

Supporting Information for

The Nonradiative Decay Mechanism of Dinuclear Iridium Complexes: A Density Functional Theory Study

Guo-Jun Kang¹, Yong-Fei Wu¹, Xue-Feng Ren^{1*}, Jie-Qiong Mei¹, Shi-Jian Lu¹

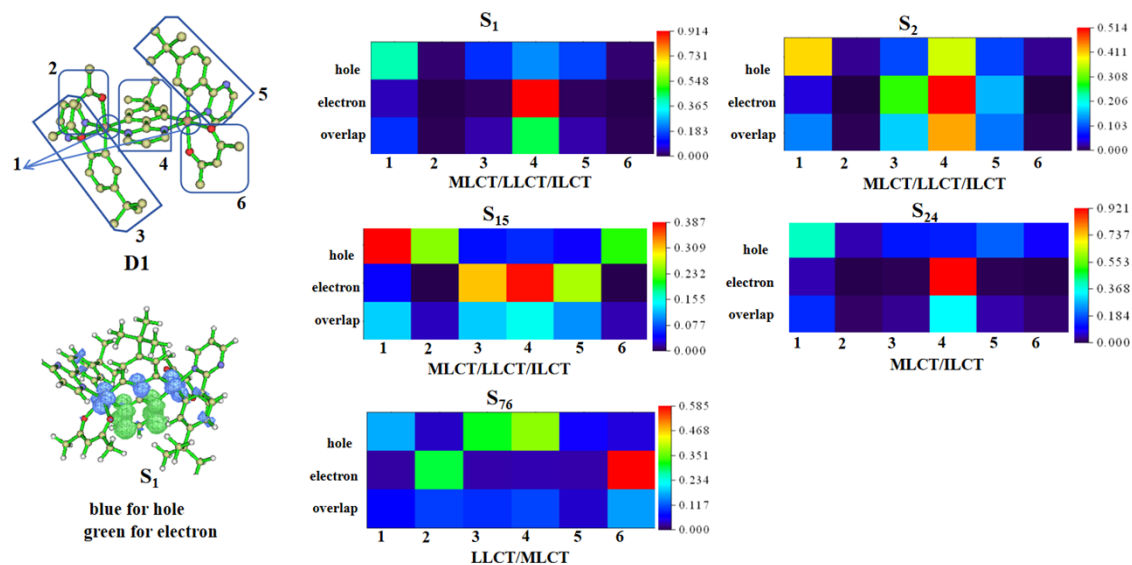
Xi Zeng^{2*}

¹ Carbon neutrality institute and School of Chemical Engineering & Technology,
China University of Mining and Technology, Xuzhou 221008, China.

² School of Light Industry Science and Engineering, Beijing Technology and Business
University, Beijing 100048, China

**Corresponding author:* Xue-Feng Ren; E-mail: renxf@cumt.edu.cn; Xi-Zeng, zengxi@btbu.edu.cn

Figure S1. The contribution of each fragment (%) to hole and electron of the strong absorption peaks of **D1** and **D2**.



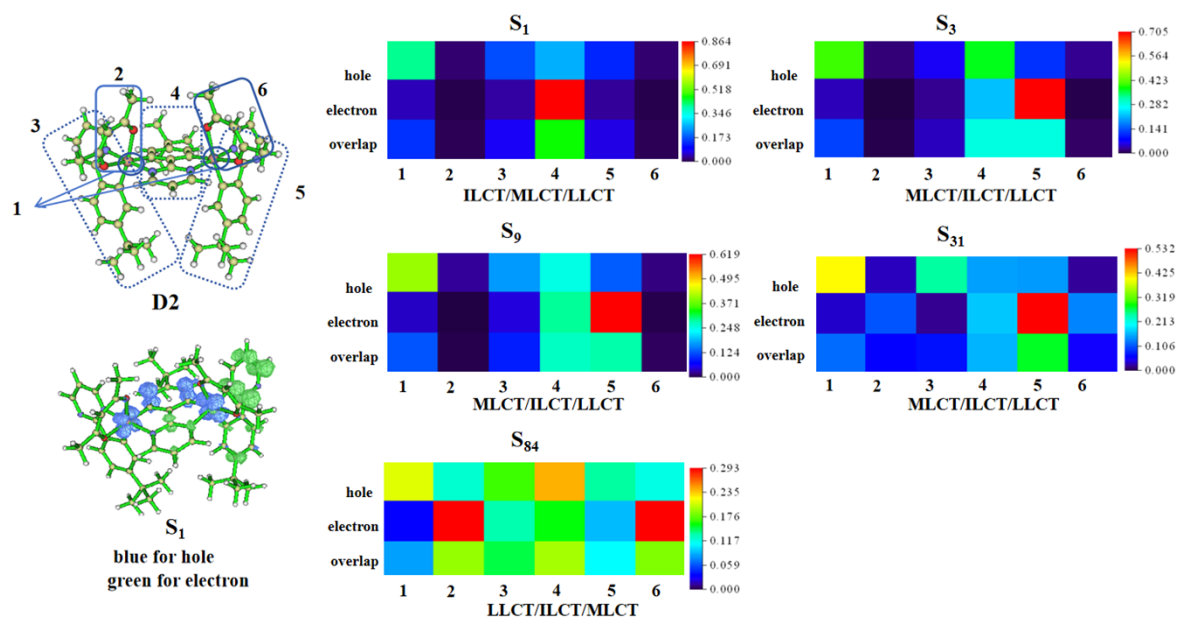


Table S1. The absorption spectra of **M1** calculated by ROCIS, s-TDDFT, SF-TDDFT, as well as LR-TDDFT with SOC correction with def2-TZVP(-f) basis set by ORCA.

| | s-TDDFT/B3LYP | | s-TDDFT/PBE0 | | s-TDDFT/M062X | | Exp. | | |
|----------|------------------------|---------|---------------|-------|---------------|-----------|-------|---------|-----|
| S_1 | 480.9 | 0.01408 | S_1 | 469.0 | 0.02227 | S_1 | 413.4 | 0.00588 | 460 |
| S_2 | 452.3 | 0.03215 | S_2 | 439.2 | 0.03091 | S_2 | 377.2 | 0.03778 | 411 |
| S_5 | 401.3 | 0.05117 | S_5 | 391.4 | 0.05390 | S_4 | 336.5 | 0.08341 | 379 |
| S_{10} | 357.8 | 0.09053 | S_9 | 350.2 | 0.08666 | S_8 | 318.0 | 0.08788 | 340 |
| S_{18} | 320.7 | 0.02696 | S_{13} | 332.4 | 0.02752 | S_9 | 316.5 | 0.08893 | 269 |
| S_{21} | 313.7 | 0.06243 | S_{18} | 312.7 | 0.02075 | S_{11} | 307.8 | 0.05828 | |
| S_{23} | 307.6 | 0.02905 | S_{20} | 308.2 | 0.02864 | S_{16} | 288.4 | 0.26425 | |
| S_{24} | 304.4 | 0.03948 | S_{21} | 304.0 | 0.08981 | | | | |
| S_{31} | 285.1 | 0.2364 | S_{23} | 299.9 | 0.02886 | | | | |
| | | | S_{24} | 295.4 | 0.02597 | | | | |
| | | | S_{27} | 286.4 | 0.06066 | | | | |
| | | | S_{31} | 279.3 | 0.43517 | | | | |
| | ROCIS/PBE0//def2-SV(P) | | SF-TDDFT/PBE0 | | TDDFT/PBE0 | | | | |
| S_1 | 44.3 | 0.00370 | S_1 | 439.3 | 0.07035 | S_7 | 439.0 | 0.02298 | |
| S_2 | 44.0 | 0.00088 | S_3 | 420.2 | 0.02395 | S_{24} | 407.5 | 0.02823 | |
| S_3 | 42.9 | 0.03068 | S_4 | 405.3 | 0.00076 | S_{32} | 369.4 | 0.03665 | |
| S_4 | 42.6 | 0.00001 | S_5 | 398.6 | 0.12155 | S_{53} | 335.1 | 0.08025 | |
| S_5 | 42.4 | 0.00046 | S_6 | 381.5 | 0.00408 | S_{119} | 273.4 | 0.22509 | |
| | | | S_7 | 371.8 | 0.01802 | | | | |
| | | | S_8 | 344.6 | 0.05821 | | | | |
| | | | S_9 | 316.0 | 0.06249 | | | | |

Table S2. Calculated phosphorescence emission wavelength (nm) of **M1** and **D2** by considering the effect of function, the transition type, and basis set.

| Basis | 6-31G(d)+LANLD2Z (Ir) | | | | 6-311G(d,p) +SDD (Ir) | | | |
|----------------------------|-----------------------|------------------|-------------------|---------------------|--------------------------|-----------------|---------------------|--------|
| | DF | TPSSh (10%HF) | B3PW91 (20%HF) | mpw1pw91 (25%HF) | mpw1pw91 (25%HF) | M06-2X (54%) | mpw1pw91 (25%HF) | Exp.15 |
| Transition Wavelength (nm) | | | | | | | | |
| M1 | 593.2 | 571.9 | 564.5 | 540.5* | 479.7 | 530.5 | 526 | |
| D2 | 664.0 | 683.9 | 642.6 | 665.9* | 457.0 | 607.5 | 606 | |

*Adiabatic. DF = Density functional

Table S3. Calculated phosphorescence emission wavelength (nm) of **M1** and **D2** with different functional with ZORA-DEF2-TZVP+SARC-ZORA-TZVP(Ir) basis set.

| | TPSSh | B3PW91 | PBE0 | BHANDHLYP | REVPBE38 | M062X | wB97X-D3 |
|-----------|-------|--------|-------|-----------|----------|-------|----------|
| M1 | 554.1 | 596.9 | 583.1 | 575.2 | 573.9 | 508.3 | 508 |
| D2 | 678.7 | | | | | 499.3 | 445.0 |

Table S4. The interfragment charge transfer between fragments in the main electron excitation process. (The ligand number is consistent with the Figure S1)

| M1 | | Contribution of each fragment to hole and electron(%) | | | | Transferred electron between fragment | | | |
|-----------------|----------|--|-------------------|--------------------|--------------------|--|--------------|--------------|--------------|
| | | Ligand 1 (Ir center) | Ligand2 (acac) | Ligand 3 (ppd1) | Ligand 4 (ppd2) | | | | |
| S ₁ | hole | 41.95% | 3.89% | 27.05% | 27.05% | 1→2 0.000 | 1→3 0.189 | 1→4 0.189 | 2→3 0.017 |
| | electron | 4.64% | 0.91% | 47.19% | 47.18% | 2→4 0.017 | 3→4 0.000 | | |
| S ₂ | hole | 41.95% | 3.93% | 27.05% | 27.06% | 1→2 0.000 | 1→3 0.204 | 1→4 0.204 | 2→3 0.018 |
| | electron | 1.02% | 0.27% | 49.33% | 49.35% | 2→4 0.018 | 3→4 0.000 | | |
| S ₅ | hole | 41.16% | 45.16% | 6.79% | 6.79% | 1→2 0.018 | 1→3 0.191 | 1→4 0.191 | 2→3 0.212 |
| | electron | 4.65% | 0.96% | 47.18% | 47.19% | 2→4 0.212 | 3→4 0.000 | | |
| S ₉ | hole | 56.59% | 4.97% | 19.14% | 19.22% | 1→2 0.002 | 1→3 0.262 | 1→4 0.262 | 2→3 0.023 |
| | electron | 4.12% | 0.34% | 47.75% | 47.77% | 2→4 0.023 | 3→4 0.000 | | |
| S ₃₁ | hole | 8.61% | 58.53% | 16.21% | 16.43% | 1→2 | 1→3 | 1→4 | 2→3 |

| | | | | | | | | | |
|--|----------|-------|-------|--------|--------|--------------|--------------|-------|-------|
| | | | | | | 0.024 | 0.034 | 0.034 | 0.275 |
| | electron | 4.40% | 0.94% | 47.30% | 47.33% | 2→4 0.275 | 3→4 0.000 | | |

| D1 | | Contribution of each fragment to hole and electron | | | | | | Transferred electron between fragment | | | | |
|-----------------|----------|---|--------------------|--------------------|--------------------|--------------------|---------------------|---------------------------------------|---------------|---------------|---------------|---------------|
| | | Ligand 1 (Ir center) | Ligand2 (acac1) | Ligand 3 (ppd1) | Ligand 4 (ppd2) | Ligand 5 (ppd3) | Ligand 6 (acac2) | | | | | |
| S ₁ | hole | 42.23% | 1.90% | 14.54% | 23.50% | 16.69% | 2.14% | 1→2 0.000 | 1→3 0.001 | 1→4 0.365 | 1→5 0.003 | 1→6 0.001 |
| | electron | 5.05% | 0.47% | 1.44% | 91.36% | 1.22% | 0.46% | 2→3 0.000 | 2→4 0.016 | 2→5 0.000 | 2→6 0.000 | 3→4 0.129 |
| | | | | | | | | 3→5 0.000 | 3→6 0.000 | 4→5 -0.150 | 4→6 0.019 | 5→6 0.000 |
| S ₂ | hole | 40.63% | 2.00% | 9.83% | 36.25% | 9.35% | 1.94% | 1→2 0.000 | 1→3 0.113 | 1→4 0.194 | 1→5 0.059 | 1→6 0.000 |
| | electron | 3.99% | 0.18% | 28.74% | 51.40% | 15.56% | 0.12% | 2→3 0.000 | 2→4 0.000 | 2→5 0.003 | 2→6 0.000 | 3→4 -0.053 |
| | | | | | | | | 3→5 0.012 | 3→6 0.005 | 4→5 0.008 | 4→6 0.010 | 5→6 0.003 |
| S ₁₅ | hole | 38.69% | 24.69% | 5.02% | 6.00% | 3.98% | 21.62% | 1→2 0.009 | 1→3 0.119 | 1→4 0.145 | 1→5 0.099 | 1→6 0.008 |
| | electron | 4.17% | 0.22% | 31.27% | 38.21% | 25.94% | 0.20% | 2→3 0.077 | 2→4 0.094 | 2→5 0.063 | 2→6 0.000 | 3→4 0.004 |
| | | | | | | | | 3→5 0.000 | 3→6 -0.067 | 4→5 0.000 | 4→6 -0.083 | 5→6 -0.056 |
| S ₂₄ | hole | 40.14% | 4.97% | 12.51% | 13.11% | 19.92% | 9.35% | 1→2 0.000 | 1→3 0.003 | 1→4 0.363 | 1→5 0.006 | 1→6 0.003 |
| | electron | 5.06% | 0.47% | 0.96% | 92.09% | 0.96% | 0.46% | 2→3 0.000 | 2→4 -0.045 | 2→5 0.000 | 2→6 0.000 | 3→4 -0.114 |
| | | | | | | | | 3→5 0.000 | 3→6 0.000 | 4→5 0.182 | 4→6 0.085 | 5→6 0.000 |
| S ₃₁ | hole | 40.84% | 3.03% | 21.37% | 25.65% | 8.14% | 0.97% | 1→2 0.004 | 1→3 0.004 | 1→4 0.003 | 1→5 0.001 | 1→6 0.387 |
| | electron | 2.25% | 1.28% | 0.24% | 0.67% | 0.79% | 94.77% | 2→3 0.003 | 2→4 0.003 | 2→5 0.000 | 2→6 -0.029 | 3→4 0.000 |
| | | | | | | | | 3→5 0.001 | 3→6 0.203 | 4→5 0.001 | 4→6 0.243 | 5→6 0.077 |
| S ₇₆ | hole | 17.26% | 3.73% | 30.96% | 37.59% | 5.92% | 4.55% | 1→2 0.051 | 1→3 0.003 | 1→4 0.004 | 1→5 0.003 | 1→6 0.010 |
| | electron | 2.61% | 29.95% | 2.86% | 3.18% | 2.90% | 58.50% | 2→3 -0.092 | 2→4 -0.111 | 2→5 0.017 | 2→6 0.008 | 3→4 0.001 |
| | | | | | | | | 3→5 0.007 | 3→6 0.180 | 4→5 0.009 | 4→6 0.218 | 5→6 -0.033 |

| D2 | | Contribution of each fragment to hole and electron | | | | | | Transferred electron between fragment | | | | |
|-----|----------|---|--------------------|--------------------|--------------------|--------------------|---------------------|---------------------------------------|---------------|---------------|---------------|---------------|
| | | Ligand 1 (Ir center) | Ligand2 (acac1) | Ligand 3 (ppd1) | Ligand 4 (ppd2) | Ligand 5 (ppd3) | Ligand 6 (acac2) | | | | | |
| S1 | hole | 40.72% | 1.87% | 39.22% | 25.69% | 0.75% | 1.70% | 1→2 0.000 | 1→3 0.064 | 1→4 0.339 | 1→5 0.004 | 1→6 0.001 |
| | electron | 4.97% | 0.35% | 20.61% | 86.39% | 1.01% | 0.37% | 2→3 0.003 | 2→4 0.015 | 2→5 0.000 | 2→6 0.000 | 3→4 0.286 |
| | | | | | | | | 3→5 0.002 | 3→6 -0.002 | 4→5 -0.004 | 4→6 -0.014 | 5→6 0.000 |
| S3 | hole | 40.18% | 1.93% | 6.40% | 37.26% | 11.64% | 2.59% | 1→2 0.000 | 1→3 0.008 | 1→4 0.074 | 1→5 0.278 | 1→6 0.001 |
| | electron | 4.05% | 0.08% | 2.71% | 22.14% | 70.47% | 0.49% | 2→3 0.000 | 2→4 0.004 | 2→5 0.014 | 2→6 0.000 | 3→4 0.004 |
| | | | | | | | | 3→5 0.042 | 3→6 0.000 | 4→5 0.237 | 4→6 -0.004 | 5→6 -0.018 |
| S9 | hole | 40.69% | 2.52% | 16.98% | 25.02% | 13.05% | 1.74% | 1→2 -0.001 | 1→3 0.012 | 1→4 0.108 | 1→5 0.247 | 1→6 0.001 |
| | electron | 3.91% | 0.08% | 4.64% | 28.99% | 61.91% | 0.40% | 2→3 0.001 | 2→4 0.007 | 2→5 0.016 | 2→6 0.000 | 3→4 0.038 |
| | | | | | | | | 3→5 0.099 | 3→6 0.000 | 4→5 0.117 | 4→6 -0.004 | 5→6 -0.010 |
| S31 | hole | 40.26% | 3.32% | 24.61% | 15.04% | 14.60% | 2.17% | 1→2 0.042 | 1→3 -0.001 | 1→4 0.0063 | 1→5 0.209 | 1→6 0.053 |
| | electron | 3.62% | 10.87% | 2.03% | 16.97% | 53.16% | 13.36% | 2→3 0.026 | 2→4 0.011 | 2→5 0.002 | 2→6 0.002 | 3→4 0.039 |
| | | | | | | | | 3→5 0.012 | 3→6 0.032 | 4→5 0.055 | 4→6 0.016 | 5→6 0.008 |
| S84 | hole | 21.17% | 12.43% | 16.72% | 24.29% | 13.59% | 11.80% | 1→2 0.058 | 1→3 0.023 | 1→4 0.025 | 1→5 0.015 | 1→6 0.058 |
| | electron | 3.24% | 29.34% | 13.30% | 15.76% | 9.05% | 29.30% | 2→3 0.033 | 2→4 -0.052 | 2→5 -0.029 | 2→6 -0.002 | 3→4 0.006 |
| | | | | | | | | 3→5 -0.003 | 3→6 0.033 | 4→5 0.001 | 4→6 0.053 | 5→6 0.029 |

Table S5. The cartesian coordinates for all of optimized T_1 state and 3MC state.

| | M1- 3MC_1 | | | | M1- 3MC_1 | | |
|----|--------------|-----------|-----------|----|--------------|--------------|--------------|
| 77 | 0.831449 | -0.109123 | -0.231535 | 77 | 0.846114000 | -0.125204000 | -0.225119000 |
| 7 | 1.194052 | 3.69822 | -2.29718 | 7 | 1.181301000 | 3.557826000 | -2.512199000 |
| 7 | 1.595453 | 1.449587 | -1.68121 | 7 | 1.602708000 | 1.353003000 | -1.764490000 |
| 7 | 0.840362 | -1.4664 | 1.890011 | 7 | 0.829138000 | -1.359987000 | 1.971265000 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|--------------|--------------|--------------|
| 8 | 2.227801 | -1.661257 | -0.836879 | 7 | -0.322903000 | -3.207734000 | 2.903524000 |
| 8 | 2.496645 | 0.785224 | 0.91141 | 8 | 2.519292000 | 0.812812000 | 0.861005000 |
| 6 | 4.174478 | -2.937708 | -1.048158 | 8 | 2.229712000 | -1.718855000 | -0.745342000 |
| 1 | 3.763528 | -3.830645 | -0.567553 | 6 | 2.531825000 | 1.192631000 | -2.700956000 |
| 1 | 5.248842 | -2.898997 | -0.865578 | 1 | 3.035858000 | 0.230674000 | -2.716476000 |
| 1 | 3.985201 | -3.037963 | -2.119839 | 6 | 2.831802000 | 2.206905000 | -3.592143000 |
| 6 | 3.4458 | -1.727495 | -0.522433 | 1 | 3.586678000 | 2.088102000 | -4.358632000 |
| 6 | 4.171568 | -0.796754 | 0.248565 | 6 | 2.113306000 | 3.388920000 | -3.437577000 |
| 1 | 5.22816 | -1.000146 | 0.370398 | 1 | 2.297422000 | 4.239092000 | -4.091235000 |
| 6 | 3.691221 | 0.361716 | 0.874181 | 6 | 0.935534000 | 2.529709000 | -1.693354000 |
| 6 | 4.678279 | 1.234139 | 1.609273 | 6 | -0.090470000 | 2.612412000 | -0.669000000 |
| 1 | 4.712867 | 2.21351 | 1.12306 | 6 | -0.327832000 | 1.467389000 | 0.121816000 |
| 1 | 5.682792 | 0.810635 | 1.635576 | 6 | -1.324399000 | 1.563064000 | 1.100718000 |
| 1 | 4.323837 | 1.402481 | 2.62994 | 1 | -1.518496000 | 0.687872000 | 1.708492000 |
| 6 | 1.536155 | -2.427331 | 3.937793 | 6 | -2.066534000 | 2.723527000 | 1.310955000 |
| 1 | 2.186811 | -2.429863 | 4.803156 | 6 | -1.797716000 | 3.840811000 | 0.501146000 |
| 6 | 1.639705 | -1.463318 | 2.946969 | 1 | -2.358564000 | 4.759622000 | 0.637773000 |
| 1 | 2.369429 | -0.660909 | 2.991142 | 6 | -0.825580000 | 3.787886000 | -0.474387000 |
| 6 | -0.098435 | -2.423536 | 1.803876 | 6 | -3.160788000 | 2.813696000 | 2.374687000 |
| 6 | -0.983525 | -2.343912 | 0.646776 | 6 | -2.828249000 | 3.951151000 | 3.352592000 |
| 6 | -0.783376 | -1.310554 | -0.288594 | 1 | -2.761183000 | 4.917310000 | 2.845807000 |
| 6 | -2.745188 | -2.104594 | -1.528937 | 1 | -1.871952000 | 3.767456000 | 3.851198000 |
| 6 | -3.688515 | -1.919662 | -2.717618 | 1 | -3.605407000 | 4.028862000 | 4.120542000 |
| 6 | -4.370102 | -0.546359 | -2.615857 | 6 | -4.504933000 | 3.106500000 | 1.690056000 |
| 1 | -5.048819 | -0.397846 | -3.462594 | 1 | -5.303110000 | 3.176682000 | 2.436907000 |
| 1 | -4.951996 | -0.468729 | -1.692697 | 1 | -4.763384000 | 2.308639000 | 0.987586000 |
| 6 | -2.882766 | -1.994364 | -4.023392 | 1 | -4.480618000 | 4.047608000 | 1.134434000 |
| 1 | -2.387755 | -2.965154 | -4.120182 | 6 | -3.305139000 | 1.520255000 | 3.178022000 |
| 1 | -2.112805 | -1.220016 | -4.067979 | 1 | -4.095582000 | 1.640958000 | 3.925172000 |
| 1 | -3.545735 | -1.859955 | -4.884812 | 1 | -2.381915000 | 1.268288000 | 3.708238000 |
| 6 | 2.534316 | 1.341263 | -2.615776 | 1 | -3.575737000 | 0.673386000 | 2.540921000 |
| 1 | 3.033113 | 0.379099 | -2.685392 | 6 | 1.616967000 | -1.300847000 | 3.034824000 |
| 6 | 2.84996 | 2.406661 | -3.439208 | 1 | 2.361211000 | -0.510454000 | 3.034307000 |
| 1 | 3.612951 | 2.330616 | -4.203081 | 6 | 1.485321000 | -2.195331000 | 4.085939000 |
| 6 | 2.135917 | 3.581205 | -3.220479 | 1 | 2.126513000 | -2.152039000 | 4.957279000 |
| 1 | 2.331987 | 4.468893 | -3.818406 | 6 | 0.481783000 | -3.147237000 | 3.954819000 |
| 6 | 0.933962 | 2.623519 | -1.545583 | 1 | 0.313769000 | -3.891451000 | 4.730727000 |
| 6 | -0.102937 | 2.649776 | -0.52835 | 6 | -0.126105000 | -2.304316000 | 1.936859000 |
| 6 | -0.35072 | 1.458854 | 0.195599 | 6 | -0.997181000 | -2.286191000 | 0.767117000 |
| 6 | -2.099097 | 2.658561 | 1.432728 | 6 | -2.061792000 | -3.184409000 | 0.647838000 |
| 6 | -1.821236 | 3.815655 | 0.693976 | 1 | -2.209300000 | -3.919380000 | 1.431956000 |
| 6 | -0.835159 | 3.811246 | -0.275689 | 6 | -2.904860000 | -3.129037000 | -0.443333000 |
| 1 | -0.61456 | 4.704417 | -0.850829 | 1 | -3.723355000 | -3.838321000 | -0.510755000 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|--------------|--------------|--------------|
| 6 | -4.243829 | 1.571398 | 2.114175 | 6 | -2.727812000 | -2.161243000 | -1.443577000 |
| 1 | -4.711856 | 1.832566 | 1.160266 | 6 | -1.670297000 | -1.262540000 | -1.303239000 |
| 1 | -5.027849 | 1.520774 | 2.877591 | 1 | -1.533593000 | -0.486463000 | -2.047879000 |
| 1 | -3.80845 | 0.574649 | 2.009446 | 6 | -0.775101000 | -1.319389000 | -0.226532000 |
| 6 | -3.887939 | 3.964241 | 2.681903 | 6 | -3.699492000 | -2.106046000 | -2.622090000 |
| 1 | -4.385446 | 4.285616 | 1.761951 | 6 | -3.668804000 | -3.449301000 | -3.367080000 |
| 1 | -3.188135 | 4.748307 | 2.986792 | 1 | -4.366417000 | -3.429180000 | -4.211098000 |
| 1 | -4.652528 | 3.880748 | 3.460109 | 1 | -3.953409000 | -4.280744000 | -2.717255000 |
| 6 | -3.187227 | 2.615883 | 2.506748 | 1 | -2.667169000 | -3.655736000 | -3.755556000 |
| 6 | -2.558925 | 2.224382 | 3.85293 | 6 | -5.118750000 | -1.847192000 | -2.093763000 |
| 1 | -3.327485 | 2.190308 | 4.63271 | 1 | -5.166274000 | -0.892949000 | -1.560910000 |
| 1 | -1.798731 | 2.951719 | 4.153184 | 1 | -5.444206000 | -2.631687000 | -1.405675000 |
| 1 | -2.08284 | 1.241928 | 3.806221 | 1 | -5.831341000 | -1.811491000 | -2.924729000 |
| 7 | -0.268598 | -3.391585 | 2.711097 | 6 | -3.350117000 | -0.998939000 | -3.618199000 |
| 6 | 0.547585 | -3.386273 | 3.755158 | 1 | -4.070672000 | -1.008569000 | -4.441643000 |
| 1 | 0.401606 | -4.182915 | 4.481891 | 1 | -2.353644000 | -1.140238000 | -4.047405000 |
| 6 | -2.898214 | -3.133143 | -0.594858 | 1 | -3.388687000 | -0.008262000 | -3.155874000 |
| 1 | -3.643037 | 0.269509 | -2.619986 | 6 | 4.159766000 | -3.031046000 | -0.877441000 |
| 6 | -4.777988 | -2.992701 | -2.767357 | 1 | 3.740075000 | -3.889589000 | -0.344477000 |
| 1 | -4.354555 | -3.997213 | -2.862396 | 1 | 5.234762000 | -2.993418000 | -0.698357000 |
| 1 | -5.413251 | -2.96934 | -1.876792 | 1 | 3.967497000 | -3.192051000 | -1.941092000 |
| 1 | -5.419993 | -2.819988 | -3.636292 | 6 | 3.445379000 | -1.784257000 | -0.422666000 |
| 1 | -2.37623 | 4.728282 | 0.872838 | 6 | 4.179978000 | -0.821883000 | 0.299563000 |
| 1 | -3.704416 | -3.849691 | -0.693527 | 1 | 5.233521000 | -1.030385000 | 0.437862000 |
| 6 | -1.354676 | 1.505963 | 1.162985 | 6 | 3.709754000 | 0.375304000 | 0.854842000 |
| 1 | -1.563224 | 0.599721 | 1.722923 | 6 | 4.702182000 | 1.279259000 | 1.542735000 |
| 6 | -1.693145 | -1.200043 | -1.341631 | 1 | 4.749267000 | 2.227885000 | 0.999923000 |
| 1 | -1.581822 | -0.375121 | -2.039697 | 1 | 5.702081000 | 0.847858000 | 1.598969000 |
| 6 | -2.035949 | -3.243243 | 0.48363 | 1 | 4.344838000 | 1.510892000 | 2.549880000 |
| 1 | -2.165622 | -4.02813 | 1.221251 | 1 | -0.613841000 | 4.647251000 | -1.101878000 |

| D1-3MC1 | | | | D1-3MC2 | | | |
|---------|----------|-----------|-----------|---------|-----------|-----------|-----------|
| 77 | 2.850041 | 0.789182 | -0.092544 | 77 | -2.802592 | -0.563459 | -0.399586 |
| 7 | 6.717063 | -0.078415 | 1.703049 | 7 | -5.819457 | -0.724083 | 2.505959 |
| 7 | 4.802518 | 1.119056 | 0.997985 | 7 | -4.109357 | -1.320699 | 0.975184 |
| 7 | 0.824542 | 0.780336 | -1.946624 | 7 | -1.452919 | 0.257861 | -1.700032 |
| 8 | 2.306358 | 2.884754 | -0.190451 | 8 | -2.193267 | -2.525437 | -1.137265 |
| 8 | 4.027610 | 1.118906 | -1.873971 | 8 | -4.399457 | -0.663106 | -1.883465 |
| 6 | 1.979114 | 5.050641 | -1.015537 | 6 | -2.067276 | -4.479678 | -2.415299 |
| 1 | 0.891983 | 4.983408 | -1.122036 | 1 | -1.061790 | -4.271437 | -2.793250 |
| 1 | 2.365671 | 5.745002 | -1.762297 | 1 | -2.616190 | -5.057631 | -3.159488 |
| 1 | 2.176091 | 5.438399 | -0.013267 | 1 | -1.944898 | -5.074085 | -1.505891 |
| 6 | 2.568610 | 3.669947 | -1.141680 | 6 | -2.741191 | -3.175050 | -2.073633 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 6 | 3.349465 | 3.379635 | -2.277483 | 6 | -3.885875 | -2.808389 | -2.799994 |
| 1 | 3.484356 | 4.186971 | -2.986501 | 1 | -4.227168 | -3.512724 | -3.548209 |
| 6 | 4.032391 | 2.188261 | -2.555928 | 6 | -4.634794 | -1.627905 | -2.665020 |
| 6 | 4.895362 | 2.127558 | -3.790078 | 6 | -5.853466 | -1.451328 | -3.535062 |
| 1 | 5.928579 | 1.930332 | -3.490910 | 1 | -6.736262 | -1.368538 | -2.894534 |
| 1 | 4.859625 | 3.045485 | -4.377745 | 1 | -5.995434 | -2.272728 | -4.238072 |
| 1 | 4.579031 | 1.282412 | -4.407846 | 1 | -5.772343 | -0.509782 | -4.085126 |
| 6 | -0.683281 | 1.097068 | -3.759648 | 6 | -0.656062 | 1.118032 | -3.754021 |
| 1 | -0.871564 | 1.406130 | -4.779358 | 1 | -0.839371 | 1.430488 | -4.773608 |
| 6 | 0.588018 | 1.144589 | -3.197811 | 6 | -1.681205 | 0.641903 | -2.955070 |
| 1 | 1.444956 | 1.494877 | -3.766646 | 1 | -2.708038 | 0.555742 | -3.293155 |
| 6 | -0.200593 | 0.347471 | -1.210560 | 6 | -0.186020 | 0.359668 | -1.205417 |
| 6 | -0.038002 | -0.033043 | 0.160846 | 6 | -0.029005 | -0.026620 | 0.165338 |
| 6 | 1.213942 | 0.034588 | 0.805920 | 6 | -1.210376 | -0.469235 | 0.808077 |
| 6 | 0.108259 | -0.757460 | 2.838899 | 6 | 0.112436 | -0.763697 | 2.839692 |
| 6 | 0.238393 | -1.139952 | 4.314997 | 6 | 0.152730 | -1.168585 | 4.315436 |
| 6 | 1.197093 | -2.333268 | 4.448830 | 6 | -0.762366 | -0.231512 | 5.118764 |
| 1 | 1.307190 | -2.612811 | 5.502272 | 1 | -0.750717 | -0.509009 | 6.178534 |
| 1 | 0.814916 | -3.200645 | 3.902449 | 1 | -0.426419 | 0.805957 | 5.032517 |
| 6 | 0.797941 | 0.056900 | 5.099204 | 6 | -0.342328 | -2.615736 | 4.461485 |
| 1 | 0.131338 | 0.920321 | 5.016394 | 1 | 0.293395 | -3.302090 | 3.894386 |
| 1 | 1.781814 | 0.357510 | 4.730516 | 1 | -1.367308 | -2.732264 | 4.100243 |
| 1 | 0.898427 | -0.199284 | 6.159550 | 1 | -0.320043 | -2.917912 | 5.514194 |
| 6 | 5.297713 | 2.245826 | 1.499437 | 6 | -4.280786 | -2.611590 | 1.262431 |
| 1 | 4.681747 | 3.132858 | 1.380676 | 1 | -3.628344 | -3.300305 | 0.737142 |
| 6 | 6.527880 | 2.266805 | 2.130152 | 6 | -5.232552 | -3.014543 | 2.180358 |
| 1 | 6.941557 | 3.177249 | 2.544173 | 1 | -5.375333 | -4.060534 | 2.417926 |
| 6 | 7.202544 | 1.050388 | 2.195425 | 6 | -5.989339 | -2.010536 | 2.774476 |
| 1 | 8.180510 | 0.984200 | 2.667878 | 1 | -6.763008 | -2.251305 | 3.500077 |
| 6 | 5.516449 | -0.024911 | 1.115840 | 6 | -4.881826 | -0.397627 | 1.618483 |
| 6 | 4.887209 | -1.214328 | 0.572003 | 6 | -4.571317 | 0.971791 | 1.276512 |
| 6 | 3.603763 | -1.073903 | -0.004954 | 6 | -3.523052 | 1.142768 | 0.342977 |
| 6 | 3.622163 | -3.481472 | -0.470648 | 6 | -3.791270 | 3.563636 | 0.606649 |
| 6 | 4.896092 | -3.578070 | 0.104849 | 6 | -4.841877 | 3.347103 | 1.508925 |
| 6 | 5.520958 | -2.457988 | 0.621391 | 6 | -5.226309 | 2.061846 | 1.847046 |
| 1 | 6.506653 | -2.525603 | 1.069833 | 1 | -6.029169 | 1.884913 | 2.555527 |
| 6 | 1.574407 | -4.895719 | -0.252462 | 6 | -1.859361 | 5.135991 | 0.730830 |
| 1 | 1.780884 | -5.070078 | 0.807787 | 1 | -1.801678 | 5.031156 | 1.818150 |
| 1 | 1.033384 | -5.765270 | -0.642564 | 1 | -1.481305 | 6.128908 | 0.462172 |
| 1 | 0.915943 | -4.026416 | -0.325798 | 1 | -1.195524 | 4.385631 | 0.293991 |
| 6 | 3.705037 | -5.980639 | -0.931678 | 6 | -4.157910 | 6.066438 | 0.884726 |
| 1 | 3.937570 | -6.231513 | 0.107602 | 1 | -4.123873 | 6.020722 | 1.977139 |
| 1 | 4.645539 | -5.907527 | -1.486435 | 1 | -5.204084 | 6.005022 | 0.569677 |
| 1 | 3.135262 | -6.814323 | -1.353321 | 1 | -3.776667 | 7.047102 | 0.584002 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | 2.882337 | -4.695176 | -1.034657 | 6 | -3.306958 | 4.968750 | 0.243134 |
| 6 | 2.557091 | -4.452098 | -2.516347 | 6 | -3.358896 | 5.157584 | -1.280473 |
| 1 | 2.023665 | -5.314435 | -2.931412 | 1 | -3.017494 | 6.163590 | -1.547375 |
| 1 | 3.472227 | -4.304098 | -3.097494 | 1 | -4.379922 | 5.032682 | -1.653061 |
| 1 | 1.928559 | -3.568338 | -2.651712 | 1 | -2.722211 | 4.438345 | -1.801563 |
| 77 | -2.812683 | -0.571062 | -0.387736 | 77 | 2.859554 | 0.788606 | -0.075622 |
| 7 | -5.826146 | -0.719942 | 2.522006 | 7 | 6.725617 | -0.107182 | 1.705914 |
| 7 | -4.115727 | -1.322736 | 0.994130 | 7 | 4.816241 | 1.103288 | 1.009368 |
| 7 | -1.470177 | 0.244988 | -1.698549 | 7 | 0.842364 | 0.796766 | -1.934251 |
| 8 | -2.208247 | -2.535747 | -1.120778 | 8 | 2.326654 | 2.887532 | -0.161738 |
| 8 | -4.418009 | -0.676991 | -1.862448 | 8 | 4.035638 | 1.121091 | -1.858237 |
| 6 | -2.084244 | -4.492059 | -2.395617 | 6 | 2.012621 | 5.060438 | -0.972820 |
| 1 | -1.961449 | -5.085805 | -1.485816 | 1 | 2.221952 | 5.444843 | 0.028307 |
| 1 | -2.633394 | -5.070725 | -3.139070 | 1 | 2.395396 | 5.754729 | -1.721571 |
| 1 | -1.078934 | -4.283896 | -2.774061 | 1 | 0.924153 | 4.999027 | -1.068021 |
| 6 | -2.758217 | -3.187311 | -2.054640 | 6 | 2.593721 | 3.677053 | -1.108014 |
| 6 | -3.905127 | -2.822633 | -2.778372 | 6 | 3.373300 | 3.389445 | -2.245393 |
| 1 | -4.248019 | -3.528252 | -3.524637 | 1 | 3.513485 | 4.200622 | -2.948968 |
| 6 | -4.655100 | -1.642950 | -2.642006 | 6 | 4.048372 | 2.195545 | -2.532034 |
| 6 | -5.877246 | -1.468947 | -3.507657 | 6 | 4.911724 | 2.138049 | -3.766099 |
| 1 | -5.798858 | -0.528446 | -4.059917 | 1 | 4.591810 | 1.298113 | -4.389085 |
| 1 | -6.021360 | -2.291825 | -4.208494 | 1 | 4.880791 | 3.059677 | -4.348209 |
| 1 | -6.757610 | -1.385435 | -2.863897 | 1 | 5.943826 | 1.934155 | -3.467506 |
| 6 | -1.704650 | 0.624622 | -2.953689 | 6 | 0.612213 | 1.165073 | -3.185456 |
| 1 | -2.733254 | 0.538031 | -3.286230 | 1 | 1.471740 | 1.518338 | -3.748461 |
| 6 | -1.213893 | -0.471021 | 0.808954 | 6 | 1.216978 | 0.038258 | 0.813772 |
| 6 | -1.111373 | -0.805233 | 2.161751 | 6 | 1.265806 | -0.373920 | 2.148078 |
| 1 | 2.190391 | -2.104594 | 4.055091 | 1 | -1.796727 | -0.275780 | 4.769025 |
| 6 | -1.101553 | -1.531721 | 4.940681 | 6 | 1.559574 | -1.086734 | 4.910934 |
| 1 | -1.827024 | -0.714240 | 4.891871 | 1 | 2.257486 | -1.756466 | 4.399920 |
| 1 | -1.537468 | -2.408309 | 4.451915 | 1 | 1.960935 | -0.070008 | 4.863841 |
| 1 | -0.951632 | -1.781276 | 5.995613 | 1 | 1.526671 | -1.381563 | 5.964273 |
| 6 | -4.288302 | -2.612554 | 1.285350 | 6 | 5.318321 | 2.225449 | 1.514352 |
| 1 | -3.636522 | -3.303393 | 0.762021 | 1 | 4.706911 | 3.116218 | 1.400202 |
| 6 | -5.240771 | -3.011824 | 2.204048 | 6 | 6.549719 | 2.237283 | 2.142812 |
| 1 | -5.384581 | -4.056918 | 2.444905 | 1 | 6.969055 | 3.143827 | 2.559679 |
| 6 | -5.996870 | -2.005374 | 2.794816 | 6 | 7.218042 | 1.017047 | 2.201838 |
| 1 | -6.770867 | -2.243243 | 3.521011 | 1 | 8.196593 | 0.943808 | 2.672024 |
| 6 | -4.888057 | -0.397148 | 1.633805 | 6 | 5.524142 | -0.045026 | 1.121486 |
| 6 | -4.576918 | 0.971019 | 1.286998 | 6 | 4.887327 | -1.228832 | 0.574245 |
| 6 | -3.529584 | 1.138350 | 0.351832 | 6 | 3.602979 | -1.079372 | 0.001532 |
| 6 | -3.793119 | 3.560188 | 0.610735 | 6 | 3.608138 | -3.484835 | -0.475123 |
| 6 | -4.843729 | 3.347308 | 1.513838 | 6 | 4.883124 | -3.590327 | 0.096321 |
| 6 | -5.229963 | 2.063397 | 1.855208 | 6 | 5.514970 | -2.475741 | 0.616307 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 1 | -6.032587 | 1.889351 | 2.564674 | 1 | 6.501526 | -2.550243 | 1.061749 |
| 6 | -3.353844 | 5.149790 | -1.278775 | 6 | 2.534953 | -4.440632 | -2.523330 |
| 1 | -4.374352 | 5.026575 | -1.653348 | 1 | 3.449863 | -4.294100 | -3.105219 |
| 1 | -3.009577 | 6.154537 | -1.546733 | 1 | 1.996886 | -5.298475 | -2.941718 |
| 1 | -2.717680 | 4.428209 | -1.797254 | 1 | 1.910343 | -3.553287 | -2.653356 |
| 6 | -4.155783 | 6.064186 | 0.882930 | 6 | 3.678278 | -5.982183 | -0.947932 |
| 1 | -5.201528 | 6.003736 | 0.566259 | 1 | 4.618023 | -5.911077 | -1.504226 |
| 1 | -4.123654 | 6.020970 | 1.975501 | 1 | 3.911678 | -6.238923 | 0.089726 |
| 1 | -3.772402 | 7.043535 | 0.580652 | 1 | 3.103692 | -6.811219 | -1.372177 |
| 6 | -3.305552 | 4.963654 | 0.245266 | 6 | 2.861465 | -4.692358 | -1.043361 |
| 6 | -1.858653 | 5.128947 | 0.735771 | 6 | 1.553951 | -4.890505 | -0.259916 |
| 1 | -1.478131 | 6.120680 | 0.466248 | 1 | 1.007986 | -5.755332 | -0.653578 |
| 1 | -1.803572 | 5.025994 | 1.823417 | 1 | 1.761376 | -5.071831 | 0.798991 |
| 1 | -1.195167 | 4.376646 | 0.301771 | 1 | 0.899489 | -4.017739 | -0.327398 |
| 1 | 5.405527 | -4.532450 | 0.155212 | 1 | -5.358649 | 4.184944 | 1.960009 |
| 1 | -5.359002 | 4.186968 | 1.963271 | 1 | 5.388031 | -4.547396 | 0.140817 |
| 1 | -2.001830 | -1.119926 | 2.692032 | 1 | 2.224424 | -0.393412 | 2.652366 |
| 6 | 3.007135 | -2.227221 | -0.511852 | 6 | -3.154281 | 2.453238 | 0.042745 |
| 1 | 2.014858 | -2.139491 | -0.942547 | 1 | -2.333007 | 2.615784 | -0.648199 |
| 6 | -3.158587 | 2.447447 | 0.048586 | 6 | 2.999069 | -2.227355 | -0.508808 |
| 1 | -2.337281 | 2.606904 | -0.642990 | 1 | 2.006012 | -2.132807 | -0.936285 |
| 6 | 1.262969 | -0.371580 | 2.136152 | 6 | -1.108587 | -0.808080 | 2.153718 |
| 1 | 2.222333 | -0.392191 | 2.643858 | 1 | -1.998615 | -1.129724 | 2.685221 |

| D1- ³ MC3 | | | D1- ³ MC4 | | | | |
|----------------------|-----------|-----------|----------------------|----|-----------|-----------|-----------|
| 77 | 2.782359 | 0.625545 | -0.373859 | 77 | -2.819892 | -0.619172 | -0.255565 |
| 7 | 6.534926 | -0.328001 | 1.823701 | 7 | -5.815856 | -0.014815 | 2.612316 |
| 7 | 4.680382 | 0.954015 | 1.105206 | 7 | -4.142878 | -1.003152 | 1.251995 |
| 7 | 0.852948 | 0.268226 | -2.021660 | 7 | -1.442918 | -0.150945 | -1.699466 |
| 8 | 2.141873 | 2.674760 | -0.472082 | 8 | -2.313752 | -2.725396 | -0.551115 |
| 8 | 4.285141 | 1.248292 | -1.811502 | 8 | -4.429548 | -0.950876 | -1.689448 |
| 6 | 2.225569 | 5.011542 | -0.594117 | 6 | -2.345345 | -4.927841 | -1.344115 |
| 1 | 1.321472 | 5.133406 | -1.197999 | 1 | -1.397388 | -4.897053 | -1.890206 |
| 1 | 2.910374 | 5.831323 | -0.814913 | 1 | -3.006913 | -5.646500 | -1.829245 |
| 1 | 1.915503 | 5.057050 | 0.452777 | 1 | -2.115847 | -5.260778 | -0.329115 |
| 6 | 2.827681 | 3.661438 | -0.877542 | 6 | -2.929173 | -3.538295 | -1.299299 |
| 6 | 4.041360 | 3.600055 | -1.575409 | 6 | -4.070252 | -3.279530 | -2.076151 |
| 1 | 4.485438 | 4.542644 | -1.870207 | 1 | -4.472776 | -4.116945 | -2.632241 |
| 6 | 4.658180 | 2.427998 | -2.050867 | 6 | -4.739030 | -2.053471 | -2.223101 |
| 6 | 5.855506 | 2.554482 | -2.955670 | 6 | -5.957202 | -2.005509 | -3.110250 |
| 1 | 6.687194 | 1.984491 | -2.533008 | 1 | -6.822002 | -1.711687 | -2.508430 |
| 1 | 6.161861 | 3.589968 | -3.107345 | 1 | -6.164881 | -2.958884 | -3.597089 |
| 1 | 5.619415 | 2.104035 | -3.924074 | 1 | -5.821859 | -1.230239 | -3.869449 |
| 6 | -0.628470 | 0.238503 | -3.878656 | 6 | -0.604191 | 0.224662 | -3.881763 |

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|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 1 | -0.801870 | 0.332345 | -4.942578 | 1 | -0.773122 | 0.315076 | -4.946706 |
| 6 | 0.639614 | 0.371773 | -3.324721 | 6 | -1.649053 | -0.041121 | -3.010780 |
| 1 | 1.513887 | 0.566862 | -3.940689 | 1 | -2.675076 | -0.168776 | -3.338526 |
| 6 | -0.189983 | 0.027302 | -1.221114 | 6 | -0.177287 | 0.021700 | -1.221940 |
| 6 | -0.039362 | -0.049794 | 0.197885 | 6 | -0.031482 | -0.050139 | 0.197950 |
| 6 | 1.217997 | 0.168808 | 0.806804 | 6 | -1.222699 | -0.313145 | 0.913632 |
| 6 | 0.096252 | -0.144055 | 2.960567 | 6 | 0.099980 | -0.120632 | 2.960453 |
| 6 | 0.215502 | -0.185966 | 4.486165 | 6 | 0.127124 | -0.153332 | 4.490754 |
| 6 | 1.194873 | -1.300475 | 4.885455 | 6 | -0.810382 | 0.935185 | 5.036109 |
| 1 | 1.294640 | -1.344306 | 5.975647 | 1 | -0.806185 | 0.924271 | 6.131639 |
| 1 | 0.838588 | -2.273454 | 4.534382 | 1 | -0.489288 | 1.925950 | 4.701595 |
| 6 | 0.745028 | 1.164907 | 4.992063 | 6 | -0.349547 | -1.529535 | 4.980328 |
| 1 | 0.064559 | 1.975767 | 4.716042 | 1 | 0.301786 | -2.323013 | 4.602196 |
| 1 | 1.727750 | 1.395626 | 4.573721 | 1 | -1.368308 | -1.745909 | 4.648834 |
| 1 | 0.837269 | 1.150169 | 6.083644 | 1 | -0.335990 | -1.566426 | 6.075105 |
| 6 | 5.211476 | 2.044931 | 1.640019 | 6 | -4.353568 | -2.187627 | 1.827719 |
| 1 | 4.639437 | 2.962656 | 1.533513 | 1 | -3.730935 | -3.001304 | 1.472725 |
| 6 | 6.430893 | 2.008810 | 2.297479 | 6 | -5.308067 | -2.337511 | 2.816335 |
| 1 | 6.869146 | 2.894742 | 2.739488 | 1 | -5.482206 | -3.296319 | 3.286764 |
| 6 | 7.052667 | 0.767665 | 2.360917 | 6 | -6.025978 | -1.199558 | 3.167185 |
| 1 | 8.009855 | 0.648546 | 2.864385 | 1 | -6.800403 | -1.242010 | 3.929760 |
| 6 | 5.358038 | -0.203220 | 1.201318 | 6 | -4.876150 | 0.068606 | 1.672347 |
| 6 | 4.734556 | -1.376147 | 0.583294 | 6 | -4.523614 | 1.313660 | 1.029219 |
| 6 | 3.506205 | -1.224963 | -0.105726 | 6 | -3.476179 | 1.234633 | 0.082847 |
| 6 | 3.506631 | -3.643743 | -0.541168 | 6 | -3.684921 | 3.654545 | -0.230883 |
| 6 | 4.731181 | -3.744484 | 0.125909 | 6 | -4.731608 | 3.683569 | 0.700762 |
| 6 | 5.332444 | -2.628282 | 0.690015 | 6 | -5.145687 | 2.523857 | 1.331110 |
| 1 | 6.273527 | -2.715533 | 1.222118 | 1 | -5.948390 | 2.538309 | 2.061360 |
| 6 | 1.470129 | -5.068880 | -0.373083 | 6 | -1.715399 | 5.155741 | -0.545071 |
| 1 | 1.660392 | -5.256715 | 0.687795 | 1 | -1.617328 | 5.308448 | 0.533790 |
| 1 | 0.934657 | -5.933197 | -0.781670 | 1 | -1.330512 | 6.047030 | -1.053621 |
| 1 | 0.813801 | -4.197436 | -0.442861 | 1 | -1.082821 | 4.306363 | -0.814656 |
| 6 | 3.620133 | -6.136366 | -1.022078 | 6 | -3.987014 | 6.162002 | -0.543275 |
| 1 | 3.820971 | -6.403191 | 0.019776 | 1 | -3.920488 | 6.371052 | 0.528449 |
| 1 | 4.577336 | -6.045391 | -1.544923 | 1 | -5.043575 | 6.061464 | -0.809739 |
| 1 | 3.071967 | -6.968367 | -1.474250 | 1 | -3.591709 | 7.033057 | -1.074750 |
| 6 | 2.789050 | -4.856874 | -1.132513 | 6 | -3.183477 | 4.919144 | -0.930877 |
| 6 | 2.489381 | -4.609036 | -2.618364 | 6 | -3.288701 | 4.740461 | -2.453126 |
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| 8 | -2.323737 | -2.723835 | -0.549162 | 8 | 2.152384 | 2.671806 | -0.468599 |
| 8 | -4.445021 | -0.947304 | -1.672841 | 8 | 4.293209 | 1.240933 | -1.807463 |
| 6 | -2.358505 | -4.924445 | -1.346703 | 6 | 2.242921 | 5.008379 | -0.587622 |
| 1 | -2.126482 | -5.260499 | -0.333282 | 1 | 1.935074 | 5.054645 | 0.459925 |
| 1 | -3.020980 | -5.641861 | -1.832417 | 1 | 2.928867 | 5.826826 | -0.809776 |
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| 6 | -2.942663 | -3.535265 | -1.296113 | 6 | 2.841742 | 3.656998 | -0.871911 |
| 6 | -4.087702 | -3.275078 | -2.066520 | 6 | 4.056415 | 3.593012 | -1.567756 |
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| 1 | -6.190622 | -2.951416 | -3.575230 | 1 | 6.179075 | 3.579005 | -3.096683 |
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| 6 | -1.669337 | -0.031053 | -3.004182 | 6 | 0.661620 | 0.359059 | -3.323231 |
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| 6 | -1.121901 | -0.353582 | 2.307347 | 6 | 1.250732 | 0.126655 | 2.202951 |
| 1 | 2.188472 | -1.137724 | 4.461054 | 1 | -1.840208 | 0.789803 | 4.700783 |
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| 1 | -1.861436 | 0.316119 | 4.951292 | 1 | 2.240394 | -0.663502 | 4.727602 |
| 1 | -1.539549 | -1.427012 | 4.881587 | 1 | 1.910141 | 1.078218 | 4.774332 |
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| 6 | -6.031811 | -1.209837 | 3.177204 | 6 | 7.052667 | 0.765465 | 2.379713 |
| 1 | -6.806523 | -1.254781 | 3.939337 | 1 | 8.007575 | 0.645664 | 2.887326 |
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| 6 | -4.531054 | 1.309840 | 1.045819 | 6 | 4.735954 | -1.379108 | 0.601367 |
| 6 | -3.484276 | 1.234116 | 0.098542 | 6 | 3.508911 | -1.228970 | -0.090117 |
| 6 | -3.696014 | 3.654314 | -0.210234 | 6 | 3.506475 | -3.649528 | -0.516060 |
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| 1 | -4.341896 | 4.567288 | -2.730030 | 1 | 3.411737 | -4.461187 | -3.154491 |
| 1 | -2.949834 | 5.646248 | -2.941558 | 1 | 1.972130 | -5.487352 | -3.016660 |
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| 6 | -4.001811 | 6.161870 | -0.518214 | 6 | 3.618822 | -6.143461 | -0.990105 |
| 1 | -5.058582 | 6.060392 | -0.783496 | 1 | 4.576086 | -6.054056 | -1.513112 |
| 1 | -3.934180 | 6.369312 | 0.553758 | 1 | 3.819514 | -6.407834 | 0.052402 |

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| 1 | -3.608318 | 7.034279 | -1.048809 | 1 | 3.070401 | -6.976398 | -1.440241 |
| 6 | -3.197170 | 4.920687 | -0.908842 | 6 | 2.788146 | -4.863978 | -1.103747 |
| 6 | -1.728848 | 5.158598 | -0.524887 | 6 | 1.469452 | -5.073296 | -0.343210 |
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| 1 | -1.629325 | 5.310050 | 0.554021 | 1 | 1.660056 | -5.258682 | 0.718036 |
| 1 | -1.095582 | 4.310411 | -0.796553 | 1 | 0.813573 | -4.201666 | -0.414904 |
| 1 | 5.224188 | -4.704433 | 0.221975 | 1 | -5.224427 | 4.616921 | 0.942311 |
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| 6 | 2.916035 | -2.379490 | -0.628335 | 6 | -3.076256 | 2.427784 | -0.516594 |
| 1 | 1.953325 | -2.277227 | -1.119307 | 1 | -2.257838 | 2.403492 | -1.229512 |
| 6 | -3.085882 | 2.428865 | -0.498614 | 6 | 2.917287 | -2.384950 | -0.608018 |
| 1 | -2.267900 | 2.406845 | -1.212095 | 1 | 1.954849 | -2.283591 | -1.099717 |
| 6 | 1.247662 | 0.111816 | 2.196547 | 6 | -1.119908 | -0.338067 | 2.301172 |
| 1 | 2.196663 | 0.268243 | 2.700353 | 1 | -2.010493 | -0.520483 | 2.894344 |

| D2- ³ MC1 | | | | D2- ³ MC2 | | | |
|----------------------|-----------|-----------|-----------|----------------------|-----------|-----------|-----------|
| 77 | -2.886892 | -0.811709 | -0.172775 | 77 | -2.901530 | -0.742476 | 0.010001 |
| 7 | -6.749027 | -0.162091 | 1.692149 | 7 | -5.688228 | 1.059152 | 2.572426 |
| 7 | -4.820048 | -1.260700 | 0.876388 | 7 | -4.182708 | -0.480880 | 1.579246 |
| 7 | -0.756516 | -0.845105 | -1.987164 | 7 | -1.545433 | -0.899407 | -1.514170 |
| 8 | -2.358067 | -2.894337 | -0.452627 | 8 | -2.568134 | -2.850686 | 0.443902 |
| 8 | -4.035854 | -0.964232 | -1.993703 | 8 | -4.578140 | -1.404095 | -1.215750 |
| 6 | -1.988526 | -4.958238 | -1.488724 | 6 | -2.719465 | -5.181833 | 0.387011 |
| 1 | -0.898022 | -4.865654 | -1.504059 | 1 | -1.652814 | -5.260309 | 0.160440 |
| 1 | -2.307830 | -5.559717 | -2.340419 | 1 | -3.257744 | -5.999335 | -0.093729 |
| 1 | -2.252275 | -5.468344 | -0.558868 | 1 | -2.819369 | -5.275863 | 1.472583 |
| 6 | -2.589011 | -3.576236 | -1.487968 | 6 | -3.213149 | -3.822958 | -0.041648 |
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| 1 | -3.449612 | -3.900452 | -3.401657 | 1 | -4.760676 | -4.704012 | -1.193710 |
| 6 | -4.017741 | -1.957374 | -2.782185 | 6 | -4.938144 | -2.600688 | -1.404110 |
| 6 | -4.841985 | -1.767003 | -4.029387 | 6 | -6.161595 | -2.761807 | -2.270454 |
| 1 | -5.881166 | -1.582969 | -3.743025 | 1 | -7.012171 | -2.286801 | -1.772928 |
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| 1 | -4.496167 | -0.871683 | -4.553730 | 1 | -6.010220 | -2.230894 | -3.214193 |
| 6 | 0.817442 | -1.250435 | -3.725595 | 6 | -0.786423 | -1.250496 | -3.727060 |
| 1 | 1.033693 | -1.446135 | -4.767613 | 1 | -0.996773 | -1.445830 | -4.770363 |
| 6 | -0.483541 | -1.093659 | -3.258373 | 6 | -1.806392 | -1.143299 | -2.798298 |
| 1 | -1.336281 | -1.170705 | -3.927440 | 1 | -2.855282 | -1.243153 | -3.055638 |
| 6 | 0.261135 | -0.748321 | -1.129780 | 6 | -0.245151 | -0.749210 | -1.128226 |
| 6 | 0.059372 | -0.417886 | 0.251490 | 6 | -0.050098 | -0.419191 | 0.254538 |
| 6 | -1.230390 | -0.221849 | 0.795422 | 6 | -1.237888 | -0.247317 | 1.003042 |
| 6 | -1.299571 | 0.246775 | 2.105578 | 6 | -1.100761 | 0.180755 | 2.321867 |
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| 6 | -0.998375 | 2.325541 | 4.291520 | 6 | -0.534815 | 2.271923 | 4.446051 |
| 1 | -1.129754 | 2.706960 | 5.310047 | 1 | -0.494659 | 2.647556 | 5.474447 |
| 1 | -0.393588 | 3.044951 | 3.731615 | 1 | -0.089920 | 3.024668 | 3.788773 |
| 6 | -1.181558 | -0.034665 | 5.121807 | 6 | -0.424651 | -0.093898 | 5.272154 |
| 1 | -0.714060 | -1.023261 | 5.158711 | 1 | 0.096953 | -1.053724 | 5.210693 |
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| 6 | -5.298572 | -2.437635 | 1.267054 | 6 | -4.459161 | -1.382852 | 2.522121 |
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| 6 | -5.547794 | -0.142711 | 1.104261 | 6 | -4.799847 | 0.734961 | 1.634546 |
| 6 | -4.931219 | 1.100487 | 0.681625 | 6 | -4.386227 | 1.654144 | 0.598887 |
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| 6 | -4.970553 | 3.498202 | 0.458547 | 6 | -4.452750 | 3.776412 | -0.524471 |
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| 1 | -1.153245 | 5.816056 | -0.023732 | 1 | -1.052327 | 5.026116 | -3.234144 |
| 1 | -1.011796 | 4.057133 | 0.128630 | 1 | -0.917191 | 3.434201 | -2.475750 |
| 6 | -3.827263 | 6.006293 | -0.342188 | 6 | -3.592936 | 5.618151 | -2.550505 |
| 1 | -4.077945 | 6.155046 | 0.712440 | 1 | -3.382019 | 6.153345 | -1.619799 |
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| 7 | 4.187280 | -0.468700 | 1.595234 | 7 | 4.833077 | -1.242575 | 0.884921 |
| 7 | 1.563732 | -0.897900 | -1.508724 | 7 | 0.777310 | -0.845469 | -1.979712 |
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| 1 | 3.291712 | -5.991524 | -0.075209 | 1 | 2.358896 | -5.559938 | -2.324402 |
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| 1 | 2.882520 | -1.241016 | -3.042554 | 1 | 1.368435 | -1.169858 | -3.916825 |
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| 1 | 1.554678 | 0.146658 | 5.125822 | 1 | 2.249233 | 0.249770 | 4.782861 |
| 1 | 1.679532 | 1.820881 | 4.551426 | 1 | 2.171498 | 1.923135 | 4.201138 |
| 1 | 0.847280 | 1.463772 | 6.067834 | 1 | 1.650451 | 1.530767 | 5.843038 |
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| 1 | 3.933452 | -2.311051 | 2.462960 | 1 | 4.693944 | -3.281764 | 1.072419 |
| 6 | 5.373640 | -1.088384 | 3.542608 | 6 | 6.549556 | -2.506688 | 1.898659 |
| 1 | 5.602646 | -1.814894 | 4.311171 | 1 | 6.956527 | -3.455434 | 2.223724 |
| 6 | 5.970199 | 0.167317 | 3.510073 | 6 | 7.234997 | -1.307452 | 2.076058 |
| 1 | 6.700306 | 0.457267 | 4.262322 | 1 | 8.215135 | -1.294667 | 2.548471 |
| 6 | 4.803298 | 0.747723 | 1.648360 | 6 | 5.555240 | -0.120432 | 1.110294 |
| 6 | 4.388571 | 1.664992 | 0.611274 | 6 | 4.930876 | 1.119097 | 0.688373 |
| 6 | 3.406901 | 1.174368 | -0.280841 | 6 | 3.642423 | 1.043369 | 0.106225 |
| 6 | 2.969511 | 2.047981 | -1.275824 | 6 | 3.052001 | 2.248325 | -0.274404 |
| 1 | 2.208561 | 1.707585 | -1.971278 | 1 | 2.056893 | 2.212966 | -0.706635 |
| 6 | 3.474513 | 3.345326 | -1.417420 | 6 | 3.679014 | 3.487918 | -0.110137 |
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| 6 | 4.902751 | 2.955202 | 0.495379 | 6 | 5.575040 | 2.345891 | 0.860092 |
| 1 | 5.655696 | 3.289389 | 1.201934 | 1 | 6.563648 | 2.359782 | 1.307017 |
| 6 | 1.433889 | 4.397224 | -2.415251 | 6 | 1.665270 | 4.906549 | 0.289804 |
| 1 | 1.176148 | 4.866725 | -1.461687 | 1 | 1.900585 | 4.979119 | 1.355960 |
| 1 | 1.047412 | 5.027726 | -3.223274 | 1 | 1.125136 | 5.813679 | -0.002973 |
| 1 | 0.915424 | 3.436393 | -2.463036 | 1 | 0.995191 | 4.054205 | 0.153630 |
| 6 | 3.587542 | 5.624760 | -2.541627 | 6 | 3.797408 | 6.018157 | -0.335352 |
| 1 | 3.376059 | 6.160448 | -1.611333 | 1 | 4.052776 | 6.169330 | 0.717811 |

| | | | | | | | |
|---|----------|----------|-----------|---|----------|----------|-----------|
| 1 | 4.672711 | 5.579317 | -2.673729 | 1 | 4.726252 | 5.980813 | -0.912866 |
| 1 | 3.178442 | 6.217212 | -3.365598 | 1 | 3.234839 | 6.895862 | -0.667707 |
| 6 | 2.954578 | 4.231865 | -2.550827 | 6 | 2.949956 | 4.761098 | -0.540687 |
| 6 | 3.276568 | 3.569143 | -3.899184 | 6 | 2.590025 | 4.666648 | -2.031026 |
| 1 | 2.910648 | 4.191015 | -4.723377 | 1 | 2.068446 | 5.574917 | -2.351554 |
| 1 | 4.355969 | 3.439075 | -4.021112 | 1 | 3.490702 | 4.554414 | -2.642033 |
| 1 | 2.808817 | 2.585036 | -3.985590 | 1 | 1.937170 | 3.815228 | -2.236674 |

| D2- ³ MC3 | | | | D2- ³ MC4 | | | |
|----------------------|-----------|-----------|-----------|----------------------|-----------|-----------|-----------|
| 77 | -2.713244 | -0.616959 | -0.497393 | 77 | -2.923483 | -0.733314 | -0.023968 |
| 7 | -6.574957 | -0.301602 | 1.796660 | 7 | -5.710995 | 1.068567 | 2.531578 |
| 7 | -4.627743 | -1.304718 | 0.897930 | 7 | -4.220919 | -0.478749 | 1.527117 |
| 7 | -0.787857 | -0.907204 | -1.897050 | 7 | -1.537296 | -0.889305 | -1.533022 |
| 8 | -2.307196 | -2.743801 | -0.335612 | 8 | -2.637935 | -2.858085 | 0.366364 |
| 8 | -4.125336 | -1.110467 | -2.081839 | 8 | -4.578826 | -1.334456 | -1.310556 |
| 6 | -2.233869 | -5.013927 | -0.865936 | 6 | -2.831293 | -5.183757 | 0.249162 |
| 1 | -1.157135 | -4.999000 | -1.059102 | 1 | -1.764221 | -5.281916 | 0.032110 |
| 1 | -2.702236 | -5.773850 | -1.492202 | 1 | -3.381803 | -5.979391 | -0.253909 |
| 1 | -2.360650 | -5.276856 | 0.187954 | 1 | -2.945078 | -5.296503 | 1.331485 |
| 6 | -2.788077 | -3.632602 | -1.105920 | 6 | -3.289132 | -3.805680 | -0.157835 |
| 6 | -3.745894 | -3.466141 | -2.111742 | 6 | -4.374889 | -3.699820 | -1.042308 |
| 1 | -4.047130 | -4.363164 | -2.638269 | 1 | -4.823730 | -4.629917 | -1.367812 |
| 6 | -4.361165 | -2.264266 | -2.523926 | 6 | -4.956602 | -2.519344 | -1.533931 |
| 6 | -5.409284 | -2.335372 | -3.604801 | 6 | -6.162838 | -2.637987 | -2.431023 |
| 1 | -6.376955 | -2.061000 | -3.173920 | 1 | -7.019711 | -2.173770 | -1.933923 |
| 1 | -5.489346 | -3.325834 | -4.054012 | 1 | -6.408879 | -3.671741 | -2.676015 |
| 1 | -5.183819 | -1.596019 | -4.377235 | 1 | -5.987633 | -2.074578 | -3.351398 |
| 6 | 0.706991 | -1.317630 | -3.690485 | 6 | -0.684178 | -1.248364 | -3.715701 |
| 1 | 0.882517 | -1.529179 | -4.736678 | 1 | -0.855962 | -1.442490 | -4.765892 |
| 6 | -0.576457 | -1.175751 | -3.177853 | 6 | -1.742253 | -1.130972 | -2.825957 |
| 1 | -1.459732 | -1.279119 | -3.801526 | 1 | -2.779294 | -1.223859 | -3.129850 |
| 6 | 0.268615 | -0.771039 | -1.079788 | 6 | -0.255302 | -0.746094 | -1.094438 |
| 6 | 0.090193 | -0.422638 | 0.284742 | 6 | -0.081355 | -0.425658 | 0.277809 |
| 6 | -1.214447 | -0.226488 | 0.795221 | 6 | -1.275249 | -0.285907 | 1.026521 |
| 6 | -1.288593 | 0.168446 | 2.124448 | 6 | -1.125121 | 0.081429 | 2.356731 |
| 1 | -2.265818 | 0.343696 | 2.562523 | 1 | -2.006033 | 0.223823 | 2.974761 |
| 6 | -0.138611 | 0.361391 | 2.911058 | 6 | 0.144613 | 0.280302 | 2.926637 |
| 6 | -0.315037 | 0.822726 | 4.360466 | 6 | 0.230491 | 0.692056 | 4.399155 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | -1.033702 | 2.181286 | 4.372059 | 6 | -0.485928 | 2.038364 | 4.588771 |
| 1 | -1.176057 | 2.525319 | 5.402540 | 1 | -0.437328 | 2.347691 | 5.638670 |
| 1 | -0.445760 | 2.933775 | 3.838040 | 1 | -0.015012 | 2.816139 | 3.980537 |
| 6 | -1.160150 | -0.208263 | 5.124529 | 6 | -0.451474 | -0.375712 | 5.268660 |
| 1 | -0.668384 | -1.185697 | 5.129691 | 1 | 0.035898 | -1.347177 | 5.142875 |
| 1 | -2.148680 | -0.333431 | 4.676757 | 1 | -1.506834 | -0.495161 | 5.011192 |
| 1 | -1.297796 | 0.112201 | 6.163093 | 1 | -0.392011 | -0.096245 | 6.326304 |
| 6 | -5.036029 | -2.496601 | 1.308364 | 6 | -4.523823 | -1.393428 | 2.449380 |
| 1 | -4.373192 | -3.329185 | 1.094380 | 1 | -4.004876 | -2.341513 | 2.360563 |
| 6 | -6.238481 | -2.657206 | 1.978796 | 6 | -5.438969 | -1.117958 | 3.448098 |
| 1 | -6.578044 | -3.627459 | 2.318557 | 1 | -5.687978 | -1.855947 | 4.199302 |
| 6 | -6.979167 | -1.500686 | 2.190543 | 6 | -6.015734 | 0.147259 | 3.433838 |
| 1 | -7.938129 | -1.538738 | 2.703290 | 1 | -6.750891 | 0.433291 | 4.182648 |
| 6 | -5.400893 | -0.236842 | 1.159989 | 6 | -4.815814 | 0.747371 | 1.599585 |
| 6 | -4.868592 | 1.050868 | 0.729829 | 6 | -4.368946 | 1.679606 | 0.589722 |
| 6 | -3.619640 | 1.079908 | 0.076947 | 6 | -3.379538 | 1.190452 | -0.294466 |
| 6 | -3.078929 | 2.326621 | -0.242814 | 6 | -2.907466 | 2.077581 | -1.261224 |
| 1 | -2.089348 | 2.364247 | -0.688438 | 1 | -2.139418 | 1.738033 | -1.949299 |
| 6 | -3.760874 | 3.525908 | -0.002481 | 6 | -3.386157 | 3.386680 | -1.383339 |
| 6 | -5.010101 | 3.456994 | 0.620600 | 6 | -4.371689 | 3.825839 | -0.488855 |
| 1 | -5.565096 | 4.361395 | 0.837245 | 1 | -4.762840 | 4.833439 | -0.554404 |
| 6 | -5.549556 | 2.236989 | 0.994509 | 6 | -4.857583 | 2.981093 | 0.493192 |
| 1 | -6.507141 | 2.183188 | 1.501434 | 1 | -5.617236 | 3.313850 | 1.193213 |
| 6 | -1.799976 | 5.017730 | 0.400791 | 6 | -1.308638 | 4.430804 | -2.310815 |
| 1 | -1.996444 | 5.027236 | 1.477029 | 1 | -1.068755 | 4.881015 | -1.343303 |
| 1 | -1.313545 | 5.962094 | 0.133202 | 1 | -0.894002 | 5.069739 | -3.098076 |
| 1 | -1.096568 | 4.206197 | 0.198662 | 1 | -0.802535 | 3.463361 | -2.362196 |
| 6 | -4.005536 | 6.053635 | -0.086928 | 6 | -3.442431 | 5.689155 | -2.464602 |
| 1 | -4.225439 | 6.138471 | 0.981484 | 1 | -3.245053 | 6.204550 | -1.519885 |
| 1 | -4.953376 | 5.999909 | -0.631282 | 1 | -4.524858 | 5.660222 | -2.621299 |
| 1 | -3.498606 | 6.973641 | -0.392991 | 1 | -3.007532 | 6.291482 | -3.267978 |
| 6 | -3.107353 | 4.852642 | -0.389737 | 6 | -2.827756 | 4.288355 | -2.486284 |
| 6 | -2.801336 | 4.852405 | -1.894835 | 6 | -3.125214 | 3.657176 | -3.855210 |
| 1 | -2.328602 | 5.797132 | -2.183874 | 1 | -2.731883 | 4.290528 | -4.657758 |
| 1 | -3.719425 | 4.735815 | -2.478501 | 1 | -4.202877 | 3.543468 | -4.005286 |
| 1 | -2.123010 | 4.041325 | -2.170038 | 1 | -2.668141 | 2.668889 | -3.950843 |
| 77 | 2.931654 | -0.733698 | 0.000167 | 77 | 2.724098 | -0.604862 | -0.495230 |
| 7 | 5.715679 | 1.118638 | 2.522989 | 7 | 6.570726 | -0.297451 | 1.824390 |
| 7 | 4.225103 | -0.447450 | 1.549216 | 7 | 4.634767 | -1.299891 | 0.901186 |
| 7 | 1.552214 | -0.920984 | -1.511411 | 7 | 0.803898 | -0.867282 | -1.910326 |
| 8 | 2.649102 | -2.850310 | 0.433669 | 8 | 2.325405 | -2.733752 | -0.371100 |
| 8 | 4.590707 | -1.360399 | -1.269767 | 8 | 4.146087 | -1.066878 | -2.080261 |
| 6 | 2.839801 | -5.178020 | 0.360046 | 6 | 2.271024 | -4.997207 | -0.930894 |
| 1 | 1.772066 | -5.278720 | 0.147467 | 1 | 1.196673 | -4.987233 | -1.137284 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 1 | 3.388085 | -5.983531 | -0.129557 | 1 | 2.752048 | -5.746868 | -1.559904 |
| 1 | 2.956186 | -5.271008 | 1.443975 | 1 | 2.386463 | -5.271085 | 0.121475 |
| 6 | 3.298556 | -3.808413 | -0.073489 | 6 | 2.818791 | -3.609721 | -1.148499 |
| 6 | 4.383175 | -3.720327 | -0.961150 | 6 | 3.783655 | -3.424263 | -2.144054 |
| 1 | 4.830408 | -4.656734 | -1.270312 | 1 | 4.094615 | -4.312339 | -2.680012 |
| 6 | 4.966700 | -2.549446 | -1.473068 | 6 | 4.392737 | -2.212793 | -2.536768 |
| 6 | 6.172556 | -2.685216 | -2.368199 | 6 | 5.446810 | -2.261646 | -3.612969 |
| 1 | 7.029558 | -2.211265 | -1.880640 | 1 | 6.409408 | -1.981489 | -3.174574 |
| 1 | 6.418602 | -3.723472 | -2.593332 | 1 | 5.539359 | -3.246396 | -4.072211 |
| 1 | 5.996835 | -2.139795 | -3.299281 | 1 | 5.217196 | -1.516710 | -4.378820 |
| 6 | 1.761944 | -1.184108 | -2.799291 | 6 | 0.597276 | -1.114009 | -3.196251 |
| 1 | 2.800179 | -1.280418 | -3.097994 | 1 | 1.482884 | -1.205902 | -3.818459 |
| 6 | 1.278708 | -0.264280 | 1.031660 | 6 | 1.218237 | -0.245192 | 0.796712 |
| 6 | 1.128485 | 0.141761 | 2.356656 | 6 | 1.293453 | 0.110693 | 2.142912 |
| 1 | 2.009727 | 0.297333 | 2.966845 | 1 | 2.270391 | 0.265127 | 2.583592 |
| 1 | -2.014921 | 2.124828 | 3.894712 | 1 | -1.538536 | 1.982823 | 4.300755 |
| 6 | 1.015611 | 0.983588 | 5.097797 | 6 | 1.672393 | 0.848328 | 4.886388 |
| 1 | 1.568634 | 0.040586 | 5.147154 | 1 | 2.231777 | -0.088078 | 4.801870 |
| 1 | 1.655254 | 1.733544 | 4.623364 | 1 | 2.209452 | 1.619599 | 4.327110 |
| 1 | 0.825265 | 1.311177 | 6.124544 | 1 | 1.670555 | 1.141681 | 5.940880 |
| 6 | 4.527936 | -1.344104 | 2.489009 | 6 | 5.046844 | -2.494508 | 1.299662 |
| 1 | 4.008397 | -2.293400 | 2.418461 | 1 | 4.390212 | -3.328093 | 1.070740 |
| 6 | 5.443773 | -1.049739 | 3.481591 | 6 | 6.245682 | -2.656856 | 1.976037 |
| 1 | 5.692840 | -1.773023 | 4.246934 | 1 | 6.588437 | -3.629345 | 2.306071 |
| 6 | 6.020730 | 0.214826 | 3.442715 | 6 | 6.978700 | -1.499004 | 2.206627 |
| 1 | 6.756281 | 0.515103 | 4.185519 | 1 | 7.934470 | -1.538171 | 2.725211 |
| 6 | 4.820229 | 0.779574 | 1.597796 | 6 | 5.400431 | -0.231150 | 1.181038 |
| 6 | 4.373230 | 1.692287 | 0.570151 | 6 | 4.865048 | 1.058869 | 0.761320 |
| 6 | 3.385906 | 1.185598 | -0.306400 | 6 | 3.618615 | 1.090027 | 0.103762 |
| 6 | 2.912261 | 2.054781 | -1.288502 | 6 | 3.076415 | 2.337599 | -0.209828 |
| 1 | 2.145140 | 1.701630 | -1.970707 | 1 | 2.088860 | 2.376178 | -0.659934 |
| 6 | 3.387022 | 3.363217 | -1.432076 | 6 | 3.755970 | 3.536526 | 0.039604 |
| 6 | 4.371413 | 3.819692 | -0.545026 | 6 | 5.002287 | 3.465803 | 0.668211 |
| 1 | 4.759995 | 4.827082 | -0.627214 | 1 | 5.555045 | 4.369756 | 0.892281 |
| 6 | 4.859071 | 2.992890 | 0.451322 | 6 | 5.542238 | 2.244478 | 1.037195 |
| 1 | 5.617594 | 3.339331 | 1.145909 | 1 | 6.497733 | 2.189243 | 1.547873 |
| 6 | 1.305198 | 4.383607 | -2.376378 | 6 | 1.794647 | 5.028845 | 0.441160 |
| 1 | 1.062433 | 4.844953 | -1.414832 | 1 | 1.988468 | 5.037512 | 1.517882 |
| 1 | 0.888628 | 5.010836 | -3.171986 | 1 | 1.309016 | 5.973595 | 0.173560 |
| 1 | 0.803013 | 3.413582 | -2.416142 | 1 | 1.091570 | 4.217812 | 0.235989 |
| 6 | 3.432999 | 5.649474 | -2.547057 | 6 | 4.002223 | 6.064407 | -0.037685 |
| 1 | 3.232393 | 6.177298 | -1.609912 | 1 | 4.218863 | 6.146965 | 1.031569 |
| 1 | 4.515682 | 5.623617 | -2.702531 | 1 | 4.951719 | 6.011097 | -0.579169 |
| 1 | 2.995759 | 6.238095 | -3.359260 | 1 | 3.496878 | 6.985395 | -0.343419 |

| | | | | | | | |
|---|----------|----------|-----------|---|----------|----------|-----------|
| 6 | 2.825125 | 4.245570 | -2.548783 | 6 | 3.104141 | 4.864674 | -0.345903 |
| 6 | 3.126560 | 3.595570 | -3.907953 | 6 | 2.802445 | 4.868699 | -1.851900 |
| 1 | 2.730526 | 4.214879 | -4.720083 | 1 | 2.331686 | 5.814763 | -2.139752 |
| 1 | 4.204878 | 3.485070 | -4.055711 | 1 | 3.722126 | 4.752611 | -2.433143 |
| 1 | 2.674425 | 2.603712 | -3.988819 | 1 | 2.123949 | 4.059244 | -2.131379 |

| Ir1-CI-3MC | | | | Ir1-2CI-3MC | | | |
|-------------------|-----------|-----------|-----------|--------------------|-----------|-----------|-----------|
| 77 | 2.93572 | 0.836591 | -0.066313 | 77 | 2.696661 | 0.715689 | -0.3891 |
| 7 | 6.856413 | 0.048284 | 1.650942 | 7 | 6.646656 | -0.097931 | 1.279647 |
| 7 | 4.893428 | 1.201734 | 1.008847 | 7 | 4.694636 | 1.079357 | 0.656109 |
| 7 | 0.906346 | 0.828397 | -1.859727 | 7 | 0.564207 | 0.643496 | -2.030092 |
| 8 | 2.312753 | 2.913379 | -0.072559 | 8 | 2.108764 | 2.798524 | -0.467272 |
| 8 | 4.088189 | 1.292023 | -1.841073 | 8 | 3.802542 | 1.076686 | -2.203162 |
| 6 | 1.91857 | 5.108539 | -0.779154 | 6 | 1.701565 | 4.958399 | -1.270884 |
| 1 | 0.830506 | 4.995547 | -0.769063 | 1 | 0.614657 | 4.86208 | -1.194272 |
| 1 | 2.198386 | 5.825868 | -1.551232 | 1 | 1.946272 | 5.627679 | -2.09613 |
| 1 | 2.204681 | 5.498024 | 0.201484 | 1 | 2.046478 | 5.397709 | -0.331048 |
| 6 | 2.550644 | 3.755768 | -0.980116 | 6 | 2.307234 | 3.588624 | -1.430097 |
| 6 | 3.344901 | 3.55099 | -2.125295 | 6 | 3.040278 | 3.311199 | -2.600374 |
| 1 | 3.455831 | 4.397931 | -2.790914 | 1 | 3.121541 | 4.116273 | -3.319956 |
| 6 | 4.065298 | 2.396973 | -2.463193 | 6 | 3.747834 | 2.138503 | -2.896341 |
| 6 | 4.933723 | 2.42903 | -3.694566 | 6 | 4.56336 | 2.091956 | -4.162083 |
| 1 | 5.971953 | 2.251256 | -3.400553 | 1 | 5.615665 | 1.948672 | -3.90078 |
| 1 | 4.869204 | 3.374431 | -4.234117 | 1 | 4.462631 | 2.995876 | -4.763545 |
| 1 | 4.648403 | 1.60676 | -4.356665 | 1 | 4.263277 | 1.221232 | -4.751593 |
| 6 | -0.609604 | 1.435716 | -3.577736 | 6 | -1.050209 | 1.180657 | -3.67977 |
| 1 | -0.815571 | 1.873584 | -4.54389 | 1 | -1.311533 | 1.561368 | -4.656692 |
| 6 | 0.671777 | 1.318028 | -3.066156 | 6 | 0.259703 | 1.065632 | -3.24649 |
| 6 | -0.128861 | 0.402501 | -1.136999 | 1 | 1.090045 | 1.339853 | -3.890701 |
| 6 | 0.065116 | -0.045595 | 0.205405 | 6 | -0.428881 | 0.289701 | -1.214721 |
| 6 | 1.334091 | 0.007613 | 0.822224 | 6 | -0.153718 | -0.080435 | 0.137349 |
| 6 | 0.273718 | -0.828439 | 2.861419 | 6 | 1.158143 | -0.035581 | 0.6606 |
| 6 | 0.438153 | -1.243044 | 4.32495 | 6 | 0.222647 | -0.722062 | 2.813783 |
| 6 | 1.396969 | -2.440878 | 4.409533 | 6 | 0.478772 | -1.066268 | 4.282422 |
| 1 | 1.531719 | -2.7426 | 5.453847 | 6 | 1.383537 | -2.305792 | 4.361049 |
| 1 | 0.999198 | -3.295955 | 3.854916 | 1 | 1.584179 | -2.560441 | 5.407258 |
| 6 | 1.019726 | -0.064219 | 5.120548 | 1 | 0.903702 | -3.16626 | 3.885316 |
| 1 | 0.354675 | 0.80287 | 5.070262 | 6 | 1.174491 | 0.120523 | 4.966806 |
| 1 | 1.996488 | 0.240292 | 4.736422 | 1 | 0.549956 | 1.017345 | 4.917586 |
| 1 | 1.142576 | -0.342433 | 6.172897 | 1 | 2.132927 | 0.353863 | 4.496741 |
| 6 | 5.356684 | 2.327675 | 1.541531 | 1 | 1.363147 | -0.10925 | 6.020982 |
| 1 | 4.709316 | 3.196344 | 1.460155 | 6 | 5.201476 | 2.202555 | 1.155922 |
| 6 | 6.59365 | 2.370393 | 2.157675 | 1 | 4.577503 | 3.088189 | 1.075456 |
| 1 | 6.981628 | 3.280454 | 2.596655 | 6 | 6.450946 | 2.238597 | 1.742927 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | 7.310035 | 1.176411 | 2.174306 | 1 | 6.875992 | 3.143028 | 2.154486 |
| 1 | 8.295942 | 1.128404 | 2.632196 | 6 | 7.125873 | 1.018501 | 1.760063 |
| 6 | 5.647109 | 0.079696 | 1.080265 | 6 | 5.422836 | -0.055223 | 0.732985 |
| 6 | 5.051848 | -1.112946 | 0.505439 | 6 | 4.800838 | -1.249654 | 0.199862 |
| 6 | 3.757178 | -0.999373 | -0.052509 | 6 | 3.496148 | -1.129378 | -0.334717 |
| 6 | 3.85076 | -3.389982 | -0.589686 | 6 | 3.549226 | -3.532354 | -0.822045 |
| 6 | 5.134254 | -3.460313 | -0.032282 | 6 | 4.843315 | -3.608203 | -0.288586 |
| 6 | 5.727946 | -2.335056 | 0.509379 | 6 | 5.461891 | -2.480971 | 0.217431 |
| 1 | 6.721017 | -2.382323 | 0.943914 | 1 | 6.463074 | -2.534035 | 0.632299 |
| 6 | 1.844018 | -4.864896 | -0.399888 | 6 | 1.535322 | -4.984681 | -0.558016 |
| 1 | 2.058163 | -5.05776 | 0.655638 | 1 | 1.773932 | -5.167389 | 0.494023 |
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| 1 | -3.773089 | 6.799624 | 1.727985 | 1 | -3.320906 | 7.229293 | 0.69669 |
| 6 | -3.302985 | 4.787657 | 1.106367 | 6 | -3.055141 | 5.110402 | 0.387013 |
| 6 | -1.853412 | 4.889892 | 1.606704 | 6 | -1.555489 | 5.173286 | 0.714843 |
| 1 | -1.47947 | 5.911798 | 1.4784 | 1 | -1.132304 | 6.124083 | 0.371953 |
| 1 | -1.790327 | 4.634065 | 2.66845 | 1 | -1.390522 | 5.09486 | 1.793347 |
| 1 | -1.188813 | 4.211107 | 1.066185 | 1 | -1.001955 | 4.359693 | 0.238998 |
| 1 | 5.526801 | -4.482365 | -0.310867 | 1 | 4.883102 | -5.061765 | -0.07986 |
| 1 | -5.342945 | 3.775283 | 2.713659 | 1 | -4.994699 | 4.55131 | 2.309511 |
| 1 | -1.896656 | -1.547557 | 2.689042 | 1 | -2.015348 | -0.983829 | 2.960304 |
| 6 | 3.092243 | -2.154419 | -0.715015 | 6 | 2.635007 | -2.588222 | -0.659266 |
| 1 | 2.102556 | -2.031016 | -1.143546 | 1 | 1.634093 | -2.428897 | -1.048024 |
| 6 | -3.147819 | 2.322385 | 0.568162 | 6 | -3.111265 | 2.58484 | 0.280061 |
| 1 | -2.333 | 2.57984 | -0.101585 | 1 | -2.346846 | 2.658939 | -0.487064 |
| 6 | 1.347816 | -0.701655 | 2.158324 | 6 | 1.243527 | -0.54878 | 2.115776 |
| 1 | 2.321426 | -0.785935 | 2.631036 | 1 | 2.237197 | -0.644045 | 2.542141 |
| 17 | -1.117016 | 2.181616 | -4.985325 | 17 | -1.462515 | 1.397141 | -5.252226 |
| 1 | 6.903746 | 2.912834 | 2.999223 | 17 | 7.399273 | 3.021711 | 2.415808 |

Ir3-Cl-3MC

| | | | | | | | |
|----|----------|----------|-----------|----|-----------|-----------|-----------|
| 77 | 2.762338 | 0.759285 | -0.060025 | 77 | -2.676119 | -0.482155 | -0.277136 |
| 7 | 6.029268 | 0.058259 | 2.761418 | 7 | -6.130397 | 0.160036 | 2.456421 |
| 7 | 4.288626 | 1.162364 | 1.599736 | 7 | -4.315213 | -0.982909 | 1.445629 |
| 7 | 0.715712 | 0.470366 | -2.039832 | 7 | -0.673188 | 0.172559 | -2.015258 |
| 8 | 2.089374 | 2.792845 | -0.298748 | 8 | -2.06538 | -2.41201 | -0.999056 |
| 8 | 4.311682 | 1.253105 | -1.446812 | 8 | -4.381074 | -0.767991 | -1.547184 |
| 6 | 1.795775 | 4.957728 | -1.143972 | 6 | -1.874627 | -4.391733 | -2.2314 |
| 1 | 0.795164 | 4.811529 | -1.562935 | 1 | -0.894988 | -4.159131 | -2.65955 |
| 1 | 2.314234 | 5.717338 | -1.729842 | 1 | -2.42861 | -5.017574 | -2.931719 |
| 1 | 1.663072 | 5.307198 | -0.117444 | 1 | -1.696052 | -4.943544 | -1.305189 |
| 6 | 2.520899 | 3.638206 | -1.13445 | 6 | -2.592012 | -3.10772 | -1.912196 |

Ir3-2Cl-3MC

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 6 | 3.589471 | 3.453707 | -2.025968 | 6 | -3.757039 | -2.791505 | -2.628691 |
| 1 | 3.827334 | 4.283692 | -2.679102 | 1 | -4.074308 | -3.494919 | -3.387717 |
| 6 | 4.400651 | 2.317482 | -2.13166 | 6 | -4.569423 | -1.673316 | -2.413527 |
| 6 | 5.517311 | 2.314391 | -3.139779 | 6 | -5.804872 | -1.493084 | -3.252734 |
| 1 | 6.459857 | 2.095192 | -2.631303 | 1 | -6.676757 | -1.417579 | -2.597375 |
| 1 | 5.603522 | 3.258059 | -3.679283 | 1 | -5.953691 | -2.30546 | -3.964753 |
| 1 | 5.343448 | 1.502949 | -3.852699 | 1 | -5.728749 | -0.545407 | -3.793797 |
| 6 | -0.83977 | 0.69069 | -3.833026 | 6 | 0.843665 | 0.399019 | -3.83714 |
| 1 | -1.039384 | 0.919201 | -4.870029 | 1 | 1.02038 | 0.451348 | -4.901843 |
| 6 | 0.444104 | 0.724569 | -3.294418 | 6 | -0.433221 | 0.253268 | -3.299822 |
| 6 | -0.297904 | 0.13987 | -1.231393 | 6 | 0.364762 | 0.238777 | -1.17354 |
| 6 | -0.116535 | -0.13731 | 0.165477 | 6 | 0.207549 | 0.106192 | 0.244816 |
| 6 | 1.139933 | -0.034476 | 0.812048 | 6 | -1.050617 | -0.164857 | 0.840878 |
| 6 | 0.027316 | -0.727504 | 2.888706 | 6 | 0.102196 | -0.193475 | 3.010563 |
| 6 | 0.157988 | -1.043441 | 4.379568 | 6 | 0.000039 | -0.391061 | 4.524061 |
| 6 | 1.10337 | -2.24101 | 4.561586 | 6 | -0.961506 | 0.654108 | 5.110093 |
| 1 | 1.215003 | -2.475346 | 5.625797 | 1 | -1.053523 | 0.516503 | 6.192823 |
| 1 | 0.708816 | -3.126874 | 4.055297 | 1 | -0.594552 | 1.667774 | 4.923925 |
| 6 | 0.73551 | 0.180198 | 5.107448 | 6 | -0.539727 | -1.801304 | 4.809193 |
| 1 | 0.078316 | 1.047058 | 4.991419 | 1 | 0.131161 | -2.562961 | 4.401274 |
| 1 | 1.721013 | 0.4527 | 4.721165 | 1 | -1.526672 | -1.955752 | 4.365693 |
| 1 | 0.839346 | -0.031325 | 6.17713 | 1 | -0.62514 | -1.962163 | 5.889344 |
| 6 | 4.520352 | 2.281383 | 2.276935 | 6 | -4.720171 | -2.107103 | 1.995207 |
| 1 | 3.88207 | 3.127184 | 2.035891 | 6 | -5.850911 | -2.188343 | 2.794409 |
| 6 | 5.5194 | 2.346094 | 3.231219 | 1 | -6.174523 | -3.119755 | 3.237756 |
| 1 | 5.717344 | 3.251541 | 3.790418 | 6 | -6.522352 | -0.989232 | 2.986713 |
| 6 | 6.253513 | 1.17948 | 3.428528 | 1 | -7.418637 | -0.956398 | 3.602212 |
| 1 | 7.059218 | 1.148551 | 4.159196 | 6 | -5.035709 | 0.135315 | 1.691861 |
| 6 | 5.044201 | 0.072002 | 1.855738 | 6 | -4.549018 | 1.36646 | 1.08111 |
| 6 | 4.714746 | -1.116986 | 1.087064 | 6 | -3.437031 | 1.307831 | 0.212636 |
| 6 | 3.650236 | -1.033076 | 0.160973 | 6 | -3.599944 | 3.739802 | -0.081834 |
| 6 | 4.046466 | -3.382579 | -0.417315 | 6 | -4.701669 | 3.754159 | 0.780502 |
| 6 | 5.093355 | -3.426278 | 0.512193 | 6 | -5.172385 | 2.583585 | 1.352957 |
| 6 | 5.424876 | -2.307308 | 1.254806 | 1 | -6.0287 | 2.596665 | 2.018353 |
| 1 | 6.238013 | -2.33527 | 1.972564 | 6 | -1.593544 | 5.212268 | -0.279221 |
| 6 | 2.180931 | -4.959215 | -0.946825 | 1 | -1.538587 | 5.340262 | 0.805922 |
| 1 | 2.059704 | -5.219348 | 0.10891 | 1 | -1.173976 | 6.107861 | -0.750999 |
| 1 | 1.870636 | -5.820192 | -1.549357 | 1 | -0.96225 | 4.359692 | -0.542146 |
| 1 | 1.502279 | -4.130145 | -1.162436 | 6 | -3.847838 | 6.254848 | -0.353499 |
| 6 | 4.510634 | -5.822151 | -0.965616 | 1 | -3.828029 | 6.438073 | 0.725028 |
| 1 | 4.433238 | -6.137214 | 0.079424 | 1 | -4.892286 | 6.179295 | -0.671122 |
| 1 | 5.564899 | -5.635344 | -1.191353 | 1 | -3.414714 | 7.130982 | -0.845431 |
| 1 | 4.181155 | -6.659131 | -1.588775 | 6 | -3.047183 | 5.007679 | -0.73261 |
| 6 | 3.642041 | -4.596463 | -1.254941 | 6 | -3.090339 | 4.856245 | -2.260807 |

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|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | 3.779795 | -4.252011 | -2.745881 | 1 | -2.69379 | 5.757328 | -2.741075 |
| 1 | 3.491009 | -5.111165 | -3.361069 | 1 | -4.117138 | 4.707796 | -2.607777 |
| 1 | 4.813151 | -3.98841 | -2.989884 | 1 | -2.49751 | 4.003833 | -2.60174 |
| 1 | 3.145768 | -3.407328 | -3.026054 | 77 | 3.012425 | 0.685462 | -0.1081 |
| 77 | -2.916612 | -0.671609 | -0.307037 | 7 | 6.027168 | -0.261054 | 2.645792 |
| 7 | -5.914036 | -0.611634 | 2.621926 | 7 | 4.337276 | 0.879506 | 1.435059 |
| 7 | -4.217276 | -1.324969 | 1.12702 | 7 | 1.643171 | 0.427236 | -1.605902 |
| 7 | -1.581268 | 0.03484 | -1.680992 | 8 | 2.512219 | 2.809637 | -0.145756 |
| 8 | -2.356942 | -2.683037 | -0.93421 | 8 | 4.636947 | 1.196445 | -1.469086 |
| 8 | -4.55402 | -0.838733 | -1.740453 | 6 | 2.52479 | 5.089859 | -0.667372 |
| 6 | -2.279508 | -4.70999 | -2.095906 | 1 | 2.347909 | 5.316097 | 0.387123 |
| 1 | -2.166936 | -5.260471 | -1.157927 | 1 | 3.154049 | 5.862855 | -1.109806 |
| 1 | -2.838328 | -5.315654 | -2.809991 | 1 | 1.548285 | 5.100682 | -1.160958 |
| 1 | -1.270848 | -4.537215 | -2.482773 | 6 | 3.12057 | 3.71091 | -0.791778 |
| 6 | -2.931389 | -3.379268 | -1.819816 | 6 | 4.264973 | 3.552306 | -1.589942 |
| 6 | -4.087561 | -3.040597 | -2.541656 | 1 | 4.663602 | 4.450522 | -2.044483 |
| 1 | -4.454179 | -3.782624 | -3.239729 | 6 | 4.944246 | 2.355561 | -1.86919 |
| 6 | -4.820526 | -1.84552 | -2.457208 | 6 | 6.171472 | 2.416256 | -2.74235 |
| 6 | -6.059875 | -1.706015 | -3.30395 | 1 | 6.054885 | 1.722858 | -3.579666 |
| 1 | -5.988635 | -0.794375 | -3.903407 | 1 | 6.371113 | 3.418039 | -3.123825 |
| 1 | -6.223816 | -2.561728 | -3.959577 | 1 | 7.034138 | 2.072258 | -2.16441 |
| 1 | -6.92562 | -1.585329 | -2.646308 | 6 | 1.870997 | 0.492023 | -2.917999 |
| 6 | -1.840964 | 0.321895 | -2.956564 | 1 | 2.906996 | 0.621806 | -3.211049 |
| 1 | -2.880369 | 0.241688 | -3.255174 | 6 | 1.401073 | 0.244539 | 0.98371 |
| 6 | -1.294177 | -0.523524 | 0.844512 | 6 | 1.313949 | 0.073222 | 2.372351 |
| 6 | -1.191336 | -0.788852 | 2.215384 | 1 | -1.961071 | 0.577244 | 4.675194 |
| 1 | 2.097562 | -2.041604 | 4.154352 | 6 | 1.350097 | -0.246481 | 5.228086 |
| 6 | -1.184587 | -1.390895 | 5.025409 | 1 | 2.073329 | -0.988149 | 4.876233 |
| 1 | -1.900403 | -0.56745 | 4.943647 | 1 | 1.779058 | 0.749828 | 5.08325 |
| 1 | -1.632675 | -2.282639 | 4.576558 | 1 | 1.218043 | -0.396701 | 6.303895 |
| 1 | -1.034439 | -1.596628 | 6.089667 | 6 | 4.558084 | 1.989247 | 2.14108 |
| 6 | -4.409372 | -2.59401 | 1.489117 | 1 | 3.932633 | 2.838659 | 1.889766 |
| 1 | -3.770851 | -3.323156 | 1.002743 | 6 | 5.526199 | 2.022365 | 3.126988 |
| 6 | -5.365031 | -2.926554 | 2.430668 | 1 | 5.709179 | 2.919542 | 3.703576 |
| 1 | -5.524662 | -3.954277 | 2.72933 | 6 | 6.245954 | 0.850388 | 3.333091 |
| 6 | -6.103767 | -1.877029 | 2.966137 | 1 | 7.029996 | 0.803033 | 4.085418 |
| 1 | -6.879305 | -2.062151 | 3.705914 | 6 | 5.075768 | -0.233388 | 1.714448 |
| 6 | -4.973652 | -0.353384 | 1.715175 | 6 | 4.712444 | -1.393252 | 0.933137 |
| 6 | -4.641794 | 0.988445 | 1.293139 | 6 | 3.657381 | -1.201817 | 0.011383 |
| 6 | -3.595971 | 1.088954 | 0.346582 | 6 | 3.831921 | -3.577167 | -0.560296 |
| 6 | -3.811729 | 3.525173 | 0.486236 | 6 | 4.892752 | -3.714779 | 0.345353 |
| 6 | -4.864933 | 3.377401 | 1.399213 | 6 | 5.326658 | -2.634264 | 1.092132 |
| 6 | -5.273631 | 2.11995 | 1.805999 | 1 | 6.137312 | -2.735744 | 1.806494 |
| 1 | -6.077261 | 1.996926 | 2.524923 | 6 | 3.30861 | -4.423115 | -2.863272 |

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|----|------------|-----------|-----------|----|-------------|-----------|-----------|
| 6 | -3.30243 | 5.009341 | -1.472901 | 1 | 4.326502 | -4.208803 | -3.202493 |
| 1 | -4.31593 | 4.885848 | -1.865985 | 1 | 2.925769 | -5.269555 | -3.443414 |
| 1 | -2.933226 | 5.993175 | -1.78167 | 1 | 2.688452 | -3.553212 | -3.093116 |
| 1 | -2.667742 | 4.252442 | -1.940179 | 6 | 4.111623 | -6.034415 | -1.157171 |
| 6 | -4.138238 | 6.044825 | 0.619416 | 1 | 5.155262 | -5.89824 | -1.45667 |
| 1 | -5.178771 | 5.980668 | 0.28667 | 1 | 4.092533 | -6.365258 | -0.114571 |
| 1 | -4.126837 | 6.06229 | 1.713099 | 1 | 3.69314 | -6.841764 | -1.76585 |
| 1 | -3.735074 | 7.000606 | 0.27105 | 6 | 3.290763 | -4.760282 | -1.364695 |
| 6 | -3.292817 | 4.899394 | 0.05919 | 6 | 1.846858 | -5.038719 | -0.919248 |
| 6 | -1.854693 | 5.063908 | 0.575442 | 1 | 1.425941 | -5.870486 | -1.495146 |
| 1 | -1.452024 | 6.03644 | 0.270603 | 1 | 1.81398 | -5.305787 | 0.141118 |
| 1 | -1.827313 | 5.009852 | 1.667776 | 1 | 1.204206 | -4.166069 | -1.059219 |
| 1 | -1.193401 | 4.28348 | 0.190871 | 1 | -5.204572 | 4.68532 | 1.011553 |
| 1 | 5.657337 | -4.338917 | 0.660615 | 1 | 5.378927 | -4.673203 | 0.478599 |
| 1 | -5.364502 | 4.247891 | 1.805695 | 1 | 2.220203 | 0.147189 | 2.961304 |
| 1 | -2.086634 | -1.063072 | 2.759743 | 6 | -2.994702 | 2.507895 | -0.346414 |
| 6 | 3.349633 | -2.180478 | -0.570874 | 1 | -2.141884 | 2.468601 | -1.017035 |
| 1 | 2.531157 | -2.130715 | -1.282558 | 6 | 3.23602 | -2.319436 | -0.706312 |
| 6 | -3.200236 | 2.373713 | -0.021612 | 1 | 2.405235 | -2.210798 | -1.396188 |
| 1 | -2.376585 | 2.483255 | -0.719927 | 6 | -1.062211 | -0.286387 | 2.231606 |
| 6 | 1.179227 | -0.384696 | 2.162015 | 1 | -2.012017 | -0.477935 | 2.719363 |
| 1 | 2.138301 | -0.380142 | 2.669473 | 17 | -1.797459 | 0.184644 | -4.363961 |
| 17 | 1.777004 | 1.10708 | -4.335514 | 17 | -3.768931 | -3.522754 | 1.711178 |
| | Ir4-Cl-3MC | | | | Ir4-2Cl-3MC | | |
| 77 | -2.995226 | -0.786869 | -0.114647 | 77 | -2.767983 | -0.676252 | -0.361039 |
| 7 | -6.928615 | 0.060367 | 1.514528 | 7 | -6.767269 | 0.265252 | 1.056531 |
| 7 | -4.993759 | -1.130656 | 0.85774 | 7 | -4.833837 | -0.977175 | 0.508183 |
| 7 | -0.896903 | -0.902292 | -1.850905 | 7 | -0.588343 | -0.792562 | -1.97504 |
| 8 | -2.508599 | -2.89517 | -0.257546 | 8 | -2.33477 | -2.791208 | -0.529851 |
| 8 | -4.095162 | -1.019354 | -1.963423 | 8 | -3.787262 | -0.83483 | -2.258372 |
| 6 | -2.18372 | -5.032582 | -1.150608 | 6 | -2.016128 | -4.912937 | -1.462358 |
| 1 | -1.091608 | -4.973611 | -1.19518 | 1 | -0.921885 | -4.884599 | -1.477901 |
| 1 | -2.536428 | -5.688727 | -1.946969 | 1 | -2.364737 | -5.545568 | -2.279242 |
| 1 | -2.44104 | -5.459739 | -0.178439 | 1 | -2.311272 | -5.3479 | -0.504712 |
| 6 | -2.745054 | -3.637543 | -1.24834 | 6 | -2.535113 | -3.501393 | -1.552052 |
| 6 | -3.470302 | -3.289249 | -2.404543 | 6 | -3.185676 | -3.102983 | -2.736256 |
| 1 | -3.594644 | -4.068746 | -3.145926 | 1 | -3.286742 | -3.858347 | -3.505614 |
| 6 | -4.106695 | -2.070193 | -2.673847 | 6 | -3.781507 | -1.86336 | -3.001983 |
| 6 | -4.917811 | -1.949231 | -3.938639 | 6 | -4.522034 | -1.686374 | -4.302446 |
| 1 | -5.958564 | -1.742997 | -3.673255 | 1 | -5.572054 | -1.470538 | -4.085498 |
| 1 | -4.875811 | -2.84665 | -4.556812 | 1 | -4.461971 | -2.563693 | -4.947302 |
| 1 | -4.563105 | -1.089048 | -4.513251 | 1 | -4.123426 | -0.814238 | -4.82806 |
| 6 | 0.610862 | -1.174251 | -3.659321 | 6 | 1.00971 | -1.028868 | -3.70947 |
| 1 | 0.806404 | -1.321788 | -4.711728 | 1 | 1.258778 | -1.139345 | -4.755107 |

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| 6 | -0.669902 | -1.123563 | -3.134379 | 6 | -0.296415 | -0.971766 | -3.252226 |
| 1 | -1.541873 | -1.255839 | -3.768422 | 1 | -1.13498 | -1.062686 | -3.936631 |
| 6 | 0.148139 | -0.747274 | -1.038964 | 6 | 0.41449 | -0.690168 | -1.103349 |
| 6 | -0.05083 | -0.383426 | 0.328653 | 6 | 0.149926 | -0.366241 | 0.263146 |
| 6 | -1.347164 | -0.172474 | 0.854018 | 6 | -1.167521 | -0.133232 | 0.721729 |
| 6 | -1.425706 | 0.361058 | 2.136946 | 6 | -1.305018 | 0.365174 | 2.013536 |
| 1 | -2.403077 | 0.599023 | 2.544068 | 1 | -2.297182 | 0.619991 | 2.371353 |
| 6 | -0.278923 | 0.612885 | 2.912331 | 6 | -0.197772 | 0.558518 | 2.860361 |
| 6 | -0.453502 | 1.20242 | 4.313294 | 6 | -0.4359 | 1.10524 | 4.269346 |
| 6 | -1.145839 | 2.569936 | 4.199662 | 6 | -1.097825 | 2.488536 | 4.168069 |
| 1 | -1.282418 | 3.007339 | 5.194602 | 1 | -1.283808 | 2.891517 | 5.169443 |
| 1 | -0.542926 | 3.259863 | 3.601911 | 1 | -0.450246 | 3.188813 | 3.632252 |
| 6 | -1.320553 | 0.25859 | 5.160261 | 6 | -1.362868 | 0.149076 | 5.035357 |
| 1 | -0.8482 | -0.723907 | 5.254022 | 1 | -0.913815 | -0.845373 | 5.116563 |
| 1 | -2.31046 | 0.113659 | 4.721036 | 1 | -2.331078 | 0.039783 | 4.54082 |
| 1 | -1.45577 | 0.671462 | 6.165767 | 1 | -1.542795 | 0.527826 | 6.047238 |
| 6 | -5.523772 | -2.27117 | 1.287735 | 6 | -5.434613 | -2.10089 | 0.889229 |
| 1 | -4.910423 | -3.159079 | 1.163503 | 1 | -4.850136 | -3.011666 | 0.796532 |
| 6 | -6.784041 | -2.302278 | 1.855211 | 6 | -6.727693 | -2.103683 | 1.37364 |
| 1 | -7.226962 | -3.223406 | 2.21123 | 1 | -7.229794 | -3.007112 | 1.689262 |
| 6 | -7.449851 | -1.08174 | 1.934388 | 6 | -7.340061 | -0.851628 | 1.41915 |
| 1 | -8.450683 | -1.023355 | 2.357351 | 6 | -5.506061 | 0.190235 | 0.608128 |
| 6 | -5.699816 | 0.016562 | 0.988442 | 6 | -4.776316 | 1.378287 | 0.220261 |
| 6 | -5.026845 | 1.219401 | 0.53483 | 6 | -3.438116 | 1.214501 | -0.215009 |
| 6 | -3.712765 | 1.087323 | 0.024381 | 6 | -2.741956 | 2.375279 | -0.551868 |
| 6 | -3.075091 | 2.259127 | -0.382489 | 1 | -1.709 | 2.274705 | -0.869142 |
| 1 | -2.060452 | 2.18222 | -0.759844 | 6 | -3.309259 | 3.651474 | -0.482073 |
| 6 | -3.678475 | 3.518874 | -0.31063 | 6 | -4.640293 | 3.766312 | -0.058178 |
| 6 | -4.983186 | 3.603324 | 0.192406 | 1 | -5.114447 | 4.737681 | 0.006464 |
| 1 | -5.484425 | 4.560736 | 0.261977 | 6 | -5.365312 | 2.643443 | 0.290789 |
| 6 | -5.649042 | 2.466962 | 0.612279 | 1 | -6.39434 | 2.726048 | 0.624855 |
| 1 | -6.65824 | 2.524458 | 1.006561 | 6 | -1.26736 | 4.953924 | 0.118244 |
| 6 | -1.648421 | 4.904663 | 0.122788 | 1 | -1.610651 | 5.058462 | 1.151865 |
| 1 | -1.931028 | 5.032675 | 1.172084 | 1 | -0.646565 | 5.822786 | -0.125645 |
| 1 | -1.070747 | 5.783162 | -0.18517 | 1 | -0.637927 | 4.062295 | 0.064936 |
| 1 | -0.995467 | 4.030802 | 0.058239 | 6 | -3.246824 | 6.179841 | -0.74847 |
| 6 | -3.717976 | 6.038572 | -0.652912 | 1 | -3.605887 | 6.363859 | 0.26854 |
| 1 | -4.018548 | 6.243004 | 0.379075 | 1 | -4.107079 | 6.190083 | -1.424827 |
| 1 | -4.619142 | 5.999176 | -1.272613 | 1 | -2.59734 | 7.015809 | -1.025074 |
| 1 | -3.116492 | 6.886051 | -0.995438 | 6 | -2.461155 | 4.870604 | -0.845852 |
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| 6 | -2.468235 | 4.582037 | -2.226887 | 1 | -1.329537 | 5.59073 | -2.553864 |
| 1 | -1.906534 | 5.461006 | -2.560924 | 1 | -2.782226 | 4.671237 | -2.992599 |
| 1 | -3.341605 | 4.466159 | -2.875779 | 1 | -1.340619 | 3.828142 | -2.413207 |

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| 1 | -1.83047 | 3.70546 | -2.363432 | 77 | 2.991029 | -0.78402 | 0.233133 |
| 77 | 2.799208 | -0.717463 | 0.15264 | 7 | 5.589817 | 0.684194 | 3.163147 |
| 7 | 5.504628 | 0.963325 | 2.864884 | 7 | 4.082117 | -0.6774 | 1.943515 |
| 7 | 3.982322 | -0.500454 | 1.789721 | 7 | 1.742279 | -0.802057 | -1.449627 |
| 7 | 1.457967 | -0.842599 | -1.452828 | 8 | 2.396401 | -2.855161 | 0.542832 |
| 8 | 2.301789 | -2.795218 | 0.57026 | 8 | 4.841641 | -1.604257 | -0.591284 |
| 8 | 4.638043 | -1.504098 | -0.735583 | 6 | 2.331769 | -5.189281 | 0.452559 |
| 6 | 2.316539 | -5.131832 | 0.564024 | 1 | 1.345238 | -5.166698 | -0.01831 |
| 1 | 1.323724 | -5.173202 | 0.107376 | 1 | 2.888578 | -6.055587 | 0.093864 |
| 1 | 2.903211 | -5.991411 | 0.238227 | 1 | 2.1639 | -5.288659 | 1.529127 |
| 1 | 2.16681 | -5.183862 | 1.646371 | 6 | 3.03663 | -3.885179 | 0.177197 |
| 6 | 2.962038 | -3.815176 | 0.212899 | 6 | 4.304522 | -3.924115 | -0.416249 |
| 6 | 4.203057 | -3.83237 | -0.436007 | 1 | 4.706411 | -4.90502 | -0.636809 |
| 1 | 4.632189 | -4.806244 | -0.635519 | 6 | 5.123666 | -2.823329 | -0.732112 |
| 6 | 4.962404 | -2.716349 | -0.836592 | 6 | 6.485244 | -3.094105 | -1.31985 |
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| 1 | 7.062733 | -2.368679 | -0.954764 | 1 | 6.737009 | -4.155043 | -1.335838 |
| 1 | 6.594391 | -4.01278 | -1.46715 | 1 | 6.514056 | -2.704128 | -2.341953 |
| 1 | 6.27711 | -2.605244 | -2.509608 | 6 | 2.006939 | -0.933539 | -2.74797 |
| 6 | 1.655277 | -1.021649 | -2.757417 | 6 | 1.285747 | -0.194956 | 1.074849 |
| 6 | 1.123165 | -0.154358 | 1.068879 | 6 | 1.07866 | 0.273176 | 2.377883 |
| 6 | 0.976508 | 0.348699 | 2.366538 | 1 | 1.935482 | 0.436168 | 3.019334 |
| 1 | 1.862972 | 0.555416 | 2.95271 | 1 | -2.053194 | 2.445874 | 3.639127 |
| 1 | -2.128367 | 2.491636 | 3.727589 | 6 | 0.860029 | 1.254573 | 5.068085 |
| 6 | 0.87959 | 1.401471 | 5.036931 | 1 | 1.371251 | 0.295351 | 5.195636 |
| 1 | 1.415969 | 0.456294 | 5.166309 | 1 | 1.55332 | 1.95371 | 4.591457 |
| 1 | 1.532796 | 2.097753 | 4.502966 | 1 | 0.630325 | 1.643242 | 6.064811 |
| 1 | 0.695153 | 1.817265 | 6.03218 | 6 | 4.173013 | -1.636521 | 2.864909 |
| 6 | 4.167637 | -1.419624 | 2.737485 | 1 | 3.575102 | -2.52209 | 2.681322 |
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| 1 | 5.187618 | -1.926788 | 4.563317 | 6 | 5.680656 | -0.278442 | 4.069122 |
| 6 | 5.687322 | 0.040643 | 3.798019 | 1 | 6.340773 | -0.083764 | 4.911332 |
| 1 | 6.387565 | 0.292833 | 4.591164 | 6 | 4.791282 | 0.475059 | 2.118425 |
| 6 | 4.654401 | 0.683761 | 1.878722 | 6 | 4.580384 | 1.460254 | 1.083913 |
| 6 | 4.343128 | 1.61883 | 0.823283 | 6 | 3.679213 | 1.083507 | 0.061538 |
| 6 | 3.400147 | 1.166778 | -0.128379 | 6 | 3.435587 | 2.023083 | -0.938984 |
| 6 | 3.055148 | 2.057525 | -1.143936 | 1 | 2.739401 | 1.770684 | -1.732833 |
| 1 | 2.324143 | 1.747817 | -1.884535 | 6 | 4.056864 | 3.276437 | -0.964382 |
| 6 | 3.616056 | 3.334797 | -1.249413 | 6 | 4.947 | 3.604459 | 0.067785 |
| 6 | 4.553094 | 3.737118 | -0.287558 | 1 | 5.442042 | 4.567354 | 0.078637 |
| 1 | 5.004399 | 4.719921 | -0.340279 | 6 | 5.205321 | 2.706164 | 1.087142 |
| 6 | 4.912873 | 2.888577 | 0.743763 | 1 | 5.890929 | 2.95246 | 1.891529 |
| 1 | 5.634328 | 3.193054 | 1.49516 | 6 | 2.250031 | 4.550399 | -2.137601 |

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|----|----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | 1.680803 | 4.472256 | -2.356346 | 1 | 1.934638 | 5.017518 | -1.200128 |
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| 1 | 1.367171 | 5.119791 | -3.18221 | 1 | 1.649765 | 3.647889 | -2.277214 |
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| Ir5-Cl-3MC | | | | Ir5-2Cl-3MC | | | |
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| 77 | -2.909085 | -0.812553 | 0.013649 | 77 | -2.75589 | -0.416533 | -0.335861 |
| 7 | -6.787922 | 0.018618 | 1.763126 | 7 | -6.642435 | 0.498172 | 1.377671 |
| 7 | -4.832806 | -1.142723 | 1.113242 | 7 | -4.763062 | -0.731799 | 0.647618 |
| 7 | -0.707965 | -1.088958 | -1.744425 | 7 | -0.501343 | -0.611877 | -1.983657 |
| 8 | -2.315964 | -2.895887 | 0.036858 | 8 | -2.379389 | -2.523433 | -0.641966 |
| 8 | -4.022557 | -1.261325 | -1.775074 | 8 | -3.838435 | -0.446826 | -2.193053 |
| 6 | -1.880698 | -5.079761 | -0.679297 | 6 | -2.124172 | -4.590397 | -1.706896 |
| 1 | -0.794033 | -4.958498 | -0.636672 | 1 | -1.038188 | -4.599353 | -1.574064 |
| 1 | -2.131855 | -5.792744 | -1.465075 | 1 | -2.37974 | -5.123541 | -2.622904 |
| 1 | -2.194878 | -5.47752 | 0.2893 | 1 | -2.554435 | -5.113947 | -0.848916 |
| 6 | -2.511451 | -3.727951 | -0.890623 | 6 | -2.601783 | -3.162075 | -1.707608 |
| 6 | -3.252531 | -3.510011 | -2.067401 | 6 | -3.248869 | -2.670179 | -2.856719 |
| 1 | -3.327185 | -4.345701 | -2.752008 | 1 | -3.362135 | -3.364228 | -3.680082 |
| 6 | -3.961406 | -2.353132 | -2.418737 | 6 | -3.836768 | -1.408651 | -3.021615 |
| 6 | -4.767341 | -2.36348 | -3.69149 | 6 | -4.573518 | -1.118571 | -4.302516 |
| 1 | -5.818369 | -2.185134 | -3.447767 | 1 | -5.614843 | -0.881633 | -4.067364 |
| 1 | -4.67856 | -3.301091 | -4.241012 | 1 | -4.543336 | -1.950352 | -5.006902 |
| 1 | -4.445036 | -1.53349 | -4.326439 | 1 | -4.143992 | -0.227095 | -4.768132 |
| 6 | 0.924454 | -1.75015 | -3.3258 | 6 | 1.153924 | -1.178212 | -3.577313 |
| 6 | -0.397924 | -1.535633 | -2.947921 | 6 | -0.162309 | -0.88772 | -3.230067 |
| 1 | -1.214609 | -1.730963 | -3.636775 | 1 | -0.949722 | -0.880949 | -3.977987 |
| 6 | 0.273401 | -0.847938 | -0.873081 | 6 | 0.443221 | -0.619556 | -1.041106 |
| 6 | 0.024688 | -0.307725 | 0.431767 | 6 | 0.16372 | -0.281234 | 0.32368 |
| 6 | -1.282354 | -0.047563 | 0.905891 | 6 | -1.143459 | 0.024416 | 0.770576 |
| 6 | -1.391139 | 0.621 | 2.123595 | 6 | -1.272002 | 0.482423 | 2.080189 |
| 1 | -2.378463 | 0.899251 | 2.477214 | 1 | -2.251905 | 0.792374 | 2.427891 |
| 6 | -0.266393 | 0.945805 | 2.902115 | 6 | -0.176053 | 0.552634 | 2.958388 |
| 6 | -0.474445 | 1.67085 | 4.233074 | 6 | -0.407956 | 1.04514 | 4.388278 |

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| 6 | -1.149895 | 3.025457 | 3.966831 | 6 | -0.974115 | 2.473151 | 4.345043 |
| 1 | -1.309901 | 3.559047 | 4.910165 | 1 | -1.1532 | 2.838976 | 5.361925 |
| 1 | -0.524359 | 3.649512 | 3.321832 | 1 | -0.271298 | 3.153581 | 3.855308 |
| 6 | -1.374005 | 0.821567 | 5.143791 | 6 | -1.413284 | 0.117043 | 5.087088 |
| 1 | -0.917333 | -0.152697 | 5.342539 | 1 | -1.031987 | -0.907666 | 5.129196 |
| 1 | -2.355137 | 0.646515 | 4.695736 | 1 | -2.374012 | 0.095214 | 4.566629 |
| 1 | -1.527783 | 1.330164 | 6.101616 | 1 | -1.593432 | 0.458427 | 6.112163 |
| 6 | -5.286173 | -2.261711 | 1.66953 | 6 | -5.335933 | -1.874082 | 1.00426 |
| 1 | -4.636799 | -3.129115 | 1.592908 | 1 | -4.773421 | -2.786366 | 0.829774 |
| 6 | -6.514983 | -2.295539 | 2.301649 | 6 | -6.59747 | -1.871791 | 1.570223 |
| 1 | -6.895985 | -3.19898 | 2.759892 | 6 | -7.219772 | -0.63484 | 1.73138 |
| 6 | -7.232874 | -1.1021 | 2.309246 | 1 | -8.216523 | -0.575042 | 2.161947 |
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| 6 | -5.586484 | -0.019883 | 1.177133 | 6 | -4.694106 | 1.632103 | 0.460093 |
| 6 | -4.996827 | 1.161042 | 0.575546 | 6 | -3.389775 | 1.474071 | -0.068376 |
| 6 | -3.709175 | 1.031676 | 0.001473 | 6 | -2.700756 | 2.639125 | -0.403685 |
| 6 | -3.151982 | 2.178981 | -0.561955 | 1 | -1.692046 | 2.539138 | -0.791518 |
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| 6 | -3.808206 | 3.414074 | -0.57754 | 6 | -4.544467 | 4.028199 | 0.267747 |
| 6 | -5.082965 | 3.497498 | -0.002223 | 1 | -5.00116 | 5.001017 | 0.40069 |
| 1 | -5.62212 | 4.436579 | 0.004443 | 6 | -5.260076 | 2.899389 | 0.618661 |
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| 1 | -6.657343 | 2.440733 | 1.016575 | 6 | -1.168894 | 5.18428 | 0.301734 |
| 6 | -1.81305 | 4.907681 | -0.429865 | 1 | -1.464255 | 5.25882 | 1.352621 |
| 1 | -2.025593 | 5.131504 | 0.619854 | 1 | -0.548763 | 6.053766 | 0.057878 |
| 1 | -1.296332 | 5.76993 | -0.865365 | 1 | -0.555297 | 4.287076 | 0.190875 |
| 1 | -1.130795 | 4.054705 | -0.456849 | 6 | -3.176237 | 6.452706 | -0.433334 |
| 6 | -3.978208 | 5.885081 | -1.155999 | 1 | -3.483757 | 6.60805 | 0.605145 |
| 1 | -4.219291 | 6.176487 | -0.129319 | 1 | -4.068653 | 6.487812 | -1.065855 |
| 1 | -4.914977 | 5.754511 | -1.706366 | 1 | -2.535262 | 7.293179 | -0.716192 |
| 1 | -3.43609 | 6.716562 | -1.616348 | 6 | -2.405628 | 5.142627 | -0.609539 |
| 6 | -3.112124 | 4.624951 | -1.200464 | 6 | -1.959058 | 5.046003 | -2.076085 |
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| 77 | 2.887377 | -0.613613 | 0.335286 | 7 | 5.711188 | 0.711481 | 3.081616 |
| 7 | 5.560821 | 1.659545 | 2.627621 | 7 | 4.161693 | -0.700609 | 1.973866 |
| 7 | 4.118637 | -0.062816 | 1.868936 | 7 | 1.750839 | -0.895997 | -1.316813 |
| 7 | 1.589102 | -1.042885 | -1.180733 | 8 | 2.451517 | -2.930916 | 0.708161 |
| 8 | 2.59584 | -2.624952 | 1.119172 | 8 | 4.691005 | -1.654395 | -0.783639 |
| 8 | 4.604646 | -1.431122 | -0.729092 | 6 | 2.413516 | -5.266398 | 0.646967 |
| 6 | 2.81083 | -4.923857 | 1.477091 | 1 | 1.386692 | -5.279132 | 0.270768 |
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| 1 | 3.424368 | -5.785367 | 1.211895 | 1 | 2.350633 | -5.341284 | 1.736402 |
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| 6 | 4.418898 | -3.69636 | 0.007138 | 1 | 4.618515 | -4.958604 | -0.747115 |
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| 1 | 2.969164 | -1.608603 | -2.601785 | 6 | 1.292524 | -0.228583 | 1.168675 |
| 6 | 1.182031 | -0.003778 | 1.181423 | 6 | 1.086012 | 0.192334 | 2.487753 |
| 6 | 1.00106 | 0.621778 | 2.419467 | 1 | 1.93777 | 0.257556 | 3.153292 |
| 1 | 1.874324 | 0.878624 | 3.006169 | 1 | -1.919227 | 2.519642 | 3.798792 |
| 1 | -2.119585 | 2.906858 | 3.477156 | 6 | 0.877253 | 1.066886 | 5.217625 |
| 6 | 0.840433 | 1.929702 | 4.971168 | 1 | 1.318549 | 0.069608 | 5.308408 |
| 1 | 1.363048 | 0.997397 | 5.206341 | 1 | 1.626814 | 1.738328 | 4.788565 |
| 1 | 1.514627 | 2.565893 | 4.390267 | 1 | 0.651754 | 1.423581 | 6.227194 |
| 1 | 0.632962 | 2.442283 | 5.915522 | 6 | 4.304059 | -1.627495 | 2.922643 |
| 6 | 4.396446 | -0.793144 | 2.949956 | 1 | 3.706605 | -2.523815 | 2.797448 |
| 1 | 3.887313 | -1.748464 | 3.013637 | 6 | 5.160646 | -1.426274 | 3.98832 |
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| 1 | 5.502804 | -0.918966 | 4.79151 | 6 | 5.853554 | -0.220758 | 4.012238 |
| 6 | 5.840023 | 0.919785 | 3.690763 | 1 | 6.55034 | 0.005754 | 4.816032 |
| 1 | 6.545113 | 1.34628 | 4.400634 | 6 | 4.866882 | 0.462402 | 2.082466 |
| 6 | 4.70298 | 1.163269 | 1.738214 | 6 | 4.602836 | 1.41474 | 1.028306 |
| 6 | 4.293407 | 1.890545 | 0.55857 | 6 | 3.657018 | 1.007374 | 0.059292 |
| 6 | 3.35138 | 1.234849 | -0.267648 | 6 | 3.366658 | 1.914722 | -0.958446 |
| 6 | 2.924264 | 1.921512 | -1.403193 | 1 | 2.636182 | 1.63851 | -1.712706 |
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| 1 | 4.724211 | 4.787447 | -1.124557 | 6 | 5.222681 | 2.661361 | 0.964965 |
| 6 | 4.777937 | 3.160005 | 0.248696 | 1 | 5.943222 | 2.93305 | 1.729643 |
| 1 | 5.500649 | 3.626072 | 0.910707 | 6 | 2.118702 | 4.402718 | -2.176933 |
| 6 | 1.37582 | 4.015367 | -2.961698 | 1 | 1.840001 | 4.891501 | -1.238986 |
| 1 | 1.075922 | 4.628306 | -2.10695 | 1 | 1.848585 | 5.06841 | -3.003717 |
| 1 | 1.007314 | 4.496524 | -3.874096 | 1 | 1.519164 | 3.493592 | -2.269139 |
| 1 | 0.876177 | 3.047713 | -2.869048 | 6 | 4.379267 | 5.42763 | -2.150101 |
| 6 | 3.509102 | 5.256335 | -3.225601 | 1 | 4.150863 | 5.9848 | -1.236519 |
| 1 | 3.255428 | 5.934831 | -2.405572 | 1 | 5.462438 | 5.28233 | -2.20308 |
| 1 | 4.598803 | 5.215668 | -3.314929 | 1 | 4.087543 | 6.051644 | -3.000202 |
| 1 | 3.117602 | 5.692197 | -4.149675 | 6 | 3.623654 | 4.098558 | -2.210191 |

| | | | | | | | |
|----|----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | 2.903302 | 3.866633 | -3.021011 | 6 | 3.976037 | 3.408885 | -3.537309 |
| 6 | 3.284302 | 2.996862 | -4.229349 | 1 | 3.730736 | 4.063537 | -4.380405 |
| 1 | 2.938383 | 3.465633 | -5.156901 | 1 | 5.044074 | 3.176656 | -3.583325 |
| 1 | 4.369451 | 2.872688 | -4.292143 | 1 | 3.424603 | 2.47407 | -3.666189 |
| 1 | 2.836575 | 2.001688 | -4.168289 | 17 | 1.597308 | -1.533189 | -5.208581 |
| 17 | 1.328811 | -2.322821 | -4.904904 | 17 | -7.371886 | -3.338613 | 2.050476 |

| Ir6-Cl-3MC | | | Ir6-2Cl-3MC | | | | |
|------------|-----------|-----------|-------------|----|-----------|-----------|-----------|
| 77 | -2.830811 | -0.793374 | -0.139451 | 77 | -2.718014 | -0.466312 | -0.384919 |
| 7 | -6.272531 | -0.433519 | 2.50041 | 7 | -6.109135 | -0.398905 | 2.485279 |
| 7 | -4.470461 | -1.388957 | 1.302614 | 7 | -4.340435 | -1.298008 | 1.18516 |
| 7 | -0.644304 | -0.483809 | -2.057888 | 7 | -0.611284 | 0.321123 | -1.999391 |
| 8 | -2.186706 | -2.794163 | -0.620641 | 8 | -2.069973 | -2.244417 | -1.408604 |
| 8 | -4.267481 | -1.000976 | -1.704065 | 8 | -4.354246 | -0.497807 | -1.757782 |
| 6 | -1.836106 | -4.785696 | -1.796782 | 6 | -1.753746 | -3.895142 | -3.032647 |
| 1 | -0.76666 | -4.601467 | -1.937041 | 1 | -0.694365 | -3.641931 | -3.130086 |
| 1 | -2.214773 | -5.364126 | -2.639897 | 1 | -2.135843 | -4.239738 | -3.99405 |
| 1 | -1.941999 | -5.367729 | -0.877375 | 1 | -1.82466 | -4.707379 | -2.303435 |
| 6 | -2.539537 | -3.463895 | -1.632059 | 6 | -2.499191 | -2.698213 | -2.504297 |
| 6 | -3.509044 | -3.093658 | -2.578444 | 6 | -3.593505 | -2.2042 | -3.233834 |
| 1 | -3.687461 | -3.788803 | -3.388988 | 1 | -3.832216 | -2.703985 | -4.163851 |
| 6 | -4.29989 | -1.937874 | -2.560796 | 6 | -4.448321 | -1.174165 | -2.827452 |
| 6 | -5.322166 | -1.745538 | -3.647457 | 6 | -5.620256 | -0.810862 | -3.697188 |
| 1 | -6.30584 | -1.600785 | -3.192986 | 1 | -6.542502 | -0.919178 | -3.11986 |
| 1 | -5.360899 | -2.583554 | -4.343923 | 1 | -5.682003 | -1.421259 | -4.598678 |
| 1 | -5.085493 | -0.828266 | -4.19439 | 1 | -5.540126 | 0.243679 | -3.976219 |
| 6 | 0.973168 | -0.736344 | -3.791727 | 6 | 0.953306 | 0.60453 | -3.772082 |
| 1 | 1.206313 | -0.809297 | -4.844192 | 1 | 1.160775 | 0.869581 | -4.79887 |
| 6 | -0.329414 | -0.576738 | -3.323794 | 6 | -0.334308 | 0.63075 | -3.239851 |
| 6 | 0.34602 | -0.529619 | -1.158541 | 6 | 0.396178 | -0.045034 | -1.198177 |
| 6 | 0.122468 | -0.353986 | 0.249083 | 6 | 0.19644 | -0.353678 | 0.188713 |
| 6 | -1.169803 | -0.218531 | 0.815935 | 6 | -1.095027 | -0.402709 | 0.776443 |
| 6 | -1.232703 | 0.11882 | 2.168145 | 6 | -1.137695 | -0.577571 | 2.161564 |
| 1 | -2.208375 | 0.297215 | 2.608208 | 1 | -2.109094 | -0.592903 | 2.64456 |
| 6 | -0.085694 | 0.222632 | 2.973918 | 6 | 0.017717 | -0.75042 | 2.939716 |
| 6 | -0.249416 | 0.573113 | 4.453648 | 6 | -0.124236 | -0.934363 | 4.451671 |
| 6 | -0.941252 | 1.939986 | 4.575125 | 6 | -0.815979 | 0.302317 | 5.046094 |
| 1 | -1.073177 | 2.20291 | 5.630346 | 1 | -0.934267 | 0.184523 | 6.128677 |
| 1 | -0.341295 | 2.721617 | 4.100002 | 1 | -0.224143 | 1.203764 | 4.862604 |
| 6 | -1.112941 | -0.498867 | 5.136201 | 6 | -0.975837 | -2.181833 | 4.733567 |
| 1 | -0.643072 | -1.48401 | 5.058853 | 1 | -0.506419 | -3.076703 | 4.314259 |
| 1 | -2.106526 | -0.564855 | 4.686137 | 1 | -1.975981 | -2.096581 | 4.301412 |
| 1 | -1.239668 | -0.261626 | 6.198009 | 1 | -1.087034 | -2.326097 | 5.813724 |
| 6 | -4.774524 | -2.596248 | 1.766672 | 6 | -4.713113 | -2.514214 | 1.524051 |
| 1 | -4.137017 | -3.410383 | 1.433132 | 6 | -5.799455 | -2.763369 | 2.349087 |
| 6 | -5.844151 | -2.782879 | 2.622637 | 1 | -6.095492 | -3.767551 | 2.618653 |
| 1 | -6.102181 | -3.760377 | 3.009219 | 6 | -6.467426 | -1.63395 | 2.801388 |
| 6 | -6.569277 | -1.641007 | 2.954185 | 1 | -7.332565 | -1.734125 | 3.453177 |
| 1 | -7.429464 | -1.704395 | 3.617575 | 6 | -5.051735 | -0.257862 | 1.680867 |
| 6 | -5.220214 | -0.328829 | 1.680765 | 6 | -4.597043 | 1.072311 | 1.303384 |

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|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | -4.80242 | 0.955537 | 1.148263 | 6 | -3.496997 | 1.195215 | 0.425157 |
| 6 | -3.666802 | 0.981572 | 0.304618 | 6 | -3.092001 | 2.487845 | 0.086012 |
| 6 | -3.275479 | 2.224104 | -0.192192 | 1 | -2.247835 | 2.591862 | -0.589194 |
| 1 | -2.400144 | 2.262348 | -0.833093 | 6 | -3.723186 | 3.636369 | 0.573818 |
| 6 | -3.953969 | 3.409683 | 0.10694 | 6 | -4.810474 | 3.469753 | 1.439436 |
| 6 | -5.075988 | 3.339826 | 0.943124 | 1 | -5.330823 | 4.331955 | 1.838302 |
| 1 | -5.628134 | 4.236454 | 1.196058 | 6 | -5.242723 | 2.205263 | 1.799538 |
| 6 | -5.495538 | 2.127584 | 1.458605 | 1 | -6.088265 | 2.076331 | 2.466398 |
| 1 | -6.364325 | 2.066504 | 2.105689 | 6 | -1.772211 | 5.184082 | 0.682416 |
| 6 | -2.028216 | 4.994886 | 0.06236 | 1 | -1.742364 | 5.115225 | 1.773908 |
| 1 | -2.031496 | 5.07336 | 1.153705 | 1 | -1.374729 | 6.161914 | 0.389572 |
| 1 | -1.636663 | 5.932347 | -0.347696 | 1 | -1.107152 | 4.415118 | 0.282957 |
| 1 | -1.339518 | 4.192027 | -0.211017 | 6 | -4.06046 | 6.151492 | 0.731894 |
| 6 | -4.330075 | 5.918427 | -0.080667 | 1 | -4.059423 | 6.153201 | 1.825985 |
| 1 | -4.362202 | 6.063908 | 1.003338 | 1 | -5.097638 | 6.09156 | 0.388025 |
| 1 | -5.355503 | 5.796579 | -0.442686 | 1 | -3.655493 | 7.112509 | 0.40077 |
| 1 | -3.927552 | 6.834082 | -0.52442 | 6 | -3.20782 | 5.015773 | 0.163297 |
| 6 | -3.445589 | 4.73201 | -0.468831 | 6 | -3.215455 | 5.133627 | -1.368296 |
| 6 | -3.409916 | 4.643426 | -2.002077 | 1 | -2.840251 | 6.116834 | -1.671651 |
| 1 | -3.045156 | 5.58525 | -2.426012 | 1 | -4.229401 | 5.01751 | -1.762355 |
| 1 | -4.409338 | 4.451764 | -2.403835 | 1 | -2.585934 | 4.374283 | -1.838292 |
| 1 | -2.752693 | 3.842009 | -2.347858 | 77 | 3.034983 | -0.670392 | -0.201955 |
| 77 | 2.981271 | -0.676808 | 0.026061 | 7 | 5.915854 | -0.274527 | 2.817073 |
| 7 | 5.78559 | 0.870295 | 2.73134 | 7 | 4.322459 | -1.166044 | 1.304268 |
| 7 | 4.258136 | -0.562533 | 1.618716 | 7 | 1.688634 | -0.088869 | -1.627343 |
| 7 | 1.652823 | -0.67054 | -1.523175 | 8 | 2.587545 | -2.744651 | -0.689823 |
| 8 | 2.650512 | -2.815936 | 0.259315 | 8 | 4.689078 | -0.837801 | -1.610359 |
| 8 | 4.683058 | -1.219016 | -1.223821 | 6 | 2.621807 | -4.84082 | -1.721081 |
| 6 | 2.81027 | -5.131496 | -0.00886 | 1 | 1.555237 | -4.763159 | -1.947876 |
| 1 | 1.760029 | -5.199526 | -0.305667 | 1 | 3.123618 | -5.407909 | -2.505682 |
| 1 | 3.385236 | -5.903348 | -0.521395 | 1 | 2.704364 | -5.385593 | -0.775744 |
| 1 | 2.845615 | -5.311565 | 1.069619 | 6 | 3.188041 | -3.454719 | -1.546147 |
| 6 | 3.310675 | -3.738846 | -0.297388 | 6 | 4.309028 | -3.09095 | -2.310121 |
| 6 | 4.439551 | -3.593385 | -1.119936 | 1 | 4.702241 | -3.84692 | -2.978103 |
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| 6 | 5.057111 | -2.39299 | -1.50715 | 6 | 6.213395 | -1.707824 | -3.153766 |
| 6 | 6.299245 | -2.470232 | -2.35778 | 1 | 7.0811 | -1.530778 | -2.511591 |
| 1 | 7.134154 | -2.029537 | -1.805247 | 1 | 6.402769 | -2.580599 | -3.77936 |
| 1 | 6.555972 | -3.49141 | -2.641143 | 1 | 6.101426 | -0.822336 | -3.785255 |
| 1 | 6.160811 | -1.86486 | -3.257677 | 6 | 1.953004 | 0.231568 | -2.894877 |
| 6 | 1.951466 | -0.774775 | -2.818602 | 1 | 2.997228 | 0.186902 | -3.184318 |
| 1 | 3.005495 | -0.876538 | -3.052538 | 6 | 1.38475 | -0.566937 | 0.916724 |
| 6 | 1.301554 | -0.27277 | 1.02313 | 6 | 1.258446 | -0.751239 | 2.301111 |
| 6 | 1.160974 | 0.018853 | 2.38651 | 1 | 2.15658 | -0.891926 | 2.889634 |

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|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 1 | 2.054317 | 0.105738 | 2.992663 | 1 | -1.806996 | 0.460573 | 4.61385 |
| 1 | -1.925927 | 1.94095 | 4.101671 | 6 | 1.224636 | -1.109119 | 5.151387 |
| 6 | 1.089036 | 0.647225 | 5.190273 | 1 | 1.755754 | -1.996529 | 4.793579 |
| 1 | 1.620606 | -0.308882 | 5.161267 | 1 | 1.87195 | -0.238879 | 5.008163 |
| 1 | 1.742177 | 1.417837 | 4.770378 | 1 | 1.064184 | -1.230015 | 6.227003 |
| 1 | 0.912938 | 0.898107 | 6.240752 | 6 | 4.550876 | -2.39708 | 1.764376 |
| 6 | 4.53631 | -1.548139 | 2.47337 | 1 | 3.965425 | -3.186195 | 1.305446 |
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| 6 | 5.454044 | -1.367681 | 3.490918 | 1 | 5.665135 | -3.615907 | 3.144389 |
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| 6 | 6.061848 | -0.119246 | 3.567804 | 1 | 6.889245 | -1.600383 | 4.043912 |
| 1 | 6.800284 | 0.094638 | 4.337193 | 6 | 5.009114 | -0.122879 | 1.853674 |
| 6 | 4.886951 | 0.638415 | 1.776215 | 6 | 4.653064 | 1.168998 | 1.312734 |
| 6 | 4.474437 | 1.650853 | 0.830821 | 6 | 3.647283 | 1.159103 | 0.318523 |
| 6 | 3.483464 | 1.253203 | -0.096261 | 6 | 3.273903 | 2.393097 | -0.211628 |
| 6 | 3.038212 | 2.220405 | -0.995999 | 1 | 2.496432 | 2.421215 | -0.969129 |
| 1 | 2.265635 | 1.953974 | -1.710616 | 6 | 3.866364 | 3.596509 | 0.188454 |
| 6 | 3.54909 | 3.522988 | -1.017432 | 6 | 4.860423 | 3.557839 | 1.175421 |
| 6 | 4.538849 | 3.869441 | -0.088144 | 1 | 5.33645 | 4.471137 | 1.509657 |
| 1 | 4.954704 | 4.869052 | -0.078466 | 6 | 5.249394 | 2.354959 | 1.737071 |
| 6 | 4.995857 | 2.943517 | 0.832782 | 1 | 6.017793 | 2.316104 | 2.502457 |
| 1 | 5.757267 | 3.205395 | 1.560408 | 6 | 1.916606 | 5.105259 | -0.240397 |
| 6 | 1.504738 | 4.711081 | -1.830001 | 1 | 1.68497 | 5.153558 | 0.827472 |
| 1 | 1.301537 | 5.104546 | -0.829888 | 1 | 1.583841 | 6.039154 | -0.705934 |
| 1 | 1.102361 | 5.417302 | -2.564226 | 1 | 1.331108 | 4.289486 | -0.671076 |
| 1 | 0.958353 | 3.770275 | -1.933744 | 6 | 4.154663 | 6.123035 | 0.099831 |
| 6 | 3.688431 | 5.888977 | -1.944198 | 1 | 3.97191 | 6.243541 | 1.171827 |
| 1 | 3.524501 | 6.351047 | -0.966103 | 1 | 5.234985 | 6.059215 | -0.060935 |
| 1 | 4.766722 | 5.824365 | -2.11841 | 1 | 3.798947 | 7.028649 | -0.400697 |
| 1 | 3.270119 | 6.559497 | -2.70091 | 6 | 3.421907 | 4.905629 | -0.46685 |
| 6 | 3.013254 | 4.519837 | -2.047015 | 6 | 3.705052 | 4.836302 | -1.975568 |
| 6 | 3.259942 | 3.972481 | -3.461458 | 1 | 3.391201 | 5.766065 | -2.462113 |
| 1 | 2.883307 | 4.677338 | -4.2104 | 1 | 4.77303 | 4.693384 | -2.165009 |
| 1 | 4.328871 | 3.822129 | -3.639584 | 1 | 3.167311 | 4.01072 | -2.448735 |
| 1 | 2.756378 | 3.015231 | -3.618807 | 17 | -1.65766 | 1.120247 | -4.246161 |
| 17 | -1.620431 | -0.460832 | -4.477071 | 17 | -3.783679 | -3.837858 | 0.916483 |
| | Ir-Cl-T1 | | | | Ir-2Cl-T1 | | |
| 77 | -2.537309 | -0.876497 | -0.031149 | 77 | 2.771724 | 0.755623 | 0.211759 |
| 77 | 2.686928 | 0.899702 | -0.184643 | 77 | -2.502142 | -0.652917 | -0.615125 |
| 7 | -5.728808 | -0.668384 | 2.67878 | 7 | 5.686627 | 0.030134 | 3.134964 |
| 7 | -3.85069 | -1.417271 | 1.445983 | 7 | 3.971654 | 1.034429 | 1.848803 |
| 7 | -1.135776 | -0.237562 | -1.471122 | 7 | 1.479131 | 0.382701 | -1.412558 |
| 7 | 1.188498 | 0.322007 | -1.505919 | 7 | -0.856465 | -0.024409 | -1.716053 |
| 7 | 4.103307 | 1.371156 | 1.210365 | 7 | -4.074091 | -1.183113 | 0.577091 |

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| 7 | 5.973811 | 0.513561 | 2.39152 | 7 | -5.984103 | -0.339961 | 1.698338 |
| 8 | -4.022315 | -1.612913 | -1.40476 | 8 | 4.413385 | 1.555311 | -0.924801 |
| 8 | -1.731071 | -2.871525 | -0.21667 | 8 | 2.102327 | 2.810448 | 0.211906 |
| 8 | 1.895979 | 2.928631 | -0.282566 | 8 | -1.82342 | -2.709344 | -0.868211 |
| 8 | 4.029351 | 1.4933 | -1.768084 | 8 | -3.709607 | -0.970974 | -2.375874 |
| 6 | -5.048615 | -2.73062 | -3.181736 | 6 | 5.655837 | 2.799983 | -2.464029 |
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| 1 | -5.048493 | -3.690391 | -3.699063 | 1 | 5.753685 | 3.810397 | -2.861853 |
| 1 | -4.913191 | -1.927678 | -3.912565 | 1 | 5.547498 | 2.095314 | -3.293913 |
| 6 | -3.953335 | -2.624013 | -2.159236 | 6 | 4.466754 | 2.647086 | -1.559363 |
| 6 | -2.973003 | -3.626604 | -2.100537 | 6 | 3.538874 | 3.695246 | -1.465007 |
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| 6 | -1.975011 | -3.722266 | -1.12724 | 6 | 2.468639 | 3.743542 | -0.568086 |
| 6 | -1.12432 | -4.961501 | -1.075955 | 6 | 1.687672 | 5.021201 | -0.431796 |
| 1 | -0.077671 | -4.678369 | -0.948906 | 1 | 0.619589 | 4.795366 | -0.427157 |
| 1 | -1.236199 | -5.578126 | -1.96817 | 1 | 1.912798 | 5.732308 | -1.227064 |
| 1 | -1.406821 | -5.555151 | -0.200214 | 1 | 1.923528 | 5.484795 | 0.531793 |
| 6 | -3.89004 | -2.599678 | 2.060072 | 6 | 4.017435 | 2.133713 | 2.601072 |
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| 1 | -6.552853 | -1.986059 | 4.018572 | 1 | 6.454068 | 1.129706 | 4.688114 |
| 6 | -4.774248 | -0.471842 | 1.772682 | 6 | 4.809467 | 0.000819 | 2.13512 |
| 6 | -4.618973 | 0.777368 | 1.060321 | 6 | 4.650636 | -1.145206 | 1.266362 |
| 6 | -5.454836 | 1.876741 | 1.255618 | 6 | 5.401119 | -2.313174 | 1.395903 |
| 1 | -6.272517 | 1.804862 | 1.965015 | 1 | 6.154922 | -2.378847 | 2.173369 |
| 6 | -5.226433 | 3.034315 | 0.537695 | 6 | 5.170589 | -3.363774 | 0.528784 |
| 1 | -5.882477 | 3.884646 | 0.690719 | 1 | 5.760754 | -4.268057 | 0.633817 |
| 6 | -4.168529 | 3.127769 | -0.385043 | 6 | 4.194258 | -3.281739 | -0.480818 |
| 6 | -3.344584 | 2.018053 | -0.564313 | 6 | 3.456688 | -2.104793 | -0.594149 |
| 1 | -2.526002 | 2.059477 | -1.269973 | 1 | 2.703648 | -2.00893 | -1.364329 |
| 6 | -3.547555 | 0.832177 | 0.1451 | 6 | 3.664399 | -1.024022 | 0.265406 |
| 6 | -3.96565 | 4.428188 | -1.161396 | 6 | 3.981221 | -4.471356 | -1.415512 |
| 6 | -2.773553 | 4.353119 | -2.116489 | 6 | 2.887396 | -4.204875 | -2.45084 |
| 1 | -1.83889 | 4.163561 | -1.580232 | 1 | 1.921553 | -4.008686 | -1.97575 |
| 1 | -2.669121 | 5.306319 | -2.64352 | 1 | 2.771858 | -5.08357 | -3.092432 |
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| 17 | -2.664653 | 0.192898 | -3.655461 | 17 | 3.18035 | 0.105037 | -3.492454 |
| | Ir2-Cl-T1 | | | | Ir2-2Cl-T1 | | |
| 77 | 2.648033 | 0.814815 | -0.055581 | 77 | -2.524279 | -0.38209 | -0.460674 |
| 77 | -2.621117 | -0.809086 | -0.045928 | 77 | 2.835564 | 0.601974 | 0.277858 |
| 7 | 5.888985 | 0.064694 | 2.498099 | 7 | -5.915387 | -0.027674 | 1.966503 |
| 7 | 4.092057 | 1.114204 | 1.357414 | 7 | -4.091886 | -0.898702 | 0.720536 |
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| 7 | -1.159673 | -0.274603 | -1.41638 | 7 | 1.451452 | 0.636998 | -1.253671 |
| 7 | -4.04395 | -1.239897 | 1.373115 | 7 | 4.17236 | 0.466233 | 1.819071 |
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| 8 | 4.01567 | 1.443239 | -1.59695 | 8 | -3.790514 | -0.420318 | -2.196523 |
| 8 | 1.968314 | 2.88997 | 0.001911 | 8 | -2.013681 | -2.451472 | -0.897405 |
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| | Ir4-Cl-t1 | | | | Ir4-2Cl-t1 | | |
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| 1 | -1.758367 | 6.008154 | 0.948702 | 1 | -0.395406 | 6.164959 | -0.142292 |
| 1 | -1.344283 | 4.303482 | 0.72333 | 1 | -0.340735 | 4.405124 | -0.300969 |
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| 8 | 2.585837 | -2.625494 | -0.916418 | 8 | 2.161002 | -2.574615 | -1.255462 |
| 8 | 4.31081 | -0.407288 | -1.856297 | 8 | 4.464033 | -0.903199 | -1.560616 |
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| 6 | 4.438047 | 1.307472 | 1.230497 | 6 | 3.694902 | 0.697267 | 0.778781 |
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| 6 | 1.426115 | 5.148123 | -0.109824 | 1 | 2.394273 | 4.633335 | 2.490762 |
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| 1 | 1.039714 | 6.074082 | -0.549222 | 1 | 1.850799 | 4.255192 | 0.852866 |
| 1 | 0.865125 | 4.314803 | -0.539379 | 6 | 4.952281 | 5.39736 | 1.858857 |
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| 1 | 3.477757 | 6.35285 | 1.258484 | 1 | 6.004007 | 5.220713 | 1.613619 |
| 1 | 4.70369 | 6.244304 | -0.02017 | 1 | 4.734151 | 6.446372 | 1.638747 |
| 1 | 3.215873 | 7.15397 | -0.294167 | 6 | 4.017326 | 4.5037 | 1.041686 |
| 6 | 2.930368 | 5.017669 | -0.383804 | 6 | 4.23544 | 4.813438 | -0.447517 |
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| 1 | 2.083089 | 2.4947 | -0.885421 | 6 | -1.346749 | -1.112293 | 2.078726 |
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| Ir5-CI-T1 | | | | Ir5-2CI-T1 | | | |
|-----------|-----------|-----------|-----------|------------|-----------|-----------|-----------|
| 77 | -2.632995 | -0.711182 | -0.300216 | 77 | 2.622228 | -0.033164 | 0.498273 |
| 7 | -5.846916 | -1.192553 | 2.345817 | 7 | 5.974162 | -0.048693 | -2.013852 |
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| 1 | -5.298394 | -1.681512 | -4.718858 | 1 | 5.403667 | 0.312203 | 4.935484 |
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| 6 | 0.090236 | -0.131253 | -0.954756 | 6 | -0.199315 | 0.071871 | 0.935133 |
| 6 | 0.094744 | -0.60491 | 0.395275 | 6 | -0.034908 | -0.626431 | -0.302616 |
| 6 | -1.14867 | -0.830268 | 0.995371 | 6 | 1.2624 | -0.713851 | -0.808139 |
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| 6 | -2.082553 | 4.982596 | 1.154887 | 1 | 0.933915 | 4.802373 | -3.024855 |
| 1 | -2.080676 | 4.834384 | 2.239025 | 1 | 0.165694 | 5.983995 | -1.946346 |
| 1 | -1.758367 | 6.008154 | 0.948702 | 1 | 0.169277 | 4.26198 | -1.527396 |
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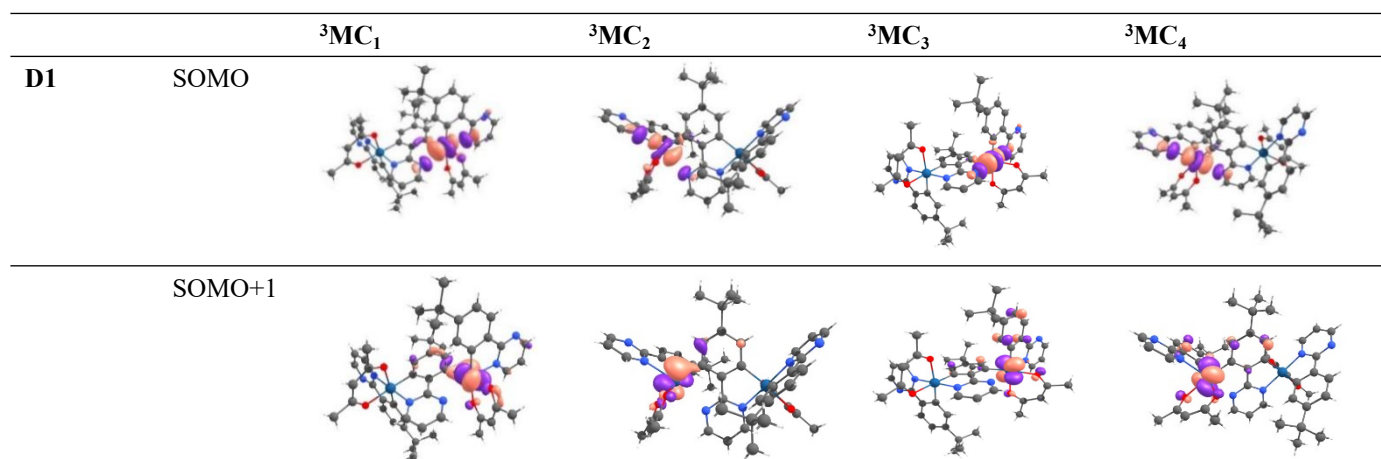
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| 1 | 0.865125 | 4.314803 | -0.539379 | 6 | -5.14647 | 5.27178 | -1.471185 |
| 6 | 3.627921 | 6.257371 | 0.17869 | 1 | -4.970219 | 5.19921 | -2.548885 |
| 1 | 3.477757 | 6.35285 | 1.258484 | 1 | -6.197291 | 5.037521 | -1.275638 |
| 1 | 4.70369 | 6.244304 | -0.02017 | 1 | -4.981966 | 6.31299 | -1.179319 |
| 1 | 3.215873 | 7.15397 | -0.294167 | 6 | -4.201276 | 4.367348 | -0.678303 |
| 6 | 2.930368 | 5.017669 | -0.383804 | 6 | -4.501711 | 4.544197 | 0.818613 |
| 6 | 3.16841 | 4.977384 | -1.901624 | 1 | -4.384314 | 5.594837 | 1.10394 |
| 1 | 2.798845 | 5.897803 | -2.366644 | 1 | -5.526613 | 4.238929 | 1.049765 |
| 1 | 4.235281 | 4.884516 | -2.125655 | 1 | -3.825331 | 3.950568 | 1.438838 |
| 1 | 2.653897 | 4.132646 | -2.366395 | 1 | 4.44183 | 4.640142 | -2.577209 |
| 1 | -5.571652 | 3.760104 | 2.120788 | 1 | -5.971186 | 3.165213 | -2.454137 |
| 1 | 4.944329 | 4.63496 | 1.501707 | 1 | -1.912898 | -2.024507 | -2.753388 |
| 1 | 2.222065 | -1.221417 | 2.918113 | 6 | 2.377094 | 2.832422 | -0.572838 |
| 6 | -3.147282 | 2.249057 | 0.287187 | 1 | 1.463837 | 2.927341 | 0.006142 |
| 1 | -2.300538 | 2.476014 | -0.350363 | 6 | -3.543788 | 1.93617 | -0.427541 |
| 6 | 2.894128 | 2.499415 | -0.164018 | 1 | -2.786848 | 2.252948 | 0.281991 |
| 1 | 2.083089 | 2.4947 | -0.885421 | 6 | 1.349195 | -1.288389 | -2.08524 |
| 6 | -1.126126 | -1.187188 | 2.361699 | 1 | 2.324077 | -1.379424 | -2.556059 |
| 1 | -2.062603 | -1.364974 | 2.880988 | 17 | -0.762895 | 2.534677 | 4.523714 |
| 17 | -2.507715 | 1.559797 | -3.297524 | 17 | 6.552511 | -3.85676 | -1.0912 |
| | Ir6-Cl-T1 | | | | Ir6-2Cl-T1 | | |
| 77 | -2.632995 | -0.711182 | -0.300216 | 77 | -2.589697 | -0.448755 | -0.320465 |
| 7 | -5.846916 | -1.192553 | 2.345817 | 7 | -6.135037 | -0.560878 | 1.938628 |
| 7 | -4.011095 | -1.608822 | 0.909909 | 7 | -4.11844 | -1.248443 | 0.860857 |
| 7 | -1.113019 | 0.155878 | -1.482331 | 7 | -1.028461 | 0.398599 | -1.437861 |
| 8 | -2.018537 | -2.572663 | -1.221746 | 8 | -1.991472 | -2.193775 | -1.467423 |
| 8 | -4.173698 | -0.751015 | -1.801047 | 8 | -4.163195 | -0.304954 | -1.781183 |
| 6 | -1.420941 | -4.064314 | -2.921304 | 6 | -1.519176 | -3.552449 | -3.306973 |
| 1 | -0.398626 | -3.697121 | -3.05615 | 1 | -0.492105 | -3.197094 | -3.4345 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 1 | -1.781522 | -4.468767 | -3.867519 | 1 | -1.918485 | -3.847675 | -4.277713 |
| 1 | -1.3843 | -4.85513 | -2.168098 | 1 | -1.484979 | -4.419406 | -2.642172 |
| 6 | -2.265085 | -2.927666 | -2.41521 | 6 | -2.323243 | -2.458773 | -2.656629 |
| 6 | -3.237505 | -2.378341 | -3.256948 | 6 | -3.353601 | -1.853516 | -3.391661 |
| 1 | -3.342629 | -2.81524 | -4.241404 | 1 | -3.527452 | -2.222824 | -4.393928 |
| 6 | -4.159817 | -1.385217 | -2.894356 | 6 | -4.225665 | -0.870115 | -2.912484 |
| 6 | -5.256368 | -1.018707 | -3.854101 | 6 | -5.365315 | -0.414429 | -3.78066 |
| 1 | -6.214332 | -1.033823 | -3.328731 | 1 | -6.300833 | -0.504859 | -3.222417 |
| 1 | -5.298394 | -1.681512 | -4.718858 | 1 | -5.437082 | -0.979288 | -4.710517 |
| 1 | -5.088436 | 0.007297 | -4.194504 | 1 | -5.227009 | 0.645924 | -4.010452 |
| 6 | 0.128122 | 0.920988 | -3.40556 | 6 | 0.243192 | 1.157577 | -3.341671 |
| 1 | 0.132647 | 1.389935 | -4.381965 | 1 | 0.269655 | 1.665919 | -4.297735 |
| 6 | -1.085061 | 0.719444 | -2.758194 | 6 | -0.971484 | 1.016571 | -2.686861 |
| 6 | 0.090236 | -0.131253 | -0.954756 | 6 | 0.157932 | 0.003841 | -0.93978 |
| 6 | 0.094744 | -0.60491 | 0.395275 | 6 | 0.137043 | -0.536313 | 0.38281 |
| 6 | -1.14867 | -0.830268 | 0.995371 | 6 | -1.117458 | -0.720298 | 0.966536 |
| 6 | 0.079927 | -1.306612 | 3.063541 | 6 | 0.084652 | -1.39858 | 3.002343 |
| 6 | 0.039299 | -1.653922 | 4.555512 | 6 | 0.018651 | -1.842137 | 4.467472 |
| 6 | -0.740995 | -0.562418 | 5.304255 | 6 | -0.685479 | -0.753658 | 5.291955 |
| 1 | -0.775401 | -0.788359 | 6.375346 | 1 | -0.7473 | -1.055084 | 6.342996 |
| 1 | -0.264038 | 0.413369 | 5.17524 | 1 | -0.136504 | 0.19092 | 5.238387 |
| 6 | -0.661462 | -3.007311 | 4.748931 | 6 | -0.772542 | -3.154951 | 4.569809 |
| 1 | -0.124588 | -3.80287 | 4.223601 | 1 | -0.28982 | -3.946905 | 3.989537 |
| 1 | -1.688057 | -2.990528 | 4.373401 | 1 | -1.794569 | -3.045272 | 4.197781 |
| 1 | -0.699293 | -3.264484 | 5.812775 | 1 | -0.830164 | -3.481558 | 5.613602 |
| 6 | -4.161251 | -2.925261 | 1.059588 | 6 | -4.414962 | -2.51732 | 1.141288 |
| 1 | -3.456566 | -3.544232 | 0.51414 | 6 | -5.587092 | -2.872414 | 1.791784 |
| 6 | -5.165051 | -3.430361 | 1.86407 | 1 | -5.811992 | -3.908603 | 2.000682 |
| 1 | -5.296437 | -4.496505 | 1.994004 | 6 | -6.431967 | -1.834088 | 2.147805 |
| 6 | -5.993098 | -2.502107 | 2.487393 | 1 | -7.381163 | -2.038205 | 2.637287 |
| 1 | -6.808746 | -2.826782 | 3.129247 | 6 | -4.988699 | -0.29069 | 1.324104 |
| 6 | -4.857527 | -0.767485 | 1.563476 | 6 | -4.532713 | 1.066267 | 1.149511 |
| 6 | -4.572376 | 0.632631 | 1.348072 | 6 | -3.291575 | 1.22272 | 0.500197 |
| 6 | -3.467789 | 0.912291 | 0.509181 | 6 | -3.442676 | 3.623851 | 0.911493 |
| 6 | -3.887425 | 3.293947 | 0.853123 | 6 | -4.691755 | 3.42914 | 1.520088 |
| 6 | -4.978253 | 2.973049 | 1.672678 | 6 | -5.235105 | 2.163345 | 1.644201 |
| 6 | -5.319717 | 1.654937 | 1.924131 | 1 | -6.193946 | 2.00729 | 2.126789 |
| 1 | -6.163313 | 1.404157 | 2.55875 | 6 | -1.526411 | 5.017396 | 1.665229 |
| 6 | -2.082553 | 4.982596 | 1.154887 | 1 | -1.764501 | 4.826235 | 2.716026 |
| 1 | -2.080676 | 4.834384 | 2.239025 | 1 | -1.032077 | 5.992254 | 1.597163 |
| 1 | -1.758367 | 6.008154 | 0.948702 | 1 | -0.816033 | 4.254412 | 1.339146 |
| 1 | -1.344283 | 4.303482 | 0.72333 | 6 | -3.724132 | 6.121104 | 1.303527 |
| 6 | -4.445829 | 5.751232 | 1.198417 | 1 | -3.973496 | 6.004732 | 2.362568 |
| 1 | -4.473087 | 5.669574 | 2.289283 | 1 | -4.655823 | 6.161254 | 0.730822 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 1 | -5.464767 | 5.632669 | 0.816938 | 1 | -3.222633 | 7.086648 | 1.189147 |
| 1 | -4.116791 | 6.765362 | 0.953513 | 6 | -2.80045 | 5.007049 | 0.806809 |
| 6 | -3.48264 | 4.74085 | 0.572168 | 6 | -2.439272 | 5.3044 | -0.656091 |
| 6 | -3.457238 | 4.981896 | -0.94485 | 1 | -1.967837 | 6.289971 | -0.730948 |
| 1 | -3.157649 | 6.014321 | -1.153403 | 1 | -3.333523 | 5.303875 | -1.286156 |
| 1 | -4.447236 | 4.818444 | -1.380978 | 1 | -1.744913 | 4.568947 | -1.067919 |
| 1 | -2.755623 | 4.318919 | -1.45625 | 77 | 2.874015 | -0.642816 | -0.305791 |
| 77 | 2.844184 | -0.556673 | -0.27773 | 7 | 6.00576 | -0.586626 | 2.482323 |
| 7 | 5.917084 | -0.119079 | 2.542973 | 7 | 4.303848 | -1.306772 | 0.996783 |
| 7 | 4.304477 | -1.040988 | 1.068045 | 7 | 1.347165 | 0.096208 | -1.5151 |
| 7 | 1.278024 | 0.011025 | -1.525702 | 8 | 2.474206 | -2.645493 | -1.05115 |
| 8 | 2.585837 | -2.625494 | -0.916418 | 8 | 4.339522 | -0.520173 | -1.888432 |
| 8 | 4.31081 | -0.407288 | -1.856297 | 6 | 2.44547 | -4.556764 | -2.39653 |
| 6 | 2.735163 | -4.60558 | -2.15197 | 1 | 1.355669 | -4.56662 | -2.324409 |
| 1 | 1.652513 | -4.706948 | -2.050755 | 1 | 2.755221 | -4.917232 | -3.378121 |
| 1 | 3.053886 | -4.979063 | -3.125897 | 1 | 2.823947 | -5.244638 | -1.633412 |
| 1 | 3.190356 | -5.22661 | -1.373272 | 6 | 2.948197 | -3.166861 | -2.101912 |
| 6 | 3.122536 | -3.165563 | -1.926144 | 6 | 3.892785 | -2.600158 | -2.968548 |
| 6 | 4.042768 | -2.580082 | -2.807074 | 1 | 4.186116 | -3.194296 | -3.824591 |
| 1 | 4.397695 | -3.200145 | -3.620531 | 6 | 4.534852 | -1.3621 | -2.810186 |
| 6 | 4.586711 | -1.2887 | -2.717837 | 6 | 5.579551 | -0.958017 | -3.817354 |
| 6 | 5.618046 | -0.871439 | -3.734038 | 1 | 6.52834 | -0.79242 | -3.299491 |
| 1 | 6.546649 | -0.617639 | -3.215099 | 1 | 5.720417 | -1.7015 | -4.602427 |
| 1 | 5.818504 | -1.645146 | -4.475854 | 1 | 5.292653 | -0.00392 | -4.268322 |
| 1 | 5.277358 | 0.036779 | -4.238825 | 6 | 1.408083 | 0.673244 | -2.778662 |
| 6 | 1.312512 | 0.538698 | -2.812569 | 1 | 2.37507 | 0.709162 | -3.25695 |
| 1 | 2.280986 | 0.619335 | -3.28272 | 6 | 1.367088 | -0.804749 | 0.977395 |
| 6 | 1.335516 | -0.757655 | 1.007043 | 6 | 1.302932 | -1.235166 | 2.327557 |
| 6 | 1.289576 | -1.106605 | 2.377948 | 1 | -1.702422 | -0.567908 | 4.936161 |
| 1 | -1.770263 | -0.479879 | 4.94548 | 6 | 1.404628 | -2.075601 | 5.071524 |
| 6 | 1.435674 | -1.748461 | 5.173662 | 1 | 1.949303 | -2.867184 | 4.547599 |
| 1 | 2.037897 | -2.532365 | 4.70407 | 1 | 2.014718 | -1.167578 | 5.055877 |
| 1 | 1.979978 | -0.802654 | 5.095937 | 1 | 1.298096 | -2.384208 | 6.115713 |
| 1 | 1.346888 | -1.992645 | 6.236488 | 6 | 4.573274 | -2.582205 | 1.279371 |
| 6 | 4.673498 | -2.275832 | 1.411449 | 1 | 3.957781 | -3.314651 | 0.767754 |
| 1 | 4.128178 | -3.077848 | 0.925392 | 6 | 5.574745 | -2.913887 | 2.172442 |
| 6 | 5.684029 | -2.485079 | 2.33116 | 1 | 5.800071 | -3.946498 | 2.404871 |
| 1 | 5.989534 | -3.484555 | 2.611936 | 6 | 6.272056 | -1.857032 | 2.748427 |
| 6 | 6.282566 | -1.350276 | 2.868492 | 1 | 7.077337 | -2.04068 | 3.456034 |
| 1 | 7.088591 | -1.435787 | 3.593803 | 6 | 5.026282 | -0.330184 | 1.617218 |
| 6 | 4.93425 | 0.018394 | 1.654348 | 6 | 4.632064 | 1.013364 | 1.258445 |
| 6 | 4.438047 | 1.307472 | 1.230497 | 6 | 3.545128 | 1.11368 | 0.358798 |
| 6 | 3.364897 | 1.275826 | 0.309598 | 6 | 3.829411 | 3.542608 | 0.393684 |
| 6 | 3.452626 | 3.719286 | 0.233498 | 6 | 4.886555 | 3.399628 | 1.303192 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| 6 | 4.49806 | 3.706491 | 1.167823 | 6 | 5.286798 | 2.146874 | 1.734682 |
| 6 | 4.988747 | 2.511778 | 1.664457 | 1 | 6.114947 | 2.03011 | 2.426202 |
| 1 | 5.809244 | 2.494406 | 2.374584 | 6 | 1.920565 | 5.145991 | 0.173115 |
| 6 | 1.426115 | 5.148123 | -0.109824 | 1 | 1.748214 | 5.130931 | 1.253214 |
| 1 | 1.225458 | 5.170142 | 0.965342 | 1 | 1.601887 | 6.121096 | -0.210692 |
| 1 | 1.039714 | 6.074082 | -0.549222 | 1 | 1.281359 | 4.384471 | -0.279806 |
| 1 | 0.865125 | 4.314803 | -0.539379 | 6 | 4.211528 | 6.057115 | 0.456178 |
| 6 | 3.627921 | 6.257371 | 0.17869 | 1 | 4.094886 | 6.108899 | 1.543077 |
| 1 | 3.477757 | 6.35285 | 1.258484 | 1 | 5.27792 | 5.969299 | 0.227517 |
| 1 | 4.70369 | 6.244304 | -0.02017 | 1 | 3.861768 | 7.006568 | 0.03988 |
| 1 | 3.215873 | 7.15397 | -0.294167 | 6 | 3.40229 | 4.907746 | -0.14741 |
| 6 | 2.930368 | 5.017669 | -0.383804 | 6 | 3.602789 | 4.924489 | -1.671087 |
| 6 | 3.16841 | 4.977384 | -1.901624 | 1 | 3.300232 | 5.894174 | -2.081018 |
| 1 | 2.798845 | 5.897803 | -2.366644 | 1 | 4.653281 | 4.757025 | -1.926928 |
| 1 | 4.235281 | 4.884516 | -2.125655 | 1 | 3.010107 | 4.149378 | -2.163452 |
| 1 | 2.653897 | 4.132646 | -2.366395 | 1 | -5.245436 | 4.275007 | 1.90788 |
| 1 | -5.571652 | 3.760104 | 2.120788 | 1 | 5.413122 | 4.271816 | 1.67016 |
| 1 | 4.944329 | 4.63496 | 1.501707 | 1 | 2.226541 | -1.445114 | 2.85435 |
| 1 | 2.222065 | -1.221417 | 2.918113 | 6 | -2.765342 | 2.509316 | 0.406293 |
| 6 | -3.147282 | 2.249057 | 0.287187 | 1 | -1.805324 | 2.637939 | -0.080827 |
| 1 | -2.300538 | 2.476014 | -0.350363 | 6 | 3.167178 | 2.391733 | -0.048653 |
| 6 | 2.894128 | 2.499415 | -0.164018 | 1 | 2.346434 | 2.486793 | -0.751989 |
| 1 | 2.083089 | 2.4947 | -0.885421 | 6 | -1.112586 | -1.156407 | 2.312155 |
| 6 | -1.126126 | -1.187188 | 2.361699 | 1 | -2.059024 | -1.306863 | 2.822758 |
| 1 | -2.062603 | -1.364974 | 2.880988 | 17 | -2.350662 | 1.936136 | -3.193651 |
| 17 | -2.507715 | 1.559797 | -3.297524 | 17 | -3.299317 | -3.744521 | 0.717649 |

Table S6. The spin densities of SOMO and SOMO+1 for other ^3MC states.



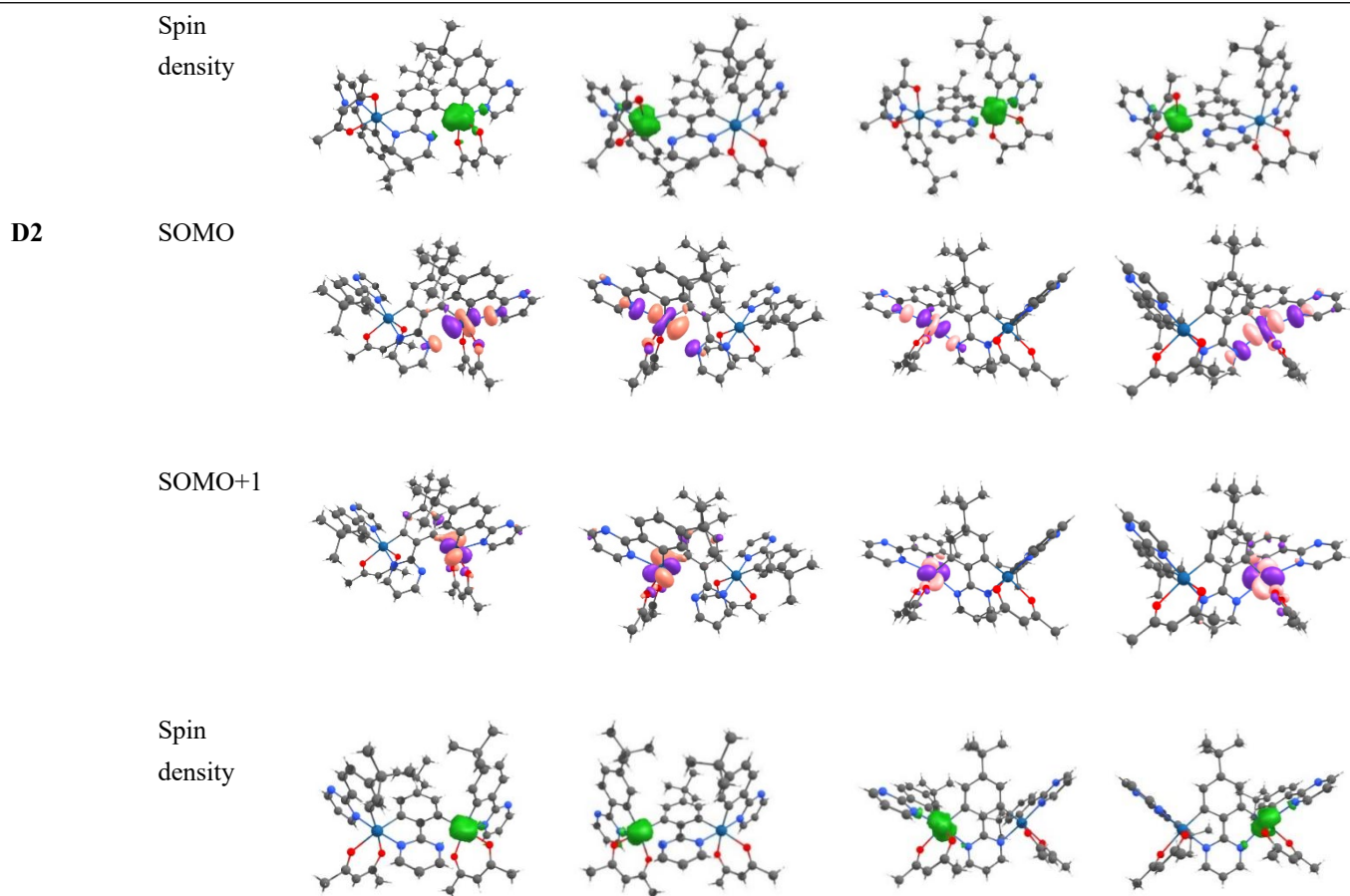


Table S7. The optimized geometries of seam crossing points for **M1**, **D1** and **D2**.

| | MESX1 | SX2 | SX3 | SX4 |
|----|-------|-----|-----|-----|
| M1 | | | | |
| D1 | | | | |
| D2 | | | | |

Table S8. The calculated $\langle T_1 | \text{SOC} | S_0 \rangle$ of the MESX state at PBE functional with ZORA-def2-tzvp (unmetal atoms)+SARC-ZORA-TZVP(Ir) basis set.

| | $\langle T_1 \text{SOC} S_0 \rangle$ |
|----|--|
| M1 | 3531 cm ⁻¹ |
| D1 | 2118 cm ⁻¹ |
| D2 | 2777 cm ⁻¹ |

Table S9. The extended transition state coupled with natural orbitals for chemical valence (ETS-NOCV) analysis of Ir₁-Cl and Ir₃-Cl in the ³MC state. Three pairs of NOCV (Pair1, Pair2, Pair3) are found at each alpha and beta. All These orbital energy contributions are collected (kcal/mol).

| | | Alpha NOCV | | | | Beta NOCV | | | |
|---|---------|--------------------------------|------------------------|----------------|---------------------|-----------------------|---------------------|------|----------------|
| | | E _{orb} (kcal/mol) | E(Alpha) (kcal/mol) | | %E _{total} | E(Beta) (kcal/mol) | %E _{total} | | |
| ³ MC state of Ir ₁ -Cl | -910.72 | E _{total} | -410.57 | | 45.1 | E _{total} | -500.15 | 54.9 | |
| | | Pair1 | -233.19 | σ-donation | 25.6 | Pair1 | -178.34 | 36.2 | d-backdonation |
| | | Pair2 | -96.09 | σ-donation | 10.6 | Pair2 | -140.76 | 19.1 | d-backdonation |
| | | Pair3 | — | — | — | Pair3 | -98.58 | 8.4 | d-backdonation |
| ³ MC state of Ir ₃ -Cl | -797.94 | E _{total} | -329.77 | | 41.3 | E _{total} | -468.17 | 58.7 | |
| | | Pair1 | -174.24 | d-backdonation | 21.8 | Pair1 | -119.98 | 15.0 | σ-donation |
| | | Pair2 | -76.28 | d-backdonation | 9.6 | Pair2 | -134.24 | 16.8 | d-backdonation |
| | | Pair3 | — | — | — | Pair3 | -99.75 | 12.5 | d-backdonation |