

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [Mn(CO)3(diphos)(HOBF3)]·(C6H5)2CH3PO

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| H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  | H   | K  | L | 10FO | 10FC |
|-----|---|---|------|-------|-----|---|---|------|------|-----|---|---|------|-------|-----|---|---|------|-------|-----|----|---|------|------|
| -5  | 1 | 3 | 607  | 633   | 5   | 2 | 3 | 240  | 228  | -4  | 4 | 3 | 979  | 935   | -6  | 6 | 3 | 619  | -572  | -1  | 6  | 3 | 108  | -105 |
| -7  | 1 | 3 | 436  | -459  | 6   | 2 | 3 | 217  | -213 | -3  | 4 | 3 | 1202 | -1088 | -5  | 6 | 3 | 323  | -299  | 0   | 6  | 3 | 135  | -143 |
| -8  | 1 | 3 | 201  | 180   | 7   | 2 | 3 | 331  | -361 | -2  | 4 | 3 | 733  | -676  | -4  | 6 | 3 | 793  | -681  | 1   | 8  | 3 | 781  | 743  |
| -5  | 1 | 3 | 138  | -213  | 8   | 2 | 3 | 299  | -275 | -1  | 4 | 3 | 885  | -961  | -3  | 6 | 3 | 617  | -608  | 2   | 8  | 3 | 265  | 271  |
| -4  | 1 | 3 | 515  | -477  | 10  | 2 | 3 | 356  | -382 | 0   | 4 | 3 | 118  | -116  | -2  | 6 | 3 | 794  | 785   | 3   | 8  | 3 | 428  | 478  |
| -3  | 1 | 3 | 982  | 929   | 11  | 2 | 3 | 501  | -485 | 3   | 4 | 3 | 207  | -240  | 0   | 6 | 3 | 346  | 387   | 4   | 8  | 3 | 221  | -265 |
| -2  | 1 | 3 | 414  | 317   | -14 | 3 | 3 | 175  | 180  | 4   | 4 | 3 | 487  | 564   | 1   | 6 | 3 | 343  | 407   | 5   | 8  | 3 | 140  | -136 |
| -1  | 1 | 3 | 1565 | 1557  | -13 | 3 | 3 | 343  | 398  | 6   | 4 | 3 | 532  | 572   | 2   | 6 | 3 | 189  | 293   | 6   | 8  | 3 | 558  | 579  |
| 0   | 1 | 3 | 164  | -185  | -12 | 3 | 3 | 241  | 282  | 7   | 4 | 3 | 284  | 360   | 3   | 6 | 3 | 308  | 351   | 7   | 8  | 3 | 629  | -637 |
| 1   | 1 | 3 | 448  | 558   | -11 | 3 | 3 | 419  | 43   | 9   | 4 | 3 | 193  | 223   | 5   | 6 | 3 | 210  | 208   | 8   | 8  | 3 | 331  | -316 |
| 2   | 1 | 3 | 334  | -324  | -10 | 3 | 3 | 154  | 218  | 11  | 4 | 3 | 269  | 269   | 6   | 6 | 3 | 316  | -364  | 11  | 8  | 3 | 275  | -293 |
| 3   | 1 | 3 | 481  | 487   | -9  | 3 | 3 | 723  | 738  | 12  | 4 | 3 | 262  | -260  | 7   | 6 | 3 | 257  | 246   | 12  | 8  | 3 | 339  | 487  |
| 4   | 1 | 3 | 279  | -268  | -8  | 3 | 3 | 241  | -225 | 13  | 4 | 3 | 174  | -125  | 10  | 6 | 3 | 550  | -506  | -3  | 9  | 3 | 196  | -140 |
| 5   | 1 | 3 | 1652 | -1329 | -7  | 3 | 3 | 219  | -198 | -12 | 5 | 3 | 258  | -248  | 12  | 6 | 3 | 383  | 287   | -8  | 9  | 3 | 287  | 231  |
| 6   | 1 | 3 | 313  | 321   | -6  | 3 | 3 | 476  | -487 | -10 | 5 | 3 | 345  | -412  | -14 | 7 | 3 | 258  | 309   | -7  | 9  | 3 | 184  | 210  |
| 7   | 1 | 3 | 739  | -708  | -5  | 3 | 3 | 294  | -289 | -9  | 5 | 3 | 196  | -241  | -12 | 7 | 3 | 448  | 277   | -5  | 9  | 3 | 212  | 187  |
| 8   | 1 | 3 | 431  | -448  | -4  | 3 | 3 | 220  | -210 | -8  | 5 | 3 | 475  | 443   | -11 | 7 | 3 | 209  | -257  | -4  | 9  | 3 | 665  | 609  |
| 12  | 1 | 3 | 284  | 269   | -3  | 3 | 3 | 253  | -198 | -7  | 5 | 3 | 190  | 187   | -9  | 7 | 3 | 356  | -346  | -1  | 9  | 3 | 350  | -361 |
| 13  | 1 | 3 | 450  | 420   | -2  | 3 | 3 | 659  | -664 | -6  | 5 | 3 | 959  | -840  | -8  | 7 | 3 | 720  | -706  | 0   | 9  | 3 | 132  | -85  |
| -13 | 2 | 3 | 295  | 261   | -1  | 3 | 3 | 32   | -75  | -5  | 5 | 3 | 194  | -175  | -6  | 7 | 3 | 425  | -389  | 2   | 9  | 3 | 418  | -435 |
| -11 | 2 | 3 | 362  | 490   | 1   | 3 | 3 | 905  | 1010 | -3  | 5 | 3 | 384  | 372   | -5  | 7 | 3 | 462  | -497  | 3   | 9  | 3 | 243  | -251 |
| -10 | 2 | 3 | 495  | -111  | 3   | 3 | 3 | 486  | 512  | -2  | 5 | 3 | 236  | -288  | -2  | 7 | 3 | 397  | 391   | 4   | 9  | 3 | 535  | -604 |
| -9  | 2 | 3 | 258  | -281  | 4   | 3 | 3 | 317  | 331  | -1  | 5 | 3 | 807  | 784   | 0   | 7 | 3 | 476  | -453  | 5   | 9  | 3 | 570  | 628  |
| -8  | 2 | 3 | 318  | -123  | 5   | 3 | 3 | 552  | 486  | 0   | 5 | 3 | 602  | 588   | 2   | 7 | 3 | 1062 | -1142 | 6   | 9  | 3 | 174  | 161  |
| -7  | 2 | 3 | 418  | -110  | 6   | 3 | 3 | 195  | 159  | 1   | 5 | 3 | 119  | 1175  | 3   | 7 | 3 | 422  | -480  | 7   | 9  | 3 | 278  | 310  |
| -6  | 2 | 3 | 379  | 360   | 7   | 3 | 3 | 234  | 240  | 2   | 5 | 3 | 482  | 593   | 4   | 7 | 3 | 371  | 426   | 8   | 9  | 3 | 279  | 280  |
| -5  | 2 | 3 | 109  | -75   | 8   | 3 | 3 | 342  | -336 | 4   | 5 | 3 | 361  | -413  | 5   | 7 | 3 | 277  | -298  | 10  | 9  | 3 | 374  | 333  |
| -4  | 2 | 3 | 786  | 715   | 8   | 3 | 3 | 370  | 356  | 5   | 5 | 3 | 238  | -227  | 6   | 7 | 3 | 332  | 272   | -11 | 10 | 3 | 360  | -392 |
| -3  | 2 | 3 | 281  | 273   | 10  | 3 | 3 | 415  | -426 | 7   | 5 | 3 | 235  | -229  | 10  | 7 | 3 | 346  | -325  | -7  | 10 | 3 | 346  | 328  |
| -2  | 2 | 3 | 1243 | 1113  | 13  | 3 | 3 | 329  | -269 | 8   | 5 | 3 | 452  | 462   | 12  | 7 | 3 | 387  | -312  | -5  | 10 | 3 | 242  | 241  |
| -1  | 2 | 3 | 479  | 437   | -14 | 4 | 3 | 163  | 251  | 9   | 5 | 3 | 140  | -85   | -10 | 8 | 3 | 596  | 621   | -4  | 10 | 3 | 129  | -78  |
| 0   | 2 | 3 | 764  | -740  | -13 | 4 | 3 | 162  | -109 | 12  | 5 | 3 | 318  | 326   | -9  | 8 | 3 | 216  | 194   | -3  | 10 | 3 | 483  | 465  |
| 1   | 2 | 3 | 727  | -643  | -10 | 4 | 3 | 180  | 202  | -12 | 6 | 3 | 307  | -378  | -8  | 8 | 3 | 229  | -240  | -2  | 10 | 3 | 708  | 684  |
| 2   | 2 | 3 | 293  | -320  | -9  | 4 | 3 | 556  | 519  | -10 | 6 | 3 | 347  | -354  | -5  | 8 | 3 | 106  | -283  | -1  | 10 | 3 | 257  | -252 |
| 3   | 2 | 3 | 260  | 230   | -8  | 4 | 3 | 567  | 538  | -8  | 6 | 3 | 691  | -666  | -3  | 8 | 3 | 228  | -205  | 0   | 10 | 3 | 180  | 220  |
| 4   | 2 | 3 | 304  | -310  | -5  | 4 | 3 | 385  | 361  | -7  | 6 | 3 | 258  | 259   | -2  | 8 | 3 | 657  | -654  | 1   | 10 | 3 | 204  | -199 |

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [MnNiCo13I01P0H0S1] (H0BF3)1.054512CH3F0

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| H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC | H   | K | L | 10FO | 10FC |
|-----|----|---|------|------|-----|----|---|------|-------|-----|---|---|------|-------|-----|---|---|------|-------|-----|---|---|------|------|-----|---|---|------|------|
| 4   | 10 | 3 | 412  | -495 | 3   | 13 | 3 | 179  | -325  | 2   | 0 | 4 | 467  | -478  | 2   | 2 | 4 | 173  | 181   | 4   | 4 | 4 | 138  | 159  | 4   | 4 | 4 | 138  | 159  |
| 5   | 10 | 3 | 303  | -316 | 5   | 13 | 3 | 337  | -397  | 4   | 0 | 4 | 175  | -148  | 3   | 2 | 4 | 339  | 510   | 5   | 4 | 4 | 209  | 259  | 5   | 4 | 4 | 209  | 259  |
| 6   | 10 | 3 | 731  | -798 | 6   | 13 | 3 | 420  | -434  | 6   | 0 | 4 | 215  | 185   | 4   | 2 | 4 | 245  | 223   | 7   | 4 | 4 | 249  | 218  | 7   | 4 | 4 | 249  | 218  |
| 7   | 10 | 3 | 613  | 615  | 7   | 13 | 3 | 425  | 431   | 8   | 0 | 4 | 574  | -563  | 8   | 2 | 4 | 351  | 296   | 9   | 4 | 4 | 185  | -232 | 9   | 4 | 4 | 185  | -232 |
| 11  | 10 | 3 | 247  | 209  | 8   | 13 | 3 | 262  | -249  | 10  | 0 | 4 | 221  | -258  | 10  | 2 | 4 | 213  | 198   | 10  | 4 | 4 | 182  | -150 | 10  | 4 | 4 | 182  | -150 |
| -11 | 11 | 3 | 207  | -212 | -7  | 14 | 3 | 225  | 196   | 12  | 0 | 4 | 427  | 336   | 11  | 2 | 4 | 193  | -106  | 12  | 4 | 4 | 178  | 118  | 12  | 4 | 4 | 178  | 118  |
| -10 | 11 | 3 | 163  | 68   | -6  | 14 | 3 | 286  | 314   | -14 | 1 | 4 | 215  | 217   | 12  | 2 | 4 | 493  | -439  | -13 | 5 | 4 | 237  | -253 | -13 | 5 | 4 | 237  | -253 |
| -9  | 11 | 3 | 657  | -622 | -4  | 14 | 3 | 296  | 283   | -11 | 1 | 4 | 231  | -286  | -13 | 3 | 4 | 319  | 394   | -11 | 5 | 4 | 369  | -358 | -11 | 5 | 4 | 369  | -358 |
| -8  | 11 | 3 | 348  | -309 | -3  | 14 | 3 | 429  | 753   | -10 | 1 | 4 | 306  | -330  | -12 | 3 | 4 | 217  | 190   | -10 | 5 | 4 | 205  | 236  | -10 | 5 | 4 | 205  | 236  |
| -7  | 11 | 3 | 161  | -89  | 0   | 14 | 3 | 212  | 190   | -8  | 1 | 4 | 742  | -778  | -11 | 3 | 4 | 254  | 271   | -9  | 2 | 4 | 913  | -500 | -9  | 2 | 4 | 913  | -500 |
| -6  | 11 | 3 | 560  | -526 | 2   | 14 | 3 | 192  | 197   | -6  | 1 | 4 | 516  | -489  | -10 | 3 | 4 | 346  | 368   | -8  | 5 | 4 | 412  | -409 | -8  | 5 | 4 | 412  | -409 |
| -5  | 11 | 3 | 336  | 275  | 3   | 14 | 3 | 387  | -486  | -5  | 1 | 4 | 295  | -287  | -8  | 3 | 4 | 619  | 606   | -6  | 5 | 4 | 703  | -660 | -6  | 5 | 4 | 703  | -660 |
| -4  | 11 | 3 | 286  | -215 | 5   | 14 | 3 | 370  | -403  | -4  | 1 | 4 | 813  | -735  | -7  | 3 | 4 | 263  | 287   | -5  | 5 | 4 | 459  | -388 | -5  | 5 | 4 | 459  | -388 |
| -3  | 11 | 3 | 200  | 163  | 6   | 14 | 3 | 161  | 168   | -3  | 1 | 4 | 573  | -567  | -6  | 3 | 4 | 125  | -100  | -4  | 5 | 4 | 315  | -308 | -4  | 5 | 4 | 315  | -308 |
| 0   | 11 | 3 | 438  | 407  | 7   | 14 | 3 | 208  | 162   | -2  | 1 | 4 | 614  | -600  | -5  | 3 | 4 | 393  | 362   | -3  | 5 | 4 | 623  | 569  | -3  | 5 | 4 | 623  | 569  |
| 1   | 11 | 3 | 194  | -182 | 9   | 14 | 3 | 164  | 131   | -1  | 1 | 4 | 139  | 154   | -3  | 3 | 4 | 1455 | -1371 | -2  | 5 | 4 | 171  | 164  | -2  | 5 | 4 | 171  | 164  |
| 2   | 11 | 3 | 374  | 402  | -10 | 15 | 3 | 235  | -230  | 0   | 1 | 4 | 253  | 292   | -2  | 3 | 4 | 512  | 518   | -1  | 5 | 4 | 587  | 580  | -1  | 5 | 4 | 587  | 580  |
| 4   | 11 | 3 | 551  | 623  | -1  | 15 | 3 | 611  | 671   | 2   | 1 | 4 | 234  | 237   | -1  | 3 | 4 | 924  | -914  | 0   | 5 | 4 | 948  | 913  | 0   | 5 | 4 | 948  | 913  |
| 5   | 11 | 3 | 129  | -124 | 4   | 15 | 3 | 160  | 212   | 3   | 1 | 4 | 697  | 736   | 0   | 3 | 4 | 185  | 190   | 1   | 5 | 4 | 417  | 416  | 1   | 5 | 4 | 417  | 416  |
| 9   | 11 | 3 | 532  | -517 | -8  | 16 | 3 | 264  | -254  | 4   | 1 | 4 | 800  | 819   | 1   | 3 | 4 | 187  | -178  | 2   | 5 | 4 | 302  | 341  | 2   | 5 | 4 | 302  | 341  |
| 10  | 11 | 3 | 258  | -224 | -1  | 16 | 3 | 335  | 273   | 6   | 1 | 4 | 438  | -377  | 4   | 3 | 4 | 142  | 136   | 3   | 5 | 4 | 103  | -127 | 3   | 5 | 4 | 103  | -127 |
| -11 | 12 | 3 | 195  | 166  | -6  | 17 | 3 | 215  | -174  | 8   | 1 | 4 | 336  | -325  | 9   | 3 | 4 | 274  | 276   | 4   | 5 | 4 | 380  | 420  | 4   | 5 | 4 | 380  | 420  |
| -7  | 12 | 3 | 498  | -413 | 0   | 17 | 3 | 241  | 254   | 9   | 1 | 4 | 156  | -174  | 10  | 3 | 4 | 502  | 454   | 5   | 5 | 4 | 287  | -306 | 5   | 5 | 4 | 287  | -306 |
| -6  | 12 | 3 | 334  | -273 | 1   | 17 | 3 | 265  | 307   | 10  | 1 | 4 | 307  | -256  | -14 | 4 | 4 | 152  | -154  | -11 | 6 | 4 | 210  | -151 | -11 | 6 | 4 | 210  | -151 |
| -5  | 12 | 3 | 178  | 202  | -2  | 18 | 3 | 187  | -215  | -14 | 2 | 4 | 377  | 461   | -11 | 4 | 4 | 288  | -283  | 7   | 5 | 4 | 252  | 247  | 7   | 5 | 4 | 252  | 247  |
| -3  | 12 | 3 | 160  | -185 | -1  | 18 | 3 | 293  | -326  | -12 | 2 | 4 | 233  | 198   | -10 | 4 | 4 | 243  | -272  | 8   | 5 | 4 | 137  | 17   | 8   | 5 | 4 | 137  | 17   |
| -2  | 12 | 3 | 368  | -373 | 2   | 18 | 3 | 430  | -709  | -10 | 2 | 4 | 483  | 512   | -8  | 4 | 4 | 190  | 236   | -11 | 5 | 4 | 269  | 249  | -11 | 5 | 4 | 269  | 249  |
| -1  | 12 | 3 | 241  | 238  | -1  | 19 | 3 | 177  | 150   | -8  | 2 | 4 | 260  | 288   | -6  | 4 | 4 | 140  | 138   | -9  | 6 | 4 | 347  | -338 | -9  | 6 | 4 | 347  | -338 |
| 2   | 12 | 3 | 135  | -148 | -1  | 19 | 3 | 374  | -407  | -7  | 2 | 4 | 357  | -347  | -6  | 4 | 4 | 380  | 927   | -6  | 6 | 4 | 267  | 237  | -6  | 6 | 4 | 267  | 237  |
| -9  | 13 | 3 | 335  | 350  | -10 | 0  | 4 | 363  | -1034 | -5  | 2 | 4 | 241  | 225   | -5  | 4 | 4 | 198  | -154  | -7  | 5 | 4 | 401  | -385 | -7  | 5 | 4 | 401  | -385 |
| -8  | 13 | 3 | 348  | 319  | -8  | 0  | 4 | 783  | -811  | -4  | 2 | 4 | 811  | -760  | -4  | 4 | 4 | 300  | 276   | -6  | 6 | 4 | 365  | 355  | -6  | 6 | 4 | 365  | 355  |
| -3  | 13 | 3 | 203  | -203 | -8  | 0  | 4 | 222  | -207  | -3  | 2 | 4 | 734  | -667  | -3  | 4 | 4 | 1195 | 1092  | -5  | 6 | 4 | 648  | -608 | -5  | 6 | 4 | 648  | -608 |
| -2  | 13 | 3 | 964  | -572 | -4  | 0  | 4 | 1105 | 1006  | -2  | 2 | 4 | 1066 | -1014 | -2  | 4 | 4 | 858  | 815   | -4  | 6 | 4 | 526  | -485 | -4  | 6 | 4 | 526  | -485 |
| -1  | 13 | 3 | 190  | -194 | -2  | 0  | 4 | 2460 | 2436  | -1  | 2 | 4 | 231  | 170   | -1  | 4 | 4 | 652  | -655  | -3  | 6 | 4 | 562  | -532 | -3  | 6 | 4 | 562  | -532 |
| 0   | 13 | 3 | 272  | -273 | 0   | 0  | 4 | 740  | 796   | 0   | 2 | 4 | 542  | 559   | 0   | 4 | 4 | 341  | -626  | -2  | 6 | 4 | 600  | -764 | -2  | 6 | 4 | 600  | -764 |

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [MN(CO)3(DIPHOS)(HMBF3)], (C25H5)2CH3PO

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| H   | K | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  |
|-----|---|---|------|------|-----|----|---|------|------|-----|----|---|------|------|-----|----|---|------|-------|-----|---|---|------|-------|
| -1  | 6 | 4 | 336  | -340 | -11 | 9  | 4 | 354  | -335 | -4  | 11 | 4 | 453  | -428 | -4  | 15 | 4 | 205  | -228  | -3  | 1 | 5 | 2300 | -2153 |
| 0   | 6 | 4 | 484  | -447 | -9  | 9  | 4 | 551  | -532 | -3  | 15 | 4 | 438  | -787 | -3  | 15 | 4 | 170  | -182  | -2  | 1 | 5 | 523  | -528  |
| 1   | 6 | 4 | 682  | -705 | -8  | 9  | 4 | 510  | 487  | -1  | 11 | 4 | 154  | -167 | -2  | 15 | 4 | 274  | 396   | -1  | 1 | 5 | 1363 | -1417 |
| 2   | 6 | 4 | 157  | -244 | -6  | 9  | 4 | 865  | 513  | 4   | 11 | 4 | 521  | 579  | 0   | 15 | 4 | 238  | 277   | 2   | 1 | 5 | 448  | 464   |
| 3   | 6 | 4 | 270  | 250  | -5  | 9  | 4 | 452  | 492  | 5   | 11 | 4 | 180  | 161  | 3   | 15 | 4 | 168  | 160   | 3   | 1 | 5 | 164  | 216   |
| 10  | 6 | 4 | 258  | 153  | -4  | 9  | 4 | 913  | 831  | 7   | 11 | 4 | 404  | 393  | 8   | 15 | 4 | 187  | 168   | 4   | 1 | 5 | 249  | 213   |
| -11 | 6 | 4 | 461  | -407 | -3  | 9  | 4 | 887  | 823  | 8   | 11 | 4 | 153  | -177 | -5  | 18 | 4 | 163  | -180  | 5   | 1 | 5 | 324  | 258   |
| -13 | 7 | 4 | 316  | 334  | -2  | 9  | 4 | 324  | 318  | 9   | 11 | 4 | 250  | 271  | 0   | 18 | 4 | 256  | 224   | 6   | 1 | 5 | 157  | 187   |
| -11 | 7 | 4 | 265  | 220  | -7  | 9  | 4 | 368  | 387  | 10  | 11 | 4 | 178  | -218 | 1   | 16 | 4 | 344  | -351  | 8   | 1 | 5 | 136  | -133  |
| -9  | 7 | 4 | 277  | 315  | 0   | 9  | 4 | 214  | -230 | -10 | 12 | 4 | 187  | 179  | -6  | 17 | 4 | 289  | -230  | 9   | 1 | 5 | 261  | 288   |
| -8  | 7 | 4 | 435  | -406 | 1   | 9  | 4 | 263  | -265 | -9  | 12 | 4 | 213  | 166  | -5  | 17 | 4 | 180  | 130   | -10 | 2 | 5 | 257  | 293   |
| -6  | 7 | 4 | 308  | -274 | 2   | 9  | 4 | 380  | -409 | -5  | 12 | 4 | 375  | -369 | -4  | 17 | 4 | 225  | -275  | -10 | 2 | 5 | 156  | 113   |
| -5  | 7 | 4 | 477  | 449  | 3   | 9  | 4 | 220  | -225 | -2  | 12 | 4 | 582  | -584 | 0   | 17 | 4 | 148  | 44    | -9  | 2 | 5 | 703  | 688   |
| -4  | 7 | 4 | 557  | -459 | 5   | 9  | 4 | 425  | -491 | -1  | 12 | 4 | 218  | -200 | 4   | 17 | 4 | 198  | -316  | -8  | 2 | 5 | 234  | 239   |
| -3  | 7 | 4 | 680  | -654 | 6   | 9  | 4 | 248  | 274  | 1   | 12 | 4 | 220  | -257 | -9  | 18 | 4 | 357  | 253   | -7  | 2 | 5 | 475  | 459   |
| 1   | 7 | 4 | 120  | 111  | 7   | 9  | 4 | 174  | 195  | 2   | 12 | 4 | 289  | -312 | -1  | 18 | 4 | 341  | -350  | -6  | 2 | 5 | 160  | 192   |
| 2   | 7 | 4 | 122  | -139 | 8   | 9  | 4 | 275  | -244 | 3   | 12 | 4 | 347  | -385 | 1   | 18 | 4 | 180  | -173  | -5  | 2 | 5 | 169  | 150   |
| 3   | 7 | 4 | 272  | -313 | 9   | 9  | 4 | 383  | -388 | 5   | 12 | 4 | 230  | -239 | 5   | 18 | 4 | 224  | -213  | -4  | 2 | 5 | 278  | -273  |
| 5   | 7 | 4 | 327  | 360  | 10  | 9  | 4 | 244  | 214  | 10  | 12 | 4 | 290  | 184  | -3  | 19 | 4 | 486  | 504   | -2  | 2 | 5 | 409  | -402  |
| 8   | 7 | 4 | 150  | -123 | -12 | 10 | 4 | 200  | -191 | -8  | 13 | 4 | 357  | 346  | -1  | 19 | 4 | 236  | 392   | -1  | 2 | 5 | 1133 | -1204 |
| 9   | 7 | 4 | 333  | 292  | -11 | 10 | 4 | 174  | 172  | -7  | 13 | 4 | 251  | 255  | -11 | 0  | 5 | 189  | -181  | 0   | 2 | 5 | 355  | -377  |
| 11  | 7 | 4 | 378  | -386 | -10 | 10 | 4 | 384  | -386 | -6  | 13 | 4 | 274  | 279  | -9  | 0  | 5 | 923  | -1015 | 1   | 2 | 5 | 355  | -419  |
| -12 | 7 | 4 | 174  | -100 | -9  | 10 | 4 | 210  | -213 | -4  | 13 | 4 | 780  | 718  | -7  | 0  | 5 | 467  | -500  | 2   | 2 | 5 | 801  | -872  |
| -10 | 8 | 4 | 564  | 583  | -7  | 10 | 4 | 711  | -509 | -3  | 13 | 4 | 144  | -103 | -5  | 0  | 5 | 1036 | -868  | 3   | 2 | 5 | 968  | -617  |
| -9  | 8 | 4 | 417  | 385  | -5  | 10 | 4 | 732  | -658 | 7   | 13 | 4 | 386  | -371 | -3  | 0  | 5 | 512  | 495   | 6   | 2 | 5 | 134  | -73   |
| -8  | 8 | 4 | 177  | 145  | -4  | 10 | 4 | 467  | 436  | 9   | 13 | 4 | 231  | -228 | -1  | 0  | 5 | 367  | 374   | 7   | 2 | 5 | 173  | 168   |
| -6  | 8 | 4 | 418  | 434  | -2  | 10 | 4 | 847  | 815  | -10 | 14 | 4 | 328  | -310 | 1   | 0  | 5 | 195  | 212   | 8   | 2 | 5 | 234  | 207   |
| -5  | 8 | 4 | 214  | -202 | -1  | 10 | 4 | 844  | 773  | -8  | 14 | 4 | 301  | -284 | 3   | 0  | 5 | 722  | 675   | -10 | 3 | 5 | 392  | 440   |
| -4  | 8 | 4 | 188  | -479 | 1   | 10 | 4 | 232  | 249  | -7  | 14 | 4 | 299  | 333  | 7   | 0  | 5 | 408  | 343   | -9  | 3 | 5 | 183  | 186   |
| -2  | 8 | 4 | 695  | -657 | 5   | 10 | 4 | 136  | -122 | -5  | 14 | 4 | 185  | 183  | 11  | 0  | 5 | 522  | -527  | -8  | 3 | 5 | 525  | 509   |
| -1  | 8 | 4 | 202  | 212  | 8   | 10 | 4 | 226  | -126 | -4  | 14 | 4 | 284  | 244  | -12 | 1  | 5 | 152  | -164  | -7  | 3 | 5 | 319  | 311   |
| 2   | 8 | 4 | 537  | 543  | -10 | 11 | 4 | 267  | -336 | -3  | 14 | 4 | 261  | 245  | -11 | 1  | 5 | 473  | 536   | -5  | 3 | 5 | 328  | 289   |
| 5   | 8 | 4 | 275  | -274 | -8  | 11 | 4 | 343  | -348 | -2  | 14 | 4 | 911  | 892  | -9  | 1  | 5 | 379  | 354   | -4  | 3 | 5 | 954  | 478   |
| 6   | 8 | 4 | 215  | -167 | -7  | 11 | 4 | 284  | -261 | 4   | 14 | 4 | 300  | -373 | -8  | 1  | 5 | 102  | -141  | -3  | 3 | 5 | 666  | 631   |
| 8   | 8 | 4 | 454  | -463 | -6  | 11 | 4 | 257  | 265  | 7   | 14 | 4 | 147  | 83   | -5  | 1  | 5 | 567  | -570  | -1  | 3 | 5 | 134  | 150   |
| 11  | 8 | 4 | 330  | 281  | -5  | 11 | 4 | 229  | -202 | -8  | 15 | 4 | 260  | -287 | -4  | 1  | 5 | 462  | -428  | 0   | 3 | 5 | 176  | 158   |

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR LMN(CO)3(DIPHOS)(HOBFB)3, IC6H5I2CH3PO

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| H   | K | L | 10FO | 10FC | H   | K | L | 10FO | 10FC  | H   | K  | L | 10FO | 10FC | H  | K  | L | 10FO | 10FC  |
|-----|---|---|------|------|-----|---|---|------|-------|-----|----|---|------|------|----|----|---|------|-------|
| 1   | 3 | 5 | 462  | 537  | 4   | 5 | 5 | 115  | -116  | -6  | 11 | 5 | 207  | 165  | -1 | 15 | 5 | 392  | 365   |
| 2   | 3 | 5 | 236  | -262 | 7   | 5 | 5 | 194  | 170   | -5  | 8  | 5 | 261  | 257  | 2  | 15 | 5 | 293  | 348   |
| 3   | 3 | 5 | 234  | -221 | 8   | 5 | 5 | 352  | 394   | -4  | 8  | 5 | 543  | 526  | 5  | 15 | 5 | 208  | 205   |
| 4   | 3 | 5 | 369  | -350 | 9   | 5 | 5 | 416  | 428   | -3  | 8  | 5 | 375  | -353 | -2 | 15 | 5 | 289  | -261  |
| -12 | 4 | 5 | 248  | -275 | -11 | 6 | 5 | 229  | -191  | -2  | 8  | 5 | 605  | 554  | -1 | 11 | 5 | 547  | -518  |
| -10 | 4 | 5 | 365  | -408 | -10 | 6 | 5 | 405  | 481   | -1  | 8  | 5 | 165  | 180  | 0  | 11 | 5 | 159  | -169  |
| -9  | 4 | 5 | 355  | -361 | -9  | 6 | 5 | 140  | 181   | 1   | 8  | 5 | 222  | 333  | 1  | 11 | 5 | 156  | 109   |
| -8  | 4 | 5 | 146  | 164  | -6  | 6 | 5 | 307  | -281  | 3   | 8  | 5 | 355  | -376 | 2  | 11 | 5 | 221  | -198  |
| -7  | 4 | 5 | 215  | 163  | -4  | 6 | 5 | 1074 | -1028 | 4   | 8  | 5 | 520  | -519 | 3  | 11 | 5 | 250  | -267  |
| -6  | 4 | 5 | 274  | 268  | -2  | 6 | 5 | 1308 | -1164 | 5   | 8  | 5 | 352  | -372 | 5  | 11 | 5 | 285  | -319  |
| -5  | 4 | 5 | 307  | -317 | -1  | 6 | 5 | 109  | -46   | 7   | 8  | 5 | 229  | -205 | -9 | 12 | 5 | 151  | -72   |
| -4  | 4 | 5 | 724  | -853 | 0   | 6 | 5 | 332  | -313  | -11 | 9  | 5 | 147  | -163 | -7 | 12 | 5 | 343  | 341   |
| -3  | 4 | 5 | 325  | -318 | 1   | 6 | 5 | 522  | 558   | -10 | 9  | 5 | 362  | -396 | -5 | 12 | 5 | 344  | 405   |
| -2  | 4 | 5 | 850  | 772  | 2   | 6 | 5 | 116  | -112  | -8  | 9  | 5 | 369  | -389 | -1 | 12 | 5 | 654  | -707  |
| -1  | 4 | 5 | 319  | 325  | 3   | 6 | 5 | 251  | -254  | -5  | 9  | 5 | 313  | 279  | -6 | 0  | 6 | 390  | 361   |
| 0   | 4 | 5 | 164  | -155 | 4   | 6 | 5 | 228  | 229   | -3  | 9  | 5 | 339  | 321  | -4 | 0  | 6 | 1312 | -1227 |
| 2   | 4 | 5 | 795  | 815  | 7   | 6 | 5 | 236  | -174  | -2  | 9  | 5 | 491  | 450  | -2 | 0  | 6 | 948  | -1031 |
| 3   | 4 | 5 | 240  | 220  | 8   | 6 | 5 | 218  | 197   | -1  | 9  | 5 | 360  | 350  | 0  | 0  | 6 | 672  | -883  |
| 4   | 4 | 5 | 869  | 826  | -12 | 7 | 5 | 147  | 44    | 0   | 9  | 5 | 201  | 206  | 6  | 12 | 5 | 738  | -642  |
| 5   | 4 | 5 | 125  | -141 | -11 | 7 | 5 | 194  | -187  | 1   | 9  | 5 | 359  | 378  | 5  | 13 | 5 | 1164 | 1095  |
| 6   | 4 | 5 | 314  | -276 | -10 | 7 | 5 | 292  | 349   | 3   | 9  | 5 | 273  | 286  | -5 | 13 | 5 | 530  | 488   |
| 7   | 4 | 5 | 130  | 126  | -8  | 7 | 5 | 153  | 134   | 4   | 9  | 5 | 376  | 358  | -3 | 13 | 5 | 357  | 314   |
| 8   | 4 | 5 | 187  | -185 | -6  | 7 | 5 | 345  | 360   | 9   | 9  | 5 | 460  | -440 | -2 | 13 | 5 | 703  | 749   |
| 9   | 4 | 5 | 229  | 225  | -5  | 7 | 5 | 345  | -389  | 10  | 9  | 5 | 317  | -338 | -1 | 13 | 5 | 447  | 418   |
| -11 | 5 | 5 | 312  | -337 | -4  | 7 | 5 | 1305 | 1197  | -12 | 10 | 5 | 292  | 261  | 1  | 13 | 5 | 260  | 242   |
| -10 | 5 | 5 | 507  | -572 | -3  | 7 | 5 | 168  | -178  | -10 | 10 | 5 | 157  | 166  | 2  | 13 | 5 | 380  | -324  |
| -9  | 5 | 5 | 388  | -351 | -2  | 7 | 5 | 227  | -247  | -9  | 10 | 5 | 549  | -569 | 6  | 13 | 5 | 836  | -832  |
| -8  | 5 | 5 | 279  | -297 | 0   | 7 | 5 | 735  | -694  | -8  | 10 | 5 | 376  | -352 | -8 | 14 | 5 | 276  | -326  |
| -7  | 5 | 5 | 324  | -270 | 1   | 7 | 5 | 163  | 128   | -7  | 10 | 5 | 356  | -381 | 2  | 1  | 6 | 1102 | -1218 |
| -6  | 5 | 5 | 858  | -791 | 2   | 7 | 5 | 297  | -362  | -6  | 10 | 5 | 350  | -327 | 4  | 1  | 6 | 808  | -568  |
| -5  | 5 | 5 | 618  | 600  | 4   | 7 | 5 | 236  | -246  | -5  | 10 | 5 | 577  | -518 | 5  | 1  | 6 | 142  | -163  |
| -4  | 5 | 5 | 489  | 490  | 6   | 7 | 5 | 428  | 461   | -4  | 10 | 5 | 545  | -518 | 1  | 1  | 6 | 257  | 230   |
| -3  | 5 | 5 | 155  | 158  | 5   | 7 | 5 | 230  | 153   | 1   | 10 | 5 | 307  | 305  | 2  | 14 | 5 | 228  | -250  |
| -2  | 5 | 5 | 139  | 127  | -10 | 8 | 5 | 370  | -382  | 3   | 10 | 5 | 272  | 250  | 5  | 14 | 5 | 363  | -413  |
| 0   | 5 | 5 | 414  | 500  | -9  | 8 | 5 | 821  | 588   | 8   | 10 | 5 | 271  | 271  | -4 | 15 | 5 | 205  | 226   |
| 2   | 5 | 5 | 356  | -371 | -7  | 8 | 5 | 334  | 316   | -9  | 11 | 5 | 286  | 247  | -3 | 15 | 5 | 639  | 622   |

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [MN(CO)3(DIPHQS)(HDBF3)], (C6H5)2CH3PO

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| H   | K | L | 10FO | 10FC | H   | K | L | 10FO | 10FC  | H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC  | H   | K  | L | 10FO | 10FC  |
|-----|---|---|------|------|-----|---|---|------|-------|-----|----|---|------|------|-----|----|---|------|-------|-----|----|---|------|-------|
| 1   | 3 | 5 | 462  | 537  | 4   | 5 | 5 | 115  | -116  | -6  | 8  | 5 | 202  | -197 | -6  | 11 | 5 | 207  | 195   | -1  | 15 | 5 | 392  | 365   |
| 2   | 3 | 5 | 236  | -242 | 7   | 5 | 5 | 164  | 170   | -6  | 8  | 5 | 261  | 257  | -6  | 11 | 5 | 202  | -186  | 2   | 15 | 5 | 293  | 346   |
| 3   | 3 | 5 | 234  | -221 | 8   | 5 | 5 | 352  | 394   | -4  | 8  | 5 | 563  | 526  | -3  | 11 | 5 | 1058 | -1010 | 5   | 15 | 5 | 208  | 205   |
| 4   | 3 | 5 | 369  | -350 | 8   | 5 | 5 | 458  | 425   | -4  | 8  | 5 | 376  | -353 | -2  | 11 | 5 | 406  | -363  | -7  | 16 | 5 | 299  | -281  |
| -12 | 4 | 5 | 248  | -275 | -11 | 6 | 5 | 229  | -191  | -2  | 8  | 5 | 608  | 554  | -1  | 11 | 5 | 391  | -610  | -2  | 16 | 5 | 547  | -518  |
| -10 | 4 | 5 | 395  | -468 | -10 | 6 | 5 | 405  | 451   | -1  | 8  | 5 | 168  | 180  | 0   | 11 | 5 | 166  | -165  | 3   | 16 | 5 | 159  | -169  |
| -9  | 4 | 5 | 355  | -361 | -9  | 6 | 5 | 140  | 181   | 1   | 8  | 5 | 322  | 333  | 1   | 11 | 5 | 269  | -301  | -1  | 17 | 5 | 156  | 109   |
| -8  | 4 | 5 | 146  | 104  | -6  | 6 | 5 | 307  | -281  | 3   | 8  | 5 | 355  | -378 | 2   | 11 | 5 | 209  | -221  | 1   | 17 | 5 | 221  | -196  |
| -7  | 4 | 5 | 215  | 163  | -4  | 6 | 5 | 1074 | -1028 | 4   | 8  | 5 | 520  | -519 | 3   | 11 | 5 | 204  | 234   | 2   | 17 | 5 | 250  | -267  |
| -6  | 4 | 5 | 274  | 268  | -2  | 6 | 5 | 1301 | -1184 | 5   | 8  | 5 | 392  | -372 | 5   | 11 | 5 | 417  | 449   | 3   | 17 | 5 | 295  | -319  |
| -5  | 4 | 5 | 307  | -317 | -1  | 6 | 5 | 109  | -46   | 7   | 8  | 5 | 228  | -205 | -9  | 12 | 5 | 278  | 238   | 4   | 17 | 5 | 151  | -72   |
| -4  | 4 | 5 | 724  | 653  | 0   | 6 | 5 | 332  | -313  | -11 | 9  | 5 | 147  | -103 | -7  | 12 | 5 | 301  | 308   | -4  | 18 | 5 | 343  | 341   |
| -3  | 4 | 5 | 325  | -318 | 1   | 6 | 5 | 522  | 596   | -10 | 8  | 5 | 362  | -386 | -5  | 12 | 5 | 446  | 400   | -12 | 0  | 6 | 344  | 405   |
| -2  | 4 | 5 | 850  | 772  | 2   | 6 | 5 | 116  | -112  | -6  | 8  | 5 | 368  | -389 | -1  | 12 | 5 | 211  | -173  | -6  | 0  | 6 | 654  | -707  |
| -1  | 4 | 5 | 319  | 325  | 3   | 6 | 5 | 251  | -204  | -5  | 9  | 5 | 313  | 278  | 0   | 12 | 5 | 193  | 193   | -6  | 0  | 6 | 390  | -361  |
| 0   | 4 | 5 | 164  | -155 | 4   | 6 | 5 | 228  | 229   | -3  | 9  | 5 | 339  | 321  | 2   | 12 | 5 | 163  | -131  | -4  | 0  | 6 | 1319 | -1227 |
| 2   | 4 | 5 | 795  | 815  | 7   | 6 | 5 | 236  | -174  | -2  | 9  | 5 | 491  | 450  | 3   | 12 | 5 | 556  | -654  | -2  | 0  | 6 | 948  | -1031 |
| 3   | 4 | 5 | 240  | 270  | 8   | 6 | 5 | 218  | 197   | -1  | 8  | 5 | 380  | 350  | 4   | 12 | 5 | 415  | -478  | 0   | 0  | 6 | 672  | -663  |
| 4   | 4 | 5 | 569  | 526  | -12 | 7 | 5 | 147  | 44    | 0   | 9  | 5 | 201  | 206  | 6   | 12 | 5 | 248  | -309  | 2   | 0  | 6 | 738  | -642  |
| 5   | 4 | 5 | 125  | -141 | -11 | 7 | 5 | 164  | -187  | 1   | 9  | 5 | 359  | 378  | -11 | 13 | 5 | 352  | -350  | 4   | 0  | 6 | 1164 | 1095  |
| 8   | 4 | 5 | 314  | -276 | -10 | 7 | 5 | 292  | 349   | 3   | 9  | 5 | 273  | 245  | -5  | 13 | 5 | 151  | 95    | 6   | 0  | 6 | 530  | 486   |
| 0   | 4 | 5 | 150  | 126  | -6  | 7 | 5 | 163  | 134   | 4   | 9  | 5 | 376  | 398  | -3  | 13 | 5 | 457  | 908   | 8   | 0  | 6 | 357  | 314   |
| -10 | 4 | 5 | 162  | -185 | -6  | 7 | 5 | 346  | 350   | 5   | 9  | 5 | 460  | -440 | -2  | 13 | 5 | 209  | 158   | -10 | 1  | 6 | 703  | 749   |
| -11 | 5 | 5 | 225  | 225  | -5  | 7 | 5 | 345  | -288  | 10  | 9  | 5 | 317  | -336 | -1  | 13 | 5 | 325  | 394   | -8  | 1  | 6 | 447  | 418   |
| -10 | 5 | 5 | 312  | -337 | -4  | 7 | 5 | 1305 | 1197  | -12 | 10 | 5 | 292  | 291  | 1   | 13 | 5 | 335  | 356   | -6  | 1  | 6 | 280  | 242   |
| -8  | 5 | 5 | 507  | -572 | -3  | 7 | 5 | 168  | -178  | -10 | 10 | 5 | 157  | 168  | -2  | 13 | 5 | 200  | 342   | -3  | 1  | 6 | 360  | -324  |
| -7  | 5 | 5 | 384  | -351 | -2  | 7 | 5 | 227  | -247  | -9  | 10 | 5 | 548  | -569 | 6   | 13 | 5 | 357  | -337  | -2  | 1  | 6 | 836  | -832  |
| -6  | 5 | 5 | 278  | -287 | 0   | 7 | 5 | 735  | -694  | -8  | 10 | 5 | 376  | -342 | -8  | 14 | 5 | 362  | -360  | 0   | 1  | 6 | 270  | -326  |
| -5  | 5 | 5 | 324  | -270 | 1   | 7 | 5 | 163  | 128   | -7  | 10 | 5 | 388  | -381 | -7  | 14 | 5 | 168  | -137  | 2   | 1  | 6 | 1102 | -1218 |
| -4  | 5 | 5 | 858  | -791 | 2   | 7 | 5 | 297  | -362  | -6  | 10 | 5 | 350  | -327 | -2  | 14 | 5 | 191  | 174   | 4   | 1  | 6 | 608  | -568  |
| -3  | 5 | 5 | 619  | 600  | 4   | 7 | 5 | 236  | -246  | -5  | 10 | 5 | 577  | -518 | 1   | 14 | 5 | 209  | -172  | 5   | 1  | 6 | 142  | -163  |
| -2  | 5 | 5 | 499  | 490  | 6   | 7 | 5 | 426  | 461   | -4  | 10 | 5 | 545  | -516 | 2   | 14 | 5 | 209  | 303   | 10  | 1  | 6 | 257  | 230   |
| -1  | 5 | 5 | 188  | 158  | 9   | 7 | 5 | 230  | 153   | 1   | 10 | 5 | 307  | 305  | 4   | 14 | 5 | 155  | 238   | -13 | 2  | 6 | 228  | -250  |
| 0   | 5 | 5 | 139  | 127  | -10 | 8 | 5 | 370  | -382  | 3   | 10 | 5 | 272  | 260  | 5   | 14 | 5 | 209  | 181   | -10 | 2  | 6 | 383  | -413  |
| 2   | 5 | 5 | 414  | 500  | -9  | 8 | 5 | 621  | 586   | 8   | 10 | 5 | 271  | 271  | -4  | 15 | 5 | 380  | -356  | -9  | 2  | 6 | 205  | 226   |
| 3   | 5 | 5 | 366  | -371 | -7  | 8 | 5 | 334  | 316   | -9  | 11 | 5 | 266  | 247  | -3  | 15 | 5 | 350  | -315  | -8  | 2  | 6 | 639  | 622   |



## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [MnClO3(DIPHOS)](HOBFF3)1.1234512CH3FO

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| H   | K | L | 10FO | 10FC | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC  |
|-----|---|---|------|------|-----|---|---|------|-------|-----|---|---|------|------|-----|----|---|------|------|-----|----|---|------|-------|
| -7  | 2 | 8 | 183  | 187  | 1   | 4 | 6 | 803  | 863   | -4  | 7 | 6 | 125  | -111 | 3   | 8  | 5 | 434  | 527  | -6  | 14 | 6 | 185  | -84   |
| -6  | 2 | 6 | 626  | 617  | 3   | 4 | 5 | 839  | 848   | -3  | 7 | 5 | 841  | 853  | 4   | 9  | 8 | 508  | 507  | -2  | 14 | 6 | 299  | -277  |
| -5  | 2 | 6 | 670  | 606  | 4   | 4 | 6 | 433  | 458   | -1  | 7 | 6 | 235  | 240  | 5   | 9  | 7 | 543  | 543  | 1   | 14 | 6 | 191  | 185   |
| -4  | 2 | 6 | 851  | 891  | 8   | 4 | 6 | 189  | 176   | 0   | 7 | 6 | 301  | -286 | 7   | 9  | 6 | 181  | 112  | 3   | 14 | 6 | 342  | 396   |
| -2  | 2 | 6 | 111  | 125  | -11 | 5 | 6 | 194  | 228   | 2   | 7 | 6 | 268  | -274 | -9  | 10 | 6 | 291  | 325  | 5   | 14 | 6 | 324  | 338   |
| -1  | 2 | 6 | 408  | -413 | -10 | 5 | 6 | 187  | 221   | 3   | 7 | 6 | 517  | -612 | -8  | 10 | 6 | 484  | -440 | 6   | 14 | 6 | 196  | 207   |
| 0   | 2 | 6 | 211  | -193 | -7  | 5 | 6 | 275  | -270  | 5   | 7 | 6 | 198  | -149 | -6  | 10 | 6 | 153  | -177 | -5  | 15 | 6 | 304  | -302  |
| 1   | 2 | 6 | 238  | -257 | -6  | 5 | 6 | 152  | 156   | 7   | 7 | 5 | 185  | 177  | -5  | 10 | 6 | 398  | 330  | -4  | 15 | 6 | 263  | 223   |
| 2   | 2 | 6 | 488  | -488 | -5  | 5 | 6 | 427  | -393  | 9   | 7 | 6 | 297  | -276 | -4  | 10 | 6 | 583  | -589 | 0   | 15 | 6 | 206  | 210   |
| 3   | 2 | 6 | 405  | -39  | -4  | 5 | 6 | 255  | 255   | 10  | 7 | 6 | 175  | -171 | -   | 10 | 6 | 493  | -482 | 2   | 15 | 6 | 381  | -382  |
| 4   | 2 | 6 | 628  | -665 | -3  | 5 | 6 | 1268 | -1138 | -9  | 6 | 6 | 357  | -355 | 1   | 10 | 6 | 811  | -610 | 4   | 16 | 6 | 223  | -237  |
| 5   | 2 | 6 | 375  | -301 | -2  | 5 | 6 | 448  | 396   | -8  | 6 | 6 | 168  | 215  | 3   | 10 | 6 | 651  | -713 | -5  | 17 | 6 | 250  | 274   |
| -12 | 3 | 6 | 213  | 275  | 1   | 5 | 6 | 280  | -281  | -7  | 8 | 6 | 185  | -183 | 7   | 10 | 6 | 257  | 268  | -13 | 0  | 7 | 259  | -273  |
| -10 | 3 | 6 | 263  | -273 | 2   | 5 | 6 | 308  | -322  | -6  | 8 | 6 | 243  | 231  | 8   | 10 | 6 | 254  | 331  | -9  | 0  | 7 | 408  | 469   |
| -8  | 3 | 6 | 151  | -39  | 3   | 6 | 6 | 211  | 249   | -5  | 8 | 6 | 354  | -298 | -9  | 10 | 6 | 224  | 229  | -5  | 0  | 7 | 226  | 184   |
| -6  | 3 | 6 | 172  | -186 | 5   | 5 | 6 | 466  | 478   | -4  | 8 | 6 | 647  | 634  | -10 | 11 | 6 | 186  | 176  | -3  | 0  | 7 | 239  | -238  |
| -5  | 3 | 6 | 244  | 223  | 7   | 5 | 6 | 439  | 474   | -3  | 8 | 6 | 480  | 470  | -6  | 11 | 6 | 270  | 250  | -1  | 0  | 7 | 457  | -457  |
| -3  | 3 | 6 | 619  | 573  | 8   | 5 | 6 | 198  | 202   | -2  | 8 | 6 | 280  | 249  | -5  | 11 | 6 | 225  | -220 | 1   | 0  | 7 | 1316 | -1362 |
| -2  | 3 | 6 | 1249 | 1151 | 10  | 5 | 6 | 219  | 144   | -1  | 8 | 6 | 160  | 137  | -4  | 11 | 6 | 368  | -335 | 2   | 0  | 7 | 350  | -320  |
| -1  | 3 | 6 | 346  | 314  | -13 | 6 | 6 | 211  | -138  | 0   | 8 | 6 | 512  | 532  | -2  | 11 | 6 | 560  | -560 | 7   | 0  | 7 | 143  | -46   |
| 0   | 3 | 6 | 282  | 284  | -9  | 6 | 6 | 536  | 544   | 1   | 8 | 6 | 264  | 289  | 0   | 12 | 6 | 181  | -184 | -11 | 1  | 7 | 232  | -214  |
| 1   | 3 | 6 | 477  | 573  | -6  | 6 | 6 | 625  | -614  | 2   | 8 | 6 | 221  | 253  | 1   | 11 | 6 | 208  | 253  | -8  | 1  | 7 | 308  | 327   |
| 2   | 3 | 6 | 515  | 518  | -5  | 6 | 6 | 257  | -225  | 3   | 8 | 6 | 374  | 403  | 1   | 11 | 6 | 227  | -223 | -6  | 1  | 7 | 235  | 256   |
| 3   | 3 | 6 | 265  | -263 | -4  | 6 | 6 | 396  | -383  | 4   | 8 | 6 | 256  | -276 | -10 | 12 | 6 | 202  | -203 | -5  | 1  | 7 | 1134 | 1084  |
| 7   | 3 | 6 | 290  | -257 | -3  | 6 | 6 | 657  | -648  | -5  | 8 | 6 | 265  | -260 | -8  | 12 | 6 | 156  | 76   | -4  | 1  | 7 | 283  | -266  |
| 8   | 3 | 6 | 207  | 152  | -2  | 6 | 6 | 298  | 300   | -7  | 8 | 6 | 580  | -544 | -5  | 12 | 6 | 429  | -446 | -3  | 1  | 7 | 623  | 625   |
| 9   | 3 | 6 | 237  | -233 | 0   | 6 | 6 | 308  | 234   | 7   | 8 | 6 | 188  | 182  | -4  | 12 | 6 | 708  | 685  | -1  | 1  | 7 | 142  | -171  |
| 11  | 3 | 6 | 168  | 130  | 1   | 6 | 6 | 139  | -102  | 6   | 8 | 6 | 333  | -347 | -3  | 12 | 6 | 244  | 213  | 2   | 1  | 7 | 225  | -211  |
| -11 | 4 | 6 | 221  | -228 | 2   | 6 | 6 | 472  | 509   | 9   | 8 | 6 | 264  | -210 | 0   | 12 | 6 | 134  | -75  | 3   | 1  | 7 | 1063 | -1033 |
| -9  | 4 | 6 | 153  | -156 | 3   | 6 | 6 | 441  | -442  | -11 | 9 | 6 | 228  | 203  | 2   | 12 | 6 | 181  | -133 | 4   | 1  | 7 | 254  | -252  |
| -8  | 4 | 6 | 143  | -170 | 7   | 8 | 6 | 233  | -237  | -5  | 9 | 6 | 310  | -281 | 3   | 12 | 6 | 280  | -322 | 5   | 1  | 7 | 436  | -466  |
| -6  | 4 | 6 | 307  | 326  | 8   | 8 | 6 | 206  | -102  | -3  | 9 | 6 | 594  | -547 | -2  | 13 | 6 | 423  | 396  | 7   | 1  | 7 | 373  | -354  |
| -4  | 4 | 6 | 282  | -368 | 5   | 6 | 6 | 164  | -93   | -2  | 9 | 6 | 196  | -224 | -1  | 15 | 6 | 384  | 391  | 10  | 1  | 7 | 302  | 266   |
| -2  | 4 | 6 | 787  | -692 | -11 | 7 | 6 | 431  | -444  | -1  | 9 | 6 | 209  | -225 | 1   | 13 | 6 | 261  | 325  | -13 | 2  | 7 | 278  | 264   |
| -1  | 4 | 6 | 450  | -389 | -7  | 7 | 6 | 393  | 432   | 0   | 9 | 6 | 264  | 261  | 2   | 13 | 6 | 478  | 531  | -11 | 2  | 7 | 295  | -340  |
| 0   | 4 | 6 | 200  | 221  | -5  | 7 | 6 | 1004 | -978  | 2   | 9 | 6 | 448  | 484  | 7   | 13 | 6 | 175  | -170 | -5  | 2  | 7 | 242  | -299  |

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [MNFeO]3[SiO4]3[OHFe3]11[CaH5]2[CH3PO]

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| H   | K | L | 10FO | 10FC | H   | K | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K | L | 10FO | 10FC |
|-----|---|---|------|------|-----|---|---|------|------|-----|----|---|------|------|-----|----|---|------|------|-----|---|---|------|------|
| -8  | 2 | 7 | 259  | 248  | 2   | 5 | 7 | 495  | -496 | 8   | 8  | 7 | 450  | 431  | -5  | 13 | 7 | 202  | -233 | -12 | 2 | 8 | 317  | 355  |
| -6  | 2 | 7 | 219  | -190 | 3   | 5 | 7 | 322  | -333 | -10 | 9  | 7 | 240  | 262  | -3  | 13 | 7 | 282  | -267 | -9  | 2 | 8 | 192  | 179  |
| -3  | 2 | 7 | 576  | 557  | 4   | 5 | 7 | 143  | 222  | -7  | 9  | 7 | 157  | 183  | 0   | 13 | 7 | 192  | 236  | -8  | 2 | 8 | 265  | 232  |
| -2  | 2 | 7 | 282  | -248 | 5   | 5 | 7 | 167  | 161  | -6  | 9  | 7 | 391  | 384  | 2   | 13 | 7 | 161  | 203  | -6  | 2 | 8 | 371  | -326 |
| -1  | 2 | 7 | 207  | -180 | 6   | 5 | 7 | 317  | 242  | -5  | 9  | 7 | 225  | -180 | 3   | 13 | 7 | 372  | 385  | -5  | 2 | 8 | 201  | -155 |
| 1   | 2 | 7 | 606  | 659  | 8   | 5 | 7 | 332  | 256  | -3  | 9  | 7 | 132  | -100 | 5   | 13 | 7 | 266  | 251  | -4  | 2 | 8 | 439  | -445 |
| 3   | 2 | 7 | 341  | 327  | 9   | 5 | 7 | 160  | 118  | -2  | 8  | 7 | 283  | -268 | -7  | 14 | 7 | 195  | 190  | -1  | 2 | 8 | 219  | 219  |
| 6   | 2 | 7 | 409  | -356 | -12 | 6 | 7 | 366  | -392 | -1  | 9  | 7 | 171  | -173 | -5  | 14 | 7 | 236  | 243  | 0   | 2 | 8 | 131  | -136 |
| 8   | 2 | 7 | 308  | -256 | -9  | 6 | 7 | 321  | 303  | 0   | 9  | 7 | 403  | -377 | -3  | 14 | 7 | 228  | -211 | 1   | 2 | 8 | 245  | 292  |
| 9   | 2 | 7 | 396  | -326 | -7  | 6 | 7 | 226  | -244 | 2   | 5  | 7 | 267  | -271 | 1   | 14 | 7 | 295  | -324 | 2   | 2 | 8 | 825  | 883  |
| -11 | 3 | 7 | 270  | 332  | -5  | 6 | 7 | 518  | -505 | 3   | 9  | 7 | 358  | 362  | -7  | 15 | 7 | 202  | -181 | 3   | 2 | 8 | 241  | -204 |
| -9  | 3 | 7 | 402  | -359 | -4  | 6 | 7 | 650  | 619  | 6   | 9  | 7 | 158  | 85   | -5  | 15 | 7 | 178  | -135 | 4   | 2 | 8 | 249  | 206  |
| -5  | 3 | 7 | 544  | -565 | -3  | 6 | 7 | 289  | -301 | -10 | 10 | 7 | 186  | -174 | -3  | 15 | 7 | 415  | 413  | 5   | 2 | 8 | 272  | -287 |
| -2  | 3 | 7 | 273  | 266  | -2  | 6 | 7 | 304  | -283 | -4  | 10 | 7 | 700  | 699  | -3  | 15 | 7 | 196  | -193 | 6   | 2 | 8 | 379  | 365  |
| -1  | 3 | 7 | 580  | 565  | 2   | 6 | 7 | 170  | -223 | -3  | 10 | 7 | 525  | -481 | -4  | 16 | 7 | 184  | 95   | 7   | 2 | 8 | 238  | -180 |
| 0   | 3 | 7 | 122  | 125  | 4   | 6 | 7 | 512  | -480 | 0   | 10 | 7 | 196  | 93   | -12 | 0  | 8 | 516  | -594 | -11 | 3 | 8 | 237  | 218  |
| 2   | 3 | 7 | 742  | 828  | 5   | 6 | 7 | 328  | -313 | 1   | 10 | 7 | 441  | -482 | -10 | 0  | 8 | 474  | -514 | -9  | 3 | 8 | 251  | 202  |
| 3   | 3 | 7 | 505  | 537  | 8   | 6 | 7 | 463  | -406 | 2   | 10 | 7 | 448  | -488 | -8  | 0  | 8 | 225  | -208 | -8  | 3 | 8 | 190  | -198 |
| 5   | 3 | 7 | 151  | 152  | -10 | 7 | 7 | 495  | -521 | 3   | 10 | 7 | 205  | -233 | -6  | 0  | 8 | 675  | 634  | -5  | 3 | 8 | 272  | -237 |
| 7   | 3 | 7 | 470  | 446  | -7  | 7 | 7 | 219  | 259  | 4   | 10 | 7 | 327  | -366 | -4  | 6  | 8 | 319  | 850  | -4  | 3 | 8 | 368  | -406 |
| 9   | 3 | 7 | 211  | 202  | -6  | 7 | 7 | 186  | 225  | 5   | 10 | 7 | 281  | 248  | 7   | 0  | 8 | 363  | -344 | -3  | 3 | 8 | 247  | 203  |
| -13 | 4 | 7 | 238  | -282 | -4  | 7 | 7 | 562  | 546  | -9  | 11 | 7 | 185  | 226  | 4   | 0  | 8 | 299  | -325 | -2  | 3 | 8 | 229  | -247 |
| -10 | 4 | 7 | 142  | 29   | -3  | 7 | 7 | 123  | -123 | -8  | 11 | 7 | 274  | -282 | 6   | 0  | 8 | 576  | -591 | 0   | 3 | 8 | 326  | -363 |
| -4  | 4 | 7 | 521  | -497 | -2  | 7 | 7 | 244  | 173  | -6  | 11 | 7 | 308  | -284 | 8   | 0  | 8 | 384  | -367 | 1   | 3 | 8 | 362  | 403  |
| -3  | 4 | 7 | 321  | -328 | 0   | 7 | 7 | 170  | 124  | -5  | 11 | 7 | 168  | 153  | -7  | 1  | 8 | 297  | -177 | 2   | 3 | 8 | 195  | -200 |
| -2  | 4 | 7 | 125  | -165 | 2   | 7 | 7 | 507  | 517  | 2   | 11 | 7 | 274  | 271  | -5  | 1  | 8 | 570  | -557 | 3   | 3 | 8 | 322  | 295  |
| 1   | 4 | 7 | 343  | -341 | 6   | 7 | 7 | 148  | 135  | 3   | 11 | 7 | 357  | -406 | -5  | 1  | 8 | 161  | 124  | 4   | 3 | 8 | 561  | 578  |
| 2   | 4 | 7 | 515  | 576  | 7   | 7 | 7 | 162  | -136 | 4   | 11 | 7 | 242  | -264 | -4  | 1  | 8 | 231  | 206  | 5   | 3 | 8 | 175  | 203  |
| 3   | 4 | 7 | 340  | -357 | 8   | 7 | 7 | 249  | -276 | 5   | 11 | 7 | 265  | -293 | 0   | 1  | 8 | 224  | 256  | 6   | 3 | 8 | 336  | 308  |
| 4   | 4 | 7 | 574  | 556  | -12 | 8 | 7 | 301  | 262  | 7   | 11 | 7 | 347  | -365 | 1   | 1  | 8 | 136  | -133 | 7   | 3 | 8 | 308  | 281  |
| 5   | 4 | 7 | 223  | 226  | -6  | 8 | 7 | 345  | -344 | -9  | 12 | 7 | 232  | -204 | 2   | 1  | 8 | 136  | 113  | 8   | 3 | 8 | 410  | 396  |
| -10 | 5 | 7 | 223  | 222  | -4  | 8 | 7 | 720  | -725 | -4  | 12 | 7 | 447  | -432 | 3   | 1  | 8 | 275  | -248 | -13 | 4 | 8 | 301  | -334 |
| -7  | 5 | 7 | 172  | -177 | -1  | 8 | 7 | 525  | 499  | -3  | 12 | 7 | 310  | 334  | 4   | 1  | 8 | 320  | -356 | -11 | 4 | 8 | 176  | 147  |
| -2  | 5 | 7 | 378  | -346 | 3   | 8 | 7 | 531  | 550  | 0   | 12 | 7 | 177  | -184 | 5   | 1  | 8 | 152  | -120 | -8  | 4 | 8 | 171  | 192  |
| 0   | 5 | 7 | 284  | -369 | 4   | 8 | 7 | 256  | 259  | 1   | 12 | 7 | 186  | 180  | 7   | 1  | 8 | 162  | -170 | -7  | 4 | 8 | 188  | 202  |
| 1   | 5 | 7 | 174  | 172  | 5   | 8 | 7 | 335  | -315 | -8  | 13 | 7 | 199  | -132 | 8   | 1  | 8 | 226  | -190 | -6  | 4 | 8 | 337  | 330  |

| H   | K | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K  | L | 10FO | 10FC | H   | K  | L  | 10FO | 10FC |
|-----|---|---|------|------|-----|----|---|------|------|-----|----|---|------|------|-----|----|---|------|------|-----|----|----|------|------|
| -5  | 4 | 8 | 143  | -34  | -6  | 8  | 8 | 179  | 207  | 2   | 15 | 8 | 218  | 181  | -1  | 4  | 9 | 275  | 302  | -8  | 12 | 9  | 178  | 148  |
| -4  | 4 | 8 | 173  | 180  | 0   | 8  | 8 | 413  | 443  | -11 | 0  | 9 | 397  | -362 | 3   | 4  | 9 | 284  | -315 | -7  | 12 | 9  | 286  | 279  |
| -3  | 4 | 8 | 548  | -507 | 1   | 8  | 8 | 476  | -508 | -7  | 0  | 8 | 470  | -419 | 6   | 4  | 9 | 262  | -247 | -3  | 12 | 9  | 233  | -179 |
| -2  | 4 | 8 | 230  | -182 | 2   | 4  | 8 | 174  | 152  | -3  | 0  | 8 | 254  | -279 | 7   | 4  | 9 | 277  | -212 | -1  | 12 | 9  | 151  | -145 |
| -1  | 4 | 8 | 258  | -243 | 5   | 8  | 8 | 199  | 271  | -1  | 0  | 8 | 249  | -461 | -8  | 5  | 9 | 200  | -199 | 2   | 12 | 9  | 195  | -247 |
| 0   | 4 | 8 | 158  | -167 | -10 | 9  | 8 | 203  | 187  | 7   | 0  | 9 | 486  | -437 | -6  | 5  | 9 | 265  | -284 | 3   | 12 | 9  | 215  | 183  |
| 2   | 4 | 8 | 367  | -386 | -8  | 8  | 8 | 183  | 199  | -11 | 1  | 9 | 231  | 227  | -2  | 5  | 9 | 191  | -169 | -5  | 13 | 9  | 330  | 319  |
| 3   | 4 | 8 | 316  | 335  | -5  | 9  | 8 | 600  | 599  | -9  | 1  | 9 | 256  | 259  | 8   | 5  | 9 | 230  | -142 | -2  | 13 | 9  | 181  | 148  |
| 4   | 4 | 8 | 222  | -224 | -4  | 9  | 8 | 366  | -335 | -5  | 1  | 9 | 368  | -350 | -10 | 6  | 9 | 198  | 132  | -1  | 13 | 9  | 204  | 183  |
| 6   | 4 | 8 | 213  | -218 | -2  | 8  | 8 | 282  | -317 | -4  | 1  | 8 | 221  | 204  | -8  | 6  | 9 | 220  | 290  | 0   | 13 | 9  | 273  | 295  |
| 7   | 4 | 8 | 177  | 61   | 0   | 9  | 8 | 212  | -164 | -1  | 1  | 8 | 351  | -358 | -5  | 6  | 9 | 293  | -212 | 1   | 14 | 9  | 209  | 184  |
| 9   | 4 | 8 | 392  | 309  | 3   | 9  | 8 | 258  | -257 | 1   | 1  | 9 | 491  | 318  | -5  | 8  | 9 | 288  | -257 | -8  | 0  | 10 | 165  | 188  |
| -5  | 5 | 8 | 375  | -342 | -9  | 10 | 8 | 217  | -222 | 7   | 1  | 9 | 184  | 153  | -4  | 8  | 9 | 219  | -204 | -8  | 0  | 10 | 497  | -479 |
| -5  | 5 | 8 | 455  | 507  | -7  | 10 | 8 | 351  | -357 | -8  | 2  | 9 | 250  | 258  | -2  | 8  | 9 | 244  | -271 | -4  | 0  | 10 | 530  | -523 |
| -4  | 5 | 8 | 327  | 288  | -3  | 10 | 8 | 473  | 489  | -7  | 2  | 9 | 515  | 488  | 1   | 8  | 9 | 170  | -170 | -2  | 0  | 10 | 434  | -418 |
| -2  | 5 | 8 | 357  | 334  | -2  | 10 | 8 | 293  | -279 | -6  | 2  | 9 | 251  | -252 | 2   | 8  | 9 | 334  | 330  | 2   | 0  | 10 | 273  | 274  |
| 3   | 5 | 8 | 331  | -370 | -1  | 10 | 8 | 200  | 150  | -4  | 2  | 9 | 361  | -402 | 6   | 8  | 9 | 255  | 214  | 6   | 0  | 10 | 171  | -83  |
| 4   | 5 | 8 | 272  | -280 | 0   | 10 | 8 | 178  | -241 | -3  | 2  | 9 | 157  | -153 | -8  | 7  | 9 | 385  | 357  | -8  | 1  | 10 | 436  | 427  |
| 6   | 5 | 8 | 334  | 272  | 1   | 10 | 8 | 204  | 184  | -1  | 2  | 9 | 339  | -372 | -6  | 7  | 9 | 700  | 674  | -6  | 1  | 10 | 288  | 306  |
| 7   | 5 | 8 | 396  | -382 | 2   | 10 | 8 | 234  | -271 | 1   | 2  | 9 | 268  | -253 | -4  | 7  | 9 | 149  | 144  | -3  | 1  | 10 | 225  | 249  |
| -11 | 6 | 8 | 174  | -218 | -4  | 10 | 8 | 148  | -182 | 3   | 2  | 9 | 417  | 408  | 0   | 7  | 9 | 187  | -189 | 0   | 1  | 10 | 427  | -446 |
| -9  | 6 | 8 | 187  | 144  | -8  | 11 | 8 | 233  | 257  | 7   | 2  | 9 | 227  | 249  | 2   | 7  | 9 | 163  | 208  | 1   | 1  | 10 | 158  | -176 |
| -6  | 6 | 8 | 431  | -405 | -5  | 11 | 8 | 611  | -608 | -8  | 3  | 9 | 302  | -334 | 4   | 7  | 9 | 236  | 254  | 6   | 1  | 10 | 285  | 234  |
| 1   | 6 | 8 | 287  | 274  | -2  | 11 | 8 | 192  | 101  | -8  | 3  | 9 | 312  | 273  | -6  | 8  | 9 | 508  | 530  | -6  | 2  | 10 | 410  | 406  |
| 4   | 6 | 8 | 213  | -200 | 0   | 11 | 8 | 241  | 212  | -8  | 3  | 9 | 409  | 402  | 2   | 8  | 9 | 392  | -409 | 2   | 2  | 10 | 199  | -184 |
| 8   | 6 | 8 | 183  | 225  | 6   | 11 | 8 | 261  | -187 | -5  | 3  | 9 | 448  | 439  | -7  | 8  | 9 | 218  | 180  | 3   | 2  | 10 | 268  | -243 |
| 9   | 6 | 8 | 280  | -218 | -4  | 12 | 8 | 285  | -275 | -2  | 3  | 9 | 158  | -63  | -3  | 8  | 9 | 216  | -235 | 5   | 2  | 10 | 170  | -115 |
| -7  | 7 | 8 | 550  | 544  | -3  | 12 | 8 | 208  | -211 | -1  | 3  | 9 | 259  | -325 | -7  | 10 | 9 | 214  | -184 | -6  | 3  | 10 | 214  | -218 |
| -7  | 7 | 8 | 138  | 46   | 1   | 12 | 8 | 203  | -213 | 1   | 3  | 9 | 473  | -488 | -6  | 10 | 9 | 215  | -184 | -7  | 3  | 10 | 261  | 266  |
| -1  | 7 | 8 | 163  | -160 | 4   | 12 | 8 | 216  | 273  | 3   | 3  | 9 | 237  | -224 | -3  | 10 | 9 | 175  | -152 | -6  | 3  | 10 | 214  | 217  |
| 1   | 7 | 8 | 191  | 180  | -4  | 14 | 8 | 274  | 308  | 7   | 3  | 9 | 222  | 91   | 3   | 10 | 9 | 231  | -172 | -5  | 3  | 10 | 259  | 244  |
| 3   | 7 | 8 | 430  | 436  | 2   | 14 | 8 | 235  | -255 | -12 | 4  | 9 | 240  | -262 | 5   | 10 | 9 | 185  | -160 | -3  | 3  | 10 | 232  | 192  |
| 5   | 7 | 8 | 312  | 281  | -6  | 15 | 8 | 266  | -245 | -8  | 4  | 9 | 165  | -167 | -5  | 11 | 9 | 486  | -538 | -1  | 3  | 10 | 369  | 410  |
| 6   | 7 | 8 | 204  | -200 | -3  | 15 | 8 | 171  | 159  | -7  | 4  | 9 | 337  | -341 | -4  | 11 | 9 | 353  | -336 | -11 | 4  | 10 | 228  | -234 |
| 7   | 7 | 8 | 268  | 240  | 0   | 15 | 8 | 196  | 169  | -5  | 4  | 9 | 235  | 220  | 0   | 11 | 9 | 226  | -239 | -10 | 4  | 10 | 282  | -299 |
| -7  | 8 | 8 | 332  | 308  | 1   | 15 | 8 | 177  | -84  | -3  | 4  | 9 | 273  | 273  | 3   | 11 | 9 | 189  | 261  | -7  | 4  | 10 | 372  | -363 |



## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [Mn(CO)3(DIPHOS)(HOBF3)], (C6H5)2CH3FO

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| H  | K | L  | 10FO | 10FC | H  | K  | L  | 10FO | 10FC | H  | K | L  | 10FO | 10FC | H  | K  | L  | 10FO | 10FC | H  | K | L  | 10FO | 10FC |
|----|---|----|------|------|----|----|----|------|------|----|---|----|------|------|----|----|----|------|------|----|---|----|------|------|
| -3 | 4 | 10 | 180  | -225 | -5 | 7  | 10 | 344  | 335  | 1  | 1 | 11 | 267  | -243 | 5  | 3  | 11 | 340  | 315  | -8 | 0 | 12 | 247  | 255  |
| -1 | 4 | 10 | 423  | 443  | 0  | 8  | 10 | 221  | 174  | 1  | 1 | 11 | 243  | -266 | -6 | 4  | 11 | 446  | -430 | -3 | 1 | 12 | 180  | 157  |
| 1  | 4 | 10 | 441  | 436  | 1  | 9  | 10 | 430  | 223  | 3  | 1 | 11 | 188  | -179 | -1 | 4  | 11 | 313  | -240 | -2 | 1 | 12 | 207  | 203  |
| 6  | 4 | 10 | 250  | 260  | -4 | 10 | 10 | 419  | -272 | 5  | 1 | 11 | 177  | -231 | -2 | 5  | 11 | 203  | -177 | 0  | 2 | 12 | 247  | 246  |
| -7 | 5 | 10 | 493  | -327 | -2 | 10 | 10 | 273  | -285 | -6 | 2 | 11 | 221  | 184  | 0  | 5  | 11 | 219  | -208 | -7 | 3 | 12 | 273  | -300 |
| -5 | 5 | 10 | 337  | -336 | -1 | 10 | 10 | 320  | -331 | -3 | 2 | 11 | 182  | 86   | -6 | 6  | 11 | 201  | 261  | -6 | 3 | 12 | 185  | -269 |
| -3 | 5 | 10 | 368  | -375 | 1  | 10 | 10 | 210  | -126 | -2 | 2 | 11 | 364  | 437  | -6 | 6  | 11 | 284  | 286  | -2 | 3 | 12 | 266  | -210 |
| -1 | 5 | 10 | 132  | -247 | -4 | 11 | 10 | 314  | -339 | 1  | 2 | 11 | 259  | 256  | -2 | 8  | 11 | 208  | 240  | -3 | 4 | 12 | 205  | -124 |
| 0  | 5 | 10 | 318  | -312 | 0  | 11 | 10 | 197  | -172 | -8 | 3 | 11 | 206  | -217 | -6 | 7  | 11 | 265  | 226  | -7 | 5 | 12 | 267  | 302  |
| 2  | 5 | 10 | 223  | -202 | 1  | 11 | 10 | 185  | -249 | -7 | 3 | 11 | 319  | -370 | 0  | 7  | 11 | 281  | 293  | 1  | 5 | 12 | 183  | -163 |
| -7 | 6 | 10 | 343  | 361  | -6 | 12 | 10 | 349  | 316  | -3 | 3 | 11 | 242  | -260 | 3  | 8  | 11 | 193  | -191 | -2 | 6 | 12 | 170  | -125 |
| -2 | 6 | 10 | 267  | 262  | -3 | 12 | 10 | 177  | 168  | -2 | 3 | 11 | 292  | 313  | -7 | 9  | 11 | 257  | -191 | -1 | 6 | 12 | 208  | 256  |
| -1 | 6 | 10 | 182  | -180 | -7 | 0  | 11 | 212  | -146 | -1 | 3 | 11 | 200  | -216 | -2 | 9  | 11 | 262  | -187 | -1 | 7 | 12 | 184  | 202  |
| 3  | 6 | 10 | 164  | 200  | -1 | 0  | 11 | 419  | -416 | 0  | 3 | 11 | 332  | 309  | 0  | 9  | 11 | 255  | -256 | -2 | 2 | 13 | 220  | 151  |
| -7 | 7 | 10 | 360  | 336  | -9 | 1  | 11 | 197  | 271  | 1  | 3 | 11 | 220  | 241  | -1 | 10 | 11 | 257  | -247 |    |   |    |      |      |
| -6 | 7 | 10 | 158  | 115  | -7 | 1  | 11 | 347  | 424  | 2  | 3 | 11 | 289  | 230  | 0  | 10 | 11 | 253  | -256 |    |   |    |      |      |

8.

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR

REIC015.ASF6

NOVEMBER 1981

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| H  | K  | L | 10FO | 10FC | H  | K | L | 10FO | 10FC | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  |
|----|----|---|------|------|----|---|---|------|------|-----|---|---|------|-------|-----|---|---|------|-------|-----|---|---|------|-------|
| 2  | 0  | 0 | 981  | 800  | 1  | 3 | 0 | 1707 | 1657 | 10  | 6 | 0 | 443  | 410   | -18 | 2 | 1 | 457  | 463   | 11  | 3 | 1 | 1408 | 1358  |
| 4  | 10 | 0 | 2718 | 2841 | 3  | 3 | 0 | 2336 | 2485 | 1   | 7 | 0 | 1002 | 989   | -18 | 2 | 1 | 2175 | 2118  | 13  | 3 | 1 | 2130 | 2135  |
| 6  | 0  | 0 | 1028 | 1037 | 5  | 3 | 0 | 1919 | 2004 | 3   | 7 | 0 | 688  | -678  | -14 | 2 | 1 | 1374 | 1365  | 15  | 3 | 1 | 384  | 327   |
| 8  | 0  | 0 | 4877 | 8128 | 7  | 3 | 0 | 625  | 811  | 5   | 7 | 0 | 817  | -819  | -12 | 2 | 1 | 1489 | 1560  | 17  | 3 | 1 | 1138 | 1111  |
| 10 | 0  | 0 | 2551 | 2580 | 9  | 3 | 0 | 1858 | 1885 | 7   | 7 | 0 | 884  | 892   | -8  | 2 | 1 | 1701 | 1713  | 19  | 3 | 1 | 740  | 780   |
| 12 | 0  | 0 | 3427 | 3288 | 11 | 3 | 0 | 1840 | 1898 | 9   | 7 | 0 | 1004 | 1020  | -6  | 2 | 1 | 2278 | 2312  | 21  | 3 | 1 | 1153 | 1131  |
| 14 | 10 | 0 | 882  | -841 | 13 | 3 | 0 | 2271 | 2221 | 13  | 7 | 0 | 745  | -717  | -4  | 2 | 1 | 884  | -781  | -24 | 4 | 1 | 1287 | 1263  |
| 16 | 0  | 0 | 4418 | 4471 | 17 | 3 | 0 | 978  | 975  | -27 | 1 | 1 | 1893 | 1826  | -2  | 2 | 1 | 736  | -700  | -20 | 4 | 1 | 158  | 1168  |
| 18 | 0  | 0 | 1784 | 1758 | 19 | 3 | 0 | 411  | -337 | -25 | 1 | 1 | 1447 | -1444 | 0   | 2 | 1 | 2317 | 2453  | -16 | 4 | 1 | 2286 | 2200  |
| 20 | 0  | 0 | 674  | -687 | 21 | 3 | 0 | 1807 | 1848 | -23 | 1 | 1 | 741  | -775  | 2   | 2 | 1 | 3851 | 3851  | -14 | 4 | 1 | 891  | -893  |
| 22 | 0  | 0 | 1336 | 1288 | 23 | 3 | 0 | 780  | 782  | -21 | 1 | 1 | 847  | 1073  | 4   | 2 | 1 | 456  | 853   | -12 | 4 | 1 | 1822 | 1816  |
| 24 | 10 | 0 | 2215 | 2115 | 25 | 3 | 0 | 707  | 887  | -19 | 1 | 1 | 3176 | 3186  | 8   | 2 | 1 | 1893 | -1770 | -10 | 4 | 1 | 612  | 860   |
| 26 | 0  | 0 | 1025 | 1044 | 2  | 4 | 0 | 1543 | 1588 | -17 | 1 | 1 | 1054 | -1828 | 8   | 2 | 1 | 1331 | 1370  | -8  | 4 | 1 | 2156 | -2204 |
| 3  | 1  | 0 | 2307 | 2388 | 4  | 4 | 0 | 1685 | 1725 | -15 | 1 | 1 | 2268 | -2203 | 10  | 2 | 1 | 2603 | 2622  | -8  | 4 | 1 | 1871 | 1891  |
| 5  | 1  | 0 | 1557 | 1588 | 6  | 4 | 0 | 1481 | 1480 | -13 | 1 | 1 | 1888 | 1706  | 12  | 2 | 1 | 893  | 708   | -4  | 4 | 1 | 1826 | 1866  |
| 7  | 1  | 0 | 848  | -875 | 8  | 4 | 0 | 1133 | 1155 | -11 | 1 | 1 | 4715 | 4701  | 14  | 2 | 1 | 1687 | -1058 | -2  | 4 | 1 | 1135 | 1156  |
| 9  | 1  | 0 | 938  | -944 | 10 | 4 | 0 | 953  | -814 | -9  | 1 | 1 | 1727 | -1844 | 16  | 2 | 1 | 947  | 935   | 0   | 4 | 1 | 2456 | -2503 |
| 11 | 1  | 0 | 1844 | 1888 | 12 | 4 | 0 | 1017 | -830 | -7  | 1 | 1 | 2253 | -2140 | 18  | 2 | 1 | 1875 | 1901  | 2   | 4 | 1 | 2438 | -2596 |
| 13 | 1  | 0 | 1248 | 1283 | 14 | 4 | 0 | 1415 | 1324 | -5  | 1 | 1 | 381  | 316   | 20  | 2 | 1 | 510  | -561  | 4   | 4 | 1 | 1031 | 861   |
| 15 | 1  | 0 | 585  | -578 | 16 | 4 | 0 | 884  | 881  | -1  | 1 | 1 | 747  | -719  | 22  | 2 | 1 | 1035 | 1035  | 6   | 4 | 1 | 1958 | 1953  |
| 17 | 1  | 0 | 417  | 408  | 18 | 4 | 0 | 489  | -483 | 1   | 1 | 1 | 2360 | -2356 | -25 | 3 | 1 | 837  | 882   | 8   | 4 | 1 | 1748 | 1816  |
| 19 | 1  | 0 | 815  | 899  | 20 | 4 | 0 | 512  | -550 | 3   | 1 | 1 | 886  | -745  | -23 | 3 | 1 | 537  | 498   | 10  | 4 | 1 | 2387 | -2472 |
| 21 | 1  | 0 | 382  | -396 | 22 | 4 | 0 | 751  | -804 | 5   | 1 | 1 | 5867 | 9874  | -18 | 3 | 1 | 1438 | -1428 | 12  | 4 | 1 | 750  | 806   |
| 23 | 1  | 0 | 3407 | 3455 | 1  | 5 | 0 | 2243 | 2182 | 7   | 1 | 1 | 1025 | 1065  | -17 | 3 | 1 | 1450 | 1433  | 14  | 4 | 1 | 1579 | 1644  |
| 25 | 1  | 0 | 1884 | 1892 | 3  | 5 | 0 | 1620 | 1660 | 9   | 1 | 1 | 3848 | -3830 | -15 | 3 | 1 | 1107 | 1041  | 16  | 4 | 1 | 488  | -659  |
| 27 | 1  | 0 | 1586 | 1511 | 5  | 5 | 0 | 1986 | 1953 | 11  | 1 | 1 | 498  | -860  | -11 | 3 | 1 | 2872 | -2836 | 18  | 4 | 1 | 1801 | 1789  |
| 29 | 1  | 0 | 785  | 804  | 7  | 5 | 0 | 1364 | 1382 | 13  | 1 | 1 | 4489 | 4586  | -9  | 3 | 1 | 1684 | 1746  | 22  | 4 | 1 | 978  | 883   |
| 31 | 1  | 0 | 4058 | 4122 | 9  | 5 | 0 | 1838 | 1880 | 15  | 1 | 1 | 1722 | 1870  | -7  | 3 | 1 | 1651 | 1682  | -13 | 5 | 1 | 840  | -863  |
| 10 | 2  | 0 | 388  | 282  | 11 | 5 | 0 | 731  | 780  | 17  | 1 | 1 | 1686 | 1843  | -5  | 3 | 1 | 187  | 207   | -9  | 5 | 1 | 403  | -401  |
| 12 | 2  | 0 | 1787 | 1767 | 13 | 5 | 0 | 1711 | 1748 | 19  | 1 | 1 | 1244 | -1278 | -3  | 3 | 1 | 2802 | -2670 | -7  | 5 | 1 | 472  | -455  |
| 14 | 2  | 0 | 1248 | 1230 | 15 | 5 | 0 | 882  | -886 | 21  | 1 | 1 | 2375 | 2321  | -1  | 3 | 1 | 515  | 524   | -5  | 5 | 1 | 1085 | 1060  |
| 16 | 2  | 0 | 3033 | 3075 | 17 | 5 | 0 | 1347 | 1302 | 23  | 1 | 1 | 430  | 861   | 1   | 3 | 1 | 2927 | 2959  | -1  | 5 | 1 | 701  | -673  |
| 18 | 2  | 0 | 855  | 858  | 21 | 5 | 0 | 1048 | 1087 | 27  | 1 | 1 | 1101 | -1080 | 3   | 3 | 1 | 440  | 481   | 1   | 5 | 1 | 584  | -627  |
| 20 | 2  | 0 | 1112 | 1114 | 2  | 6 | 0 | 608  | 628  | -28 | 2 | 1 | 415  | -449  | 5   | 3 | 1 | 2428 | -2521 | 3   | 5 | 1 | 812  | -848  |
| 22 | 2  | 0 | 1848 | 1931 | 4  | 6 | 0 | 383  | -305 | -24 | 2 | 1 | 1343 | 1264  | 7   | 3 | 1 | 368  | 334   | 7   | 5 | 1 | 489  | -513  |
| 24 | 2  | 0 | 815  | -804 | 6  | 6 | 0 | 516  | 542  | -20 | 2 | 1 | 567  | -563  | 9   | 3 | 1 | 1409 | 1433  | 11  | 5 | 1 | 989  | -925  |

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR

REIC015.ASF6

NOVEMBER 1981

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| H   | K  | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  | H   | K | L | 10FO | 10FC  |
|-----|----|---|------|-------|-----|---|---|------|-------|-----|---|---|------|-------|-----|---|---|------|-------|-----|---|---|------|-------|
| 15  | 5  | 1 | 516  | -403  | 15  | 0 | 2 | 875  | 883   | -2  | 2 | 2 | 3595 | -3561 | -20 | 4 | 2 | 693  | 693   | 15  | 5 | 2 | 1317 | -1338 |
| -18 | 5  | 1 | 1025 | 1030  | 14  | 0 | 2 | 8908 | -2469 | 0   | 2 | 2 | 693  | 693   | -14 | 4 | 2 | 830  | 778   | 15  | 5 | 2 | 1045 | -1127 |
| -12 | 5  | 1 | 1439 | -1414 | 20  | 0 | 2 | 609  | -806  | 2   | 2 | 2 | 4621 | 4929  | -16 | 4 | 2 | 529  | 511   | -5  | 6 | 2 | 532  | -493  |
| -10 | 6  | 1 | 943  | -921  | 22  | 0 | 2 | 458  | 510   | 4   | 2 | 2 | 1225 | -1236 | -14 | 4 | 2 | 1018 | -1064 | 0   | 6 | 2 | 576  | -923  |
| -8  | 6  | 1 | 1240 | 1148  | 24  | 0 | 2 | 1146 | 1135  | 6   | 2 | 2 | 2461 | -2474 | -12 | 4 | 2 | 1062 | 990   | 8   | 6 | 2 | 483  | -485  |
| -6  | 6  | 1 | 642  | 666   | 28  | 0 | 2 | 1589 | -1554 | 8   | 2 | 2 | 1068 | -1191 | -10 | 4 | 2 | 922  | 937   | -13 | 7 | 2 | 608  | -587  |
| -4  | 6  | 1 | 1533 | -1492 | -27 | 1 | 2 | 636  | -648  | 10  | 2 | 2 | 4088 | 1210  | -8  | 4 | 2 | 678  | 682   | -11 | 7 | 2 | 738  | 772   |
| -2  | 6  | 1 | 1347 | -1313 | -25 | 1 | 2 | 418  | -418  | 14  | 2 | 2 | 1785 | -1778 | -6  | 4 | 2 | 1011 | -970  | -7  | 7 | 2 | 1149 | -1148 |
| 0   | 6  | 1 | 684  | 934   | -19 | 1 | 2 | 815  | -816  | 16  | 2 | 2 | 1396 | -1369 | -4  | 4 | 2 | 791  | 791   | -5  | 7 | 2 | 864  | -888  |
| 2   | 6  | 1 | 1103 | 1095  | -17 | 1 | 2 | 1392 | -1315 | 18  | 2 | 2 | 2362 | 2401  | -2  | 4 | 2 | 1687 | 1721  | -1  | 7 | 2 | 810  | 782   |
| 4   | 6  | 1 | 1288 | -1317 | -15 | 1 | 2 | 305  | 279   | 20  | 2 | 2 | 572  | 542   | 0   | 4 | 2 | 953  | 848   | -1  | 7 | 2 | 504  | 566   |
| 6   | 6  | 1 | 1473 | -1511 | -13 | 1 | 2 | 515  | 513   | 22  | 2 | 2 | 794  | -771  | 2   | 4 | 2 | 1086 | -1044 | 1   | 7 | 2 | 1144 | -1103 |
| 8   | 6  | 1 | 592  | 574   | -11 | 1 | 2 | 722  | -746  | 24  | 2 | 2 | 1085 | -1161 | 4   | 4 | 2 | 1211 | 1204  | 3   | 7 | 2 | 1035 | -864  |
| 10  | 6  | 1 | 1235 | 1184  | -9  | 1 | 2 | 1568 | -1472 | 26  | 2 | 2 | 1185 | 1195  | 6   | 4 | 2 | 1063 | 1078  | 5   | 7 | 2 | 585  | 606   |
| 12  | 6  | 1 | 782  | -681  | -7  | 1 | 2 | 358  | -343  | -27 | 3 | 2 | 1132 | 1124  | 8   | 4 | 2 | 1344 | 1328  | 7   | 7 | 2 | 761  | 693   |
| 14  | 6  | 1 | 1370 | -1389 | -3  | 1 | 2 | 2339 | -2317 | -23 | 3 | 2 | 856  | -782  | 10  | 4 | 2 | 1151 | -1160 | 9   | 7 | 2 | 734  | -739  |
| 16  | 6  | 1 | 825  | 698   | -1  | 1 | 2 | 1861 | -1892 | -19 | 3 | 2 | 2045 | 2034  | 12  | 4 | 2 | 725  | 676   | 11  | 7 | 2 | 1000 | -885  |
| 1   | 7  | 1 | 655  | -651  | 3   | 1 | 2 | 324  | -366  | -17 | 3 | 2 | 921  | 890   | 14  | 4 | 2 | 777  | 828   | -7  | 1 | 3 | 1083 | -1063 |
| -20 | 10 | 2 | 1081 | 1114  | 5   | 1 | 2 | 1378 | -1307 | -15 | 3 | 2 | 1487 | -1579 | 16  | 4 | 2 | 798  | 804   | -6  | 1 | 3 | 1833 | -1838 |
| -26 | 0  | 2 | 723  | 711   | 7   | 1 | 2 | 1218 | -1194 | -11 | 3 | 2 | 2869 | 2815  | 18  | 4 | 2 | 711  | -664  | -23 | 1 | 3 | 1352 | 1248  |
| -24 | 0  | 2 | 1083 | -1104 | 13  | 1 | 2 | 1127 | -1118 | -9  | 3 | 2 | 2289 | 2250  | 2   | 4 | 2 | 383  | 358   | -21 | 1 | 3 | 567  | 560   |
| -22 | 0  | 2 | 2527 | -2445 | 15  | 1 | 2 | 1219 | -1239 | -7  | 3 | 2 | 1890 | -1923 | -19 | 5 | 2 | 1301 | -1344 | -19 | 1 | 3 | 1276 | -1235 |
| -20 | 0  | 2 | 1289 | 1245  | 23  | 1 | 2 | 686  | -837  | -5  | 3 | 2 | 886  | -880  | -15 | 5 | 2 | 1740 | 1689  | -17 | 1 | 3 | 3619 | -3509 |
| -18 | 0  | 2 | 1808 | 1856  | -28 | 2 | 2 | 906  | -857  | -3  | 3 | 2 | 3878 | 3773  | -13 | 5 | 2 | 1021 | 975   | -15 | 1 | 3 | 1868 | 1826  |
| -16 | 0  | 2 | 1924 | -1944 | -26 | 2 | 2 | 550  | -587  | -1  | 3 | 2 | 3122 | 3134  | -11 | 5 | 2 | 1890 | -1953 | -13 | 1 | 3 | 1958 | 1866  |
| -14 | 0  | 2 | 4768 | -4804 | -24 | 2 | 2 | 757  | 739   | 1   | 3 | 2 | 1283 | -1289 | -9  | 5 | 2 | 1151 | -1084 | -11 | 1 | 3 | 744  | -733  |
| -12 | 0  | 2 | 1361 | 1359  | -22 | 2 | 2 | 1636 | 1606  | 3   | 3 | 2 | 2129 | -2092 | -7  | 5 | 2 | 2082 | 2106  | -9  | 1 | 3 | 4628 | -4672 |
| -10 | 0  | 2 | 4633 | 4750  | -20 | 2 | 2 | 1227 | -1254 | 5   | 3 | 2 | 2265 | 2422  | -5  | 5 | 2 | 1498 | 1565  | -7  | 1 | 3 | 1049 | 1032  |
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| -2  | 0  | 2 | 2516 | 2665  | -12 | 2 | 2 | 1762 | -1819 | 15  | 3 | 2 | 4472 | 2512  | 3   | 5 | 2 | 1795 | 1667  | 5   | 1 | 3 | 937  | 952   |
| 0   | 0  | 2 | 1369 | 1338  | -10 | 2 | 2 | 2130 | -2129 | 17  | 3 | 2 | 1030 | -1023 | 5   | 5 | 2 | 1255 | -1273 | 7   | 1 | 3 | 5175 | -5365 |
| 10  | 0  | 2 | 4189 | -4270 | -8  | 2 | 2 | 1045 | 981   | 21  | 3 | 2 | 475  | 346   | 7   | 5 | 2 | 1471 | -1466 | 8   | 1 | 3 | 524  | -807  |
| 12  | 0  | 2 | 170  | -1667 | -6  | 2 | 2 | 3745 | 3811  | 23  | 3 | 2 | 1313 | 1352  | 9   | 5 | 2 | 1034 | 1036  | 11  | 1 | 3 | 1846 | 1743  |
| 14  | 0  | 2 | 1012 | 988   | -4  | 2 | 2 | 1808 | -1557 | -22 | 4 | 2 | 541  | -543  | 11  | 5 | 2 | 1512 | 1539  | 13  | 1 | 3 | 1011 | 993   |