 | 9 | 13 | 417 | 415 | 12 |
| 4 | 9 | 13 | 860 | 840 | 10 |
| 5 | 9 | 13 | 550 | -567 | 13 |
| 6 | 9 | 13 | 933 | -920 | 11 |
| 7 | 9 | 13 | 284 | 315 | 20 |
| 8 | 9 | 13 | 881 | 858 | 12 |
| -7 | 10 | 13 | 393 | -402 | 17 |
| -6 | 10 | 13 | 156 | -66 | 42 |
| -5 | 10 | 13 | 673 | 709 | 13 |
| -3 | 10 | 13 | 483 | -505 | 14 |
| -2 | 10 | 13 | 95 | 83 | 45 |
| -1 | 10 | 13 | 496 | 506 | 13 |
| 0 | 10 | 13 | 79 | -28 | 37 |
| 1 | 10 | 13 | 623 | -585 | 12 |
| 2 | 10 | 13 | 243 | 235 | 20 |
| 3 | 10 | 13 | 504 | 507 | 14 |
| 5 | 10 | 13 | 400 | -429 | 14 |
| 7 | 10 | 13 | 560 | 536 | 15 |
| -6 | 11 | 13 | 121 | -109 | 45 |
| -5 | 11 | 13 | 98 | -4 | 51 |
| -4 | 11 | 13 | 102 | 89 | 48 |
| -2 | 11 | 13 | 122 | -117 | 41 |
| 0 | 11 | 13 | 189 | 140 | 54 |
| 2 | 11 | 13 | 147 | -141 | 37 |
| 3 | 11 | 13 | 71 | 77 | 59 |
| 4 | 11 | 13 | 64 | 180 | 67 |
| 5 | 11 | 13 | 189 | -196 | 29 |
| -4 | 12 | 13 | 150 | -220 | 28 |
| -3 | 12 | 13 | 600 | -581 | 14 |
| -2 | 12 | 13 | 257 | 296 | 22 |
| -1 | 12 | 13 | 561 | 571 | 15 |
| 0 | 12 | 13 | 272 | -273 | 22 |
| 1 | 12 | 13 | 574 | -530 | 14 |
| 2 | 12 | 13 | 292 | 299 | 20 |
| 3 | 12 | 13 | 628 | 606 | 14 |
| -12 | 0 | 14 | 231 | 110 | 37 |
| -11 | 0 | 14 | 947 | 846 | 12 |
| -9 | 0 | 14 | 1022 | -987 | 11 |
| -8 | 0 | 14 | 220 | 189 | 28 |
| -7 | 0 | 14 | 1108 | 1065 | 11 |
| -6 | 0 | 14 | 371 | -366 | 13 |
| -5 | 0 | 14 | 1447 | -1396 | 9 |
| -4 | 0 | 14 | 231 | 243 | 15 |
| -3 | 0 | 14 | 1919 | 1878 | 8 |
| -2 | 0 | 14 | 210 | 185 | 13 |
| -1 | 0 | 14 | 1415 | -1416 | 8 |
| 0 | 0 | 14 | 735 | 718 | 28 |
| 1 | 0 | 14 | 1455 | 1368 | 8 |
| 2 | 0 | 14 | 244 | -241 | 16 |
| 3 | 0 | 14 | 2154 | -2109 | 8 |
| 4 | 0 | 14 | 601 | -582 | 12 |
| 5 | 0 | 14 | 1819 | 1795 | 9 |
| 6 | 0 | 14 | 246 | 241 | 27 |
| 7 | 0 | 14 | 1388 | -1368 | 11 |
| 8 | 0 | 14 | 119 | 137 | 43 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 9 | 0 | 14 | 1501 | 1495 | 11 |
| 10 | 0 | 14 | 63 | -17 | 67 |
| 11 | 0 | 14 | 971 | -990 | 13 |
| -12 | 1 | 14 | 762 | 707 | 14 |
| -11 | 1 | 14 | 244 | -203 | 21 |
| -10 | 1 | 14 | 949 | -883 | 11 |
| -8 | 1 | 14 | 890 | 859 | 11 |
| -7 | 1 | 14 | 109 | -68 | 40 |
| -6 | 1 | 14 | 911 | -893 | 10 |
| -5 | 1 | 14 | 442 | 448 | 12 |
| -4 | 1 | 14 | 1160 | 1143 | 9 |
| -3 | 1 | 14 | 122 | -115 | 32 |
| -2 | 1 | 14 | 1198 | -1173 | 9 |
| -1 | 1 | 14 | 260 | 244 | 12 |
| 0 | 1 | 14 | 1400 | 1395 | 57 |
| 1 | 1 | 14 | 490 | -462 | 11 |
| 2 | 1 | 14 | 1367 | -1325 | 9 |
| 3 | 1 | 14 | 404 | 420 | 15 |
| 4 | 1 | 14 | 1368 | 1317 | 9 |
| 5 | 1 | 14 | 226 | -192 | 23 |
| 6 | 1 | 14 | 1356 | -1297 | 10 |
| 8 | 1 | 14 | 1171 | 1181 | 11 |
| 9 | 1 | 14 | 88 | 27 | 54 |
| 10 | 1 | 14 | 1016 | -994 | 14 |
| 11 | 1 | 14 | 138 | -70 | 44 |
| -11 | 2 | 14 | 365 | -342 | 16 |
| -10 | 2 | 14 | 97 | 30 | 48 |
| -9 | 2 | 14 | 666 | 628 | 13 |
| -8 | 2 | 14 | 149 | -128 | 28 |
| -7 | 2 | 14 | 635 | -628 | 12 |
| -6 | 2 | 14 | 201 | 198 | 17 |
| -5 | 2 | 14 | 427 | 430 | 11 |
| -4 | 2 | 14 | 220 | -230 | 13 |
| -3 | 2 | 14 | 490 | -491 | 11 |
| -1 | 2 | 14 | 637 | 643 | 9 |
| 0 | 2 | 14 | 115 | -104 | 40 |
| 1 | 2 | 14 | 445 | -424 | 12 |
| 2 | 2 | 14 | 186 | -181 | 25 |
| 3 | 2 | 14 | 330 | 316 | 16 |
| 5 | 2 | 14 | 257 | -242 | 16 |
| 6 | 2 | 14 | 201 | 227 | 19 |
| 7 | 2 | 14 | 421 | 415 | 13 |
| 8 | 2 | 14 | 116 | 20 | 42 |
| 9 | 2 | 14 | 595 | -587 | 14 |
| 10 | 2 | 14 | 213 | -192 | 25 |
| 11 | 2 | 14 | 379 | 363 | 17 |
| -11 | 3 | 14 | 155 | 23 | 37 |
| -10 | 3 | 14 | 176 | -158 | 26 |
| -8 | 3 | 14 | 221 | -199 | 21 |
| -6 | 3 | 14 | 184 | 120 | 27 |
| -4 | 3 | 14 | 56 | 112 | 58 |
| -3 | 3 | 14 | 120 | 127 | 32 |
| -2 | 3 | 14 | 356 | -358 | 11 |
| -1 | 3 | 14 | 197 | -188 | 19 |
| 0 | 3 | 14 | 592 | 606 | 15 |
| 1 | 3 | 14 | 94 | 56 | 39 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 2 | 3 | 14 | 323 | -292 | 17 |
| 3 | 3 | 14 | 230 | 203 | 24 |
| 4 | 3 | 14 | 380 | 358 | 13 |
| 5 | 3 | 14 | 68 | 76 | 50 |
| 6 | 3 | 14 | 87 | -150 | 47 |
| 8 | 3 | 14 | 172 | 181 | 34 |
| 10 | 3 | 14 | 236 | -256 | 21 |
| 11 | 3 | 14 | 77 | -50 | 63 |
| -11 | 4 | 14 | 632 | -616 | 14 |
| -10 | 4 | 14 | 188 | 197 | 33 |
| -9 | 4 | 14 | 567 | 527 | 14 |
| -8 | 4 | 14 | 138 | -68 | 35 |
| -7 | 4 | 14 | 912 | -901 | 10 |
| -6 | 4 | 14 | 122 | 117 | 37 |
| -5 | 4 | 14 | 1048 | 1056 | 10 |
| -4 | 4 | 14 | 315 | -328 | 15 |
| -3 | 4 | 14 | 684 | -677 | 10 |
| -2 | 4 | 14 | 91 | -62 | 39 |
| -1 | 4 | 14 | 739 | 722 | 9 |
| 0 | 4 | 14 | 201 | 169 | 15 |
| 1 | 4 | 14 | 1302 | -1230 | 9 |
| 2 | 4 | 14 | 153 | 182 | 32 |
| 3 | 4 | 14 | 1157 | 1094 | 9 |
| 5 | 4 | 14 | 1187 | -1163 | 9 |
| 6 | 4 | 14 | 306 | -303 | 16 |
| 7 | 4 | 14 | 1136 | 1154 | 10 |
| 9 | 4 | 14 | 874 | -895 | 11 |
| 10 | 4 | 14 | 24 | -108 | 98 |
| -11 | 5 | 14 | 151 | 132 | 44 |
| -10 | 5 | 14 | 961 | 897 | 12 |
| -9 | 5 | 14 | 150 | -148 | 36 |
| -8 | 5 | 14 | 1068 | -1030 | 11 |
| -7 | 5 | 14 | 64 | -58 | 57 |
| -6 | 5 | 14 | 1466 | 1439 | 10 |
| -5 | 5 | 14 | 202 | -208 | 22 |
| -4 | 5 | 14 | 1394 | -1366 | 9 |
| -3 | 5 | 14 | 229 | 222 | 17 |
| -2 | 5 | 14 | 1247 | 1219 | 9 |
| -1 | 5 | 14 | 171 | 120 | 23 |
| 0 | 5 | 14 | 1684 | -1630 | 65 |
| 1 | 5 | 14 | 144 | -142 | 33 |
| 2 | 5 | 14 | 1254 | 1196 | 9 |
| 4 | 5 | 14 | 1399 | -1346 | 9 |
| 5 | 5 | 14 | 177 | -134 | 35 |
| 6 | 5 | 14 | 1475 | 1468 | 9 |
| 7 | 5 | 14 | 126 | -52 | 38 |
| 8 | 5 | 14 | 1197 | -1177 | 10 |
| 10 | 5 | 14 | 898 | 885 | 12 |
| -10 | 6 | 14 | 96 | -120 | 53 |
| -9 | 6 | 14 | 848 | -815 | 12 |
| -7 | 6 | 14 | 1050 | 1052 | 11 |
| -5 | 6 | 14 | 1281 | -1291 | 10 |
| -3 | 6 | 14 | 1181 | 1142 | 10 |
| -2 | 6 | 14 | 18 | -60 | 71 |
| -1 | 6 | 14 | 1499 | -1537 | 9 |
| 0 | 6 | 14 | 38 | -38 | 62 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 1 | 6 | 14 | 1832 | 1691 | 9 |
| 3 | 6 | 14 | 1194 | -1135 | 9 |
| 4 | 6 | 14 | 246 | 206 | 17 |
| 5 | 6 | 14 | 1059 | 1022 | 10 |
| 6 | 6 | 14 | 147 | -161 | 33 |
| 7 | 6 | 14 | 1100 | -1082 | 10 |
| 8 | 6 | 14 | 107 | 37 | 28 |
| 9 | 6 | 14 | 1045 | 1042 | 11 |
| -8 | 7 | 14 | 636 | 569 | 14 |
| -7 | 7 | 14 | 196 | 161 | 29 |
| -6 | 7 | 14 | 527 | -516 | 13 |
| -5 | 7 | 14 | 133 | -55 | 34 |
| -4 | 7 | 14 | 652 | 614 | 11 |
| -3 | 7 | 14 | 63 | -105 | 53 |
| -2 | 7 | 14 | 746 | -731 | 11 |
| -1 | 7 | 14 | 118 | 171 | 36 |
| 0 | 7 | 14 | 919 | 884 | 35 |
| 1 | 7 | 14 | 367 | -365 | 14 |
| 2 | 7 | 14 | 908 | -898 | 10 |
| 3 | 7 | 14 | 119 | -121 | 37 |
| 4 | 7 | 14 | 812 | 820 | 11 |
| 5 | 7 | 14 | 73 | -3 | 52 |
| 6 | 7 | 14 | 711 | -716 | 11 |
| 7 | 7 | 14 | 63 | -35 | 64 |
| 8 | 7 | 14 | 614 | 625 | 13 |
| -9 | 8 | 14 | 107 | 66 | 50 |
| -8 | 8 | 14 | 79 | 21 | 56 |
| -7 | 8 | 14 | 160 | 74 | 33 |
| -6 | 8 | 14 | 161 | 108 | 37 |
| -5 | 8 | 14 | 164 | 193 | 24 |
| -4 | 8 | 14 | 203 | -209 | 33 |
| -3 | 8 | 14 | 155 | -183 | 30 |
| -2 | 8 | 14 | 101 | 82 | 39 |
| -1 | 8 | 14 | 75 | -72 | 47 |
| 0 | 8 | 14 | 194 | -227 | 24 |
| 2 | 8 | 14 | 66 | 152 | 58 |
| 3 | 8 | 14 | 141 | 124 | 34 |
| 6 | 8 | 14 | 157 | 154 | 27 |
| 7 | 8 | 14 | 119 | 114 | 44 |
| 8 | 8 | 14 | 136 | 63 | 38 |
| -8 | 9 | 14 | 432 | 412 | 19 |
| -7 | 9 | 14 | 102 | 36 | 48 |
| -6 | 9 | 14 | 477 | -466 | 15 |
| -5 | 9 | 14 | 49 | -120 | 69 |
| -4 | 9 | 14 | 377 | 363 | 16 |
| -3 | 9 | 14 | 43 | -56 | 69 |
| -2 | 9 | 14 | 600 | -636 | 12 |
| -1 | 9 | 14 | 168 | 138 | 29 |
| 0 | 9 | 14 | 859 | 844 | 52 |
| 1 | 9 | 14 | 264 | 287 | 20 |
| 2 | 9 | 14 | 710 | -672 | 12 |
| 3 | 9 | 14 | 64 | -1 | 59 |
| 4 | 9 | 14 | 593 | 551 | 12 |
| 6 | 9 | 14 | 511 | -518 | 13 |
| -7 | 10 | 14 | 808 | -797 | 13 |
| -5 | 10 | 14 | 895 | 909 | 12 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -4 | 10 | 14 | 270 | 228 | 26 |
| -3 | 10 | 14 | 830 | -834 | 12 |
| -1 | 10 | 14 | 1056 | 1080 | 11 |
| 0 | 10 | 14 | 119 | 66 | 37 |
| 1 | 10 | 14 | 1054 | -997 | 10 |
| 3 | 10 | 14 | 990 | 931 | 11 |
| 4 | 10 | 14 | 123 | 34 | 41 |
| 5 | 10 | 14 | 1101 | -1100 | 11 |
| 6 | 10 | 14 | 279 | -268 | 27 |
| -5 | 11 | 14 | 84 | -11 | 55 |
| -4 | 11 | 14 | 920 | -914 | 12 |
| -2 | 11 | 14 | 966 | 981 | 11 |
| -1 | 11 | 14 | 170 | 181 | 27 |
| 0 | 11 | 14 | 1019 | -975 | 52 |
| 2 | 11 | 14 | 1073 | 1034 | 11 |
| 3 | 11 | 14 | 54 | -40 | 70 |
| 4 | 11 | 14 | 968 | -923 | 11 |
| -2 | 12 | 14 | 135 | -23 | 40 |
| -1 | 12 | 14 | 774 | -785 | 14 |
| 0 | 12 | 14 | 129 | -133 | 26 |
| 1 | 12 | 14 | 766 | 748 | 13 |
| -11 | 1 | 15 | 164 | 124 | 29 |
| -10 | 1 | 15 | 479 | -482 | 16 |
| -9 | 1 | 15 | 212 | -222 | 22 |
| -8 | 1 | 15 | 635 | 628 | 12 |
| -7 | 1 | 15 | 468 | 462 | 13 |
| -6 | 1 | 15 | 516 | -506 | 12 |
| -5 | 1 | 15 | 251 | -239 | 16 |
| -4 | 1 | 15 | 595 | 609 | 10 |
| -2 | 1 | 15 | 590 | -617 | 10 |
| -1 | 1 | 15 | 123 | -99 | 30 |
| 0 | 1 | 15 | 920 | 927 | 11 |
| 1 | 1 | 15 | 319 | 292 | 15 |
| 2 | 1 | 15 | 1245 | -1218 | 9 |
| 3 | 1 | 15 | 450 | -397 | 15 |
| 4 | 1 | 15 | 1274 | 1253 | 9 |
| 5 | 1 | 15 | 530 | 528 | 12 |
| 6 | 1 | 15 | 779 | -756 | 11 |
| 7 | 1 | 15 | 406 | -412 | 16 |
| 8 | 1 | 15 | 670 | 684 | 14 |
| 9 | 1 | 15 | 356 | 356 | 17 |
| 10 | 1 | 15 | 521 | -516 | 14 |
| -11 | 2 | 15 | 695 | -653 | 14 |
| -10 | 2 | 15 | 374 | -354 | 16 |
| -9 | 2 | 15 | 951 | 894 | 11 |
| -8 | 2 | 15 | 431 | 436 | 14 |
| -7 | 2 | 15 | 809 | -791 | 11 |
| -6 | 2 | 15 | 374 | -379 | 15 |
| -5 | 2 | 15 | 1135 | 1147 | 10 |
| -4 | 2 | 15 | 249 | 224 | 17 |
| -3 | 2 | 15 | 1337 | -1346 | 9 |
| -2 | 2 | 15 | 241 | -179 | 16 |
| -1 | 2 | 15 | 1362 | 1386 | 9 |
| 0 | 2 | 15 | 431 | 419 | 29 |
| 1 | 2 | 15 | 1482 | -1399 | 9 |
| 2 | 2 | 15 | 233 | -202 | 19 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 3 | 2 | 15 | 1391 | 1327 | 9 |
| 4 | 2 | 15 | 225 | 193 | 20 |
| 5 | 2 | 15 | 1318 | -1281 | 9 |
| 6 | 2 | 15 | 433 | -408 | 12 |
| 7 | 2 | 15 | 1081 | 1061 | 11 |
| 8 | 2 | 15 | 401 | 367 | 19 |
| 9 | 2 | 15 | 1051 | -1042 | 12 |
| 10 | 2 | 15 | 462 | -457 | 16 |
| -11 | 3 | 15 | 240 | -231 | 30 |
| -10 | 3 | 15 | 917 | 864 | 13 |
| -9 | 3 | 15 | 270 | 248 | 18 |
| -8 | 3 | 15 | 1077 | -1046 | 11 |
| -7 | 3 | 15 | 387 | -359 | 14 |
| -6 | 3 | 15 | 1413 | 1396 | 10 |
| -5 | 3 | 15 | 307 | 305 | 17 |
| -4 | 3 | 15 | 1532 | -1526 | 9 |
| -3 | 3 | 15 | 623 | -589 | 11 |
| -2 | 3 | 15 | 1381 | 1378 | 9 |
| -1 | 3 | 15 | 701 | 700 | 10 |
| 0 | 3 | 15 | 1404 | -1374 | 52 |
| 1 | 3 | 15 | 454 | -437 | 14 |
| 2 | 3 | 15 | 961 | 898 | 9 |
| 3 | 3 | 15 | 404 | 376 | 13 |
| 4 | 3 | 15 | 1021 | -960 | 10 |
| 5 | 3 | 15 | 537 | -525 | 12 |
| 6 | 3 | 15 | 993 | 953 | 10 |
| 7 | 3 | 15 | 303 | 311 | 16 |
| 8 | 3 | 15 | 1130 | -1131 | 10 |
| 9 | 3 | 15 | 548 | -545 | 13 |
| 10 | 3 | 15 | 844 | 863 | 12 |
| -10 | 4 | 15 | 432 | 393 | 17 |
| -9 | 4 | 15 | 825 | -799 | 12 |
| -8 | 4 | 15 | 250 | -253 | 20 |
| -7 | 4 | 15 | 763 | 745 | 12 |
| -6 | 4 | 15 | 228 | 245 | 16 |
| -5 | 4 | 15 | 1136 | -1141 | 10 |
| -4 | 4 | 15 | 570 | -542 | 11 |
| -3 | 4 | 15 | 932 | 918 | 10 |
| -2 | 4 | 15 | 595 | 592 | 11 |
| -1 | 4 | 15 | 812 | -831 | 9 |
| 0 | 4 | 15 | 341 | -345 | 17 |
| 1 | 4 | 15 | 1367 | 1278 | 9 |
| 2 | 4 | 15 | 394 | 370 | 14 |
| 3 | 4 | 15 | 903 | -864 | 10 |
| 4 | 4 | 15 | 790 | -766 | 10 |
| 5 | 4 | 15 | 523 | 489 | 13 |
| 6 | 4 | 15 | 374 | 409 | 13 |
| 7 | 4 | 15 | 747 | -731 | 11 |
| 8 | 4 | 15 | 380 | -391 | 14 |
| 9 | 4 | 15 | 716 | 674 | 13 |
| 10 | 4 | 15 | 490 | 451 | 16 |
| -10 | 5 | 15 | 259 | -233 | 30 |
| -9 | 5 | 15 | 215 | -220 | 24 |
| -8 | 5 | 15 | 184 | 155 | 23 |
| -7 | 5 | 15 | 132 | 188 | 38 |
| -6 | 5 | 15 | 373 | -370 | 16 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$ 

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 5 | 15 | 350 | -345 | 13 |
| -4 | 5 | 15 | 190 | 139 | 21 |
| -3 | 5 | 15 | 314 | 305 | 14 |
| -2 | 5 | 15 | 212 | -236 | 17 |
| -1 | 5 | 15 | 373 | -386 | 13 |
| 0 | 5 | 15 | 352 | 346 | 47 |
| 1 | 5 | 15 | 164 | 175 | 21 |
| 2 | 5 | 15 | 190 | -202 | 22 |
| 3 | 5 | 15 | 325 | -292 | 20 |
| 4 | 5 | 15 | 280 | 274 | 19 |
| 5 | 5 | 15 | 218 | 230 | 19 |
| 6 | 5 | 15 | 259 | -246 | 19 |
| 8 | 5 | 15 | 211 | 194 | 18 |
| 9 | 5 | 15 | 226 | 272 | 20 |
| -9 | 6 | 15 | 127 | -140 | 43 |
| -8 | 6 | 15 | 139 | 0 | 35 |
| -7 | 6 | 15 | 437 | 454 | 14 |
| -5 | 6 | 15 | 443 | -420 | 14 |
| -3 | 6 | 15 | 419 | 371 | 14 |
| -2 | 6 | 15 | 177 | 154 | 22 |
| -1 | 6 | 15 | 609 | -623 | 11 |
| 0 | 6 | 15 | 156 | -167 | 23 |
| 1 | 6 | 15 | 355 | 334 | 15 |
| 3 | 6 | 15 | 226 | -209 | 29 |
| 4 | 6 | 15 | 140 | 205 | 27 |
| 5 | 6 | 15 | 376 | 362 | 15 |
| 6 | 6 | 15 | 255 | 237 | 23 |
| 7 | 6 | 15 | 140 | -138 | 38 |
| 9 | 6 | 15 | 400 | 403 | 15 |
| -9 | 7 | 15 | 209 | -131 | 35 |
| -8 | 7 | 15 | 696 | 667 | 14 |
| -7 | 7 | 15 | 272 | 232 | 20 |
| -6 | 7 | 15 | 779 | -759 | 12 |
| -5 | 7 | 15 | 366 | -398 | 15 |
| -4 | 7 | 15 | 951 | 961 | 11 |
| -3 | 7 | 15 | 419 | 432 | 15 |
| -2 | 7 | 15 | 703 | -712 | 12 |
| -1 | 7 | 15 | 207 | -247 | 20 |
| 0 | 7 | 15 | 998 | 945 | 43 |
| 1 | 7 | 15 | 549 | 512 | 12 |
| 2 | 7 | 15 | 1164 | -1109 | 10 |
| 3 | 7 | 15 | 362 | -401 | 14 |
| 4 | 7 | 15 | 1048 | 1016 | 10 |
| 5 | 7 | 15 | 531 | 527 | 13 |
| 6 | 7 | 15 | 840 | -834 | 11 |
| 7 | 7 | 15 | 491 | -509 | 13 |
| 8 | 7 | 15 | 867 | 876 | 12 |
| -8 | 8 | 15 | 330 | 326 | 17 |
| -7 | 8 | 15 | 956 | -889 | 12 |
| -6 | 8 | 15 | 398 | -381 | 16 |
| -5 | 8 | 15 | 1048 | 1041 | 11 |
| -4 | 8 | 15 | 383 | 388 | 16 |
| -3 | 8 | 15 | 1000 | -1002 | 11 |
| -2 | 8 | 15 | 488 | -515 | 14 |
| -1 | 8 | 15 | 1057 | 1091 | 10 |
| 0 | 8 | 15 | 721 | 764 | 41 |
| 1 | 8 | 15 | 1153 | -1070 | 10 |
| 2 | 8 | 15 | 863 | -866 | 11 |
| 3 | 8 | 15 | 1191 | 1153 | 10 |
| 4 | 8 | 15 | 501 | 501 | 13 |
| 5 | 8 | 15 | 1130 | -1104 | 11 |
| 6 | 8 | 15 | 491 | -507 | 15 |
| 7 | 8 | 15 | 911 | 918 | 11 |
| -7 | 9 | 15 | 338 | -312 | 20 |
| -6 | 9 | 15 | 803 | 795 | 13 |
| -5 | 9 | 15 | 474 | 448 | 15 |
| -4 | 9 | 15 | 846 | -863 | 12 |
| -3 | 9 | 15 | 275 | -298 | 23 |
| -2 | 9 | 15 | 845 | 869 | 12 |
| -1 | 9 | 15 | 502 | 516 | 14 |
| 0 | 9 | 15 | 996 | -983 | 52 |
| 1 | 9 | 15 | 594 | -601 | 12 |
| 2 | 9 | 15 | 998 | 970 | 11 |
| 3 | 9 | 15 | 380 | 377 | 17 |
| 4 | 9 | 15 | 911 | -909 | 11 |
| 5 | 9 | 15 | 351 | -326 | 16 |
| 6 | 9 | 15 | 787 | 778 | 12 |
| -6 | 10 | 15 | 220 | 214 | 29 |
| -5 | 10 | 15 | 359 | -365 | 18 |
| -4 | 10 | 15 | 120 | -134 | 42 |
| -3 | 10 | 15 | 309 | 330 | 20 |
| -2 | 10 | 15 | 258 | 250 | 18 |
| -1 | 10 | 15 | 417 | -454 | 16 |
| 0 | 10 | 15 | 241 | -246 | 18 |
| 1 | 10 | 15 | 342 | 336 | 19 |
| 2 | 10 | 15 | 230 | 253 | 21 |
| 3 | 10 | 15 | 366 | -385 | 16 |
| 4 | 10 | 15 | 394 | -398 | 16 |
| 5 | 10 | 15 | 337 | 306 | 16 |
| -3 | 11 | 15 | 77 | -79 | 58 |
| -2 | 11 | 15 | 131 | 116 | 41 |
| -1 | 11 | 15 | 62 | -68 | 63 |
| 0 | 11 | 15 | 124 | -156 | 34 |
| 1 | 11 | 15 | 180 | -95 | 45 |
| 2 | 11 | 15 | 138 | 176 | 42 |
| 3 | 11 | 15 | 121 | 14 | 43 |
| -10 | 0 | 16 | 465 | -414 | 15 |
| -9 | 0 | 16 | 775 | 728 | 12 |
| -8 | 0 | 16 | 706 | 669 | 12 |
| -7 | 0 | 16 | 718 | -669 | 11 |
| -6 | 0 | 16 | 762 | -755 | 11 |
| -5 | 0 | 16 | 1270 | 1255 | 10 |
| -4 | 0 | 16 | 796 | 765 | 11 |
| -3 | 0 | 16 | 1116 | -1085 | 9 |
| -2 | 0 | 16 | 860 | -813 | 9 |
| -1 | 0 | 16 | 952 | 963 | 9 |
| 0 | 0 | 16 | 1032 | 1012 | 31 |
| 1 | 0 | 16 | 1495 | -1432 | 9 |
| 2 | 0 | 16 | 789 | -731 | 10 |
| 3 | 0 | 16 | 825 | 777 | 10 |
| 4 | 0 | 16 | 600 | 572 | 12 |
| 5 | 0 | 16 | 1092 | -1030 | 11 |
| 6 | 0 | 16 | 935 | -906 | 11 |
| 7 | 0 | 16 | 1103 | 1120 | 12 |
| 8 | 0 | 16 | 667 | 661 | 14 |
| 9 | 0 | 16 | 784 | -799 | 14 |
| 10 | 0 | 16 | 584 | -595 | 17 |
| -10 | 1 | 16 | 580 | 532 | 14 |
| -9 | 1 | 16 | 437 | 417 | 15 |
| -8 | 1 | 16 | 616 | -577 | 12 |
| -7 | 1 | 16 | 642 | -623 | 12 |
| -6 | 1 | 16 | 720 | 712 | 11 |
| -5 | 1 | 16 | 360 | 346 | 13 |
| -4 | 1 | 16 | 917 | -882 | 10 |
| -3 | 1 | 16 | 637 | -630 | 11 |
| -2 | 1 | 16 | 797 | 797 | 10 |
| -1 | 1 | 16 | 783 | 785 | 10 |
| 0 | 1 | 16 | 1487 | -1484 | 58 |
| 1 | 1 | 16 | 549 | -540 | 11 |
| 2 | 1 | 16 | 1051 | 1005 | 10 |
| 3 | 1 | 16 | 528 | 488 | 12 |
| 4 | 1 | 16 | 1003 | -978 | 10 |
| 5 | 1 | 16 | 621 | -611 | 11 |
| 6 | 1 | 16 | 988 | 999 | 11 |
| 7 | 1 | 16 | 484 | 513 | 15 |
| 8 | 1 | 16 | 766 | -765 | 12 |
| 9 | 1 | 16 | 671 | -691 | 14 |
| 10 | 1 | 16 | 553 | 548 | 15 |
| -10 | 2 | 16 | 252 | 190 | 23 |
| -9 | 2 | 16 | 294 | -274 | 21 |
| -8 | 2 | 16 | 327 | -304 | 18 |
| -7 | 2 | 16 | 296 | 305 | 18 |
| -6 | 2 | 16 | 251 | 241 | 18 |
| -5 | 2 | 16 | 545 | -553 | 11 |
| -4 | 2 | 16 | 272 | -273 | 14 |
| -3 | 2 | 16 | 256 | 252 | 15 |
| -2 | 2 | 16 | 321 | 307 | 13 |
| -1 | 2 | 16 | 153 | -165 | 20 |
| 0 | 2 | 16 | 306 | -319 | 12 |
| 1 | 2 | 16 | 691 | 688 | 11 |
| 2 | 2 | 16 | 213 | 219 | 22 |
| 3 | 2 | 16 | 498 | -485 | 14 |
| 4 | 2 | 16 | 434 | -425 | 15 |
| 5 | 2 | 16 | 496 | 512 | 12 |
| 6 | 2 | 16 | 416 | 433 | 14 |
| 7 | 2 | 16 | 426 | -428 | 14 |
| 8 | 2 | 16 | 241 | -273 | 22 |
| 9 | 2 | 16 | 347 | 308 | 21 |
| 10 | 2 | 16 | 339 | 377 | 20 |
| -10 | 3 | 16 | 91 | 56 | 55 |
| -8 | 3 | 16 | 82 | -126 | 54 |
| -7 | 3 | 16 | 86 | -41 | 52 |
| -5 | 3 | 16 | 170 | 167 | 24 |
| -3 | 3 | 16 | 132 | -118 | 31 |
| -2 | 3 | 16 | 127 | 142 | 22 |
| -1 | 3 | 16 | 271 | 263 | 14 |
| 1 | 3 | 16 | 338 | -349 | 15 |
| 2 | 3 | 16 | 211 | 163 | 29 |
| 3 | 3 | 16 | 416 | -413 | 15 |
| 4 | 3 | 16 | 392 | -387 | 15 |
| 6 | 3 | 16 | 134 | 53 | 37 |
| 7 | 3 | 16 | 228 | 246 | 18 |
| -10 | 4 | 16 | 277 | 283 | 20 |
| -9 | 4 | 16 | 529 | -520 | 15 |
| -8 | 4 | 16 | 520 | -481 | 13 |
| -7 | 4 | 16 | 478 | 476 | 14 |
| -6 | 4 | 16 | 365 | 368 | 14 |
| -5 | 4 | 16 | 450 | -454 | 13 |
| -4 | 4 | 16 | 398 | -429 | 13 |
| -3 | 4 | 16 | 494 | 491 | 12 |
| -2 | 4 | 16 | 600 | 605 | 11 |
| -1 | 4 | 16 | 588 | -579 | 11 |
| 0 | 4 | 16 | 569 | -578 | 16 |
| 1 | 4 | 16 | 598 | 554 | 12 |
| 2 | 4 | 16 | 856 | 799 | 11 |
| 3 | 4 | 16 | 655 | -664 | 12 |
| 4 | 4 | 16 | 892 | -851 | 11 |
| 5 | 4 | 16 | 857 | 869 | 11 |
| 6 | 4 | 16 | 740 | 772 | 12 |
| 7 | 4 | 16 | 756 | -762 | 11 |
| 8 | 4 | 16 | 560 | -560 | 14 |
| 9 | 4 | 16 | 634 | 605 | 14 |
| -9 | 5 | 16 | 508 | -499 | 17 |
| -8 | 5 | 16 | 791 | 742 | 12 |
| -7 | 5 | 16 | 712 | 688 | 12 |
| -6 | 5 | 16 | 805 | -784 | 12 |
| -5 | 5 | 16 | 622 | -650 | 12 |
| -4 | 5 | 16 | 932 | 970 | 11 |
| -3 | 5 | 16 | 666 | 662 | 12 |
| -2 | 5 | 16 | 833 | -826 | 10 |
| -1 | 5 | 16 | 628 | -631 | 11 |
| 0 | 5 | 16 | 911 | 869 | 46 |
| 1 | 5 | 16 | 1148 | 1080 | 10 |
| 2 | 5 | 16 | 764 | -729 | 11 |
| 3 | 5 | 16 | 928 | -909 | 11 |
| 4 | 5 | 16 | 824 | 795 | 11 |
| 5 | 5 | 16 | 884 | 893 | 11 |
| 6 | 5 | 16 | 855 | -831 | 11 |
| 7 | 5 | 16 | 600 | -599 | 13 |
| 8 | 5 | 16 | 953 | 939 | 11 |
| 9 | 5 | 16 | 603 | 572 | 14 |
| -9 | 6 | 16 | 780 | 741 | 13 |
| -8 | 6 | 16 | 450 | 424 | 15 |
| -7 | 6 | 16 | 789 | -756 | 12 |
| -6 | 6 | 16 | 503 | -527 | 14 |
| -5 | 6 | 16 | 886 | 920 | 12 |
| -4 | 6 | 16 | 705 | 738 | 12 |
| -3 | 6 | 16 | 834 | -869 | 11 |
| -2 | 6 | 16 | 655 | -700 | 11 |
| -1 | 6 | 16 | 847 | 853 | 10 |
| 0 | 6 | 16 | 551 | 557 | 35 |
| 1 | 6 | 16 | 1144 | -1089 | 10 |
| 2 | 6 | 16 | 555 | -558 | 13 |
| 3 | 6 | 16 | 997 | 997 | 11 |
| 4 | 6 | 16 | 628 | 620 | 12 |
| 5 | 6 | 16 | 785 | -764 | 11 |
| 6 | 6 | 16 | 609 | -585 | 12 |
| 7 | 6 | 16 | 674 | 653 | 12 |
| 8 | 6 | 16 | 527 | 565 | 13 |
| -8 | 7 | 16 | 345 | -348 | 20 |
| -7 | 7 | 16 | 173 | -198 | 39 |
| -6 | 7 | 16 | 496 | 475 | 14 |
| -5 | 7 | 16 | 392 | 388 | 16 |
| -4 | 7 | 16 | 702 | -727 | 13 |
| -3 | 7 | 16 | 426 | -444 | 13 |
| -2 | 7 | 16 | 470 | 529 | 15 |
| -1 | 7 | 16 | 290 | 345 | 20 |
| 0 | 7 | 16 | 562 | -591 | 35 |
| 1 | 7 | 16 | 457 | -466 | 15 |
| 2 | 7 | 16 | 777 | 771 | 12 |
| 3 | 7 | 16 | 425 | 437 | 15 |
| 4 | 7 | 16 | 495 | -459 | 14 |
| 5 | 7 | 16 | 313 | -291 | 18 |
| 6 | 7 | 16 | 412 | 416 | 16 |
| 7 | 7 | 16 | 538 | 562 | 14 |
| -6 | 8 | 16 | 80 | 65 | 56 |
| -5 | 8 | 16 | 19 | 10 | 77 |
| -4 | 8 | 16 | 198 | -158 | 25 |
| -3 | 8 | 16 | 143 | 156 | 30 |
| -1 | 8 | 16 | 122 | -118 | 38 |
| 0 | 8 | 16 | 106 | 38 | 40 |
| 1 | 8 | 16 | 70 | 127 | 58 |
| 5 | 8 | 16 | 178 | 164 | 30 |
| 6 | 8 | 16 | 84 | 122 | 57 |
| -6 | 9 | 16 | 369 | 397 | 19 |
| -5 | 9 | 16 | 265 | 263 | 23 |
| -4 | 9 | 16 | 369 | -417 | 16 |
| -3 | 9 | 16 | 348 | -352 | 17 |
| -2 | 9 | 16 | 338 | 346 | 17 |
| -1 | 9 | 16 | 356 | 373 | 15 |
| 0 | 9 | 16 | 436 | -400 | 14 |
| 1 | 9 | 16 | 331 | -301 | 16 |
| 2 | 9 | 16 | 380 | 373 | 16 |
| 3 | 9 | 16 | 147 | 163 | 25 |
| 4 | 9 | 16 | 440 | -444 | 15 |
| 5 | 9 | 16 | 507 | -503 | 16 |
| -4 | 10 | 16 | 485 | -488 | 15 |
| -3 | 10 | 16 | 548 | 550 | 15 |
| -2 | 10 | 16 | 592 | 583 | 15 |
| -1 | 10 | 16 | 761 | -751 | 13 |
| 0 | 10 | 16 | 680 | -685 | 31 |
| 1 | 10 | 16 | 730 | 679 | 13 |
| 2 | 10 | 16 | 662 | 648 | 14 |
| 3 | 10 | 16 | 644 | -662 | 13 |
| -10 | 1 | 17 | 143 | 128 | 41 |
| -9 | 1 | 17 | 411 | 380 | 16 |
| -8 | 1 | 17 | 199 | -231 | 28 |
| -7 | 1 | 17 | 527 | -507 | 13 |
| -6 | 1 | 17 | 426 | 410 | 14 |
| -5 | 1 | 17 | 573 | 567 | 12 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -4 | 1 | 17 | 577 | -578 | 12 |
| -3 | 1 | 17 | 468 | -431 | 12 |
| -2 | 1 | 17 | 366 | 390 | 13 |
| -1 | 1 | 17 | 419 | 403 | 13 |
| 0 | 1 | 17 | 523 | -549 | 19 |
| 1 | 1 | 17 | 763 | -789 | 12 |
| 2 | 1 | 17 | 231 | 260 | 17 |
| 3 | 1 | 17 | 504 | 514 | 14 |
| 5 | 1 | 17 | 435 | -438 | 14 |
| 6 | 1 | 17 | 174 | 184 | 24 |
| 7 | 1 | 17 | 641 | 648 | 14 |
| 8 | 1 | 17 | 215 | -242 | 28 |
| 9 | 1 | 17 | 555 | -545 | 15 |
| -10 | 2 | 17 | 598 | 545 | 14 |
| -9 | 2 | 17 | 392 | -392 | 17 |
| -8 | 2 | 17 | 791 | -762 | 12 |
| -7 | 2 | 17 | 509 | 479 | 14 |
| -6 | 2 | 17 | 1000 | 1017 | 11 |
| -5 | 2 | 17 | 656 | -671 | 12 |
| -4 | 2 | 17 | 864 | -859 | 10 |
| -3 | 2 | 17 | 742 | 726 | 11 |
| -2 | 2 | 17 | 746 | 727 | 11 |
| -1 | 2 | 17 | 656 | -686 | 11 |
| 0 | 2 | 17 | 990 | -984 | 42 |
| 1 | 2 | 17 | 858 | 798 | 11 |
| 2 | 2 | 17 | 970 | 926 | 11 |
| 3 | 2 | 17 | 611 | -602 | 13 |
| 4 | 2 | 17 | 880 | -867 | 11 |
| 5 | 2 | 17 | 366 | 337 | 15 |
| 6 | 2 | 17 | 796 | 797 | 12 |
| 7 | 2 | 17 | 559 | -538 | 13 |
| 8 | 2 | 17 | 841 | -831 | 12 |
| 9 | 2 | 17 | 442 | 402 | 16 |
| -9 | 3 | 17 | 783 | -722 | 13 |
| -8 | 3 | 17 | 586 | 553 | 14 |
| -7 | 3 | 17 | 894 | 878 | 12 |
| -6 | 3 | 17 | 503 | -510 | 12 |
| -5 | 3 | 17 | 1131 | -1138 | 11 |
| -4 | 3 | 17 | 552 | 573 | 12 |
| -3 | 3 | 17 | 1259 | 1223 | 10 |
| -2 | 3 | 17 | 363 | -329 | 16 |
| -1 | 3 | 17 | 1001 | -1021 | 10 |
| 0 | 3 | 17 | 706 | 662 | 27 |
| 1 | 3 | 17 | 1288 | 1241 | 10 |
| 2 | 3 | 17 | 874 | -831 | 11 |
| 3 | 3 | 17 | 1201 | -1148 | 10 |
| 4 | 3 | 17 | 711 | 675 | 12 |
| 5 | 3 | 17 | 1011 | 1001 | 11 |
| 6 | 3 | 17 | 695 | -674 | 11 |
| 7 | 3 | 17 | 1035 | -1055 | 11 |
| 8 | 3 | 17 | 502 | 515 | 14 |
| 9 | 3 | 17 | 894 | 898 | 12 |
| -9 | 4 | 17 | 357 | 345 | 20 |
| -8 | 4 | 17 | 618 | 577 | 13 |
| -7 | 4 | 17 | 319 | -275 | 20 |
| -6 | 4 | 17 | 597 | -579 | 12 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -5 | 4 | 17 | 424 | 450 | 14 |
| -4 | 4 | 17 | 752 | 760 | 12 |
| -3 | 4 | 17 | 522 | -557 | 12 |
| -2 | 4 | 17 | 1213 | -1203 | 10 |
| -1 | 4 | 17 | 381 | 368 | 14 |
| 0 | 4 | 17 | 1261 | 1260 | 50 |
| 1 | 4 | 17 | 612 | -541 | 13 |
| 2 | 4 | 17 | 915 | -903 | 11 |
| 3 | 4 | 17 | 593 | 594 | 14 |
| 4 | 4 | 17 | 821 | 820 | 11 |
| 5 | 4 | 17 | 488 | -468 | 13 |
| 6 | 4 | 17 | 779 | -792 | 11 |
| 7 | 4 | 17 | 398 | 403 | 21 |
| 8 | 4 | 17 | 752 | 746 | 13 |
| -9 | 5 | 17 | 269 | 254 | 17 |
| -8 | 5 | 17 | 81 | -74 | 57 |
| -7 | 5 | 17 | 176 | -144 | 25 |
| -6 | 5 | 17 | 153 | 192 | 32 |
| -5 | 5 | 17 | 232 | 260 | 19 |
| -4 | 5 | 17 | 282 | -280 | 16 |
| -3 | 5 | 17 | 170 | -193 | 23 |
| -2 | 5 | 17 | 299 | 293 | 17 |
| -1 | 5 | 17 | 339 | 355 | 16 |
| 0 | 5 | 17 | 308 | -306 | 39 |
| 1 | 5 | 17 | 352 | -375 | 17 |
| 2 | 5 | 17 | 407 | 407 | 15 |
| 3 | 5 | 17 | 479 | 472 | 13 |
| 4 | 5 | 17 | 58 | -24 | 60 |
| 5 | 5 | 17 | 336 | -317 | 17 |
| 6 | 5 | 17 | 63 | 96 | 63 |
| 7 | 5 | 17 | 349 | 338 | 17 |
| -8 | 6 | 17 | 258 | 244 | 21 |
| -6 | 6 | 17 | 194 | -176 | 24 |
| -4 | 6 | 17 | 229 | 247 | 24 |
| -3 | 6 | 17 | 105 | -30 | 41 |
| -2 | 6 | 17 | 246 | -233 | 16 |
| -1 | 6 | 17 | 146 | 186 | 29 |
| 0 | 6 | 17 | 245 | 281 | 17 |
| 2 | 6 | 17 | 146 | -133 | 27 |
| 3 | 6 | 17 | 276 | 306 | 20 |
| 5 | 6 | 17 | 320 | -312 | 20 |
| 6 | 6 | 17 | 176 | -206 | 32 |
| 7 | 6 | 17 | 23 | 136 | 90 |
| -7 | 7 | 17 | 593 | -570 | 14 |
| -6 | 7 | 17 | 445 | 395 | 16 |
| -5 | 7 | 17 | 386 | 366 | 15 |
| -4 | 7 | 17 | 691 | -687 | 13 |
| -3 | 7 | 17 | 563 | -539 | 14 |
| -2 | 7 | 17 | 562 | 587 | 14 |
| -1 | 7 | 17 | 708 | 689 | 12 |
| 0 | 7 | 17 | 477 | -448 | 23 |
| 1 | 7 | 17 | 782 | -760 | 12 |
| 2 | 7 | 17 | 477 | 480 | 15 |
| 3 | 7 | 17 | 738 | 719 | 12 |
| 4 | 7 | 17 | 529 | -527 | 13 |
| 5 | 7 | 17 | 948 | -952 | 12 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 6 | 7 | 17 | 259 | 256 | 19 |
| -6 | 8 | 17 | 675 | 639 | 13 |
| -5 | 8 | 17 | 790 | -725 | 13 |
| -4 | 8 | 17 | 755 | -746 | 13 |
| -3 | 8 | 17 | 733 | 750 | 13 |
| -2 | 8 | 17 | 722 | 739 | 13 |
| -1 | 8 | 17 | 521 | -521 | 16 |
| 0 | 8 | 17 | 922 | -896 | 25 |
| 1 | 8 | 17 | 541 | 513 | 13 |
| 2 | 8 | 17 | 959 | 917 | 11 |
| 3 | 8 | 17 | 444 | -447 | 16 |
| 4 | 8 | 17 | 995 | -948 | 12 |
| 5 | 8 | 17 | 433 | 440 | 16 |
| -5 | 9 | 17 | 743 | -724 | 13 |
| -4 | 9 | 17 | 373 | 384 | 18 |
| -3 | 9 | 17 | 677 | 685 | 14 |
| -2 | 9 | 17 | 487 | -503 | 15 |
| -1 | 9 | 17 | 764 | -809 | 13 |
| 0 | 9 | 17 | 505 | 484 | 19 |
| 1 | 9 | 17 | 802 | 801 | 12 |
| 2 | 9 | 17 | 518 | -527 | 13 |
| 3 | 9 | 17 | 806 | -809 | 12 |
| 4 | 9 | 17 | 301 | 330 | 19 |
| -2 | 10 | 17 | 400 | -394 | 19 |
| 0 | 10 | 17 | 349 | 362 | 18 |
| 1 | 10 | 17 | 100 | -188 | 54 |
| -9 | 0 | 18 | 140 | -151 | 27 |
| -8 | 0 | 18 | 921 | -855 | 12 |
| -7 | 0 | 18 | 125 | 89 | 42 |
| -6 | 0 | 18 | 940 | 935 | 12 |
| -5 | 0 | 18 | 293 | -311 | 15 |
| -4 | 0 | 18 | 1276 | -1283 | 10 |
| -2 | 0 | 18 | 1326 | 1302 | 10 |
| -1 | 0 | 18 | 160 | 163 | 26 |
| 0 | 0 | 18 | 1654 | -1608 | 64 |
| 1 | 0 | 18 | 70 | 63 | 57 |
| 2 | 0 | 18 | 1520 | 1518 | 10 |
| 3 | 0 | 18 | 106 | 51 | 35 |
| 4 | 0 | 18 | 1308 | -1320 | 10 |
| 5 | 0 | 18 | 125 | 131 | 41 |
| 6 | 0 | 18 | 1374 | 1349 | 12 |
| 7 | 0 | 18 | 303 | -304 | 22 |
| 8 | 0 | 18 | 1033 | -1039 | 13 |
| -9 | 1 | 18 | 752 | -670 | 13 |
| -8 | 1 | 18 | 208 | 214 | 21 |
| -7 | 1 | 18 | 743 | 722 | 12 |
| -6 | 1 | 18 | 112 | -98 | 43 |
| -5 | 1 | 18 | 1031 | -1051 | 11 |
| -4 | 1 | 18 | 193 | 226 | 20 |
| -3 | 1 | 18 | 1042 | 1065 | 10 |
| -2 | 1 | 18 | 183 | -160 | 22 |
| -1 | 1 | 18 | 1010 | -999 | 10 |
| 0 | 1 | 18 | 86 | 70 | 41 |
| 1 | 1 | 18 | 1615 | 1553 | 10 |
| 2 | 1 | 18 | 371 | -351 | 15 |
| 3 | 1 | 18 | 1071 | -1070 | 11 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 4 | 1 | 18 | 172 | 152 | 24 |
| 5 | 1 | 18 | 862 | 837 | 12 |
| 6 | 1 | 18 | 107 | -169 | 52 |
| 7 | 1 | 18 | 943 | -913 | 12 |
| 8 | 1 | 18 | 306 | 301 | 19 |
| -9 | 2 | 18 | 158 | 125 | 37 |
| -8 | 2 | 18 | 409 | 388 | 15 |
| -7 | 2 | 18 | 65 | -56 | 62 |
| -6 | 2 | 18 | 474 | -504 | 13 |
| -4 | 2 | 18 | 539 | 569 | 12 |
| -3 | 2 | 18 | 111 | -149 | 42 |
| -2 | 2 | 18 | 337 | -359 | 14 |
| -1 | 2 | 18 | 262 | 255 | 17 |
| 0 | 2 | 18 | 477 | 469 | 12 |
| 1 | 2 | 18 | 295 | -297 | 20 |
| 2 | 2 | 18 | 555 | -565 | 13 |
| 3 | 2 | 18 | 191 | 153 | 32 |
| 4 | 2 | 18 | 335 | 343 | 18 |
| 5 | 2 | 18 | 143 | -154 | 26 |
| 6 | 2 | 18 | 397 | -400 | 15 |
| 7 | 2 | 18 | 51 | 72 | 76 |
| 8 | 2 | 18 | 417 | 411 | 19 |
| -9 | 3 | 18 | 178 | -142 | 32 |
| -7 | 3 | 18 | 265 | 265 | 21 |
| -5 | 3 | 18 | 105 | 115 | 46 |
| -4 | 3 | 18 | 106 | -16 | 42 |
| -3 | 3 | 18 | 41 | 52 | 71 |
| -2 | 3 | 18 | 37 | 49 | 70 |
| -1 | 3 | 18 | 374 | -387 | 16 |
| 0 | 3 | 18 | 326 | 324 | 14 |
| 2 | 3 | 18 | 46 | -89 | 70 |
| 3 | 3 | 18 | 342 | -347 | 19 |
| 4 | 3 | 18 | 207 | -170 | 36 |
| 5 | 3 | 18 | 118 | 139 | 41 |
| -8 | 4 | 18 | 632 | 604 | 14 |
| -7 | 4 | 18 | 223 | -223 | 23 |
| -6 | 4 | 18 | 761 | -752 | 12 |
| -5 | 4 | 18 | 262 | 266 | 20 |
| -4 | 4 | 18 | 818 | 828 | 11 |
| -3 | 4 | 18 | 214 | -193 | 22 |
| -2 | 4 | 18 | 710 | -726 | 12 |
| -1 | 4 | 18 | 232 | 214 | 18 |
| 0 | 4 | 18 | 767 | 766 | 28 |
| 1 | 4 | 18 | 183 | -132 | 36 |
| 2 | 4 | 18 | 779 | -750 | 12 |
| 4 | 4 | 18 | 791 | 773 | 12 |
| 5 | 4 | 18 | 225 | -154 | 33 |
| 6 | 4 | 18 | 683 | -695 | 13 |
| 7 | 4 | 18 | 169 | 157 | 24 |
| -8 | 5 | 18 | 197 | -199 | 35 |
| -7 | 5 | 18 | 1001 | -960 | 12 |
| -6 | 5 | 18 | 171 | 177 | 30 |
| -5 | 5 | 18 | 989 | 991 | 11 |
| -4 | 5 | 18 | 162 | -200 | 27 |
| -3 | 5 | 18 | 1078 | -1080 | 11 |
| -2 | 5 | 18 | 177 | 176 | 20 |

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| -1 | 5 | 18 | 1067 | 1079 | 11 |
| 0 | 5 | 18 | 256 | -231 | 16 |
| 1 | 5 | 18 | 895 | -844 | 11 |
| 3 | 5 | 18 | 922 | 887 | 11 |
| 4 | 5 | 18 | 255 | -204 | 28 |
| 5 | 5 | 18 | 992 | -1000 | 12 |
| 6 | 5 | 18 | 313 | 329 | 19 |
| 7 | 5 | 18 | 959 | 958 | 12 |
| -7 | 6 | 18 | 141 | 118 | 40 |
| -6 | 6 | 18 | 841 | 835 | 12 |
| -5 | 6 | 18 | 142 | -143 | 37 |
| -4 | 6 | 18 | 818 | -844 | 12 |
| -3 | 6 | 18 | 195 | 195 | 25 |
| -2 | 6 | 18 | 962 | 987 | 12 |
| 0 | 6 | 18 | 1178 | -1181 | 60 |
| 1 | 6 | 18 | 312 | 280 | 15 |
| 2 | 6 | 18 | 1161 | 1139 | 11 |
| 3 | 6 | 18 | 203 | -193 | 27 |
| 4 | 6 | 18 | 1077 | -1066 | 12 |
| 5 | 6 | 18 | 197 | 188 | 23 |
| 6 | 6 | 18 | 1061 | 1074 | 12 |
| -6 | 7 | 18 | 247 | -255 | 21 |
| -5 | 7 | 18 | 533 | -527 | 14 |
| -4 | 7 | 18 | 110 | 134 | 47 |
| -3 | 7 | 18 | 629 | 649 | 13 |
| -1 | 7 | 18 | 706 | -720 | 13 |
| 0 | 7 | 18 | 141 | 152 | 36 |
| 1 | 7 | 18 | 809 | 774 | 12 |
| 2 | 7 | 18 | 139 | -88 | 38 |
| 3 | 7 | 18 | 719 | -703 | 13 |
| 4 | 7 | 18 | 21 | 18 | 85 |
| 5 | 7 | 18 | 815 | 818 | 13 |
| -5 | 8 | 18 | 65 | 108 | 67 |
| -3 | 8 | 18 | 141 | -156 | 22 |
| -2 | 8 | 18 | 76 | -93 | 56 |
| -1 | 8 | 18 | 76 | 60 | 54 |
| 0 | 8 | 18 | 102 | 95 | 37 |
| 1 | 8 | 18 | 103 | -62 | 49 |
| 2 | 8 | 18 | 24 | -91 | 95 |
| 3 | 8 | 18 | 105 | -65 | 49 |
| -1 | 9 | 18 | 473 | -501 | 17 |
| 0 | 9 | 18 | 52 | 123 | 75 |
| 1 | 9 | 18 | 428 | 438 | 17 |
| 2 | 9 | 18 | 192 | -182 | 33 |
| -8 | 1 | 19 | 53 | -4 | 70 |
| -7 | 1 | 19 | 524 | 490 | 14 |
| -6 | 1 | 19 | 135 | 1 | 39 |
| -5 | 1 | 19 | 690 | -663 | 12 |
| -4 | 1 | 19 | 80 | -137 | 56 |
| -3 | 1 | 19 | 638 | 644 | 12 |
| -2 | 1 | 19 | 253 | 294 | 23 |
| -1 | 1 | 19 | 482 | -470 | 14 |
| 0 | 1 | 19 | 244 | -249 | 12 |
| 1 | 1 | 19 | 440 | 442 | 15 |
| 3 | 1 | 19 | 603 | -621 | 14 |
| 4 | 1 | 19 | 311 | -313 | 19 |

Observed and calculated structure factors for $C_{28}H_{31}NO_4F_{12}W$

| h | k | l | 10Fo | 10Fc | 10s |
|---|---|---|---|---|---|
| 5 | 1 | 19 | 607 | 618 | 14 |
| 6 | 1 | 19 | 379 | 368 | 17 |
| 7 | 1 | 19 | 528 | -526 | 16 |
| -8 | 2 | 19 | 832 | 764 | 13 |
| -7 | 2 | 19 | 154 | 174 | 37 |
| -6 | 2 | 19 | 927 | -922 | 12 |
| -5 | 2 | 19 | 179 | -160 | 24 |
| -4 | 2 | 19 | 979 | 962 | 11 |
| -3 | 2 | 19 | 138 | 86 | 36 |
| -2 | 2 | 19 | 891 | -893 | 11 |
| -1 | 2 | 19 | 237 | -255 | 19 |
| 0 | 2 | 19 | 971 | 948 | 31 |
| 1 | 2 | 19 | 258 | 254 | 20 |
| 2 | 2 | 19 | 1017 | -1005 | 11 |
| 3 | 2 | 19 | 370 | -361 | 19 |
| 4 | 2 | 19 | 818 | 801 | 12 |
| 5 | 2 | 19 | 329 | 337 | 18 |
| 6 | 2 | 19 | 885 | -862 | 11 |
| 7 | 2 | 19 | 135 | -169 | 31 |
| -8 | 3 | 19 | 180 | 167 | 33 |
| -7 | 3 | 19 | 793 | -777 | 12 |
| -6 | 3 | 19 | 252 | -258 | 23 |
| -5 | 3 | 19 | 1015 | 1000 | 12 |
| -4 | 3 | 19 | 207 | 181 | 19 |
| -3 | 3 | 19 | 967 | -962 | 11 |
| -2 | 3 | 19 | 285 | -273 | 20 |
| -1 | 3 | 19 | 922 | 896 | 11 |
| 0 | 3 | 19 | 434 | 474 | 11 |
| 1 | 3 | 19 | 1287 | -1219 | 11 |
| 2 | 3 | 19 | 173 | -197 | 34 |
| 3 | 3 | 19 | 1104 | 1061 | 12 |
| 4 | 3 | 19 | 333 | 319 | 23 |
| 5 | 3 | 19 | 805 | -778 | 12 |
| 7 | 3 | 19 | 1079 | 1050 | 11 |
| -7 | 4 | 19 | 133 | -142 | 25 |
| -6 | 4 | 19 | 641 | 644 | 13 |
| -5 | 4 | 19 | 308 | 326 | 19 |
| -4 | 4 | 19 | 644 | -623 | 13 |
| -3 | 4 | 19 | 239 | -250 | 19 |
| -2 | 4 | 19 | 539 | 553 | 13 |
| -1 | 4 | 19 | 231 | 280 | 22 |
| 0 | 4 | 19 | 825 | -805 | 28 |
| 1 | 4 | 19 | 125 | -158 | 42 |
| 2 | 4 | 19 | 848 | 839 | 13 |
| 3 | 4 | 19 | 83 | 6 | 53 |
| 4 | 4 | 19 | 603 | -578 | 14 |
| 5 | 4 | 19 | 146 | 103 | 36 |
| 6 | 4 | 19 | 816 | 793 | 12 |
| -6 | 5 | 19 | 143 | 159 | 38 |
| -5 | 5 | 19 | 127 | -97 | 40 |
| -4 | 5 | 19 | 93 | -32 | 30 |
| -3 | 5 | 19 | 223 | 191 | 23 |
| -2 | 5 | 19 | 91 | -48 | 47 |
| -1 | 5 | 19 | 91 | -120 | 48 |
| 1 | 5 | 19 | 323 | 364 | 19 |
| 3 | 5 | 19 | 257 | -281 | 21 |
| 4 | 5 | 19 | 168 | -134 | 43 |
| 5 | 5 | 19 | 140 | 199 | 35 |
| 6 | 5 | 19 | 101 | -62 | 49 |
| -6 | 6 | 19 | 266 | 258 | 22 |
| -5 | 6 | 19 | 20 | -66 | 80 |
| -4 | 6 | 19 | 277 | -241 | 18 |
| -2 | 6 | 19 | 323 | 324 | 18 |
| -1 | 6 | 19 | 85 | -21 | 50 |
| 0 | 6 | 19 | 349 | -360 | 17 |
| 2 | 6 | 19 | 366 | 377 | 18 |
| 3 | 6 | 19 | 160 | -229 | 38 |
| 4 | 6 | 19 | 206 | -216 | 25 |
| 5 | 6 | 19 | 84 | -160 | 58 |
| -4 | 7 | 19 | 74 | 63 | 59 |
| -3 | 7 | 19 | 649 | 633 | 13 |
| -1 | 7 | 19 | 809 | -816 | 13 |
| 0 | 7 | 19 | 132 | 43 | 37 |
| 1 | 7 | 19 | 815 | 779 | 13 |
| 3 | 7 | 19 | 745 | -743 | 13 |
| 4 | 7 | 19 | 114 | -58 | 46 |
| -2 | 8 | 19 | 915 | -930 | 12 |
| -1 | 8 | 19 | 135 | -79 | 39 |
| 0 | 8 | 19 | 913 | 894 | 30 |
| 2 | 8 | 19 | 895 | -871 | 12 |
| -7 | 0 | 20 | 95 | 112 | 54 |
| -6 | 0 | 20 | 887 | -855 | 12 |
| -5 | 0 | 20 | 465 | -483 | 14 |
| -4 | 0 | 20 | 904 | 919 | 11 |
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| -1 | 0 | 20 | 428 | -441 | 13 |
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| 4 | 0 | 20 | 1214 | 1221 | 12 |
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| 6 | 0 | 20 | 880 | -863 | 13 |
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| -6 | 2 | 20 | 162 | 218 | 39 |
| -5 | 2 | 20 | 150 | 185 | 38 |
| -4 | 2 | 20 | 312 | -303 | 19 |
| -2 | 2 | 20 | 230 | 251 | 21 |
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| 0 | 2 | 20 | 241 | -247 | 14 |
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| 3 | 2 | 20 | 113 | 207 | 49 |
| 4 | 2 | 20 | 288 | -307 | 19 |
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| -5 | 3 | 20 | 101 | 149 | 52 |
| -3 | 3 | 20 | 270 | -311 | 19 |
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| 1 | 3 | 20 | 276 | -323 | 23 |
| 2 | 3 | 20 | 50 | -68 | 73 |
| 3 | 3 | 20 | 213 | 202 | 26 |
| 4 | 3 | 20 | 143 | 55 | 21 |
| -6 | 4 | 20 | 590 | 581 | 15 |
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| 2 | 4 | 20 | 715 | 678 | 14 |
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| 0 | 2 | 22 | 282 | 278 | 28 |
| 1 | 2 | 22 | 193 | 286 | 26 |
| 2 | 2 | 22 | 91 | -116 | 60 |
| -2 | 3 | 22 | 181 | 189 | 34 |
| -1 | 3 | 22 | 74 | 1 | 59 |
| 0 | 3 | 22 | 83 | -131 | 43 |