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# Okenite, $Ca_{10}Si_{18}O_{46} \cdot 18H_2O$: the first example of a chain and sheet silicate

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**Abstract**

The crystal structure of okenite, $Ca_{10}Si_{18}O_{46} \cdot 18H_2O$, was solved with triclinic space group $P\bar{1}$ $a = 9.69$, $b = 7.28$, $c = 22.02$Å, $\alpha = 92.7°$, $\beta = 100.1°$, $\gamma = 110.9°$. The structure is composed of the following structural units: (a) tetrahedral sheets S, with composition $(Si_6O_{15})^{-6}$, characterized by five- and eight-membered rings of silicate tetrahedra, with five tetrahedra pointing in one direction and one tetrahedron pointing in the other direction; (b) three-repeat double chains C, with composition $(Si_6O_{16})^{-8}$ and characterized by four- and six-membered rings, made up by pairing two wollastonite chains, which point in opposite directions; (c) octahedral double chains O, formed by two strands of octahedra. These structural units are connected by corner sharing to give the complex layer SOCOS, with composition $[Ca_8(Si_6O_{16})(Si_6O_{15})_2(H_2O)_6]^{-4}$. Such complex layers alternate in the structure with sheets $[Ca_2(H_2O)_9 \cdot 3H_2O]^{+4}$. Weak supercell reflections revealed a larger unit cell with doubled $a$ and $b$ parameters in the unconventional space group $C\bar{1}$.

## Introduction

Okenite, a hydrated calcium silicate, has long been of interest to a large number of mineralogists and crystal chemists: its consistent association with gyrolite and zeolites in basalts seemed indicative of some structural relations among them. Of particular interest is the role of water molecules in the structure of okenite, the definition of which could lead to an understanding of the dehydration mechanism which, according to Heller's X-ray studies (Gard and Taylor, 1956), leads topotactically to the formation of wollastonite.

Okenite was first described from Disko Island (Greenland) and was subsequently found in various other localities, such as Crestmore (California), Scawt Hill (Northern Ireland), Bordö (Faröer Islands), Bombay (India), usually in basalts. The most comprehensive account of its crystallographic properties was given by Gard and Taylor (1956) who studied a specimen from Bombay, India, consisting of fibrous aggregates. These authors studied okenite by electron diffraction, as single crystals of sufficient size for X-ray diffraction were not available. The results indicated that the crystals were triclinic with $a = 9.84$, $b = 7.20$, $c = 21.33$Å, $\alpha = 90.0°$, $\beta = 103.9°$, $\gamma = 111.5°$. The fiber direction was [010], with repeated lamellar twinning across the cleavage plane {001}. On the basis of the cell volume and a chemical analysis by Christie (1925), Gard and Taylor (1956) proposed that the cell contents are $Ca_9Si_{18}O_{63}H_{36}$, or $Ca_9(Si_6O_{15})_3 \cdot 18H_2O$.

Gard and Taylor (1956) also studied a mineral from Crestmore, California, which was previously characterized as okenite on the basis of its chemical composition and optical properties, and demonstrated that it was in fact a new species for which they proposed the name nekoite. Crystal structures for both minerals were hypothesized by Mamedov and Belov (1958) on the basis of the chemical composition and unit cell dimensions. The crystal structure of nekoite was recently solved by Alberti and Galli (1980) who showed that it was in many respects different from the structural model of Mamedov and Belov (1958).

The present work was undertaken to determine the crystal structure of okenite in order to further our understanding of the crystal chemistry of the hydrated calcium silicates.

## Experimental

A specimen of okenite from Kolhapur District, Maharastra State, India, donated by Prof. E. Passaglia, was used in this study. Careful examination of a large number of crystals from this specimen and testing by preliminary Weissenberg photographs resulted in the selection of crystals of sufficient quality for intensity measurement. By means of Weissenberg and precession photographs the lattice parameters were determined on a small fragment cut from a long lath-shaped crystal. The same crystal fragment was used to collect intensity data with a Philips PW 1100 single crystal diffractometer, after obtaining refined lattice parameters by least squares fitting of 20 medium range $\theta$ values: $a = 9.69(1)$, $b = 7.28(1)$, $c = 22.02(4)$Å, $\alpha = 92.7(2)°$, $\beta = 100.1(3)°$, $\gamma = 110.9(1)°$.

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TRUE CELL OF OKENITE



| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 0 | 0 | 276 | 274 | 4 | -4 | 1 | 318 | 305 | 0 | 6 | 1 | 154 | -189 | -8 | 0 | 2 | 430 | -498 | -4 | -6 | 3 | 426 | 422 |
| -10 | 2 | 0 | 258 | 272 | 2 | -4 | 1 | 478 | -314 | -2 | 6 | 1 | 105 | -159 | -6 | 0 | 2 | 638 | -713 | 10 | -4 | 3 | 327 | -311 |
| -8 | 2 | 0 | 102 | 89 | 0 | -4 | 1 | 230 | -276 | -4 | 6 | 1 | 180 | -226 | -4 | 0 | 2 | 203 | -203 | 8 | -4 | 3 | 148 | -106 |
| -6 | 2 | 0 | 181 | -264 | -2 | -4 | 1 | 204 | -233 | -8 | 6 | 1 | 182 | -174 | 2 | 0 | 2 | 293 | 315 | 6 | -4 | 3 | 306 | 310 |
| -4 | 2 | 0 | 101 | 84 | -4 | -4 | 1 | 215 | -193 | -10 | 6 | 1 | 251 | 244 | 4 | 0 | 2 | 110 | -74 | 4 | -4 | 3 | 1013 | -900 |
| -2 | 2 | 0 | 62 | -125 | -6 | -4 | 1 | 282 | 317 | -2 | 8 | 1 | 96 | 107 | 6 | 0 | 2 | 206 | 209 | 2 | -4 | 3 | 91 | 73 |
| 2 | 2 | 0 | 194 | 194 | 10 | -2 | 1 | 173 | -154 | -4 | 8 | 1 | 154 | 77 | 8 | 0 | 2 | 119 | -213 | 0 | -4 | 3 | 215 | 128 |
| 4 | 2 | 0 | 111 | 28 | 8 | -2 | 1 | 75 | -84 | -6 | 8 | 1 | 283 | -304 | -10 | 2 | 2 | 85 | -115 | -2 | -4 | 3 | 309 | 291 |
| 6 | 2 | 0 | 198 | -269 | 6 | -2 | 1 | 121 | -64 | 2 | -8 | 2 | 241 | -194 | -8 | 2 | 2 | 189 | -190 | -4 | -4 | 3 | 189 | 227 |
| 8 | 2 | 0 | 136 | -185 | 4 | -2 | 1 | 399 | 426 | 4 | -8 | 2 | 261 | 33 | -6 | 2 | 2 | 71 | 39 | -6 | -4 | 3 | 347 | -372 |
| -10 | 4 | 0 | 532 | 553 | 2 | -2 | 1 | 136 | -78 | 6 | -8 | 2 | 99 | 92 | -4 | 2 | 2 | 95 | 130 | 10 | -2 | 3 | 74 | -7 |
| -6 | 4 | 0 | 125 | -47 | 0 | -2 | 1 | 255 | -314 | -2 | -6 | 2 | 134 | -213 | -2 | 2 | 2 | 242 | 312 | 6 | -2 | 3 | 170 | -171 |
| -4 | 4 | 0 | 107 | 151 | -2 | -2 | 1 | 141 | 137 | 0 | -6 | 2 | 74 | 80 | 0 | 2 | 2 | 153 | 123 | 2 | -2 | 3 | 92 | 102 |
| -2 | 4 | 0 | 149 | 70 | -8 | -2 | 1 | 69 | 59 | 2 | -6 | 2 | 86 | 18 | 2 | 2 | 2 | 374 | 402 | 0 | -2 | 3 | 97 | 48 |
| 0 | 4 | 0 | 245 | 331 | 10 | 0 | 1 | 226 | 260 | 4 | -6 | 2 | 323 | -265 | 4 | 2 | 2 | 151 | -215 | -4 | -2 | 3 | 163 | -202 |
| 2 | 4 | 0 | 215 | 263 | 6 | 0 | 1 | 92 | -111 | 6 | -6 | 2 | 330 | -353 | 8 | 2 | 2 | 119 | 115 | 8 | 0 | 3 | 326 | -373 |
| 4 | 4 | 0 | 305 | 305 | 4 | 0 | 1 | 254 | -329 | 8 | -6 | 2 | 131 | -110 | -10 | 4 | 2 | 200 | -215 | 6 | 0 | 3 | 106 | 117 |
| 6 | 4 | 0 | 606 | 660 | -4 | 0 | 1 | 309 | 387 | -6 | -4 | 2 | 298 | -306 | -6 | 4 | 2 | 283 | 322 | 2 | 0 | 3 | 121 | 118 |
| -10 | 6 | 0 | 362 | 320 | -6 | 0 | 1 | 170 | 193 | -4 | -4 | 2 | 105 | -97 | -2 | 4 | 2 | 195 | -182 | -2 | 0 | 3 | 69 | 47 |
| -8 | 6 | 0 | 86 | 140 | -8 | 0 | 1 | 304 | -353 | -2 | -4 | 2 | 299 | 324 | 0 | 4 | 2 | 752 | -769 | -4 | 0 | 3 | 210 | -228 |
| -4 | 6 | 0 | 85 | 101 | -10 | 0 | 1 | 131 | 188 | 0 | -4 | 2 | 153 | -167 | 2 | 4 | 2 | 313 | 274 | -6 | 0 | 3 | 861 | -854 |
| 0 | 6 | 0 | 87 | 154 | 6 | 2 | 1 | 71 | -149 | 2 | -4 | 2 | 230 | -142 | 4 | 4 | 2 | 302 | -316 | 8 | 2 | 3 | 182 | -307 |
| 2 | 6 | 0 | 88 | 9 | 4 | 2 | 1 | 344 | -379 | 4 | -4 | 2 | 582 | -543 | 6 | 4 | 2 | 89 | -72 | 6 | 2 | 3 | 83 | -139 |
| 4 | 6 | 0 | 428 | 405 | 2 | 2 | 1 | 191 | -218 | 6 | -4 | 2 | 248 | 234 | -10 | 6 | 2 | 233 | 185 | 4 | 2 | 3 | 138 | -124 |
| -6 | 8 | 0 | 103 | -104 | 0 | 2 | 1 | 103 | -171 | 8 | -4 | 2 | 165 | -196 | -4 | 6 | 2 | 140 | 67 | 2 | 2 | 3 | 263 | 223 |
| -2 | 8 | 0 | 100 | 76 | -4 | 2 | 1 | 60 | -82 | 10 | -4 | 2 | 256 | 244 | -2 | 6 | 2 | 128 | 158 | 0 | 2 | 3 | 157 | -114 |
| 6 | -8 | 1 | 186 | 199 | -6 | 2 | 1 | 432 | -421 | -8 | -2 | 2 | 81 | 32 | 0 | 6 | 2 | 96 | -112 | -2 | 2 | 3 | 162 | -194 |
| 4 | -8 | 1 | 1678 | 1047 | -8 | 2 | 1 | 88 | 60 | -6 | -2 | 2 | 96 | -105 | 2 | 6 | 2 | 77 | 71 | -4 | 2 | 3 | 259 | 322 |
| 10 | -6 | 1 | 128 | -143 | -10 | 2 | 1 | 241 | -226 | -4 | -2 | 2 | 351 | -405 | -6 | 8 | 2 | 129 | -173 | -6 | 2 | 3 | 123 | 132 |
| 6 | -6 | 1 | 89 | 88 | 6 | 4 | 1 | 233 | 250 | -2 | -2 | 2 | 278 | 274 | -4 | 8 | 2 | 186 | -195 | -8 | 2 | 3 | 122 | 141 |
| 4 | -6 | 1 | 173 | 153 | 0 | 4 | 1 | 84 | 26 | 0 | -2 | 2 | 66 | -18 | -2 | 8 | 2 | 112 | 184 | -10 | 2 | 3 | 140 | 136 |
| -2 | -6 | 1 | 140 | 172 | -2 | 4 | 1 | 131 | -168 | 2 | -2 | 2 | 230 | 207 | 6 | -8 | 3 | 198 | 216 | 6 | 4 | 3 | 314 | -401 |
| -4 | -6 | 1 | 180 | 144 | -8 | 4 | 1 | 87 | 24 | 6 | -2 | 2 | 101 | -76 | 2 | -8 | 3 | 166 | -129 | 4 | 4 | 3 | 210 | -184 |
| 10 | -4 | 1 | 395 | 385 | -10 | 4 | 1 | 125 | -103 | 8 | -2 | 2 | 206 | -148 | 8 | -6 | 3 | 95 | -164 | 2 | 4 | 3 | 133 | -85 |
| 8 | -4 | 1 | 97 | 74 | 4 | 6 | 1 | 102 | 76 | 10 | -2 | 2 | 103 | -81 | 4 | -6 | 3 | 253 | -175 | 0 | 4 | 3 | 1368 | -1167 |
| 6 | -4 | 1 | 125 | 111 | 2 | 6 | 1 | 336 | -381 | -10 | 0 | 2 | 130 | 124 | 2 | -6 | 3 | 99 | -32 | -2 | 4 | 3 | 217 | -186 |

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -8 | 4 | 3 | 104 | -81 | 4 | 2 | 4 | 67 | -84 | -8 | -2 | 5 | 190 | 229 | 4 | -4 | 6 | 361 | 277 | 6 | -6 | 7 | 73 | 112 |
| -10 | 4 | 3 | 489 | -518 | -10 | 4 | 4 | 224 | -263 | 8 | 0 | 5 | 117 | 117 | 6 | -4 | 6 | 160 | -137 | 4 | -6 | 7 | 83 | 40 |
| 2 | 6 | 3 | 118 | 72 | -8 | 4 | 4 | 192 | 242 | 4 | 0 | 5 | 487 | 427 | 8 | -4 | 6 | 232 | 183 | 2 | -6 | 7 | 247 | 153 |
| -4 | 6 | 3 | 87 | 173 | -6 | 4 | 4 | 86 | -83 | 2 | 0 | 5 | 441 | 346 | -8 | -2 | 6 | 156 | -182 | 0 | -6 | 7 | 143 | -117 |
| -8 | 6 | 3 | 64 | -17 | -4 | 4 | 4 | 309 | -384 | 0 | 0 | 5 | 154 | -200 | -6 | -2 | 6 | 118 | -36 | -2 | -6 | 7 | 369 | -258 |
| -10 | 6 | 3 | 83 | -115 | -2 | 4 | 4 | 108 | 107 | -2 | 0 | 5 | 153 | -140 | -4 | -2 | 6 | 369 | -325 | 8 | -4 | 7 | 98 | 130 |
| -4 | 8 | 3 | 189 | -197 | 0 | 4 | 4 | 353 | -225 | -4 | 0 | 5 | 77 | 35 | -2 | -2 | 6 | 279 | 203 | 6 | -4 | 7 | 101 | 5 |
| -6 | 8 | 3 | 77 | -69 | 2 | 4 | 4 | 286 | -271 | -6 | 0 | 5 | 449 | 405 | 0 | -2 | 6 | 233 | 217 | 4 | -4 | 7 | 758 | 644 |
| 2 | -8 | 4 | 333 | -235 | 4 | 4 | 4 | 233 | 224 | -8 | 0 | 5 | 720 | 706 | 2 | -2 | 6 | 322 | 281 | 2 | -4 | 7 | 156 | 161 |
| 4 | -8 | 4 | 159 | -124 | -10 | 6 | 4 | 220 | 245 | 6 | 2 | 5 | 123 | 180 | 4 | -2 | 6 | 275 | -238 | -2 | -4 | 7 | 388 | 277 |
| -4 | -6 | 4 | 306 | 290 | -6 | 6 | 4 | 242 | 287 | 4 | 2 | 5 | 70 | 19 | 6 | -2 | 6 | 245 | -231 | -4 | -4 | 7 | 284 | -206 |
| 4 | -6 | 4 | 195 | 150 | -4 | 6 | 4 | 97 | -6 | 2 | 2 | 5 | 376 | 323 | -10 | 0 | 6 | 360 | 381 | -6 | -4 | 7 | 181 | 158 |
| -6 | -4 | 4 | 348 | -313 | -2 | 6 | 4 | 186 | -117 | 0 | 2 | 5 | 238 | 179 | -8 | 0 | 6 | 107 | 1 | 6 | -2 | 7 | 86 | -134 |
| -2 | -4 | 4 | 269 | -206 | 0 | 6 | 4 | 153 | -139 | -2 | 2 | 5 | 275 | 305 | -6 | 0 | 6 | 497 | 459 | 4 | -2 | 7 | 134 | 64 |
| 2 | -4 | 4 | 352 | -318 | 2 | 6 | 4 | 165 | -199 | -4 | 2 | 5 | 154 | 177 | -4 | 0 | 6 | 346 | -335 | 2 | -2 | 7 | 296 | -196 |
| 6 | -4 | 4 | 490 | -463 | 8 | -6 | 5 | 75 | 26 | -6 | 2 | 5 | 190 | 204 | -2 | 0 | 6 | 639 | 665 | 0 | -2 | 7 | 296 | -263 |
| 8 | -4 | 4 | 115 | -130 | 6 | -6 | 5 | 167 | -54 | -8 | 2 | 5 | 69 | -82 | 0 | 0 | 6 | 506 | 498 | -2 | -2 | 7 | 335 | -239 |
| -8 | -2 | 4 | 148 | -165 | 4 | -6 | 5 | 464 | 339 | -10 | 2 | 5 | 217 | -241 | 2 | 0 | 6 | 422 | 392 | -4 | -2 | 7 | 186 | -174 |
| -4 | -2 | 4 | 107 | 53 | 2 | -6 | 5 | 228 | 132 | 4 | 4 | 5 | 146 | 135 | 4 | 0 | 6 | 413 | 411 | -8 | -2 | 7 | 85 | -85 |
| 2 | -2 | 4 | 188 | -157 | 0 | -6 | 5 | 257 | 180 | 2 | 4 | 5 | 349 | -267 | 6 | 0 | 6 | 234 | -260 | 6 | 0 | 7 | 265 | 267 |
| 4 | -2 | 4 | 267 | 206 | -2 | -6 | 5 | 104 | 14 | 0 | 4 | 5 | 210 | 196 | -10 | 2 | 6 | 117 | 167 | 4 | 0 | 7 | 372 | 324 |
| 6 | -2 | 4 | 307 | -300 | 8 | -4 | 5 | 82 | 97 | -2 | 4 | 5 | 218 | 169 | -8 | 2 | 6 | 142 | -159 | 2 | 0 | 7 | 327 | -262 |
| 8 | -2 | 4 | 126 | -121 | 6 | -4 | 5 | 260 | -233 | -4 | 4 | 5 | 114 | -167 | -6 | 2 | 6 | 132 | -56 | 0 | 0 | 7 | 804 | 750 |
| -10 | 0 | 4 | 162 | -203 | 4 | -4 | 5 | 156 | 89 | -6 | 4 | 5 | 471 | 522 | -4 | 2 | 6 | 80 | 162 | -2 | 0 | 7 | 116 | 133 |
| -8 | 0 | 4 | 371 | 416 | 2 | -4 | 5 | 171 | 162 | -8 | 4 | 5 | 335 | 375 | 0 | 2 | 6 | 116 | -104 | -4 | 0 | 7 | 694 | -608 |
| -6 | 0 | 4 | 398 | -429 | -2 | -4 | 5 | 234 | 131 | -10 | 4 | 5 | 100 | 127 | 2 | 2 | 6 | 296 | 249 | -6 | 0 | 7 | 329 | 264 |
| -4 | 0 | 4 | 199 | -211 | -4 | -4 | 5 | 175 | 135 | -2 | 6 | 5 | 89 | 81 | 4 | 2 | 6 | 183 | -191 | 6 | 2 | 7 | 176 | -190 |
| 0 | 0 | 4 | 311 | 359 | -6 | -4 | 5 | 72 | -135 | -4 | 6 | 5 | 187 | 199 | -8 | 4 | 6 | 204 | -246 | 4 | 2 | 7 | 95 | -127 |
| 4 | 0 | 4 | 518 | -483 | 8 | -2 | 5 | 95 | 111 | -6 | 6 | 5 | 70 | 72 | -6 | 4 | 6 | 259 | 323 | -2 | 2 | 7 | 482 | -483 |
| 6 | 0 | 4 | 82 | 53 | 6 | -2 | 5 | 209 | 210 | 0 | -6 | 6 | 313 | 218 | -4 | 4 | 6 | 82 | 73 | -4 | 2 | 7 | 180 | -157 |
| 8 | 0 | 4 | 131 | -105 | 4 | -2 | 5 | 511 | 439 | 4 | -6 | 6 | 478 | -408 | -2 | 4 | 6 | 169 | 152 | -6 | 2 | 7 | 128 | -178 |
| -6 | 2 | 4 | 641 | -692 | 2 | -2 | 5 | 251 | 224 | 6 | -6 | 6 | 84 | -58 | 2 | 4 | 6 | 102 | -57 | 0 | 4 | 7 | 527 | 363 |
| -4 | 2 | 4 | 129 | -167 | 0 | -2 | 5 | 203 | -174 | -6 | -4 | 6 | 74 | 44 | -8 | 6 | 6 | 155 | -145 | -4 | 4 | 7 | 139 | 168 |
| -2 | 2 | 4 | 215 | -222 | -2 | -2 | 5 | 273 | 203 | -4 | -4 | 6 | 283 | 228 | -6 | 6 | 6 | 102 | -100 | -6 | 4 | 7 | 263 | 274 |
| 0 | 2 | 4 | 298 | 236 | -4 | -2 | 5 | 221 | -180 | 0 | -4 | 6 | 419 | 320 | -4 | 6 | 6 | 73 | -62 | -8 | 4 | 7 | 245 | -209 |
| 2 | 2 | 4 | 277 | -191 | -6 | -2 | 5 | 106 | 33 | 2 | -4 | 6 | 279 | 203 | -2 | 6 | 6 | 172 | 132 | 0 | 6 | 7 | 224 | -183 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TRUE CELL OF OKENITE



| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -2 | 6 | 7 | 144 | -146 | 6 | -2 | 9 | 128 | -163 | 14 | 0 | 0 | 313 | 351 | 14 | -8 | 1 | 321 | 348 | -10 | 10 | 1 | 239 | -213 |
| -6 | 6 | 7 | 145 | 193 | 2 | -2 | 9 | 81 | 45 | 16 | 0 | 0 | 160 | 209 | 12 | -8 | 1 | 185 | 177 | -4 | 12 | 1 | 211 | -224 |
| 0 | -6 | 8 | 158 | 86 | 0 | -2 | 9 | 96 | -125 | -14 | 2 | 0 | 209 | 243 | 8 | -8 | 1 | 146 | 102 | -8 | 12 | 1 | 188 | -200 |
| 4 | -6 | 8 | 105 | 64 | -2 | -2 | 9 | 162 | 161 | -12 | 2 | 0 | 242 | 238 | 0 | -8 | 1 | 192 | 242 | -10 | 12 | 1 | 202 | -221 |
| -6 | -4 | 8 | 75 | -67 | -6 | -2 | 9 | 81 | -26 | 12 | 2 | 0 | 198 | 284 | -2 | -8 | 1 | 132 | 141 | -14 | 12 | 1 | 186 | -154 |
| 0 | -4 | 8 | 72 | -4 | 4 | 0 | 9 | 251 | -193 | -12 | 4 | 0 | 154 | 119 | -4 | -8 | 1 | 229 | -238 | 6 | -12 | 2 | 192 | 124 |
| 2 | -4 | 8 | 535 | -441 | 2 | 0 | 9 | 182 | 186 | 8 | 4 | 0 | 278 | 317 | -6 | -8 | 1 | 215 | 175 | 8 | -12 | 2 | 248 | -209 |
| 6 | -4 | 8 | 339 | -277 | -2 | 0 | 9 | 156 | 86 | 12 | 4 | 0 | 161 | 225 | -10 | -8 | 1 | 203 | 229 | 12 | -12 | 2 | 193 | -165 |
| -8 | -2 | 8 | 85 | -91 | -6 | 0 | 9 | 113 | -105 | -16 | 6 | 0 | 148 | 157 | 18 | -6 | 1 | 206 | -227 | -2 | -10 | 2 | 234 | -245 |
| -6 | -2 | 8 | 323 | -266 | -8 | 0 | 9 | 319 | -311 | -12 | 6 | 0 | 353 | 420 | 12 | -6 | 1 | 107 | -132 | 4 | -10 | 2 | 226 | -186 |
| 4 | -2 | 8 | 139 | 165 | 4 | 2 | 9 | 325 | -209 | -14 | 8 | 0 | 182 | 183 | -6 | -6 | 1 | 144 | 99 | 12 | -10 | 2 | 196 | -201 |
| 6 | -2 | 8 | 142 | -176 | 2 | 2 | 9 | 103 | 57 | -12 | 8 | 0 | 154 | -77 | -8 | -6 | 1 | 147 | 167 | 14 | -10 | 2 | 154 | -170 |
| -8 | 0 | 8 | 347 | -399 | -4 | 2 | 9 | 114 | 181 | 6 | 8 | 0 | 252 | 292 | -10 | -6 | 1 | 173 | 223 | -8 | -8 | 2 | 154 | -110 |
| -6 | 0 | 8 | 112 | -75 | -6 | 2 | 9 | 164 | 192 | 8 | 8 | 0 | 142 | 92 | 14 | -4 | 1 | 192 | -216 | -6 | -8 | 2 | 180 | 187 |
| -4 | 0 | 8 | 295 | -293 | 0 | 4 | 9 | 610 | -497 | -10 | 10 | 0 | 309 | -331 | 12 | -4 | 1 | 313 | 318 | -4 | -8 | 2 | 366 | -361 |
| -2 | 0 | 8 | 308 | -271 | -2 | 4 | 9 | 499 | -449 | -6 | 10 | 0 | 157 | 148 | -8 | -4 | 1 | 184 | -172 | -2 | -8 | 2 | 148 | -139 |
| 0 | 0 | 8 | 317 | 401 | -6 | 4 | 9 | 292 | -333 | -4 | 10 | 0 | 276 | 185 | -14 | -4 | 1 | 151 | -149 | 0 | -8 | 2 | 110 | 186 |
| 6 | 0 | 8 | 198 | 144 | -8 | 4 | 9 | 194 | -183 | 4 | 10 | 0 | 201 | -231 | 12 | -2 | 1 | 136 | -145 | 8 | -8 | 2 | 119 | 76 |
| -6 | 2 | 8 | 422 | -415 | -2 | -4 | 10 | 291 | -226 | -14 | 12 | 0 | 137 | 204 | 16 | 0 | 1 | 280 | 317 | 12 | -8 | 2 | 212 | -176 |
| -4 | 2 | 8 | 100 | 145 | 0 | -4 | 10 | 281 | 210 | -8 | 12 | 0 | 120 | 89 | 14 | 0 | 1 | 133 | -140 | 14 | -8 | 2 | 187 | 121 |
| -2 | 2 | 8 | 176 | 206 | 2 | -4 | 10 | 269 | -284 | -6 | 12 | 0 | 151 | -88 | -16 | 2 | 1 | 217 | -213 | -8 | -6 | 2 | 153 | -163 |
| 0 | 2 | 8 | 78 | 128 | 4 | -4 | 10 | 831 | -737 | 2 | 12 | 0 | 149 | 158 | 10 | 4 | 1 | 185 | -237 | 10 | -6 | 2 | 238 | 213 |
| 2 | 2 | 8 | 169 | -101 | -4 | -2 | 10 | 189 | -168 | 14 | -12 | 1 | 273 | 249 | -12 | 4 | 1 | 463 | -523 | 12 | -6 | 2 | 128 | -216 |
| 4 | 2 | 8 | 128 | -88 | -2 | -2 | 10 | 79 | -29 | 10 | -12 | 1 | 159 | 233 | -16 | 4 | 1 | 339 | -300 | -14 | -4 | 2 | 261 | -349 |
| -6 | 4 | 8 | 278 | -288 | 4 | -2 | 10 | 246 | -196 | 8 | -12 | 1 | 389 | 333 | -18 | 4 | 1 | 294 | -275 | -12 | -4 | 2 | 424 | -569 |
| -4 | 4 | 8 | 115 | -94 | -8 | 0 | 10 | 194 | -199 | 6 | -12 | 1 | 269 | 176 | 8 | 6 | 1 | 216 | -205 | -8 | -4 | 2 | 409 | -527 |
| -2 | 4 | 8 | 374 | -315 | -6 | 0 | 10 | 502 | -464 | 4 | -12 | 1 | 280 | 248 | 6 | 6 | 1 | 129 | -130 | 12 | -4 | 2 | 618 | 660 |
| 2 | 4 | 8 | 441 | -351 | -4 | 0 | 10 | 241 | -227 | -2 | -12 | 1 | 259 | 337 | -12 | 6 | 1 | 132 | -132 | -10 | -2 | 2 | 151 | 223 |
| -2 | 6 | 8 | 298 | -201 | 0 | 0 | 10 | 223 | 226 | 14 | -10 | 1 | 164 | -161 | 6 | 8 | 1 | 190 | 155 | 14 | -2 | 2 | 85 | 97 |
| 4 | -6 | 9 | 249 | -207 | 2 | 0 | 10 | 106 | -97 | 12 | -10 | 1 | 262 | -244 | -10 | 8 | 1 | 231 | -248 | 12 | 0 | 2 | 250 | 321 |
| 0 | -6 | 9 | 380 | 260 | 4 | 0 | 10 | 325 | -280 | 10 | -10 | 1 | 193 | -194 | -12 | 8 | 1 | 542 | -589 | 14 | 0 | 2 | 158 | 187 |
| 6 | -4 | 9 | 163 | -138 | -8 | 2 | 10 | 109 | -140 | 8 | -10 | 1 | 252 | 249 | -16 | 8 | 1 | 157 | -176 | 16 | 0 | 2 | 158 | 184 |
| 4 | -4 | 9 | 123 | -76 | -4 | 2 | 10 | 132 | -167 | 6 | -10 | 1 | 138 | -91 | -18 | 8 | 1 | 151 | 113 | 12 | 2 | 2 | 158 | -167 |
| 2 | -4 | 9 | 309 | -288 | 2 | 2 | 10 | 292 | 257 | 2 | -10 | 1 | 176 | 191 | 0 | 10 | 1 | 327 | -429 | -18 | 4 | 2 | 253 | -224 |
| 0 | -4 | 9 | 134 | 94 | -6 | 4 | 10 | 139 | -160 | -2 | -10 | 1 | 143 | -148 | -6 | 10 | 1 | 123 | 150 | -16 | 4 | 2 | 391 | -446 |
| -4 | -4 | 9 | 91 | -57 | -4 | 4 | 10 | 290 | 291 | -6 | -10 | 1 | 152 | 137 | -8 | 10 | 1 | 164 | 123 | -12 | 4 | 2 | 120 | -95 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TRUE CELL OF OKENITE



| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -18 | 6 | 2 | 159 | -152 | -12 | -4 | 3 | 193 | -281 | 14 | -10 | 4 | 187 | -168 | 8 | -10 | 5 | 367 | 282 | -6 | 8 | 5 | 158 | 223 |
| 6 | 6 | 2 | 349 | 371 | -12 | -2 | 3 | 214 | 292 | -10 | -8 | 4 | 146 | 174 | 4 | -10 | 5 | 374 | -283 | -8 | 8 | 5 | 141 | 129 |
| -16 | 8 | 2 | 132 | -119 | 14 | 0 | 3 | 242 | 267 | -8 | -8 | 4 | 226 | 213 | 2 | -10 | 5 | 161 | -90 | -14 | 8 | 5 | 199 | 226 |
| -14 | 8 | 2 | 151 | 186 | 12 | 0 | 3 | 222 | 211 | -6 | -8 | 4 | 173 | -140 | 0 | -10 | 5 | 236 | -180 | -16 | 8 | 5 | 204 | 254 |
| -10 | 8 | 2 | 302 | -342 | 10 | 0 | 3 | 376 | -455 | -2 | -8 | 4 | 628 | -675 | -2 | -10 | 5 | 186 | -151 | 0 | 10 | 5 | 223 | -199 |
| -8 | 8 | 2 | 142 | 150 | -12 | 2 | 3 | 123 | 158 | 0 | -8 | 4 | 191 | -222 | -4 | -10 | 5 | 113 | 95 | -2 | 10 | 5 | 166 | 138 |
| 4 | 8 | 2 | 208 | -221 | -16 | 2 | 3 | 165 | 156 | 8 | -8 | 4 | 274 | -260 | 16 | -8 | 5 | 262 | -224 | -4 | 10 | 5 | 122 | 48 |
| 8 | 8 | 2 | 260 | 238 | -14 | 4 | 3 | 233 | -241 | 14 | -8 | 4 | 296 | -300 | 10 | -8 | 5 | 153 | -114 | -12 | 10 | 5 | 158 | -122 |
| -14 | 10 | 2 | 176 | -172 | -18 | 4 | 3 | 277 | 269 | -8 | -6 | 4 | 154 | 142 | 8 | -8 | 5 | 229 | 168 | 0 | 12 | 5 | 99 | 155 |
| -12 | 10 | 2 | 129 | -180 | 4 | 6 | 3 | 97 | 79 | 14 | -6 | 4 | 151 | -134 | 0 | -8 | 5 | 115 | 76 | -4 | 12 | 5 | 257 | 212 |
| -8 | 10 | 2 | 144 | 184 | -16 | 6 | 3 | 214 | 217 | -10 | -4 | 4 | 134 | -183 | -2 | -8 | 5 | 150 | 38 | -6 | 12 | 5 | 474 | 405 |
| -2 | 10 | 2 | 234 | 304 | 6 | 8 | 3 | 309 | -401 | -8 | -4 | 4 | 182 | 197 | -4 | -8 | 5 | 260 | 227 | -10 | 12 | 5 | 147 | 199 |
| 0 | 10 | 2 | 174 | -240 | 4 | 8 | 3 | 355 | -327 | 10 | -4 | 4 | 454 | -467 | -6 | -8 | 5 | 117 | -146 | 2 | -12 | 6 | 204 | 205 |
| 2 | 10 | 2 | 136 | -183 | 0 | 8 | 3 | 175 | -196 | 14 | -4 | 4 | 495 | -502 | 12 | -4 | 5 | 168 | 210 | 4 | -12 | 6 | 215 | -128 |
| -14 | 12 | 2 | 195 | -246 | -8 | 8 | 3 | 158 | -193 | -14 | -2 | 4 | 146 | -257 | 10 | -4 | 5 | 271 | -252 | 6 | -12 | 6 | 374 | 263 |
| -6 | 12 | 2 | 272 | 271 | -10 | 8 | 3 | 535 | -607 | -14 | 0 | 4 | 321 | 380 | -14 | -4 | 5 | 199 | 268 | 8 | -12 | 6 | 128 | -4 |
| -4 | 12 | 2 | 225 | -267 | -12 | 8 | 3 | 107 | 191 | -12 | 0 | 4 | 304 | 335 | -10 | -2 | 5 | 157 | 210 | 10 | -12 | 6 | 185 | -155 |
| 10 | -12 | 3 | 138 | 127 | -16 | 8 | 3 | 169 | 208 | 12 | 0 | 4 | 241 | -302 | -14 | -2 | 5 | 117 | -142 | 12 | -12 | 6 | 189 | 195 |
| 8 | -12 | 3 | 446 | -347 | -18 | 8 | 3 | 168 | 138 | -12 | 2 | 4 | 203 | 192 | 14 | 0 | 5 | 145 | 173 | -6 | -10 | 6 | 180 | 175 |
| 4 | -12 | 3 | 316 | -234 | 4 | 10 | 3 | 199 | -212 | 12 | 2 | 4 | 142 | 251 | 12 | 0 | 5 | 227 | -267 | 0 | -10 | 6 | 507 | -429 |
| -2 | -12 | 3 | 181 | -180 | 2 | 10 | 3 | 145 | -123 | -18 | 4 | 4 | 250 | 277 | -12 | 0 | 5 | 245 | 341 | 2 | -10 | 6 | 159 | 125 |
| 6 | -10 | 3 | 310 | 231 | 0 | 10 | 3 | 198 | 179 | -14 | 4 | 4 | 251 | -280 | -14 | 0 | 5 | 239 | 304 | 4 | -10 | 6 | 152 | 99 |
| 4 | -10 | 3 | 302 | 163 | -6 | 10 | 3 | 192 | -204 | 6 | 4 | 4 | 372 | -408 | 8 | 2 | 5 | 207 | 317 | 6 | -10 | 6 | 286 | 196 |
| 2 | -10 | 3 | 135 | 64 | -10 | 10 | 3 | 268 | -274 | 4 | 6 | 4 | 270 | 268 | -12 | 2 | 5 | 105 | -144 | 8 | -10 | 6 | 219 | 193 |
| 0 | -10 | 3 | 247 | -233 | -16 | 10 | 3 | 166 | 235 | -14 | 8 | 4 | 207 | -222 | 10 | 4 | 5 | 153 | 199 | 10 | -10 | 6 | 134 | 133 |
| 16 | -8 | 3 | 246 | 223 | -2 | 12 | 3 | 230 | -273 | -12 | 8 | 4 | 234 | 285 | 8 | 4 | 5 | 145 | 231 | 12 | -10 | 6 | 157 | 158 |
| 12 | -8 | 3 | 320 | -341 | -4 | 12 | 3 | 323 | -442 | -8 | 8 | 4 | 91 | -52 | -12 | 4 | 5 | 127 | 168 | -8 | -8 | 6 | 278 | 245 |
| 8 | -8 | 3 | 244 | -243 | -12 | 12 | 3 | 143 | 155 | 4 | 8 | 4 | 140 | 181 | -18 | 4 | 5 | 248 | 265 | -6 | -8 | 6 | 342 | 310 |
| -2 | -8 | 3 | 464 | -493 | -14 | 12 | 3 | 152 | -164 | 8 | 8 | 4 | 131 | -128 | 10 | 6 | 5 | 168 | 244 | -4 | -8 | 6 | 383 | 377 |
| 16 | -6 | 3 | 181 | 173 | -2 | -12 | 4 | 275 | -313 | -10 | 10 | 4 | 253 | -310 | 6 | 6 | 5 | 165 | 165 | -2 | -8 | 6 | 534 | 478 |
| 14 | -6 | 3 | 127 | 85 | 2 | -12 | 4 | 162 | -123 | -4 | 10 | 4 | 343 | 256 | 4 | 6 | 5 | 311 | 293 | 6 | -8 | 6 | 282 | 207 |
| 10 | -6 | 3 | 329 | 320 | 8 | -12 | 4 | 382 | -276 | -6 | 12 | 4 | 227 | 206 | -10 | 6 | 5 | 240 | 303 | 8 | -8 | 6 | 352 | 320 |
| -8 | -6 | 3 | 239 | -241 | 6 | -10 | 4 | 181 | 92 | 0 | 12 | 4 | 148 | 201 | 8 | 8 | 5 | 225 | -198 | 12 | -8 | 6 | 186 | -169 |
| 14 | -4 | 3 | 197 | -212 | 8 | -10 | 4 | 138 | 138 | 10 | -12 | 5 | 250 | -253 | 0 | 8 | 5 | 390 | 375 | 16 | -8 | 6 | 266 | -239 |
| 12 | -4 | 3 | 170 | 179 | 10 | -10 | 4 | 309 | -296 | 4 | -12 | 5 | 241 | -90 | -2 | 8 | 5 | 432 | 318 | -8 | -6 | 6 | 206 | -174 |
| -10 | -4 | 3 | 150 | -204 | 12 | -10 | 4 | 197 | -209 | 12 | -10 | 5 | 235 | -196 | -4 | 8 | 5 | 114 | 100 | -6 | -6 | 6 | 125 | 132 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TRUE CELL OF OKENITE



| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -4 | -6 | 6 | 177 | 105 | -4 | 12 | 6 | 335 | 267 | -14 | 4 | 7 | 465 | -492 | 6 | -6 | 8 | 283 | -253 | -2 | -10 | 9 | 280 | -225 |
| 10 | -6 | 6 | 452 | 419 | 8 | -12 | 7 | 422 | 333 | 6 | 6 | 7 | 159 | -155 | -14 | -4 | 8 | 267 | -323 | -4 | -10 | 9 | 213 | 120 |
| 14 | -6 | 6 | 143 | 160 | 6 | -12 | 7 | 334 | 201 | 2 | 6 | 7 | 137 | -114 | -10 | -4 | 8 | 268 | -263 | -6 | -10 | 9 | 170 | 152 |
| -14 | -4 | 6 | 167 | 217 | 2 | -12 | 7 | 316 | 204 | -14 | 6 | 7 | 205 | -210 | -8 | -4 | 8 | 136 | -97 | 12 | -8 | 9 | 234 | -241 |
| 12 | -4 | 6 | 262 | 278 | -2 | -12 | 7 | 103 | 119 | 6 | 8 | 7 | 323 | 316 | 10 | -4 | 8 | 229 | 232 | 4 | -8 | 9 | 117 | 123 |
| 14 | -4 | 6 | 211 | 232 | 10 | -10 | 7 | 197 | -226 | 0 | 8 | 7 | 290 | 241 | 12 | -4 | 8 | 207 | 207 | 2 | -8 | 9 | 126 | -62 |
| 16 | -4 | 6 | 277 | -288 | 6 | -10 | 7 | 231 | 223 | -2 | 8 | 7 | 154 | -120 | 14 | -4 | 8 | 142 | 97 | 0 | -8 | 9 | 176 | 117 |
| -14 | -2 | 6 | 157 | 132 | 4 | -10 | 7 | 200 | 140 | -4 | 8 | 7 | 359 | 312 | -14 | -2 | 8 | 183 | -190 | -2 | -8 | 9 | 129 | 135 |
| -12 | -2 | 6 | 128 | 152 | -2 | -10 | 7 | 182 | 122 | -8 | 8 | 7 | 264 | -334 | 10 | -2 | 8 | 129 | -102 | -4 | -8 | 9 | 225 | -186 |
| -10 | -2 | 6 | 160 | 186 | 14 | -8 | 7 | 322 | 293 | -12 | 8 | 7 | 239 | -319 | 10 | 0 | 8 | 150 | 165 | -6 | -8 | 9 | 197 | 148 |
| 14 | -2 | 6 | 184 | 219 | 12 | -8 | 7 | 107 | -122 | 4 | 10 | 7 | 204 | -213 | -14 | 2 | 8 | 134 | 144 | -8 | -8 | 9 | 177 | -155 |
| -14 | 0 | 6 | 156 | -100 | 4 | -8 | 7 | 463 | 325 | 0 | 10 | 7 | 169 | 153 | -12 | 2 | 8 | 97 | 51 | 6 | -6 | 9 | 273 | -238 |
| -12 | 0 | 6 | 257 | 277 | 2 | -8 | 7 | 194 | 121 | -10 | 10 | 7 | 223 | -302 | -10 | 2 | 8 | 148 | -140 | -6 | -6 | 9 | 112 | 64 |
| 10 | 0 | 6 | 199 | 232 | 0 | -8 | 7 | 382 | -301 | -16 | 10 | 7 | 136 | 183 | -18 | 4 | 8 | 285 | -294 | -10 | -6 | 9 | 180 | 199 |
| 14 | 0 | 6 | 276 | 363 | -2 | -8 | 7 | 139 | 147 | -6 | 12 | 7 | 264 | -254 | 8 | 4 | 8 | 100 | 130 | 12 | -4 | 9 | 209 | 193 |
| 8 | 2 | 6 | 101 | -156 | -4 | -8 | 7 | 132 | -65 | 4 | -12 | 8 | 209 | 149 | -12 | 6 | 8 | 101 | 120 | 10 | -4 | 9 | 159 | 112 |
| 6 | 4 | 6 | 115 | 140 | -6 | -8 | 7 | 213 | 215 | 8 | -12 | 8 | 327 | 263 | 0 | 6 | 8 | 201 | -166 | 8 | -4 | 9 | 386 | -340 |
| 8 | 4 | 6 | 143 | 132 | -8 | -8 | 7 | 311 | 295 | -2 | -10 | 8 | 286 | -242 | 2 | 6 | 8 | 289 | -232 | -6 | -4 | 9 | 320 | -225 |
| 10 | 4 | 6 | 197 | 224 | 8 | -6 | 7 | 148 | -133 | 4 | -10 | 8 | 368 | -271 | 4 | 6 | 8 | 302 | 231 | -8 | -4 | 9 | 220 | -230 |
| 12 | 4 | 6 | 166 | -205 | -4 | -6 | 7 | 93 | 152 | 6 | -10 | 8 | 156 | -111 | -16 | 8 | 8 | 114 | -124 | -12 | -4 | 9 | 166 | -190 |
| 2 | 6 | 6 | 128 | 68 | -8 | -6 | 7 | 168 | -135 | 8 | -10 | 8 | 209 | 172 | -12 | 8 | 8 | 311 | -362 | 10 | -2 | 9 | 295 | -299 |
| -14 | 8 | 6 | 238 | 266 | -8 | -4 | 7 | 122 | 123 | 10 | -10 | 8 | 224 | -203 | -4 | 8 | 8 | 206 | 185 | 8 | -2 | 9 | 103 | -149 |
| -10 | 8 | 6 | 166 | 200 | -10 | -4 | 7 | 161 | -170 | 12 | -10 | 8 | 145 | -142 | -10 | 10 | 8 | 198 | -196 | -8 | -2 | 9 | 176 | 180 |
| -8 | 8 | 6 | 228 | -226 | 14 | -2 | 7 | 137 | 139 | -10 | -8 | 8 | 318 | -296 | -6 | 10 | 8 | 167 | 123 | -10 | -2 | 9 | 278 | 265 |
| -6 | 8 | 6 | 130 | 172 | -10 | -2 | 7 | 116 | -80 | -6 | -8 | 8 | 184 | -167 | -4 | 10 | 8 | 170 | 107 | 8 | 0 | 9 | 433 | -430 |
| -4 | 8 | 6 | 236 | 238 | -14 | -2 | 7 | 138 | -149 | -4 | -8 | 8 | 501 | -404 | -2 | 10 | 8 | 219 | -179 | -10 | 0 | 9 | 256 | 239 |
| 0 | 8 | 6 | 202 | 145 | 14 | 0 | 7 | 249 | 266 | -2 | -8 | 8 | 106 | 71 | 0 | 10 | 8 | 389 | -329 | -12 | 0 | 9 | 204 | -205 |
| 4 | 8 | 6 | 311 | -289 | 10 | 0 | 7 | 239 | 330 | 0 | -8 | 8 | 291 | -230 | 2 | 10 | 8 | 134 | -160 | -14 | 0 | 9 | 162 | -177 |
| 6 | 8 | 6 | 291 | 283 | -10 | 0 | 7 | 226 | 183 | 2 | -8 | 8 | 88 | -91 | -10 | 12 | 8 | 316 | -404 | 12 | 2 | 9 | 155 | -210 |
| -12 | 10 | 6 | 164 | -175 | -14 | 0 | 7 | 234 | -245 | 4 | -8 | 8 | 380 | 262 | -4 | 12 | 8 | 141 | -119 | 10 | 2 | 9 | 124 | -129 |
| -8 | 10 | 6 | 143 | -130 | 12 | 2 | 7 | 112 | 183 | 6 | -8 | 8 | 114 | -144 | 6 | -12 | 9 | 186 | -107 | -14 | 2 | 9 | 155 | 170 |
| -6 | 10 | 6 | 307 | -306 | 8 | 2 | 7 | 121 | -130 | 8 | -8 | 8 | 209 | 195 | 2 | -12 | 9 | 257 | -167 | 8 | 4 | 9 | 102 | 53 |
| -2 | 10 | 6 | 271 | 257 | 12 | 4 | 7 | 147 | 118 | 10 | -8 | 8 | 201 | 189 | 0 | -12 | 9 | 175 | -165 | 4 | 4 | 9 | 726 | -614 |
| 2 | 10 | 6 | 142 | -149 | 6 | 4 | 7 | 153 | 160 | 12 | -8 | 8 | 244 | 173 | 8 | -10 | 9 | 262 | 231 | 2 | 4 | 9 | 252 | -165 |
| -10 | 12 | 6 | 159 | 216 | 4 | 4 | 7 | 248 | 240 | 14 | -8 | 8 | 249 | 248 | 4 | -10 | 9 | 100 | -99 | -10 | 4 | 9 | 404 | -441 |
| -6 | 12 | 6 | 140 | 34 | -12 | 4 | 7 | 157 | -168 | -6 | -6 | 8 | 228 | -168 | 2 | -10 | 9 | 109 | 7 | -12 | 4 | 9 | 218 | -273 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TRUE CELL OF OKENITE

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -14 | 4 | 9 | 217 | 228 | -12 | -4 | 10 | 182 | -202 | 8 | -8 | 11 | 291 | -270 | -10 | 10 | 11 | 110 | -88 | 2 | 0 | 12 | 320 | 300 |
| -2 | 6 | 9 | 314 | 259 | -8 | -4 | 10 | 210 | -193 | -2 | -8 | 11 | 230 | -179 | -4 | -10 | 12 | 193 | 144 | 4 | 0 | 12 | 298 | 260 |
| -4 | 6 | 9 | 210 | 188 | -6 | -4 | 10 | 521 | -424 | 8 | -6 | 11 | 190 | -139 | -2 | -10 | 12 | 154 | -85 | 6 | 0 | 12 | 247 | -240 |
| -8 | 6 | 9 | 145 | -145 | 8 | -4 | 10 | 416 | -418 | 4 | -6 | 11 | 383 | 384 | 2 | -10 | 12 | 132 | -99 | 8 | 0 | 12 | 303 | 257 |
| 6 | 8 | 9 | 312 | -284 | 14 | -4 | 10 | 166 | -257 | 2 | -6 | 11 | 497 | 389 | 4 | -10 | 12 | 227 | -143 | 10 | 0 | 12 | 212 | -195 |
| 4 | 8 | 9 | 533 | -466 | 6 | -2 | 10 | 129 | -111 | 0 | -6 | 11 | 183 | 117 | 6 | -10 | 12 | 244 | 208 | -14 | 2 | 12 | 115 | 110 |
| 0 | 8 | 9 | 350 | -248 | -14 | 0 | 10 | 166 | 139 | -2 | -6 | 11 | 182 | 137 | 8 | -10 | 12 | 563 | 481 | -10 | 2 | 12 | 216 | -223 |
| -4 | 8 | 9 | 93 | -88 | -10 | 0 | 10 | 500 | 476 | 4 | -4 | 11 | 230 | -246 | -8 | -8 | 12 | 174 | 152 | -8 | 2 | 12 | 128 | -139 |
| -6 | 8 | 9 | 170 | -188 | 6 | 0 | 10 | 154 | 165 | -4 | -4 | 11 | 533 | 428 | -6 | -8 | 12 | 148 | 78 | -6 | 2 | 12 | 133 | -136 |
| -12 | 8 | 9 | 182 | -221 | 8 | 0 | 10 | 485 | -423 | -8 | -4 | 11 | 235 | 191 | -4 | -8 | 12 | 457 | 319 | 8 | 2 | 12 | 99 | 127 |
| -14 | 8 | 9 | 324 | 365 | 10 | 0 | 10 | 246 | -282 | 10 | -2 | 11 | 158 | 206 | -2 | -8 | 12 | 342 | 266 | -14 | 4 | 12 | 125 | 176 |
| 2 | 10 | 9 | 156 | 82 | -10 | 2 | 10 | 279 | 248 | 8 | -2 | 11 | 173 | 204 | 0 | -8 | 12 | 354 | 246 | -10 | 4 | 12 | 298 | -343 |
| -2 | 10 | 9 | 249 | 218 | 8 | 2 | 10 | 175 | -163 | 6 | -2 | 11 | 171 | 210 | 6 | -8 | 12 | 193 | 167 | -8 | 4 | 12 | 286 | 324 |
| -6 | 10 | 9 | 236 | -237 | -16 | 4 | 10 | 268 | -275 | -6 | -2 | 11 | 130 | 157 | 8 | -8 | 12 | 364 | 295 | -2 | 4 | 12 | 229 | 258 |
| -8 | 10 | 9 | 196 | -258 | -10 | 4 | 10 | 353 | -393 | -8 | -2 | 11 | 121 | 150 | 12 | -8 | 12 | 287 | 232 | 2 | 4 | 12 | 304 | -291 |
| -4 | 12 | 9 | 435 | -359 | 2 | 4 | 10 | 309 | 246 | -10 | -2 | 11 | 88 | -103 | -10 | -6 | 12 | 220 | 213 | 4 | 4 | 12 | 205 | -158 |
| 2 | -12 | 10 | 357 | -259 | 4 | 4 | 10 | 186 | -152 | -12 | -2 | 11 | 159 | 177 | -2 | -6 | 12 | 293 | 174 | 6 | 4 | 12 | 202 | -192 |
| 6 | -12 | 10 | 203 | -106 | 6 | 4 | 10 | 246 | 236 | 12 | 0 | 11 | 108 | -115 | 0 | -6 | 12 | 294 | 235 | 8 | 4 | 12 | 288 | 283 |
| 8 | -12 | 10 | 373 | -262 | -12 | 6 | 10 | 172 | 155 | 10 | 0 | 11 | 324 | -329 | 6 | -6 | 12 | 267 | -185 | -14 | 6 | 12 | 236 | -272 |
| 0 | -10 | 10 | 217 | -159 | -8 | 6 | 10 | 137 | 152 | 6 | 0 | 11 | 272 | 248 | 10 | -6 | 12 | 129 | 88 | -12 | 6 | 12 | 141 | -161 |
| 2 | -10 | 10 | 224 | 151 | -6 | 6 | 10 | 234 | 263 | -8 | 0 | 11 | 273 | 454 | 12 | -6 | 12 | 220 | 254 | -10 | 6 | 12 | 129 | -146 |
| 6 | -10 | 10 | 141 | 63 | -4 | 6 | 10 | 108 | 77 | -14 | 0 | 11 | 427 | 564 | -6 | -4 | 12 | 153 | -145 | -4 | 6 | 12 | 109 | 116 |
| -6 | -8 | 10 | 432 | 343 | -2 | 6 | 10 | 110 | 123 | -16 | 2 | 11 | 100 | -68 | -2 | -4 | 12 | 365 | 270 | 4 | 6 | 12 | 165 | 174 |
| -4 | -8 | 10 | 343 | -252 | 0 | 6 | 10 | 143 | -130 | 8 | 4 | 11 | 149 | 119 | 2 | -4 | 12 | 322 | 268 | -10 | 8 | 12 | 190 | 206 |
| 0 | -8 | 10 | 255 | -195 | 6 | 6 | 10 | 274 | 238 | 4 | 4 | 11 | 186 | 109 | 6 | -4 | 12 | 182 | -173 | -2 | 8 | 12 | 307 | 250 |
| 2 | -8 | 10 | 229 | -161 | 8 | 6 | 10 | 147 | 171 | -2 | 4 | 11 | 311 | 286 | 12 | -4 | 12 | 368 | 369 | 0 | 8 | 12 | 449 | 334 |
| 8 | -8 | 10 | 368 | -342 | -14 | 8 | 10 | 224 | 242 | -6 | 4 | 11 | 149 | 142 | -14 | -2 | 12 | 161 | -165 | 2 | 8 | 12 | 272 | -227 |
| 12 | -8 | 10 | 484 | -418 | -10 | 8 | 10 | 192 | -211 | -12 | 4 | 11 | 197 | 196 | -12 | -2 | 12 | 158 | 109 | -12 | 10 | 12 | 146 | -126 |
| 14 | -8 | 10 | 262 | -205 | 0 | 8 | 10 | 248 | -195 | -2 | 6 | 11 | 131 | -125 | -6 | -2 | 12 | 248 | -204 | -10 | 10 | 12 | 186 | -243 |
| -8 | -6 | 10 | 299 | -263 | 4 | 8 | 10 | 195 | -129 | -6 | 6 | 11 | 311 | 312 | 4 | -2 | 12 | 171 | 115 | -8 | 10 | 12 | 242 | -227 |
| -6 | -6 | 10 | 107 | 90 | -4 | 10 | 10 | 275 | 254 | -16 | 6 | 11 | 163 | 180 | 6 | -2 | 12 | 150 | -95 | -6 | 10 | 12 | 169 | -202 |
| -4 | -6 | 10 | 118 | 88 | 0 | 10 | 10 | 193 | 151 | 4 | 8 | 11 | 291 | 258 | 10 | -2 | 12 | 175 | -129 | 4 | -10 | 13 | 136 | -101 |
| 4 | -6 | 10 | 224 | -201 | 2 | -12 | 11 | 389 | -285 | 0 | 8 | 11 | 231 | 228 | -14 | 0 | 12 | 266 | 300 | -2 | -10 | 13 | 264 | -184 |
| 10 | -6 | 10 | 249 | 232 | 6 | -10 | 11 | 189 | 155 | -12 | 8 | 11 | 163 | 227 | -12 | 0 | 12 | 130 | 110 | -4 | -10 | 13 | 174 | 69 |
| 12 | -6 | 10 | 167 | -160 | 2 | -10 | 11 | 275 | -187 | -4 | 10 | 11 | 165 | 89 | -8 | 0 | 12 | 229 | 224 | 10 | -8 | 13 | 366 | -287 |
| -14 | -4 | 10 | 150 | 143 | -2 | -10 | 11 | 197 | 143 | -8 | 10 | 11 | 182 | 202 | -6 | 0 | 12 | 111 | 125 | 8 | -8 | 13 | 354 | 312 |

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | -8 | 13 | 296 | 220 | -16 | 2 | 13 | 152 | -89 | -2 | -2 | 14 | 99 | 65 | 6 | -6 | 15 | 327 | -332 | -4 | 8 | 15 | 183 | 197 |
| 0 | -8 | 13 | 225 | -159 | 8 | 4 | 13 | 352 | 297 | -14 | 0 | 14 | 171 | -146 | -2 | -6 | 15 | 151 | -124 | -6 | 8 | 15 | 291 | -313 |
| -6 | -8 | 13 | 159 | 107 | 4 | 4 | 13 | 134 | -61 | -12 | 0 | 14 | 175 | 131 | 8 | -4 | 15 | 170 | -213 | -8 | 8 | 15 | 167 | -189 |
| 0 | -6 | 13 | 147 | 100 | -2 | 4 | 13 | 144 | 153 | -10 | 0 | 14 | 338 | 294 | 6 | -4 | 15 | 272 | -284 | 0 | -8 | 16 | 243 | -201 |
| -2 | -6 | 13 | 375 | -301 | -6 | 4 | 13 | 465 | 474 | -4 | 0 | 14 | 437 | -381 | 4 | -4 | 15 | 148 | -42 | 2 | -8 | 16 | 525 | -383 |
| -4 | -6 | 13 | 415 | -322 | -10 | 4 | 13 | 432 | -479 | -2 | 0 | 14 | 412 | 377 | 2 | -4 | 15 | 97 | 94 | -6 | -6 | 16 | 241 | -182 |
| -6 | -6 | 13 | 94 | -122 | -12 | 4 | 13 | 135 | -150 | 0 | 0 | 14 | 173 | 145 | 0 | -4 | 15 | 208 | -182 | 0 | -6 | 16 | 388 | 279 |
| -8 | -6 | 13 | 360 | -278 | -14 | 4 | 13 | 215 | -225 | 2 | 0 | 14 | 202 | -213 | -2 | -4 | 15 | 256 | -215 | 2 | -6 | 16 | 203 | -189 |
| -10 | -6 | 13 | 127 | -89 | 2 | 6 | 13 | 162 | -88 | 4 | 0 | 14 | 506 | 460 | -6 | -4 | 15 | 263 | -180 | -6 | -4 | 16 | 222 | -206 |
| 12 | -4 | 13 | 274 | 274 | -2 | 6 | 13 | 199 | 161 | 6 | 0 | 14 | 225 | 142 | 10 | -2 | 15 | 135 | -130 | 0 | -4 | 16 | 319 | 270 |
| 10 | -4 | 13 | 191 | -192 | 0 | 8 | 13 | 601 | 455 | 8 | 0 | 14 | 167 | -131 | 8 | -2 | 15 | 158 | -124 | 2 | -4 | 16 | 204 | 182 |
| 8 | -4 | 13 | 173 | -138 | -2 | 8 | 13 | 176 | 109 | -10 | 2 | 14 | 163 | 158 | 6 | -2 | 15 | 205 | -194 | 4 | -4 | 16 | 176 | 169 |
| -6 | -4 | 13 | 539 | -441 | -4 | 8 | 13 | 14, | -122 | -6 | 2 | 14 | 199 | -214 | 0 | -2 | 15 | 156 | -125 | 6 | -4 | 16 | 359 | -304 |
| 12 | -2 | 13 | 164 | 174 | -8 | 8 | 13 | 191 | -223 | 4 | 2 | 14 | 281 | -235 | -2 | -2 | 15 | 131 | -114 | 8 | -4 | 16 | 340 | -320 |
| 10 | -2 | 13 | 198 | -176 | -14 | 8 | 13 | 216 | 207 | 8 | 2 | 14 | 201 | -218 | -10 | -2 | 15 | 137 | -90 | -12 | -2 | 16 | 178 | 194 |
| 6 | -2 | 13 | 141 | -91 | -6 | 10 | 13 | 238 | -258 | -14 | 4 | 14 | 343 | -373 | 4 | 0 | 15 | 149 | -151 | -10 | -2 | 16 | 258 | 210 |
| 0 | -2 | 13 | 284 | -266 | -8 | 10 | 13 | 262 | -259 | -12 | 4 | 14 | 134 | 159 | 2 | 0 | 15 | 702 | -619 | -8 | -2 | 16 | 120 | 90 |
| -2 | -2 | 13 | 228 | -219 | -2 | -10 | 14 | 190 | 90 | -10 | 4 | 14 | 160 | -161 | -2 | 0 | 15 | 544 | -448 | -4 | -2 | 16 | 115 | 104 |
| -4 | -2 | 13 | 504 | -478 | 2 | -10 | 14 | 137 | -112 | -8 | 4 | 14 | 297 | -333 | -4 | 0 | 15 | 464 | -455 | -2 | 0 | 16 | 384 | -410 |
| -14 | -2 | 13 | 231 | -197 | -4 | -8 | 14 | 143 | -89 | -4 | 4 | 14 | 130 | -141 | -8 | 0 | 15 | 214 | 214 | 0 | 0 | 16 | 266 | 242 |
| 4 | 0 | 13 | 935 | 824 | 0 | -8 | 14 | 353 | -270 | 0 | 4 | 14 | 212 | -181 | -12 | 0 | 15 | 157 | -156 | 4 | 0 | 16 | 206 | 184 |
| 2 | 0 | 13 | 500 | 434 | 2 | -8 | 14 | 273 | 217 | -12 | 6 | 14 | 109 | 54 | -14 | 0 | 15 | 248 | -262 | -14 | 2 | 16 | 210 | 218 |
| 0 | 0 | 13 | 128 | -125 | 8 | -8 | 14 | 404 | 348 | -6 | 6 | 14 | 221 | 201 | 4 | 2 | 15 | 163 | -130 | -8 | 2 | 16 | 224 | 223 |
| -2 | 0 | 13 | 144 | 151 | 10 | -8 | 14 | 152 | 122 | -2 | 6 | 14 | 170 | -158 | 2 | 2 | 15 | 157 | -158 | -6 | 2 | 16 | 117 | 157 |
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| -10 | 0 | 13 | 182 | 215 | 0 | -6 | 14 | 168 | 111 | 4 | 6 | 14 | 155 | -123 | -10 | 2 | 15 | 160 | -169 | 2 | 2 | 16 | 153 | 177 |
| -14 | 0 | 13 | 275 | -273 | 2 | -6 | 14 | 352 | 279 | -8 | 8 | 14 | 347 | -390 | -12 | 2 | 15 | 138 | -117 | 4 | 2 | 16 | 123 | 183 |
| 4 | 2 | 13 | 160 | -106 | -10 | -4 | 14 | 362 | -294 | -2 | 8 | 14 | 392 | -330 | 4 | 4 | 15 | 368 | -334 | 6 | 2 | 16 | 156 | 132 |
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| 0 | 2 | 13 | 181 | -155 | -6 | -4 | 14 | 279 | -221 | 4 | -10 | 15 | 335 | -267 | -2 | 4 | 15 | 263 | 206 | -4 | 4 | 16 | 220 | 198 |
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| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -2 | 6 | 16 | 215 | 235 | -10 | 0 | 18 | 227 | 244 | -4 | 0 | 21 | 138 | -152 | 0 | 6 | 0 | 191 | 154 | -6 | -4 | 1 | 363 | 317 |
| 0 | 6 | 16 | 190 | 149 | -8 | 0 | 18 | 153 | 109 | 18 | 0 | 0 | 307 | -253 | 4 | 6 | 0 | 589 | 405 | -8 | -4 | 1 | 215 | -172 |
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| 4 | -8 | 17 | 259 | 212 | 6 | 0 | 18 | 288 | 235 | 0 | 2 | 0 | 418 | 389 | -10 | 10 | 0 | 329 | -331 | 16 | 0 | 1 | 319 | 317 |
| 2 | -8 | 17 | 176 | -188 | -12 | 2 | 18 | 155 | -142 | 2 | 2 | 0 | 238 | 194 | 2 | 10 | 0 | 195 | -179 | 10 | 0 | 1 | 249 | 260 |
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| 0 | 0 | 17 | 126 | 175 | -2 | -4 | 19 | 134 | -156 | 14 | 0 | 0 | 308 | 351 | 14 | -8 | 1 | 297 | 348 | 10 | 4 | 1 | 271 | -237 |
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| -6 | 0 | 17 | 220 | 224 | 0 | -2 | 19 | 205 | -190 | -12 | 2 | 0 | 237 | 238 | 0 | -8 | 1 | 366 | 242 | 6 | 4 | 1 | 298 | 250 |
| -10 | 0 | 17 | 494 | 484 | -2 | -2 | 19 | 158 | -178 | -10 | 2 | 0 | 238 | 272 | -2 | -8 | 1 | 223 | 141 | -4 | 4 | 1 | 212 | -282 |
| 4 | 2 | 17 | 98 | -45 | -8 | -2 | 19 | 170 | 111 | 0 | 2 | 0 | 381 | 389 | -4 | -8 | 1 | 395 | -238 | -12 | 4 | 1 | 515 | -523 |
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| 2 | 4 | 17 | 249 | 248 | -8 | 2 | 19 | 137 | 112 | 6 | 2 | 0 | 241 | -269 | -10 | -8 | 1 | 270 | 229 | -18 | 4 | 1 | 285 | -275 |
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| -2 | 6 | 17 | 197 | 168 | -4 | 4 | 19 | 94 | 124 | -10 | 4 | 0 | 514 | 553 | -10 | -6 | 1 | 225 | 223 | 0 | 6 | 1 | 258 | -189 |
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| 2 | -6 | 18 | 212 | 208 | -4 | -4 | 20 | 304 | 266 | 2 | 4 | 0 | 367 | 263 | 10 | -4 | 1 | 339 | 385 | -8 | 6 | 1 | 215 | -174 |
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| -6 | -2 | 18 | 92 | 79 | -6 | 0 | 20 | 123 | -79 | -12 | 6 | 0 | 354 | 420 | -2 | -4 | 1 | 342 | -233 | -10 | 8 | 1 | 252 | -248 |
| -2 | -2 | 18 | 164 | 175 | -2 | 2 | 20 | 290 | -305 | -10 | 6 | 0 | 317 | 320 | -4 | -4 | 1 | 287 | -193 | -12 | 8 | 1 | 540 | -589 |

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
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| 4 | 12 | 1 | 266 | 238 | -4 | 0 | 2 | 250 | -203 | -4 | -12 | 3 | 369 | -257 | -16 | 2 | 3 | 219 | 156 | 0 | -4 | 4 | 423 | -347 |
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| -10 | 0 | 2 | 176 | 124 | 0 | -14 | 3 | 289 | 240 | -4 | 2 | 3 | 316 | 322 | 6 | -4 | 4 | 402 | -463 | -10 | 4 | 4 | 257 | -263 |

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -14 | 4 | 4 | 241 | -280 | 0 | -2 | 5 | 169 | -174 | -6 | 8 | 5 | 165 | 223 | -8 | -2 | 6 | 184 | -182 | -2 | -2 | 7 | 276 | -239 |
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| 4 | 8 | 4 | 194 | 181 | -8 | 0 | 5 | 811 | 706 | -4 | 12 | 5 | 262 | 212 | 2 | 0 | 6 | 337 | 392 | -10 | 0 | 7 | 221 | 183 |
| -12 | 8 | 4 | 243 | 285 | -6 | 0 | 5 | 460 | 405 | 6 | -12 | 6 | 251 | 263 | -2 | 0 | 6 | 640 | 665 | -6 | 0 | 7 | 359 | 264 |
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| 0 | 12 | 4 | 263 | 201 | 4 | 0 | 5 | 415 | 427 | 0 | -10 | 6 | 402 | -429 | -10 | 0 | 6 | 406 | 381 | 0 | 0 | 7 | 623 | 750 |
| 0 | 14 | 4 | 331 | 302 | 12 | 0 | 5 | 264 | -267 | -6 | -10 | 6 | 210 | 175 | -12 | 0 | 6 | 268 | 277 | 2 | 0 | 7 | 240 | -262 |
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| 8 | -12 | 5 | 284 | -278 | -6 | 2 | 5 | 253 | 204 | 6 | -8 | 6 | 181 | 207 | -8 | 2 | 6 | 208 | -159 | 6 | 0 | 7 | 241 | 267 |
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| -2 | -10 | 5 | 259 | -151 | 0 | 2 | 5 | 218 | 179 | -4 | -8 | 6 | 361 | 377 | -6 | 4 | 6 | 302 | 323 | -6 | 2 | 7 | 182 | -178 |
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| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
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| 10 | -8 | 8 | 175 | 189 | 12 | -8 | 9 | 222 | -241 | -6 | 8 | 9 | 230 | -188 | -10 | 2 | 10 | 301 | 248 | -4 | 4 | 11 | 239 | 214 |
| 8 | -8 | 8 | 198 | 195 | -14 | -6 | 9 | 257 | 235 | 0 | 8 | 9 | 287 | -248 | 6 | 4 | 10 | 208 | 236 | -2 | 4 | 11 | 271 | 286 |
| 4 | -8 | 8 | 266 | 262 | 0 | -6 | 9 | 280 | 260 | 4 | 8 | 9 | 557 | -466 | 2 | 4 | 10 | 271 | 246 | -6 | 6 | 11 | 342 | 312 |
| 0 | -8 | 8 | 234 | -230 | 4 | -6 | 9 | 224 | -207 | 6 | 8 | 9 | 318 | -284 | 0 | 4 | 10 | 606 | -579 | 4 | 6 | 11 | 233 | 204 |
| -4 | -8 | 8 | 417 | -404 | 6 | -6 | 9 | 178 | -238 | -8 | 10 | 9 | 260 | -258 | -4 | 4 | 10 | 298 | 291 | -18 | 8 | 11 | 309 | 335 |
| -10 | -8 | 8 | 276 | -296 | -8 | -4 | 9 | 222 | -230 | -2 | 10 | 9 | 225 | 218 | -6 | 4 | 10 | 179 | -160 | -2 | 8 | 11 | 280 | 247 |
| -14 | -8 | 8 | 317 | -336 | -6 | -4 | 9 | 271 | -225 | -4 | 12 | 9 | 348 | -359 | -10 | 4 | 10 | 422 | -393 | 4 | 8 | 11 | 297 | 258 |
| 6 | -6 | 8 | 235 | -253 | -2 | -4 | 9 | 397 | -304 | 8 | -12 | 10 | 284 | -262 | -16 | 4 | 10 | 261 | -275 | -12 | 12 | 11 | 351 | 368 |
| 10 | -4 | 8 | 157 | 232 | 2 | -4 | 9 | 264 | -288 | 2 | -12 | 10 | 258 | -259 | 6 | 6 | 10 | 261 | 238 | 4 | -14 | 12 | 259 | 219 |
| 6 | -4 | 8 | 260 | -277 | 8 | -4 | 9 | 294 | -340 | -4 | -12 | 10 | 251 | -281 | -6 | 6 | 10 | 212 | 263 | 0 | -12 | 12 | 401 | 368 |
| 2 | -4 | 8 | 388 | -441 | -10 | -2 | 9 | 254 | 265 | 12 | -8 | 10 | 383 | -418 | -14 | 8 | 10 | 271 | 242 | -4 | -12 | 12 | 316 | 294 |
| -4 | -4 | 8 | 300 | -268 | -8 | -2 | 9 | 201 | 180 | 8 | -8 | 10 | 309 | -342 | -2 | 10 | 10 | 397 | 368 | 8 | -10 | 12 | 438 | 481 |
| -10 | -4 | 8 | 254 | -263 | 10 | -2 | 9 | 202 | -299 | 0 | -8 | 10 | 223 | -195 | -12 | 12 | 10 | 306 | 324 | 8 | -8 | 12 | 295 | 295 |
| -14 | -4 | 8 | 350 | -323 | -12 | 0 | 9 | 262 | -205 | -2 | -8 | 10 | 435 | -359 | 2 | -12 | 11 | 338 | -285 | 0 | -8 | 12 | 212 | 246 |
| -6 | -2 | 8 | 270 | -266 | -10 | 0 | 9 | 285 | 239 | -4 | -8 | 10 | 263 | -252 | 8 | -12 | 11 | 251 | -212 | -2 | -8 | 12 | 303 | 266 |
| 16 | 0 | 8 | 350 | 372 | -8 | 0 | 9 | 333 | -311 | -6 | -8 | 10 | 359 | 343 | 8 | -8 | 11 | 208 | -270 | -4 | -8 | 12 | 379 | 319 |
| -2 | 0 | 8 | 338 | -271 | -2 | 0 | 9 | 146 | 86 | 10 | -6 | 10 | 204 | 232 | -4 | -6 | 11 | 267 | 204 | -10 | -8 | 12 | 245 | 256 |
| -4 | 0 | 8 | 278 | -293 | 4 | 0 | 9 | 189 | -193 | 4 | -6 | 10 | 190 | -201 | 2 | -6 | 11 | 342 | 389 | 6 | -6 | 12 | 158 | -185 |
| -8 | 0 | 8 | 392 | -399 | 8 | 0 | 9 | 366 | -430 | -8 | -6 | 10 | 256 | -263 | 4 | -6 | 11 | 305 | 384 | -2 | -6 | 12 | 226 | 174 |
| -18 | 0 | 8 | 392 | -350 | -18 | 2 | 9 | 207 | 169 | 8 | -4 | 10 | 321 | -418 | -14 | -4 | 11 | 324 | 277 | -10 | -6 | 12 | 250 | 213 |
| -2 | 2 | 8 | 213 | 206 | -6 | 2 | 9 | 196 | 192 | 4 | -4 | 10 | 656 | -737 | -4 | -4 | 11 | 418 | 428 | 12 | -4 | 12 | 279 | 369 |
| -6 | 2 | 8 | 443 | -415 | 4 | 2 | 9 | 214 | -209 | 2 | -4 | 10 | 296 | -284 | -2 | -4 | 11 | 221 | -222 | 2 | -4 | 12 | 209 | 268 |
| 2 | 4 | 8 | 332 | -351 | -14 | 4 | 9 | 248 | 228 | 0 | -4 | 10 | 210 | 210 | 4 | -4 | 11 | 205 | -246 | -2 | -4 | 12 | 315 | 270 |
| -2 | 4 | 8 | 363 | -315 | -12 | 4 | 9 | 291 | -273 | -2 | -4 | 10 | 225 | -226 | 2 | -2 | 11 | 299 | 305 | -4 | -4 | 12 | 720 | 659 |
| -6 | 4 | 8 | 315 | -288 | -10 | 4 | 9 | 467 | -441 | -6 | -4 | 10 | 421 | -424 | 4 | -2 | 11 | 455 | 488 | -2 | -2 | 12 | 189 | 177 |
| -18 | 4 | 8 | 340 | -294 | -8 | 4 | 9 | 213 | -183 | -8 | -4 | 10 | 197 | -193 | -14 | 0 | 11 | 610 | 564 | -6 | -2 | 12 | 226 | -204 |
| 4 | 6 | 8 | 300 | 231 | -6 | 4 | 9 | 339 | -333 | 4 | -2 | 10 | 204 | -196 | -10 | 0 | 11 | 295 | 266 | 8 | 0 | 12 | 246 | 257 |
| 2 | 6 | 8 | 202 | -232 | -2 | 4 | 9 | 467 | -449 | 10 | 0 | 10 | 246 | -282 | -8 | 0 | 11 | 502 | 454 | 4 | 0 | 12 | 157 | 260 |
| -2 | 6 | 8 | 222 | -201 | 0 | 4 | 9 | 507 | -497 | 8 | 0 | 10 | 355 | -423 | 0 | 0 | 11 | 292 | 277 | 2 | 0 | 12 | 228 | 300 |
| -12 | 8 | 8 | 362 | -362 | 2 | 4 | 9 | 188 | -165 | 4 | 0 | 10 | 268 | -280 | 6 | 0 | 11 | 233 | 248 | -8 | 0 | 12 | 230 | 224 |
| 4 | 10 | 8 | 224 | -154 | 4 | 4 | 9 | 587 | -614 | -4 | 0 | 10 | 258 | -227 | 10 | 0 | 11 | 293 | -329 | -14 | 0 | 12 | 329 | 300 |
| 0 | 10 | 8 | 395 | -329 | -4 | 6 | 9 | 206 | 188 | -6 | 0 | 10 | 523 | -464 | 0 | 2 | 11 | 299 | 298 | -10 | 2 | 12 | 279 | -223 |
| 0 | 12 | 8 | 253 | -223 | -2 | 6 | 9 | 276 | 259 | -8 | 0 | 10 | 167 | -199 | 10 | 2 | 11 | 221 | 253 | 8 | 4 | 12 | 271 | 283 |

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TRUE CELL OF OKENITE

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 4 | 12 | 227 | -291 | -8 | 8 | 13 | 230 | -223 | -10 | -4 | 15 | 456 | -428 | 8 | -4 | 17 | 323 | -370 | 7 | -7 | 1 | 71 | 77 |
| -2 | 4 | 12 | 236 | 258 | 0 | 8 | 13 | 462 | 455 | -4 | -4 | 15 | 481 | -464 | -10 | 0 | 17 | 518 | 484 | -5 | -5 | 1 | 95 | 111 |
| -8 | 4 | 12 | 340 | 324 | -8 | 10 | 13 | 264 | -259 | -2 | -4 | 15 | 208 | -215 | -6 | 0 | 17 | 219 | 224 | -3 | -5 | 1 | 101 | 110 |
| -10 | 4 | 12 | 316 | -343 | -6 | 10 | 13 | 278 | -258 | -14 | 0 | 15 | 307 | -262 | -10 | 2 | 17 | 281 | 275 | 1 | -5 | 1 | 109 | -70 |
| -8 | 6 | 12 | 288 | -338 | -10 | 12 | 13 | 323 | 328 | -8 | 0 | 15 | 234 | 214 | -14 | 4 | 17 | 339 | 327 | 3 | -5 | 1 | 68 | -33 |
| -14 | 6 | 12 | 282 | -272 | 0 | -10 | 14 | 256 | -226 | -4 | 0 | 15 | 452 | -455 | -6 | -8 | 18 | 261 | 200 | 5 | -5 | 1 | 70 | -30 |
| 2 | 8 | 12 | 212 | -227 | 8 | -8 | 14 | 278 | 348 | -2 | 0 | 15 | 472 | -448 | -10 | -2 | 18 | 257 | -237 | 7 | -5 | 1 | 79 | 32 |
| 0 | 8 | 12 | 420 | 334 | 0 | -8 | 14 | 221 | -270 | 2 | 0 | 15 | 551 | -619 | -4 | 0 | 18 | 272 | 312 | -3 | -3 | 1 | 99 | 84 |
| -2 | 8 | 12 | 256 | 250 | 2 | -6 | 14 | 250 | 279 | 12 | 0 | 15 | 218 | -235 | -10 | 0 | 18 | 302 | 244 | 9 | -3 | 1 | 114 | -31 |
| -10 | 8 | 12 | 241 | 206 | -6 | -6 | 14 | 240 | 221 | -14 | 4 | 15 | 321 | -279 | 2 | 4 | 18 | 217 | 262 | -9 | -1 | 1 | 107 | -91 |
| -6 | 12 | 12 | 318 | 290 | 4 | -4 | 14 | 240 | -233 | -8 | 4 | 15 | 299 | -281 | 0 | -8 | 19 | 249 | 258 | 7 | -1 | 1 | 66 | 38 |
| -10 | -10 | 13 | 314 | -294 | -2 | -4 | 14 | 343 | 375 | -6 | 4 | 15 | 276 | -317 | 2 | -4 | 19 | 409 | 451 | -3 | 1 | 1 | 81 | -6 |
| 0 | -10 | 13 | 228 | -187 | -6 | -4 | 14 | 244 | -221 | -2 | 4 | 15 | 252 | 206 | -8 | 0 | 19 | 353 | 358 | 3 | 1 | 1 | 62 | 73 |
| 8 | -8 | 13 | 326 | 312 | -10 | -4 | 14 | 330 | -294 | 2 | 4 | 15 | 432 | -452 | -2 | 4 | 19 | 290 | 345 | 9 | 1 | 1 | 95 | -63 |
| 10 | -8 | 13 | 214 | -287 | 4 | 0 | 14 | 330 | 460 | 4 | 4 | 15 | 318 | -334 | -8 | 6 | 19 | 249 | -240 | 5 | 3 | 1 | 76 | 124 |
| -8 | -6 | 13 | 273 | -278 | -4 | 0 | 14 | 368 | -381 | -8 | 8 | 15 | 237 | -189 | -10 | 0 | 20 | 247 | -217 | 7 | 3 | 1 | 90 | -64 |
| -4 | -6 | 13 | 326 | -322 | -10 | 0 | 14 | 362 | 294 | -6 | 8 | 15 | 332 | -313 | -2 | 2 | 20 | 276 | -305 | -1 | 5 | 1 | 106 | -16 |
| -2 | -6 | 13 | 274 | -301 | -6 | 2 | 14 | 229 | -214 | -2 | 8 | 15 | 203 | -251 | -10 | 4 | 20 | 285 | -342 | 3 | 5 | 1 | 115 | 126 |
| -6 | -4 | 13 | 444 | -441 | -8 | 4 | 14 | 240 | -333 | 2 | -8 | 16 | 356 | -383 | 18 | 8 | 0 | 562 | 116 | -9 | 7 | 1 | 71 | 54 |
| -2 | -4 | 13 | 304 | 369 | -10 | 4 | 14 | 201 | -161 | 0 | -6 | 16 | 159 | 279 | -18 | -8 | 3 | 672 | -140 | -7 | 7 | 1 | 81 | 88 |
| 2 | -4 | 13 | 243 | 320 | -14 | 4 | 14 | 358 | -373 | 6 | -4 | 16 | 263 | -304 | 9 | 1 | 0 | 113 | 81 | -1 | 7 | 1 | 99 | -68 |
| -4 | -2 | 13 | 460 | -478 | 0 | 6 | 14 | 283 | -317 | 0 | -4 | 16 | 163 | 270 | 5 | 1 | 0 | 74 | 34 | 7 | -7 | 2 | 91 | -76 |
| -2 | -2 | 13 | 187 | -219 | -6 | 6 | 14 | 215 | 201 | -8 | -4 | 16 | 356 | -289 | -3 | 3 | 0 | 74 | 79 | 3 | -7 | 2 | 156 | 87 |
| 0 | -2 | 13 | 225 | -266 | -2 | 8 | 14 | 369 | -330 | -2 | 0 | 16 | 328 | -410 | 5 | 5 | 0 | 64 | -92 | 5 | -5 | 2 | 76 | 13 |
| -16 | 0 | 13 | 387 | -392 | -8 | 8 | 14 | 366 | -390 | -4 | 2 | 16 | 216 | 267 | 3 | 5 | 0 | 94 | -120 | 3 | -5 | 2 | 88 | 18 |
| -14 | 0 | 13 | 296 | -273 | -18 | 8 | 14 | 291 | -298 | -8 | 2 | 16 | 299 | 223 | 1 | 5 | 0 | 65 | 40 | 1 | -5 | 2 | 147 | 86 |
| -4 | 0 | 13 | 252 | -319 | 4 | 10 | 14 | 263 | -231 | 4 | 4 | 16 | 301 | -346 | -1 | 5 | 0 | 67 | 43 | -1 | -5 | 2 | 78 | -1 |
| 2 | 0 | 13 | 387 | 434 | -12 | 12 | 14 | 278 | -281 | -14 | 4 | 16 | 291 | 315 | -7 | 5 | 0 | 66 | -52 | -5 | -5 | 2 | 104 | -122 |
| 4 | 0 | 13 | 708 | 824 | 2 | -10 | 15 | 257 | -255 | -16 | 4 | 16 | 272 | 285 | -9 | 5 | 0 | 70 | -7 | 9 | -3 | 2 | 110 | 41 |
| -10 | 2 | 13 | 219 | 200 | -10 | -8 | 15 | 281 | -265 | -4 | 6 | 16 | 344 | 354 | 1 | 7 | 0 | 81 | 38 | 1 | -3 | 2 | 78 | 30 |
| -4 | 2 | 13 | 139 | -179 | 0 | -8 | 15 | 212 | -230 | -6 | 8 | 16 | 277 | -241 | -3 | 7 | 0 | 179 | 118 | 7 | -1 | 2 | 101 | -39 |
| -2 | 2 | 13 | 286 | -305 | 6 | -8 | 15 | 311 | -321 | -10 | 8 | 16 | 226 | 245 | -5 | 7 | 0 | 76 | -8 | -5 | -1 | 2 | 71 | 12 |
| -14 | 4 | 13 | 250 | -225 | -12 | -6 | 15 | 245 | 210 | -14 | 8 | 16 | 267 | 296 | -9 | 7 | 0 | 81 | -52 | -9 | -1 | 2 | 85 | 86 |
| -10 | 4 | 13 | 523 | -479 | -10 | -6 | 15 | 284 | 259 | -6 | -8 | 17 | 309 | 255 | -1 | -7 | 1 | 90 | -58 | -7 | 1 | 2 | 87 | 12 |
| -6 | 4 | 13 | 507 | 474 | 6 | -6 | 15 | 285 | -332 | 0 | -6 | 17 | 318 | 387 | 1 | -7 | 1 | 102 | -61 | 5 | 3 | 2 | 97 | -114 |
| 8 | 4 | 13 | 296 | 297 | 8 | -6 | 15 | 317 | -384 | -10 | -4 | 17 | 420 | 476 | 3 | -7 | 1 | 185 | -109 | 3 | 3 | 2 | 106 | -123 |

| H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC | H | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 5 | 2 | 64 | -64 | -9 | -1 | 4 | 77 | 46 | -3 | 5 | 5 | 71 | -84 | 1 | -1 | 7 | 64 | 35 | -1 | -1 | 9 | 69 | 12 |
| 3 | 5 | 2 | 91 | -122 | 7 | 1 | 4 | 109 | 107 | 5 | -7 | 6 | 67 | -4 | 7 | -1 | 7 | 114 | -113 | 3 | 1 | 9 | 127 | 109 |
| -1 | 5 | 2 | 89 | 5 | -9 | 1 | 4 | 83 | 58 | 1 | -7 | 6 | 146 | 82 | -9 | 1 | 7 | 63 | -53 | -7 | 3 | 9 | 72 | 44 |
| -5 | 5 | 2 | 70 | 35 | 3 | 3 | 4 | 164 | -152 | 1 | -5 | 6 | 66 | 42 | 3 | 1 | 7 | 70 | 125 | -5 | 3 | 9 | 101 | -88 |
| -9 | 5 | 2 | 71 | -48 | -3 | 3 | 4 | 72 | 129 | -3 | -5 | 6 | 145 | -118 | 5 | 1 | 7 | 69 | 16 | 1 | 3 | 9 | 65 | 72 |
| -7 | 7 | 2 | 63 | -95 | -1 | 5 | 4 | 66 | 39 | 3 | -3 | 6 | 78 | 3 | -7 | 3 | 7 | 60 | 34 | -3 | 5 | 9 | 114 | -105 |
| 1 | -7 | 3 | 88 | -83 | -5 | 5 | 4 | 75 | 38 | -5 | -3 | 6 | 90 | -48 | -5 | 3 | 7 | 73 | -78 | 3 | -3 | 10 | 81 | 14 |
| 3 | -7 | 3 | 122 | -60 | -9 | 5 | 4 | 73 | -74 | -7 | -3 | 6 | 68 | -3 | 1 | 3 | 7 | 62 | 56 | -5 | -3 | 10 | 79 | -55 |
| 7 | -7 | 3 | 91 | 74 | -3 | 7 | 4 | 80 | 76 | -3 | -1 | 6 | 65 | -37 | 3 | 3 | 7 | 103 | 73 | 3 | -1 | 10 | 79 | -73 |
| -5 | -5 | 3 | 112 | 120 | -5 | 7 | 4 | 67 | 37 | -5 | -1 | 6 | 97 | -69 | 5 | 3 | 7 | 66 | 50 | 1 | -1 | 10 | 64 | -29 |
| -1 | -5 | 3 | 68 | -5 | 1 | -7 | 5 | 75 | -91 | -7 | -1 | 6 | 63 | 5 | -5 | 5 | 7 | 67 | -62 | -5 | -1 | 10 | 91 | -39 |
| 1 | -5 | 3 | 128 | -83 | 7 | -7 | 5 | 75 | 60 | -9 | -1 | 6 | 73 | 30 | -1 | 5 | 7 | 110 | -65 | 3 | 1 | 10 | 83 | -85 |
| -5 | -1 | 3 | 105 | 19 | -5 | -5 | 5 | 96 | 84 | 3 | 1 | 6 | 92 | -106 | -1 | -5 | 8 | 93 | 27 | -3 | 1 | 10 | 66 | 52 |
| 7 | -1 | 3 | 83 | 17 | -3 | -5 | 5 | 113 | 128 | -3 | 1 | 6 | 62 | 52 | -3 | -5 | 8 | 106 | -61 | -5 | 1 | 10 | 94 | 31 |
| 9 | -1 | 3 | 92 | -82 | -1 | -5 | 5 | 67 | -44 | -9 | 1 | 6 | 67 | 67 | 7 | -3 | 8 | 76 | 38 | 1 | 3 | 10 | 71 | -65 |
| 5 | 1 | 3 | 68 | 21 | 1 | -5 | 5 | 70 | -52 | 3 | 3 | 6 | 147 | -108 | 3 | -3 | 8 | 70 | 11 | -3 | 11 | 0 | 95 | 20 |
| 7 | 1 | 3 | 79 | -116 | -5 | -3 | 5 | 64 | 24 | -9 | 3 | 6 | 68 | -3 | -5 | -3 | 8 | 83 | -75 | -13 | -3 | 3 | 144 | -7 |
| -7 | 3 | 3 | 76 | 9 | -1 | -3 | 5 | 67 | -37 | 3 | 5 | 6 | 72 | -42 | 5 | -1 | 8 | 78 | -19 | -11 | 11 | 3 | 93 | -9 |
| 3 | 3 | 3 | 139 | 144 | 3 | -3 | 5 | 84 | -13 | -1 | 5 | 6 | 136 | 73 | -1 | -1 | 8 | 75 | -8 | -5 | -11 | 6 | 124 | -4 |
| 5 | 3 | 3 | 72 | 89 | 5 | -3 | 5 | 62 | -11 | -3 | 5 | 6 | 62 | 79 | -5 | -1 | 8 | 106 | -53 | -13 | 7 | 6 | 82 | 29 |
| 1 | 5 | 3 | 61 | -56 | 7 | -3 | 5 | 80 | 23 | -7 | 5 | 6 | 102 | -76 | 3 | 1 | 8 | 155 | -125 | 5 | -11 | 7 | 126 | 54 |
| 3 | 5 | 3 | 114 | 105 | 9 | -3 | 5 | 76 | -57 | -3 | 7 | 6 | 103 | 91 | -7 | 1 | 8 | 71 | 35 | -3 | 7 | 7 | 92 | -97 |
| -9 | 7 | 3 | 90 | 44 | -9 | -1 | 5 | 84 | -32 | 1 | -7 | 7 | 121 | -70 | 3 | 3 | 8 | 91 | -46 | 9 | 1 | 8 | 130 | 72 |
| -5 | 7 | 3 | 72 | -37 | -5 | -1 | 5 | 76 | 66 | 3 | -7 | 7 | 77 | -38 | -1 | 3 | 8 | 65 | -21 | -3 | 7 | 8 | 101 | 93 |
| -1 | 7 | 3 | 72 | -81 | -1 | -1 | 5 | 82 | 47 | -3 | -5 | 7 | 125 | 93 | -5 | 3 | 8 | 72 | 87 | 7 | -1 | 9 | 98 | -94 |
| 1 | -7 | 4 | 113 | 92 | 5 | -1 | 5 | 84 | 42 | -1 | -5 | 7 | 85 | -44 | -9 | 3 | 8 | 94 | -32 | 7 | -5 | 10 | 115 | -9 |
| 1 | -5 | 4 | 147 | 68 | 7 | 1 | 5 | 101 | -86 | 1 | -5 | 7 | 95 | -42 | -5 | 5 | 8 | 87 | 59 | -5 | -5 | 11 | 133 | 55 |
| -1 | -5 | 4 | 70 | 24 | -5 | 3 | 5 | 89 | -63 | -5 | -3 | 7 | 105 | 68 | 1 | -5 | 9 | 64 | -51 | -15 | 9 | 11 | 106 | -35 |
| 9 | -3 | 4 | 80 | 62 | 3 | 3 | 5 | 141 | 138 | -3 | -3 | 7 | 77 | -6 | -3 | -3 | 9 | 71 | -16 | 1 | -7 | 12 | 131 | 59 |
| 7 | -3 | 4 | 90 | -31 | -9 | 5 | 5 | 64 | 70 | -5 | -1 | 7 | 87 | 62 | 5 | -3 | 9 | 92 | -16 | 3 | 3 | 12 | 109 | -58 |
| 1 | -3 | 4 | 78 | 36 | -7 | 5 | 5 | 63 | 67 | -1 | -1 | 7 | 75 | 15 | -3 | -1 | 9 | 63 | 26 | -9 | 7 | 14 | 100 | -55 |