

Functionality Optimization for Effective Singlet Fission Coupling Screening in the Full-Dimensional Molecular and Intermolecular Coordinate Space - Supporting Information

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1 Validation of Overlap Approximation

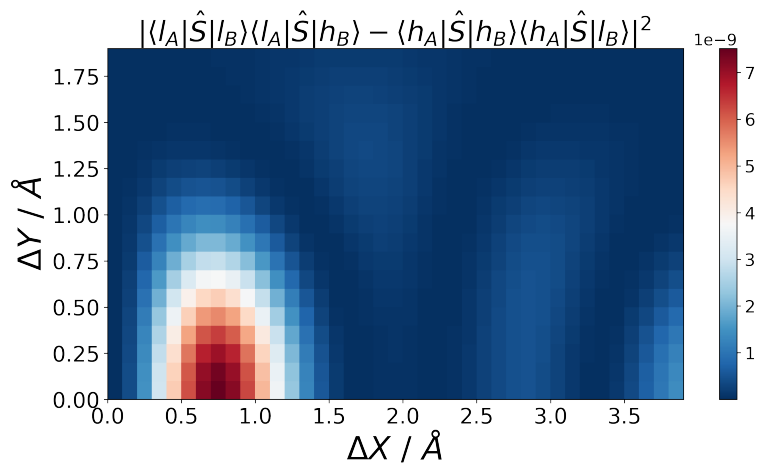


Figure 1: Overlap scan covers the region from $\Delta X = 0.0 \text{\AA}$ to 4.0\AA and from $\Delta Y = 0.0 \text{\AA}$ to 2.0\AA with a step size of 0.1\AA at an interplanar distance of $\Delta Z = 3.5 \text{\AA}$.

We performed scans of $|T_{RP}|^2$ as a function of the parallel displacement of two perylene bisimide molecules stacked cofacially (see 1). The scan covers the region from $\Delta X = 0.0 \text{\AA}$ to 4.0\AA and from $\Delta Y = 0.0 \text{\AA}$ to 2.0\AA with a step size of 0.1\AA at an interplanar distance of $\Delta Z = 3.5 \text{\AA}$. The orbitals were generated using AM1-HF calculation.

2 Analysis of all 500 optimized PBI dimers

Table 1: 500 optimized PBI dimer configurations, ordered from highest to lowest effective SF coupling. **id**: index of the original trajectory. **translation (x,y,z)**: Relative intermolecular translation in Å. **rotation (x,y,z)**: Relative intermolecular rotation in degree (due to symmetry the angle is always positive and lower than 180°). **curvature (A,B)**: mean curvature measured along two parallel lines along the long axis of PBI in $1 \times 10^{-3} \text{Å}^{-2}$. **twist (A,B)**: dihedral angle between outer carbons along the long axis of PBI in degrees. **rate**: effective SF coupling calculated with the overlap approximation. ΔE : AM1 stabilization energy of the dimer with respect to two non-interacting monomers. **steps**: Optimisation steps until convergence. Maximal step number has been set to 300.

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|------|----------|------|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 1 | 114 | -0.40 | -0.67 | 3.07 | 6.1 | 6.9 | 53.8 | 10.6 | -0.7 | 24.3 | 15.7 | 4.06×10^{-7} | 0.19 | 51 |
| 2 | 222 | -0.40 | -0.67 | 3.07 | 7.7 | 7.9 | 53.5 | 12.5 | -0.8 | 26.0 | 14.9 | 3.99×10^{-7} | 0.19 | 53 |
| 3 | 252 | -0.48 | 0.34 | 3.40 | 174.9 | 7.0 | 178.7 | -22.6 | 23.5 | 9.5 | 1.8 | 3.95×10^{-7} | 0.33 | 89 |
| 4 | 22 | -0.52 | 0.29 | 3.38 | 174.6 | 6.4 | 178.5 | -20.3 | 23.6 | 9.0 | 2.8 | 3.92×10^{-7} | 0.32 | 77 |
| 5 | 31 | 0.47 | -0.70 | 3.11 | 172.0 | 8.0 | 125.6 | 8.9 | 1.0 | 27.0 | 15.3 | 3.90×10^{-7} | 0.12 | 58 |
| 6 | 489 | 0.50 | -0.66 | 3.13 | 172.3 | 10.6 | 124.8 | 10.2 | 2.8 | 28.1 | 14.6 | 3.90×10^{-7} | 0.10 | 113 |
| 7 | 498 | -0.43 | -0.74 | 3.07 | 7.8 | 7.6 | 53.6 | 9.6 | -1.1 | 28.6 | 13.0 | 3.88×10^{-7} | 0.18 | 92 |
| 8 | 395 | -0.14 | 0.73 | 3.13 | 1.3 | 0.9 | 54.6 | 9.8 | 1.1 | 26.3 | 15.3 | 3.80×10^{-7} | 0.18 | 59 |
| 9 | 192 | -0.08 | 0.66 | 3.19 | 0.6 | 5.2 | 53.2 | 10.0 | 3.7 | 27.3 | 18.0 | 3.79×10^{-7} | 0.16 | 61 |
| 10 | 224 | -0.48 | -0.70 | 3.14 | 9.3 | 11.1 | 55.0 | 8.9 | 2.3 | 27.0 | 16.3 | 3.78×10^{-7} | 0.15 | 65 |
| 11 | 316 | 0.12 | 0.68 | 3.18 | 179.9 | 4.7 | 126.4 | 8.7 | 1.5 | 28.2 | 17.1 | 3.75×10^{-7} | 0.10 | 52 |
| 12 | 351 | 0.50 | -0.70 | 3.14 | 170.7 | 11.2 | 124.4 | 9.4 | 2.7 | 26.6 | 17.2 | 3.73×10^{-7} | 0.09 | 54 |
| 13 | 495 | 0.51 | -0.67 | 3.14 | 170.4 | 11.6 | 125.0 | 7.6 | 0.9 | 29.1 | 15.8 | 3.71×10^{-7} | 0.09 | 54 |
| 14 | 55 | -0.14 | 0.62 | 3.20 | 0.7 | 4.6 | 54.6 | 8.8 | 2.2 | 27.5 | 16.6 | 3.63×10^{-7} | 0.15 | 76 |
| 15 | 141 | -0.49 | 0.26 | 3.42 | 174.0 | 7.7 | 179.5 | -23.4 | 22.6 | 7.4 | 4.9 | 3.54×10^{-7} | 0.25 | 70 |
| 16 | 339 | 1.04 | 0.22 | 3.34 | 171.7 | 8.7 | 179.5 | -20.2 | 24.2 | 8.2 | 9.5 | 3.48×10^{-7} | 0.27 | 43 |
| 17 | 256 | -0.90 | -0.15 | 3.36 | 6.8 | 6.5 | 0.7 | -19.9 | 25.4 | 5.0 | 8.7 | 3.46×10^{-7} | 0.34 | 95 |
| 18 | 84 | 1.04 | 0.19 | 3.36 | 172.4 | 8.8 | 179.7 | -20.9 | 26.8 | 7.1 | 9.8 | 3.44×10^{-7} | 0.26 | 60 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------------------------|-----|-------------|-------|-------|----------|-----|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 19 | 177 | 1.00 | 0.10 | 3.34 | 173.6 | 8.0 | 178.7 | -19.5 | 25.7 | 3.9 | 11.6 | 3.40×10^{-7} | 0.26 | 227 |
| 20 | 451 | -0.42 | -1.02 | 2.84 | 178.7 | 2.3 | 121.8 | 18.1 | 1.4 | 20.8 | 4.1 | 3.34×10^{-7} | 0.30 | 105 |
| 21 | 5 | -0.42 | -1.07 | 2.82 | 175.0 | 0.4 | 122.6 | 15.4 | -1.6 | 22.2 | 3.6 | 3.33×10^{-7} | 0.30 | 66 |
| 22 | 32 | 1.87 | -1.69 | 3.00 | 5.1 | 0.9 | 56.1 | 3.0 | 3.8 | 25.6 | 9.4 | 3.22×10^{-7} | 0.13 | 52 |
| 23 | 44 | -1.80 | -1.71 | 2.93 | 7.3 | 3.8 | 64.3 | -7.6 | 10.2 | 0.3 | 1.6 | 3.22×10^{-7} | 0.28 | 69 |
| 24 | 361 | -1.79 | -1.62 | 2.94 | 9.4 | 4.4 | 65.0 | -3.8 | 6.8 | 0.4 | 1.6 | 3.22×10^{-7} | 0.28 | 65 |
| 25 | 207 | -0.14 | 1.10 | 2.86 | 175.4 | 7.3 | 121.9 | 15.4 | 0.6 | 24.2 | 2.2 | 3.22×10^{-7} | 0.27 | 61 |
| 26 | 480 | 1.88 | -1.69 | 3.00 | 4.5 | 0.5 | 55.9 | 3.6 | 4.6 | 25.9 | 9.8 | 3.20×10^{-7} | 0.13 | 59 |
| 27 | 317 | -1.79 | -1.67 | 2.93 | 8.7 | 4.3 | 65.4 | -3.3 | 7.9 | 0.8 | 1.7 | 3.19×10^{-7} | 0.28 | 63 |
| 28 | 302 | 1.88 | -1.69 | 2.99 | 5.3 | 0.9 | 56.0 | 3.6 | 3.7 | 25.6 | 9.1 | 3.18×10^{-7} | 0.13 | 73 |
| 29 | 402 | 1.87 | -1.68 | 3.00 | 4.7 | 0.7 | 56.1 | 3.1 | 4.4 | 25.5 | 9.7 | 3.17×10^{-7} | 0.13 | 56 |
| 30 | 284 | 1.87 | -1.68 | 3.01 | 5.1 | 0.9 | 56.0 | 3.2 | 4.4 | 25.8 | 10.0 | 3.15×10^{-7} | 0.13 | 62 |
| 31 | 138 | 2.18 | 1.66 | 2.80 | 5.1 | 5.2 | 57.2 | 1.4 | 3.1 | 24.9 | 9.6 | 3.15×10^{-7} | 0.13 | 47 |
| 32 | 312 | -2.12 | 1.68 | 2.84 | 177.1 | 3.7 | 122.5 | 4.7 | 7.3 | 25.2 | 9.2 | 3.11×10^{-7} | 0.16 | 138 |
| 33 | 238 | 1.86 | -1.52 | 3.08 | 9.5 | 6.0 | 56.6 | -2.9 | 1.7 | 21.4 | 13.4 | 3.11×10^{-7} | 0.14 | 86 |
| 34 | 86 | 1.79 | 1.70 | 2.93 | 172.4 | 4.0 | 114.9 | -6.1 | 8.1 | 0.3 | 1.2 | 3.09×10^{-7} | 0.19 | 97 |
| 35 | 124 | -1.78 | -1.74 | 2.90 | 5.7 | 3.5 | 65.4 | -4.9 | 8.0 | 0.5 | 1.4 | 3.04×10^{-7} | 0.27 | 53 |
| 36 | 375 | 1.86 | -1.46 | 3.11 | 7.9 | 5.7 | 57.1 | -5.0 | 1.8 | 20.2 | 13.6 | 3.02×10^{-7} | 0.13 | 76 |
| 37 | 441 | -1.75 | -1.58 | 2.98 | 14.0 | 5.3 | 64.5 | -3.2 | 8.6 | 4.8 | 3.6 | 2.96×10^{-7} | 0.21 | 45 |
| 38 | 250 | 2.20 | 1.65 | 2.83 | 0.0 | 1.6 | 56.1 | -1.3 | 3.0 | 25.9 | 14.6 | 2.96×10^{-7} | 0.12 | 53 |
| 39 | 233 | -1.83 | -1.57 | 3.10 | 169.9 | 6.4 | 124.0 | 2.2 | 4.0 | 25.6 | 13.6 | 2.93×10^{-7} | 0.15 | 66 |
| 40 | 328 | -1.92 | -1.66 | 2.97 | 6.0 | 0.4 | 54.3 | 2.6 | 4.4 | 29.1 | 14.9 | 2.89×10^{-7} | 0.36 | 71 |
| 41 | 381 | -1.83 | -1.58 | 3.10 | 168.9 | 6.8 | 123.5 | -0.2 | 2.1 | 23.5 | 13.5 | 2.89×10^{-7} | 0.14 | 61 |
| 42 | 64 | 1.86 | -1.51 | 3.11 | 8.9 | 6.0 | 57.2 | -5.3 | 2.8 | 19.9 | 14.2 | 2.89×10^{-7} | 0.12 | 86 |
| 43 | 146 | 1.91 | -0.48 | -3.08 | 166.3 | 2.2 | 115.5 | -1.6 | -2.6 | 9.9 | 13.0 | 2.86×10^{-7} | 0.41 | 97 |
| 44 | 230 | 2.16 | 1.58 | 2.88 | 0.3 | 0.9 | 56.6 | -1.3 | 4.0 | 24.1 | 13.5 | 2.86×10^{-7} | 0.11 | 66 |
| Continued on next page | | | | | | | | | | | | | | |

Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|------|----------|------|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 45 | 53 | 1.79 | 1.69 | 2.97 | 169.3 | 4.7 | 115.0 | -5.8 | 7.5 | 0.6 | 4.3 | 2.84×10^{-7} | 0.13 | 65 |
| 46 | 194 | -1.76 | -1.57 | 3.01 | 15.6 | 5.8 | 64.8 | -0.8 | 8.3 | 1.4 | 4.6 | 2.84×10^{-7} | 0.20 | 93 |
| 47 | 333 | -1.92 | -1.64 | 2.97 | 7.0 | 0.4 | 54.1 | 3.3 | 5.7 | 30.0 | 12.6 | 2.83×10^{-7} | 0.36 | 73 |
| 48 | 82 | -0.67 | -2.62 | 2.72 | 8.3 | 0.2 | 66.5 | -1.7 | 8.5 | 5.5 | 2.1 | 2.83×10^{-7} | 0.21 | 50 |
| 49 | 163 | -3.99 | 0.07 | 3.19 | 179.2 | 2.2 | 179.9 | -19.1 | 18.9 | 2.9 | 5.4 | 2.82×10^{-7} | 0.29 | 42 |
| 50 | 404 | -2.27 | 1.66 | 2.70 | 3.9 | 7.0 | 54.5 | 3.3 | 5.3 | 30.0 | 14.4 | 2.81×10^{-7} | 0.34 | 56 |
| 51 | 1 | 0.76 | 2.66 | 2.66 | 166.2 | 2.2 | 113.5 | -1.4 | 7.8 | 7.2 | 2.5 | 2.79×10^{-7} | 0.14 | 49 |
| 52 | 386 | -3.96 | 0.05 | 3.21 | 178.7 | 2.3 | 179.8 | -18.1 | 17.2 | 1.4 | 3.8 | 2.77×10^{-7} | 0.29 | 74 |
| 53 | 154 | 4.05 | 0.16 | 3.15 | 0.1 | 0.9 | 0.8 | -22.8 | 19.0 | 4.9 | 6.9 | 2.75×10^{-7} | 0.23 | 65 |
| 54 | 349 | 1.90 | -0.45 | 3.09 | 165.0 | 2.6 | 115.1 | 2.4 | 1.6 | 11.2 | 13.7 | 2.74×10^{-7} | 0.40 | 62 |
| 55 | 346 | -4.00 | 0.06 | 3.19 | 176.0 | 2.1 | 179.9 | -20.8 | 19.8 | 3.0 | 7.2 | 2.74×10^{-7} | 0.28 | 65 |
| 56 | 314 | 4.06 | 0.16 | 3.12 | 5.5 | 0.8 | 0.6 | -20.8 | 20.2 | 7.2 | 6.5 | 2.72×10^{-7} | 0.23 | 53 |
| 57 | 490 | -0.68 | 2.46 | 2.89 | 2.7 | 2.1 | 65.9 | -5.6 | 11.0 | 2.0 | 1.5 | 2.68×10^{-7} | 0.17 | 39 |
| 58 | 3 | -4.01 | 0.07 | 3.17 | 179.3 | 1.9 | 179.4 | -19.0 | 18.4 | 3.9 | 5.4 | 2.65×10^{-7} | 0.28 | 50 |
| 59 | 418 | -3.98 | 0.03 | 3.21 | 178.2 | 1.9 | 179.4 | -20.6 | 19.2 | 2.2 | 3.3 | 2.65×10^{-7} | 0.27 | 39 |
| 60 | 376 | -2.29 | 1.68 | 2.71 | 2.1 | 6.7 | 54.7 | 2.9 | 6.7 | 29.9 | 13.5 | 2.65×10^{-7} | 0.33 | 72 |
| 61 | 283 | -3.96 | -0.07 | 3.23 | 176.7 | 3.0 | 179.3 | -20.5 | 19.3 | 0.6 | 8.4 | 2.64×10^{-7} | 0.27 | 54 |
| 62 | 83 | -3.96 | 0.06 | 3.22 | 177.2 | 2.4 | 179.8 | -18.7 | 17.7 | 1.6 | 3.2 | 2.62×10^{-7} | 0.27 | 85 |
| 63 | 178 | -3.97 | -0.04 | 3.23 | 177.5 | 2.0 | 179.3 | -19.9 | 18.2 | 2.0 | 3.1 | 2.59×10^{-7} | 0.27 | 104 |
| 64 | 214 | 4.01 | 0.15 | 3.18 | 0.6 | 1.5 | 0.1 | -22.0 | 18.5 | 3.5 | 6.7 | 2.59×10^{-7} | 0.22 | 43 |
| 65 | 301 | -2.24 | 1.71 | 2.72 | 2.8 | 6.6 | 55.9 | 3.2 | 7.3 | 28.5 | 12.1 | 2.58×10^{-7} | 0.32 | 59 |
| 66 | 481 | 0.75 | 2.62 | 2.77 | 173.9 | 0.1 | 113.8 | -2.9 | 9.8 | 3.7 | 1.4 | 2.57×10^{-7} | 0.10 | 43 |
| 67 | 266 | 4.07 | 0.14 | 3.13 | 1.1 | 0.0 | 0.8 | -23.3 | 18.8 | 6.4 | 2.6 | 2.57×10^{-7} | 0.21 | 86 |
| 68 | 118 | 2.28 | 1.74 | 2.68 | 175.3 | 10.2 | 124.0 | 2.3 | 5.1 | 29.5 | 12.8 | 2.56×10^{-7} | 0.24 | 53 |
| 69 | 388 | 1.95 | -0.53 | 3.11 | 161.4 | 5.9 | 115.2 | -1.8 | 4.2 | 11.7 | 14.7 | 2.54×10^{-7} | 0.34 | 66 |
| 70 | 111 | 2.30 | 1.76 | 2.67 | 177.7 | 9.0 | 125.1 | 7.7 | 4.8 | 30.9 | 12.6 | 2.53×10^{-7} | 0.23 | 53 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 71 | 151 | -2.26 | 1.72 | 2.71 | 2.8 | 8.5 | 56.3 | 2.2 | 5.6 | 28.3 | 11.3 | 2.52×10^{-7} | 0.29 | 37 |
| 72 | 52 | 4.06 | 0.00 | 3.20 | 3.7 | 1.3 | 1.8 | -23.0 | 22.5 | 1.9 | 4.5 | 2.50×10^{-7} | 0.21 | 65 |
| 73 | 29 | -1.80 | 0.63 | 3.13 | 8.7 | 1.9 | 64.5 | -0.8 | 1.4 | 6.9 | 14.2 | 2.50×10^{-7} | 0.40 | 56 |
| 74 | 446 | 1.94 | -1.69 | 2.98 | 174.1 | 2.1 | 125.8 | 5.0 | 6.3 | 28.0 | 12.6 | 2.49×10^{-7} | 0.24 | 92 |
| 75 | 343 | 1.97 | -0.48 | 3.11 | 160.9 | 5.8 | 115.5 | 0.0 | 1.6 | 12.7 | 14.9 | 2.47×10^{-7} | 0.33 | 52 |
| 76 | 94 | -3.96 | -0.09 | 3.24 | 177.3 | 2.9 | 178.9 | -20.5 | 20.1 | 1.0 | 6.8 | 2.46×10^{-7} | 0.25 | 173 |
| 77 | 476 | -1.92 | -0.53 | 3.11 | 15.8 | 4.5 | 64.8 | 0.1 | 1.0 | 10.6 | 15.0 | 2.45×10^{-7} | 0.40 | 111 |
| 78 | 293 | -2.30 | 1.73 | 2.72 | 2.8 | 9.1 | 55.3 | 1.5 | 8.6 | 29.5 | 11.7 | 2.44×10^{-7} | 0.28 | 105 |
| 79 | 71 | 4.02 | 0.07 | 3.18 | 3.9 | 1.5 | 0.4 | -22.4 | 18.6 | 4.4 | 6.1 | 2.43×10^{-7} | 0.20 | 70 |
| 80 | 269 | -1.95 | -0.43 | 3.12 | 16.5 | 4.4 | 64.4 | 2.1 | 3.6 | 9.7 | 13.4 | 2.43×10^{-7} | 0.40 | 45 |
| 81 | 42 | -1.91 | -0.56 | -3.11 | 13.9 | 3.8 | 65.0 | 0.1 | -4.1 | 9.8 | 13.5 | 2.41×10^{-7} | 0.40 | 60 |
| 82 | 143 | -3.15 | 1.50 | 2.93 | 179.0 | 0.8 | 118.5 | -9.6 | 8.6 | 12.3 | 4.8 | 2.38×10^{-7} | 0.29 | 97 |
| 83 | 364 | 2.29 | 1.71 | 2.74 | 175.2 | 9.7 | 124.4 | 0.0 | 9.3 | 28.5 | 11.4 | 2.38×10^{-7} | 0.21 | 60 |
| 84 | 150 | -3.07 | 1.49 | 2.97 | 178.4 | 0.8 | 117.7 | -8.3 | 6.0 | 11.4 | 6.6 | 2.37×10^{-7} | 0.29 | 91 |
| 85 | 100 | 2.94 | 0.65 | 3.17 | 10.5 | 0.5 | 6.9 | -17.0 | 36.1 | 19.0 | 7.0 | 2.35×10^{-7} | 0.28 | 69 |
| 86 | 298 | -1.92 | -0.57 | 3.11 | 14.7 | 4.4 | 64.7 | -1.6 | 3.0 | 9.9 | 14.6 | 2.32×10^{-7} | 0.39 | 61 |
| 87 | 119 | -0.14 | 0.96 | 2.97 | 166.6 | 11.3 | 118.8 | 7.8 | -1.5 | 11.8 | 13.0 | 2.31×10^{-7} | 0.17 | 46 |
| 88 | 228 | -2.97 | -1.48 | 3.11 | 174.0 | 3.2 | 117.7 | -7.3 | 8.9 | 13.4 | 5.1 | 2.31×10^{-7} | 0.28 | 50 |
| 89 | 204 | 1.95 | -0.56 | 3.11 | 162.4 | 5.6 | 115.4 | -1.9 | 3.5 | 10.0 | 14.6 | 2.30×10^{-7} | 0.31 | 65 |
| 90 | 13 | -0.29 | -0.96 | 2.94 | 172.0 | 7.9 | 119.3 | 12.2 | 0.1 | 13.1 | 10.1 | 2.30×10^{-7} | 0.18 | 114 |
| 91 | 329 | 2.66 | -0.63 | 3.40 | 9.5 | 4.5 | 6.1 | -17.8 | 34.9 | 19.6 | 8.1 | 2.30×10^{-7} | 0.28 | 46 |
| 92 | 10 | -2.95 | -1.50 | 3.13 | 173.0 | 3.6 | 118.1 | -6.9 | 8.8 | 14.4 | 7.7 | 2.30×10^{-7} | 0.28 | 40 |
| 93 | 179 | 1.97 | -0.48 | 3.13 | 162.6 | 5.2 | 115.7 | -2.9 | 3.3 | 11.8 | 12.7 | 2.29×10^{-7} | 0.31 | 68 |
| 94 | 15 | 2.73 | -0.65 | 3.39 | 9.5 | 3.3 | 4.6 | -22.8 | 35.6 | 17.1 | 7.8 | 2.29×10^{-7} | 0.28 | 91 |
| 95 | 374 | -0.28 | -0.97 | 2.95 | 173.3 | 7.5 | 118.3 | 4.8 | -2.5 | 10.2 | 10.5 | 2.27×10^{-7} | 0.18 | 46 |
| 96 | 221 | -2.95 | -1.50 | 3.13 | 173.2 | 3.4 | 118.4 | -9.5 | 9.2 | 12.5 | 7.4 | 2.27×10^{-7} | 0.28 | 58 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 97 | 142 | -3.01 | 0.63 | 3.00 | 12.7 | 6.7 | 8.1 | -15.0 | 26.4 | 22.0 | 1.3 | 2.27×10^{-7} | 0.53 | 68 |
| 98 | 57 | -3.12 | 1.48 | 2.99 | 177.0 | 2.4 | 118.5 | -9.0 | 10.6 | 11.8 | 9.3 | 2.25×10^{-7} | 0.26 | 77 |
| 99 | 21 | -1.53 | 1.65 | 3.01 | 162.8 | 9.9 | 114.7 | -6.0 | 12.7 | 11.2 | 1.6 | 2.25×10^{-7} | 0.30 | 58 |
| 100 | 67 | 2.72 | -0.56 | 3.40 | 3.9 | 3.6 | 5.6 | -19.9 | 32.9 | 16.6 | 2.6 | 2.22×10^{-7} | 0.27 | 68 |
| 101 | 473 | 1.60 | 1.64 | 3.01 | 20.3 | 10.9 | 66.3 | -10.4 | 4.7 | 5.0 | 5.2 | 2.21×10^{-7} | 0.27 | 45 |
| 102 | 265 | -1.52 | 1.62 | 3.04 | 162.7 | 9.9 | 114.8 | -5.9 | 13.8 | 12.1 | 2.7 | 2.14×10^{-7} | 0.28 | 76 |
| 103 | 367 | -2.92 | 0.57 | 3.22 | 174.5 | 0.2 | 173.8 | -16.5 | 34.5 | 19.1 | 1.9 | 2.13×10^{-7} | 0.28 | 37 |
| 104 | 275 | -4.15 | -0.01 | 3.07 | 0.6 | 5.3 | 0.0 | -25.5 | 18.9 | 0.6 | 1.7 | 2.13×10^{-7} | 0.49 | 59 |
| 105 | 168 | -2.92 | 0.54 | 3.24 | 175.8 | 0.0 | 174.6 | -18.0 | 33.9 | 17.7 | 2.8 | 2.12×10^{-7} | 0.28 | 43 |
| 106 | 416 | -4.13 | 0.04 | -3.07 | 0.3 | 4.7 | 0.3 | 25.2 | -16.7 | 0.6 | 2.5 | 2.06×10^{-7} | 0.48 | 82 |
| 107 | 365 | 4.15 | 0.04 | 3.06 | 179.2 | 5.7 | 179.5 | -25.9 | 16.8 | 0.6 | 0.3 | 2.06×10^{-7} | 0.41 | 68 |
| 108 | 313 | -1.89 | 4.03 | 2.75 | 0.2 | 7.1 | 0.1 | -14.5 | 3.0 | 13.6 | 1.3 | 2.05×10^{-7} | 0.43 | 68 |
| 109 | 326 | 1.93 | 4.05 | 2.67 | 178.7 | 6.7 | 178.9 | -13.4 | 2.1 | 15.0 | 2.1 | 2.04×10^{-7} | 0.40 | 99 |
| 110 | 237 | 1.75 | -4.06 | 2.79 | 178.9 | 3.5 | 179.3 | -16.3 | 2.0 | 16.5 | 0.5 | 2.02×10^{-7} | 0.41 | 54 |
| 111 | 8 | -0.06 | 1.01 | 3.04 | 163.9 | 13.4 | 117.2 | 1.5 | 1.3 | 11.8 | 12.8 | 2.01×10^{-7} | 0.13 | 82 |
| 112 | 188 | -4.15 | 0.04 | 3.07 | 0.6 | 5.5 | 0.1 | -26.0 | 18.6 | 0.8 | 1.8 | 1.99×10^{-7} | 0.47 | 72 |
| 113 | 270 | 4.15 | 0.04 | 3.03 | 178.7 | 5.6 | 179.5 | -24.0 | 18.4 | 4.1 | 2.7 | 1.98×10^{-7} | 0.40 | 89 |
| 114 | 474 | -4.14 | 0.03 | -3.09 | 0.4 | 4.8 | 0.5 | 24.3 | -18.5 | 1.3 | 1.2 | 1.98×10^{-7} | 0.47 | 104 |
| 115 | 345 | -1.87 | 4.04 | 2.74 | 0.1 | 6.7 | 0.3 | -14.0 | 2.6 | 13.2 | 0.7 | 1.96×10^{-7} | 0.32 | 59 |
| 116 | 232 | 1.63 | 4.12 | 2.83 | 1.6 | 0.5 | 2.3 | -4.8 | 16.4 | 7.5 | 8.7 | 1.95×10^{-7} | 0.29 | 108 |
| 117 | 323 | -1.60 | 4.05 | 2.91 | 179.5 | 3.3 | 177.9 | -4.1 | 14.1 | 6.5 | 9.8 | 1.95×10^{-7} | 0.20 | 63 |
| 118 | 38 | -4.14 | -0.01 | 3.08 | 0.1 | 5.5 | 0.3 | -24.7 | 18.5 | 0.8 | 2.8 | 1.95×10^{-7} | 0.46 | 55 |
| 119 | 213 | -1.58 | 4.10 | 2.79 | 179.6 | 1.3 | 175.6 | 0.6 | 11.4 | 11.8 | 10.3 | 1.91×10^{-7} | 0.20 | 72 |
| 120 | 492 | -1.56 | 4.19 | 2.70 | 176.7 | 0.5 | 175.6 | -2.0 | 12.3 | 10.2 | 6.4 | 1.91×10^{-7} | 0.29 | 121 |
| 121 | 241 | 1.56 | 4.15 | -2.78 | 2.6 | 0.8 | 3.6 | 2.5 | -16.1 | 7.9 | 8.3 | 1.90×10^{-7} | 0.29 | 73 |
| 122 | 305 | -1.59 | 4.17 | 2.73 | 177.9 | 0.7 | 175.8 | -0.2 | 13.4 | 11.0 | 8.9 | 1.89×10^{-7} | 0.28 | 86 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------------------------|-----|-------------|-------|-------|----------|------|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 123 | 488 | -1.54 | 4.17 | 2.78 | 177.7 | 1.2 | 176.4 | -1.6 | 16.2 | 7.3 | 10.5 | 1.86×10^{-7} | 0.28 | 95 |
| 124 | 400 | -1.67 | 4.07 | 2.89 | 179.2 | 1.4 | 177.4 | -4.1 | 14.0 | 11.1 | 10.2 | 1.83×10^{-7} | 0.18 | 63 |
| 125 | 486 | 1.56 | 4.16 | 2.76 | 2.9 | 0.2 | 4.6 | -1.4 | 15.4 | 10.0 | 7.5 | 1.83×10^{-7} | 0.28 | 40 |
| 126 | 417 | -2.53 | 0.94 | 3.11 | 166.8 | 9.6 | 116.9 | -0.7 | 19.2 | 0.6 | 10.8 | 1.83×10^{-7} | 0.27 | 70 |
| 127 | 363 | 3.10 | -1.55 | 2.98 | 177.3 | 1.1 | 119.0 | -11.9 | 5.8 | 14.7 | 6.9 | 1.82×10^{-7} | 0.46 | 82 |
| 128 | 272 | -2.55 | -0.99 | 3.08 | 167.6 | 9.3 | 118.4 | -3.0 | 16.9 | 2.3 | 11.4 | 1.82×10^{-7} | 0.28 | 83 |
| 129 | 432 | 1.58 | 4.12 | 2.80 | 2.1 | 3.0 | 3.0 | -1.5 | 15.6 | 8.8 | 9.4 | 1.81×10^{-7} | 0.17 | 78 |
| 130 | 107 | -3.25 | 1.55 | 2.82 | 1.7 | 3.0 | 60.8 | -12.0 | 6.8 | 14.4 | 6.3 | 1.68×10^{-7} | 0.49 | 64 |
| 131 | 338 | 2.58 | 1.01 | 3.12 | 13.7 | 11.5 | 62.7 | -4.9 | 15.6 | 0.3 | 12.9 | 1.62×10^{-7} | 0.14 | 56 |
| 132 | 287 | -2.47 | -0.91 | 3.20 | 162.8 | 11.1 | 118.9 | -4.2 | 13.3 | 0.6 | 13.1 | 1.60×10^{-7} | 0.24 | 47 |
| 133 | 390 | -2.69 | 1.08 | 2.92 | 8.3 | 6.0 | 60.1 | 0.3 | 4.7 | 5.9 | 10.1 | 1.58×10^{-7} | 0.32 | 58 |
| 134 | 456 | -2.70 | 1.13 | 2.91 | 9.2 | 6.8 | 59.2 | -1.5 | 3.8 | 4.7 | 12.0 | 1.57×10^{-7} | 0.32 | 65 |
| 135 | 262 | 1.75 | 1.80 | 3.02 | 3.9 | 2.3 | 64.1 | -7.4 | 18.0 | 2.2 | 6.1 | 1.55×10^{-7} | 0.15 | 50 |
| 136 | 33 | -2.49 | 0.94 | 3.22 | 161.0 | 13.6 | 117.7 | -6.1 | 13.8 | 0.4 | 12.7 | 1.55×10^{-7} | 0.17 | 25 |
| 137 | 258 | -2.47 | 0.94 | 3.21 | 160.8 | 13.8 | 118.1 | -5.6 | 12.6 | 4.1 | 12.0 | 1.53×10^{-7} | 0.17 | 54 |
| 138 | 436 | -2.61 | -1.13 | 3.02 | 13.6 | 9.1 | 59.3 | -1.7 | 5.2 | 5.1 | 13.2 | 1.53×10^{-7} | 0.31 | 55 |
| 139 | 229 | -2.59 | -1.11 | 3.08 | 15.4 | 9.5 | 58.2 | -7.0 | 0.2 | 4.3 | 10.0 | 1.51×10^{-7} | 0.31 | 88 |
| 140 | 246 | -0.87 | 2.58 | 2.67 | 170.0 | 8.1 | 127.0 | 15.0 | -1.6 | 22.4 | 6.2 | 1.51×10^{-7} | 0.13 | 46 |
| 141 | 89 | -0.62 | -2.49 | 2.82 | 175.5 | 2.5 | 127.7 | 16.7 | 0.4 | 22.3 | 6.0 | 1.49×10^{-7} | 0.13 | 41 |
| 142 | 392 | 2.61 | -1.03 | 3.16 | 157.3 | 11.7 | 122.0 | -8.8 | -1.4 | 0.3 | 2.1 | 1.48×10^{-7} | 0.18 | 71 |
| 143 | 477 | -3.87 | 2.18 | 3.38 | 178.7 | 2.6 | 111.1 | -13.2 | 16.3 | 1.0 | 5.5 | 1.43×10^{-7} | 0.34 | 50 |
| 144 | 358 | -0.60 | 2.92 | 2.71 | 165.8 | 1.1 | 114.2 | 3.2 | 17.7 | 6.2 | 4.9 | 1.43×10^{-7} | 0.19 | 65 |
| 145 | 340 | 2.62 | -1.12 | 3.21 | 157.2 | 10.1 | 125.0 | -15.0 | -7.1 | 1.0 | 3.2 | 1.41×10^{-7} | 0.17 | 78 |
| 146 | 122 | -0.66 | 2.97 | 2.66 | 152.8 | 2.9 | 114.7 | 6.3 | 17.8 | 1.0 | 6.5 | 1.40×10^{-7} | 0.14 | 43 |
| 147 | 431 | -1.97 | -5.03 | 2.16 | 167.9 | 9.5 | 119.2 | 8.1 | 1.3 | 11.9 | 15.8 | 1.40×10^{-7} | 0.15 | 43 |
| 148 | 421 | 0.66 | -2.72 | -2.73 | 2.3 | 3.8 | 53.8 | -9.5 | -1.7 | 17.9 | 5.0 | 1.40×10^{-7} | 0.19 | 150 |
| Continued on next page | | | | | | | | | | | | | | |

Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 149 | 105 | -0.86 | 2.60 | 2.68 | 169.7 | 8.0 | 126.9 | 15.2 | -2.1 | 20.5 | 7.4 | 1.40×10^{-7} | 0.11 | 61 |
| 150 | 347 | -2.59 | 0.93 | 3.15 | 19.4 | 10.8 | 58.7 | -7.2 | 1.6 | 4.3 | 4.1 | 1.39×10^{-7} | 0.22 | 90 |
| 151 | 140 | 3.99 | -2.18 | 3.35 | 5.4 | 3.8 | 67.0 | -16.3 | 18.4 | 0.3 | 10.5 | 1.39×10^{-7} | 0.25 | 69 |
| 152 | 92 | 3.92 | -2.27 | 3.29 | 1.3 | 1.8 | 67.9 | -14.2 | 14.0 | 2.8 | 5.5 | 1.39×10^{-7} | 0.25 | 101 |
| 153 | 350 | -3.90 | 2.10 | 3.42 | 170.8 | 6.5 | 111.6 | -13.8 | 14.4 | 1.4 | 11.6 | 1.39×10^{-7} | 0.30 | 55 |
| 154 | 261 | 0.23 | 6.54 | 1.69 | 8.4 | 0.4 | 86.6 | -8.5 | -4.2 | 0.5 | 0.3 | 1.38×10^{-7} | 0.23 | 58 |
| 155 | 201 | -0.97 | 2.48 | 2.78 | 9.1 | 12.0 | 53.7 | 5.7 | 11.4 | 24.5 | 1.3 | 1.37×10^{-7} | 0.35 | 174 |
| 156 | 413 | -2.57 | 1.06 | 3.16 | 19.9 | 11.3 | 57.2 | -7.7 | -2.9 | 0.7 | 4.3 | 1.36×10^{-7} | 0.22 | 67 |
| 157 | 247 | 0.31 | 6.52 | 1.74 | 18.2 | 2.7 | 85.6 | -10.5 | -4.4 | 1.2 | 3.8 | 1.36×10^{-7} | 0.22 | 99 |
| 158 | 165 | 0.31 | -6.51 | 1.78 | 50.4 | 3.6 | 85.3 | -9.6 | -4.0 | 1.9 | 6.3 | 1.35×10^{-7} | 0.24 | 92 |
| 159 | 108 | -0.30 | 6.47 | 1.74 | 150.1 | 1.5 | 95.5 | -8.1 | -3.9 | 3.1 | 0.7 | 1.34×10^{-7} | 0.22 | 40 |
| 160 | 50 | -2.08 | 5.06 | 2.05 | 169.2 | 10.0 | 119.4 | 6.9 | 2.4 | 8.8 | 13.0 | 1.33×10^{-7} | 0.12 | 100 |
| 161 | 48 | 2.15 | 5.07 | 2.00 | 13.6 | 11.7 | 60.3 | 7.7 | 0.7 | 12.3 | 15.6 | 1.33×10^{-7} | 0.10 | 125 |
| 162 | 380 | -1.96 | -5.05 | 2.14 | 167.0 | 9.9 | 118.8 | 7.5 | 1.7 | 11.2 | 16.8 | 1.32×10^{-7} | 0.14 | 59 |
| 163 | 243 | 1.32 | 5.74 | 2.05 | 2.3 | 12.1 | 36.7 | -9.7 | 2.1 | 9.1 | 2.2 | 1.32×10^{-7} | 0.20 | 98 |
| 164 | 315 | 1.45 | 5.72 | 2.04 | 1.4 | 11.5 | 34.2 | -8.3 | 2.4 | 8.9 | 0.3 | 1.31×10^{-7} | 0.20 | 119 |
| 165 | 483 | 1.03 | 5.73 | 2.23 | 4.4 | 11.6 | 41.3 | -10.9 | 0.9 | 8.2 | 2.3 | 1.31×10^{-7} | 0.20 | 70 |
| 166 | 20 | 2.08 | 5.05 | 2.02 | 14.8 | 13.9 | 61.7 | 7.3 | 0.6 | 11.1 | 15.0 | 1.31×10^{-7} | 0.11 | 53 |
| 167 | 457 | 1.43 | 5.66 | -2.03 | 176.9 | 15.0 | 144.9 | 15.1 | 3.1 | 8.1 | 4.9 | 1.30×10^{-7} | 0.48 | 96 |
| 168 | 216 | 2.07 | 5.06 | 1.99 | 14.6 | 13.8 | 62.1 | 7.4 | 1.0 | 11.5 | 14.2 | 1.30×10^{-7} | 0.11 | 99 |
| 169 | 166 | 1.50 | 5.61 | 2.16 | 4.1 | 12.5 | 33.8 | -9.8 | 0.2 | 6.8 | 0.9 | 1.29×10^{-7} | 0.15 | 79 |
| 170 | 319 | 1.51 | 5.65 | 2.00 | 2.1 | 13.4 | 33.7 | -7.2 | -0.7 | 9.7 | 3.1 | 1.29×10^{-7} | 0.15 | 53 |
| 171 | 322 | 1.59 | 5.63 | 1.92 | 178.7 | 15.1 | 147.6 | -12.7 | -1.1 | 10.8 | 6.1 | 1.29×10^{-7} | 0.48 | 120 |
| 172 | 372 | 1.40 | 5.74 | 1.89 | 1.1 | 10.9 | 34.6 | -5.9 | 1.7 | 10.0 | 2.5 | 1.28×10^{-7} | 0.20 | 96 |
| 173 | 63 | 2.19 | 5.05 | 1.99 | 11.5 | 11.5 | 59.4 | 5.7 | 1.2 | 11.3 | 10.0 | 1.26×10^{-7} | 0.08 | 72 |
| 174 | 103 | -0.66 | 3.01 | 2.65 | 153.1 | 2.2 | 114.5 | 6.4 | 17.5 | 2.6 | 7.2 | 1.26×10^{-7} | 0.11 | 48 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------------------------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 175 | 75 | 2.14 | 5.07 | 2.04 | 12.2 | 10.8 | 60.2 | 7.7 | 1.9 | 10.8 | 14.3 | 1.25×10^{-7} | 0.08 | 48 |
| 176 | 159 | -1.97 | -0.59 | 3.49 | 25.9 | 7.7 | 23.5 | 1.4 | -6.8 | 11.5 | 8.1 | 1.25×10^{-7} | 0.27 | 62 |
| 177 | 453 | 1.82 | -0.53 | 3.40 | 5.5 | 2.8 | 11.5 | -23.3 | 25.8 | 5.2 | 21.1 | 1.23×10^{-7} | 0.29 | 179 |
| 178 | 273 | 1.47 | 5.62 | -2.03 | 176.5 | 15.8 | 145.6 | 14.9 | 1.3 | 11.2 | 5.2 | 1.22×10^{-7} | 0.46 | 85 |
| 179 | 341 | 1.58 | 5.66 | 1.86 | 179.1 | 15.4 | 147.7 | -12.6 | -1.7 | 11.2 | 9.3 | 1.22×10^{-7} | 0.46 | 103 |
| 180 | 420 | 2.20 | 5.08 | 2.04 | 14.1 | 12.0 | 59.9 | 4.6 | 2.5 | 12.1 | 13.8 | 1.21×10^{-7} | 0.07 | 81 |
| 181 | 18 | 0.96 | 5.11 | 2.13 | 179.5 | 2.6 | 112.5 | 13.0 | 4.2 | 8.2 | 10.3 | 1.21×10^{-7} | 0.08 | 79 |
| 182 | 176 | 1.54 | 5.57 | -2.04 | 176.6 | 16.8 | 146.1 | 11.8 | 2.8 | 11.2 | 6.1 | 1.21×10^{-7} | 0.37 | 69 |
| 183 | 126 | 0.88 | 5.05 | 2.27 | 176.1 | 3.8 | 112.9 | 12.1 | 4.6 | 3.1 | 10.8 | 1.20×10^{-7} | 0.08 | 72 |
| 184 | 148 | 1.43 | -5.66 | 2.06 | 179.5 | 12.3 | 146.8 | -13.1 | -0.9 | 9.9 | 8.5 | 1.20×10^{-7} | 0.47 | 105 |
| 185 | 210 | 1.52 | 5.69 | -1.92 | 178.0 | 16.1 | 146.2 | 11.1 | 0.5 | 10.4 | 5.4 | 1.20×10^{-7} | 0.37 | 62 |
| 186 | 113 | -2.04 | 0.63 | 3.36 | 28.1 | 8.9 | 24.0 | 5.7 | -11.8 | 9.7 | 8.3 | 1.20×10^{-7} | 0.29 | 69 |
| 187 | 387 | -2.21 | 0.59 | 3.37 | 26.7 | 10.6 | 22.9 | 3.8 | -4.1 | 14.5 | 7.1 | 1.20×10^{-7} | 0.25 | 63 |
| 188 | 102 | 5.34 | 0.86 | 3.11 | 5.4 | 1.7 | 5.2 | -25.0 | 16.3 | 6.8 | 16.6 | 1.19×10^{-7} | 0.24 | 90 |
| 189 | 357 | 0.93 | 5.07 | 2.20 | 179.5 | 3.4 | 113.1 | 11.2 | 4.6 | 6.4 | 9.6 | 1.19×10^{-7} | 0.11 | 81 |
| 190 | 123 | 0.92 | 5.07 | -2.20 | 179.3 | 3.3 | 113.1 | -11.1 | -4.4 | 6.1 | 9.4 | 1.19×10^{-7} | 0.11 | 74 |
| 191 | 69 | 0.92 | 5.06 | 2.18 | 177.1 | 2.6 | 113.3 | 11.0 | 4.0 | 6.1 | 8.2 | 1.19×10^{-7} | 0.11 | 94 |
| 192 | 172 | 0.92 | 5.06 | 2.21 | 178.9 | 3.2 | 113.1 | 10.9 | 4.6 | 5.8 | 9.5 | 1.18×10^{-7} | 0.10 | 56 |
| 193 | 156 | 0.93 | 5.07 | 2.20 | 180.0 | 3.6 | 112.9 | 10.5 | 4.2 | 5.7 | 9.9 | 1.17×10^{-7} | 0.10 | 82 |
| 194 | 35 | -0.82 | 5.04 | 2.22 | 6.5 | 5.2 | 67.6 | 12.5 | 1.3 | 1.2 | 11.5 | 1.17×10^{-7} | 0.12 | 117 |
| 195 | 128 | 5.34 | 0.83 | 3.13 | 5.2 | 1.3 | 5.9 | -25.8 | 17.6 | 6.8 | 13.5 | 1.17×10^{-7} | 0.23 | 98 |
| 196 | 440 | 0.91 | 5.06 | 2.20 | 175.6 | 1.1 | 113.5 | 11.1 | 5.6 | 7.4 | 8.2 | 1.17×10^{-7} | 0.07 | 98 |
| 197 | 73 | -0.88 | 5.07 | 2.20 | 0.5 | 4.0 | 67.0 | 11.9 | 4.2 | 3.9 | 10.1 | 1.16×10^{-7} | 0.15 | 126 |
| 198 | 132 | -0.89 | 5.08 | 2.19 | 0.1 | 3.9 | 67.0 | 11.9 | 4.3 | 4.1 | 10.0 | 1.16×10^{-7} | 0.15 | 80 |
| 199 | 257 | 1.14 | 4.46 | 2.73 | 173.2 | 7.9 | 170.3 | -10.8 | 24.2 | 13.4 | 6.5 | 1.16×10^{-7} | 0.30 | 74 |
| 200 | 16 | 0.97 | 5.08 | 2.20 | 177.5 | 3.5 | 112.4 | 11.3 | 4.1 | 5.6 | 11.8 | 1.16×10^{-7} | 0.07 | 58 |
| Continued on next page | | | | | | | | | | | | | | |

Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 201 | 11 | 1.39 | 5.68 | 1.96 | 177.8 | 15.1 | 144.4 | -13.7 | -1.2 | 10.4 | 8.2 | 1.16×10^{-7} | 0.45 | 100 |
| 202 | 470 | -0.85 | 5.04 | 2.30 | 0.8 | 2.7 | 66.5 | 11.3 | 5.1 | 4.8 | 10.5 | 1.16×10^{-7} | 0.12 | 82 |
| 203 | 2 | 0.68 | 3.43 | -2.43 | 8.6 | 1.7 | 55.3 | -17.5 | -12.9 | 5.0 | 5.7 | 1.15×10^{-7} | 0.09 | 48 |
| 204 | 385 | 2.08 | 0.90 | 3.24 | 179.7 | 4.5 | 168.7 | -29.6 | 18.3 | 8.5 | 23.0 | 1.15×10^{-7} | 0.32 | 113 |
| 205 | 91 | 1.57 | 5.72 | 1.75 | 178.4 | 15.1 | 148.1 | -9.5 | 1.3 | 12.0 | 5.9 | 1.14×10^{-7} | 0.35 | 98 |
| 206 | 342 | 1.55 | 5.58 | -2.09 | 175.6 | 17.1 | 146.5 | 13.6 | -1.7 | 10.0 | 6.0 | 1.14×10^{-7} | 0.35 | 92 |
| 207 | 487 | -2.99 | -1.73 | 3.04 | 15.0 | 2.5 | 61.7 | -15.0 | 9.4 | 7.9 | 3.7 | 1.14×10^{-7} | 0.38 | 60 |
| 208 | 77 | 1.55 | 5.70 | 1.80 | 179.9 | 16.7 | 147.1 | -8.6 | -0.6 | 10.7 | 8.7 | 1.14×10^{-7} | 0.35 | 62 |
| 209 | 373 | 2.76 | -0.77 | 3.02 | 176.0 | 0.4 | 121.2 | -4.6 | 15.7 | 11.6 | 17.1 | 1.14×10^{-7} | 0.18 | 69 |
| 210 | 344 | -0.82 | 5.04 | 2.26 | 0.2 | 2.6 | 66.1 | 12.9 | 6.4 | 3.2 | 8.9 | 1.13×10^{-7} | 0.11 | 72 |
| 211 | 203 | -1.52 | 5.66 | -1.91 | 1.6 | 17.1 | 33.4 | 12.7 | 3.3 | 9.7 | 7.7 | 1.13×10^{-7} | 0.36 | 158 |
| 212 | 253 | 1.07 | 4.37 | 2.88 | 175.2 | 10.9 | 172.3 | -12.0 | 27.7 | 10.5 | 8.8 | 1.13×10^{-7} | 0.22 | 112 |
| 213 | 429 | 1.64 | 5.72 | 1.78 | 179.8 | 15.6 | 148.6 | -10.3 | 0.3 | 13.5 | 4.0 | 1.13×10^{-7} | 0.35 | 91 |
| 214 | 427 | 0.83 | -5.07 | 2.20 | 176.5 | 2.6 | 113.9 | 11.1 | 3.3 | 10.4 | 4.8 | 1.13×10^{-7} | 0.11 | 42 |
| 215 | 174 | -1.04 | 4.38 | -2.90 | 3.8 | 13.0 | 5.5 | 9.6 | -26.2 | 12.6 | 12.0 | 1.12×10^{-7} | 0.25 | 63 |
| 216 | 297 | -0.98 | 4.43 | 2.86 | 4.4 | 12.2 | 4.8 | -9.3 | 26.1 | 11.3 | 10.9 | 1.12×10^{-7} | 0.25 | 67 |
| 217 | 244 | -1.06 | 4.44 | 2.84 | 4.9 | 10.1 | 5.7 | -11.8 | 24.8 | 13.8 | 12.0 | 1.12×10^{-7} | 0.32 | 123 |
| 218 | 454 | 2.12 | 0.86 | 3.29 | 179.9 | 5.4 | 168.8 | -34.9 | 21.6 | 7.2 | 22.8 | 1.12×10^{-7} | 0.32 | 80 |
| 219 | 424 | 1.20 | 4.44 | 2.73 | 173.5 | 5.9 | 166.6 | -13.4 | 24.2 | 9.2 | 8.2 | 1.12×10^{-7} | 0.29 | 69 |
| 220 | 479 | 1.07 | 4.37 | 2.90 | 175.8 | 10.6 | 171.7 | -12.5 | 27.2 | 9.8 | 9.9 | 1.11×10^{-7} | 0.22 | 46 |
| 221 | 439 | 2.09 | 0.88 | 3.26 | 179.3 | 4.9 | 167.9 | -33.1 | 17.3 | 8.3 | 24.0 | 1.11×10^{-7} | 0.31 | 219 |
| 222 | 191 | 1.62 | 5.70 | 1.86 | 178.3 | 16.5 | 147.7 | -10.8 | 0.6 | 13.3 | 4.1 | 1.11×10^{-7} | 0.34 | 88 |
| 223 | 9 | -1.41 | -3.56 | 3.14 | 174.2 | 13.5 | 135.7 | -20.6 | 24.3 | 15.8 | 8.5 | 1.11×10^{-7} | 0.31 | 156 |
| 224 | 87 | 0.69 | 3.48 | 2.39 | 9.1 | 2.3 | 56.9 | 16.0 | 14.5 | 4.0 | 1.2 | 1.10×10^{-7} | 0.12 | 47 |
| 225 | 353 | -1.53 | 5.66 | 2.04 | 3.1 | 15.6 | 33.5 | -14.1 | 0.2 | 7.7 | 3.7 | 1.10×10^{-7} | 0.35 | 74 |
| 226 | 162 | -1.04 | 4.37 | 2.92 | 3.1 | 12.5 | 6.2 | -12.1 | 25.2 | 12.5 | 12.8 | 1.10×10^{-7} | 0.24 | 53 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------------------------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 227 | 59 | 1.62 | 5.69 | 1.85 | 179.3 | 16.1 | 148.0 | -11.6 | 2.0 | 13.2 | 5.6 | 1.09×10^{-7} | 0.34 | 100 |
| 228 | 455 | -1.10 | 4.43 | 2.84 | 4.7 | 9.8 | 6.9 | -10.0 | 25.3 | 13.4 | 10.6 | 1.09×10^{-7} | 0.31 | 140 |
| 229 | 26 | 0.56 | 3.55 | 2.36 | 15.8 | 0.6 | 53.7 | 22.6 | 15.6 | 1.6 | 4.0 | 1.09×10^{-7} | 0.12 | 56 |
| 230 | 239 | -1.01 | 4.39 | -2.86 | 5.8 | 11.4 | 6.9 | 12.1 | -28.0 | 9.7 | 10.7 | 1.07×10^{-7} | 0.23 | 79 |
| 231 | 289 | -1.98 | -0.78 | 3.36 | 0.3 | 8.9 | 11.7 | -30.1 | 19.8 | 6.8 | 25.9 | 1.07×10^{-7} | 0.35 | 80 |
| 232 | 444 | -0.60 | 3.50 | 2.41 | 166.3 | 0.8 | 125.1 | 19.6 | 16.3 | 1.1 | 4.7 | 1.04×10^{-7} | 0.05 | 30 |
| 233 | 93 | -1.28 | -3.87 | 3.13 | 176.8 | 6.5 | 148.6 | -26.6 | 30.1 | 12.2 | 0.8 | 1.04×10^{-7} | 0.35 | 111 |
| 234 | 99 | -1.26 | 3.62 | 3.10 | 173.2 | 15.5 | 132.1 | -16.6 | 23.9 | 16.2 | 6.9 | 1.03×10^{-7} | 0.32 | 300 |
| 235 | 62 | -1.96 | -0.74 | 3.37 | 0.8 | 8.3 | 11.4 | -28.9 | 21.7 | 5.8 | 24.9 | 1.02×10^{-7} | 0.34 | 55 |
| 236 | 496 | -0.54 | 3.57 | 2.38 | 164.7 | 1.3 | 125.1 | 20.0 | 14.8 | 3.3 | 6.4 | 1.02×10^{-7} | 0.04 | 92 |
| 237 | 468 | -0.58 | -3.57 | 2.34 | 163.8 | 0.1 | 125.2 | 21.2 | 13.6 | 3.6 | 5.7 | 1.01×10^{-7} | 0.09 | 84 |
| 238 | 320 | -1.55 | -4.95 | 2.86 | 12.1 | 6.7 | 44.4 | 4.2 | 0.4 | 6.6 | 4.9 | 1.01×10^{-7} | 0.25 | 95 |
| 239 | 278 | 1.64 | 5.06 | 2.64 | 175.1 | 5.3 | 133.9 | -0.2 | 3.2 | 5.5 | 6.3 | 1.00×10^{-7} | 0.22 | 135 |
| 240 | 310 | 1.65 | 5.19 | 2.33 | 179.8 | 3.9 | 135.0 | 3.2 | -2.9 | 3.4 | 5.9 | 9.93×10^{-8} | 0.22 | 58 |
| 241 | 472 | -1.65 | 5.16 | 2.52 | 1.2 | 1.3 | 44.0 | -1.1 | 2.9 | 4.6 | 6.4 | 9.91×10^{-8} | 0.27 | 78 |
| 242 | 27 | -1.74 | 5.16 | -2.48 | 0.0 | 2.9 | 46.2 | 1.7 | -1.8 | 1.0 | 7.1 | 9.91×10^{-8} | 0.27 | 72 |
| 243 | 200 | -1.59 | 5.17 | -2.41 | 1.1 | 4.9 | 44.3 | -2.7 | -1.3 | 1.2 | 4.6 | 9.89×10^{-8} | 0.22 | 74 |
| 244 | 202 | -1.47 | 5.01 | 2.81 | 12.0 | 8.4 | 44.5 | 3.4 | -0.8 | 6.0 | 3.1 | 9.87×10^{-8} | 0.22 | 49 |
| 245 | 195 | 2.05 | -5.08 | 1.98 | 175.7 | 10.2 | 119.8 | 5.4 | 5.2 | 11.7 | 6.8 | 9.86×10^{-8} | 0.44 | 121 |
| 246 | 157 | 1.57 | 5.06 | -2.71 | 178.3 | 2.5 | 136.8 | 4.2 | -6.4 | 0.7 | 3.5 | 9.84×10^{-8} | 0.17 | 126 |
| 247 | 423 | -1.53 | 3.50 | 2.94 | 10.1 | 11.7 | 53.7 | -9.4 | 8.6 | 9.1 | 1.0 | 9.83×10^{-8} | 0.26 | 71 |
| 248 | 65 | -1.53 | 5.13 | 2.55 | 3.9 | 5.8 | 43.9 | 4.6 | -0.5 | 0.2 | 5.0 | 9.75×10^{-8} | 0.21 | 65 |
| 249 | 336 | -1.64 | 5.15 | 2.46 | 2.3 | 5.5 | 45.1 | 1.3 | -1.9 | 2.1 | 4.8 | 9.72×10^{-8} | 0.21 | 91 |
| 250 | 330 | -0.63 | 4.65 | 2.63 | 168.0 | 2.8 | 175.9 | -13.7 | 26.8 | 3.2 | 9.9 | 9.71×10^{-8} | 0.27 | 116 |
| 251 | 41 | -4.56 | -1.01 | 3.24 | 25.8 | 16.0 | 63.7 | -2.6 | -3.9 | 13.6 | 1.6 | 9.60×10^{-8} | 0.38 | 57 |
| 252 | 56 | -0.90 | 5.63 | 2.13 | 175.6 | 7.8 | 119.8 | -4.3 | 4.6 | 0.4 | 11.2 | 9.59×10^{-8} | 0.16 | 77 |
| Continued on next page | | | | | | | | | | | | | | |

Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------------------------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 253 | 130 | -4.16 | -0.67 | 3.18 | 163.8 | 8.7 | 119.5 | -11.3 | -3.4 | 3.6 | 7.5 | 9.55×10^{-8} | 0.27 | 73 |
| 254 | 494 | -0.71 | 4.58 | 2.69 | 172.2 | 6.7 | 177.1 | -8.6 | 20.2 | 3.3 | 10.4 | 9.54×10^{-8} | 0.26 | 107 |
| 255 | 7 | -1.76 | 3.42 | 2.83 | 2.7 | 3.6 | 53.1 | 0.6 | -1.8 | 3.8 | 6.8 | 9.51×10^{-8} | 0.24 | 63 |
| 256 | 274 | 1.75 | 5.24 | 2.35 | 173.1 | 1.7 | 136.0 | -8.5 | 4.8 | 8.4 | 7.9 | 9.48×10^{-8} | 0.21 | 139 |
| 257 | 186 | -4.74 | 1.00 | 2.99 | 21.3 | 13.0 | 62.5 | -1.3 | -3.6 | 12.7 | 0.5 | 9.46×10^{-8} | 0.27 | 84 |
| 258 | 406 | 0.73 | 4.58 | 2.69 | 12.2 | 1.0 | 5.3 | -15.2 | 27.6 | 0.3 | 9.4 | 9.45×10^{-8} | 0.34 | 73 |
| 259 | 379 | -0.65 | -4.60 | 2.65 | 168.7 | 2.8 | 177.5 | -10.1 | 22.5 | 2.0 | 12.8 | 9.45×10^{-8} | 0.35 | 99 |
| 260 | 493 | 1.62 | 5.20 | 2.37 | 177.6 | 2.5 | 136.9 | -1.5 | 0.6 | 6.8 | 4.6 | 9.45×10^{-8} | 0.16 | 140 |
| 261 | 17 | -3.70 | 2.20 | 3.33 | 19.9 | 8.3 | 51.7 | -15.5 | -5.7 | 8.3 | 14.6 | 9.43×10^{-8} | 0.36 | 102 |
| 262 | 378 | 0.76 | 3.52 | 2.36 | 164.7 | 2.9 | 125.5 | 16.3 | 18.1 | 9.2 | 5.3 | 9.37×10^{-8} | 0.21 | 86 |
| 263 | 109 | -4.16 | -0.67 | 3.17 | 164.4 | 8.4 | 118.2 | -11.8 | -3.9 | 6.1 | 10.4 | 9.33×10^{-8} | 0.26 | 39 |
| 264 | 215 | -4.14 | -0.71 | 3.19 | 162.6 | 9.0 | 119.0 | -11.2 | -3.2 | 2.9 | 9.2 | 9.32×10^{-8} | 0.26 | 45 |
| 265 | 271 | -1.74 | 3.33 | 2.97 | 6.3 | 3.1 | 52.8 | -1.6 | 0.2 | 4.9 | 8.2 | 9.31×10^{-8} | 0.17 | 52 |
| 266 | 40 | -2.10 | 5.08 | -1.86 | 12.8 | 13.8 | 61.3 | -5.3 | -4.6 | 13.4 | 13.1 | 9.31×10^{-8} | 0.37 | 85 |
| 267 | 24 | -1.61 | 5.17 | -2.41 | 0.9 | 5.2 | 44.5 | -3.5 | 1.3 | 2.5 | 6.8 | 9.27×10^{-8} | 0.20 | 62 |
| 268 | 74 | -0.67 | 4.62 | -2.69 | 171.7 | 5.5 | 177.7 | 9.4 | -20.5 | 2.1 | 9.9 | 9.26×10^{-8} | 0.25 | 60 |
| 269 | 434 | -4.54 | -0.98 | 3.27 | 154.9 | 16.5 | 116.5 | 1.0 | -2.0 | 13.5 | 4.1 | 9.26×10^{-8} | 0.25 | 88 |
| 270 | 309 | 0.83 | 3.22 | 2.56 | 170.5 | 4.7 | 127.1 | 12.2 | 17.9 | 13.0 | 4.7 | 9.24×10^{-8} | 0.21 | 94 |
| 271 | 321 | -4.73 | 1.02 | 3.00 | 20.6 | 12.2 | 61.7 | -1.9 | -5.3 | 11.8 | 2.5 | 9.12×10^{-8} | 0.26 | 49 |
| 272 | 397 | 2.08 | 5.10 | 1.80 | 166.4 | 16.2 | 117.4 | 5.2 | 2.6 | 13.9 | 13.1 | 9.11×10^{-8} | 0.40 | 91 |
| 273 | 46 | -3.65 | 2.14 | 3.38 | 22.7 | 10.2 | 52.7 | -11.4 | -5.5 | 11.4 | 12.0 | 9.11×10^{-8} | 0.34 | 41 |
| 274 | 356 | 2.14 | 5.08 | 1.77 | 170.5 | 13.6 | 119.0 | 3.3 | 3.7 | 14.4 | 8.1 | 9.09×10^{-8} | 0.34 | 69 |
| 275 | 411 | -1.72 | 3.36 | 2.95 | 5.7 | 2.9 | 52.5 | -0.5 | 1.2 | 4.1 | 8.8 | 9.08×10^{-8} | 0.17 | 98 |
| 276 | 149 | -1.73 | 3.34 | 2.96 | 6.0 | 3.0 | 52.9 | -1.1 | -0.2 | 4.4 | 8.8 | 9.08×10^{-8} | 0.16 | 37 |
| 277 | 462 | 0.90 | 5.62 | 2.05 | 3.7 | 3.3 | 58.3 | 2.0 | 2.2 | 3.6 | 8.1 | 9.07×10^{-8} | 0.13 | 79 |
| 278 | 235 | -4.71 | 0.99 | 3.04 | 23.4 | 14.0 | 62.3 | -1.7 | -4.9 | 10.8 | 0.6 | 9.07×10^{-8} | 0.25 | 46 |
| Continued on next page | | | | | | | | | | | | | | |

Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 279 | 263 | -4.17 | -0.66 | 3.17 | 165.1 | 8.2 | 118.7 | -11.6 | -3.7 | 4.1 | 9.5 | 9.05×10^{-8} | 0.25 | 55 |
| 280 | 167 | -0.53 | 4.61 | 2.66 | 170.7 | 3.8 | 177.4 | -5.6 | 20.6 | 6.7 | 11.8 | 9.05×10^{-8} | 0.32 | 92 |
| 281 | 129 | -2.09 | 5.08 | 1.83 | 14.9 | 15.1 | 61.9 | 5.8 | 2.7 | 15.0 | 13.9 | 9.03×10^{-8} | 0.36 | 60 |
| 282 | 120 | -4.59 | -0.99 | 3.24 | 26.2 | 15.9 | 62.2 | -3.2 | -4.9 | 9.1 | 1.8 | 9.03×10^{-8} | 0.36 | 41 |
| 283 | 45 | -2.06 | 5.11 | 1.79 | 11.9 | 15.4 | 62.5 | 5.8 | 3.0 | 13.2 | 12.6 | 9.01×10^{-8} | 0.41 | 48 |
| 284 | 158 | -4.52 | -0.99 | 3.29 | 154.3 | 17.1 | 115.9 | -0.2 | 0.5 | 12.4 | 6.4 | 8.99×10^{-8} | 0.24 | 38 |
| 285 | 438 | -1.62 | 5.19 | -2.39 | 1.4 | 3.6 | 44.0 | -1.5 | 0.2 | 4.2 | 6.2 | 8.98×10^{-8} | 0.19 | 69 |
| 286 | 308 | -1.74 | -3.43 | 2.81 | 5.5 | 5.6 | 55.5 | 3.2 | -3.9 | 6.8 | 4.2 | 8.91×10^{-8} | 0.23 | 93 |
| 287 | 219 | -0.84 | 5.67 | 2.04 | 176.5 | 6.6 | 119.5 | -3.8 | 1.4 | 0.4 | 11.0 | 8.91×10^{-8} | 0.12 | 53 |
| 288 | 442 | -4.57 | -1.01 | 3.25 | 25.8 | 15.9 | 62.1 | -1.7 | -3.4 | 10.5 | 1.4 | 8.86×10^{-8} | 0.26 | 68 |
| 289 | 112 | -4.55 | -1.03 | 3.29 | 155.3 | 16.9 | 116.8 | -1.7 | 1.2 | 11.4 | 6.3 | 8.85×10^{-8} | 0.24 | 70 |
| 290 | 199 | -0.94 | 5.67 | 1.94 | 177.9 | 8.0 | 121.1 | -1.0 | -0.2 | 2.0 | 10.1 | 8.84×10^{-8} | 0.14 | 74 |
| 291 | 491 | 3.70 | 2.17 | 3.34 | 160.8 | 5.8 | 129.1 | -15.3 | -2.5 | 8.5 | 12.6 | 8.82×10^{-8} | 0.20 | 95 |
| 292 | 212 | 5.30 | -0.93 | 3.14 | 179.5 | 3.4 | 175.5 | -26.5 | 14.8 | 11.6 | 13.6 | 8.79×10^{-8} | 0.57 | 61 |
| 293 | 296 | -4.49 | -0.98 | 3.33 | 151.1 | 19.9 | 114.9 | 1.2 | -1.4 | 11.0 | 9.5 | 8.77×10^{-8} | 0.16 | 71 |
| 294 | 415 | 0.90 | 5.67 | 1.99 | 4.2 | 4.8 | 58.5 | -2.3 | 2.0 | 2.6 | 9.3 | 8.76×10^{-8} | 0.14 | 69 |
| 295 | 145 | -3.76 | -2.17 | 3.25 | 20.2 | 6.0 | 49.8 | -9.9 | -3.1 | 10.3 | 12.7 | 8.74×10^{-8} | 0.27 | 64 |
| 296 | 259 | 0.87 | 5.63 | 2.06 | 4.0 | 8.5 | 61.1 | -6.6 | 2.4 | 0.2 | 10.6 | 8.70×10^{-8} | 0.14 | 84 |
| 297 | 399 | 3.72 | 2.21 | 3.32 | 162.3 | 7.0 | 128.5 | -16.9 | -4.4 | 8.7 | 11.8 | 8.69×10^{-8} | 0.26 | 94 |
| 298 | 173 | -0.94 | 5.62 | 2.06 | 174.3 | 3.6 | 121.8 | -4.8 | 0.8 | 2.4 | 4.8 | 8.66×10^{-8} | 0.13 | 54 |
| 299 | 251 | -0.70 | 3.70 | -2.22 | 18.9 | 2.1 | 56.0 | -14.9 | -15.5 | 2.4 | 6.4 | 8.64×10^{-8} | 0.21 | 110 |
| 300 | 482 | -0.87 | 5.66 | 1.96 | 177.1 | 5.7 | 120.0 | -3.6 | -1.5 | 0.7 | 6.5 | 8.62×10^{-8} | 0.13 | 46 |
| 301 | 70 | -4.65 | 1.02 | 3.11 | 158.2 | 15.7 | 117.3 | 0.3 | -0.4 | 9.7 | 8.2 | 8.53×10^{-8} | 0.14 | 74 |
| 302 | 175 | 3.75 | 2.20 | 3.32 | 162.6 | 6.6 | 128.2 | -17.8 | -3.8 | 7.9 | 12.3 | 8.52×10^{-8} | 0.25 | 106 |
| 303 | 220 | -4.14 | -0.56 | 3.09 | 14.4 | 7.2 | 61.4 | -12.8 | -8.3 | 4.7 | 2.1 | 8.49×10^{-8} | 0.52 | 57 |
| 304 | 255 | -4.51 | -1.06 | 3.36 | 152.8 | 19.9 | 116.4 | -0.4 | 0.2 | 11.7 | 9.8 | 8.48×10^{-8} | 0.15 | 54 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 305 | 448 | -4.54 | -1.09 | 3.31 | 154.5 | 18.6 | 117.1 | -0.6 | -0.9 | 12.0 | 6.9 | 8.41×10^{-8} | 0.15 | 67 |
| 306 | 60 | 0.97 | 5.69 | 1.82 | 1.1 | 6.6 | 59.3 | -3.6 | 0.2 | 2.8 | 7.5 | 8.32×10^{-8} | 0.11 | 172 |
| 307 | 396 | -1.20 | 5.25 | -2.42 | 179.0 | 6.9 | 141.0 | 1.4 | 0.9 | 4.6 | 6.0 | 8.23×10^{-8} | 0.53 | 76 |
| 308 | 36 | -3.99 | 0.75 | 3.23 | 27.0 | 12.0 | 62.4 | -16.7 | -14.6 | 4.8 | 1.2 | 8.21×10^{-8} | 0.42 | 52 |
| 309 | 51 | -5.31 | -0.86 | 3.14 | 0.4 | 3.4 | 4.2 | -24.5 | 15.3 | 11.0 | 12.2 | 8.09×10^{-8} | 0.61 | 48 |
| 310 | 121 | -1.21 | 5.21 | 2.57 | 172.8 | 10.3 | 138.9 | -1.5 | -1.0 | 7.7 | 6.5 | 7.94×10^{-8} | 0.52 | 58 |
| 311 | 337 | -3.54 | 2.47 | 3.50 | 159.1 | 13.9 | 133.6 | -12.9 | 8.6 | 11.6 | 5.1 | 7.79×10^{-8} | 0.28 | 81 |
| 312 | 461 | 0.76 | 3.49 | 2.43 | 162.8 | 3.1 | 125.5 | 13.3 | 17.9 | 6.9 | 6.1 | 7.65×10^{-8} | 0.15 | 67 |
| 313 | 332 | 0.70 | 3.50 | 2.42 | 161.0 | 1.8 | 126.8 | 16.8 | 19.4 | 5.0 | 6.0 | 7.62×10^{-8} | 0.15 | 65 |
| 314 | 81 | 0.77 | 3.45 | 2.46 | 163.2 | 3.2 | 126.0 | 12.4 | 18.6 | 7.7 | 7.2 | 7.60×10^{-8} | 0.15 | 66 |
| 315 | 428 | -4.03 | 0.64 | 3.16 | 21.3 | 9.6 | 62.3 | -13.9 | -12.2 | 2.8 | 2.0 | 7.57×10^{-8} | 0.49 | 54 |
| 316 | 72 | -3.50 | 2.67 | 3.48 | 163.2 | 13.7 | 136.3 | -10.3 | 14.8 | 12.2 | 2.7 | 7.53×10^{-8} | 0.27 | 105 |
| 317 | 383 | 0.82 | 5.76 | 1.72 | 169.3 | 4.9 | 119.8 | -8.8 | 2.4 | 0.5 | 7.5 | 7.10×10^{-8} | 0.43 | 67 |
| 318 | 4 | 2.58 | 3.80 | 2.19 | 6.4 | 3.5 | 63.7 | 17.0 | 8.5 | 11.3 | 0.5 | 6.94×10^{-8} | 0.10 | 34 |
| 319 | 260 | -0.87 | 5.74 | 1.81 | 12.4 | 4.0 | 59.2 | -10.9 | 2.5 | 0.3 | 6.3 | 6.91×10^{-8} | 0.42 | 76 |
| 320 | 426 | 1.82 | -0.17 | 3.48 | 159.4 | 7.9 | 169.7 | -13.3 | 19.6 | 16.1 | 11.0 | 6.91×10^{-8} | 0.20 | 87 |
| 321 | 187 | 0.88 | 5.75 | 1.72 | 172.5 | 6.5 | 119.7 | -8.1 | 2.4 | 2.4 | 6.4 | 6.88×10^{-8} | 0.41 | 74 |
| 322 | 171 | 0.88 | 5.76 | 1.72 | 172.4 | 6.4 | 119.7 | -8.1 | 2.2 | 2.4 | 6.3 | 6.84×10^{-8} | 0.41 | 73 |
| 323 | 135 | 0.94 | 5.74 | 1.72 | 176.8 | 7.4 | 119.6 | -6.0 | 2.9 | 5.0 | 7.2 | 6.81×10^{-8} | 0.39 | 35 |
| 324 | 131 | -0.83 | 5.78 | 1.63 | 13.5 | 4.2 | 60.1 | -7.2 | 1.0 | 0.5 | 4.0 | 6.79×10^{-8} | 0.42 | 34 |
| 325 | 409 | -1.45 | -1.25 | 3.39 | 173.9 | 8.2 | 178.9 | -11.2 | 19.7 | 17.3 | 12.6 | 6.70×10^{-8} | 0.25 | 57 |
| 326 | 211 | -0.83 | 5.83 | 1.81 | 0.2 | 8.8 | 62.7 | -9.4 | 7.8 | 4.4 | 11.2 | 6.63×10^{-8} | 0.41 | 73 |
| 327 | 95 | -1.67 | 1.35 | 3.24 | 174.6 | 3.6 | 178.5 | -10.1 | 17.1 | 18.8 | 11.3 | 6.57×10^{-8} | 0.25 | 51 |
| 328 | 25 | -3.92 | 2.73 | 3.03 | 19.1 | 4.1 | 67.1 | -16.1 | 9.4 | 3.8 | 1.9 | 6.38×10^{-8} | 0.46 | 239 |
| 329 | 217 | -1.42 | 0.23 | 3.41 | 157.0 | 0.8 | 165.9 | 5.2 | 13.2 | 14.8 | 22.4 | 6.34×10^{-8} | 0.13 | 55 |
| 330 | 437 | -1.33 | 0.29 | 3.44 | 155.4 | 1.7 | 164.0 | 6.7 | 9.1 | 13.1 | 21.7 | 5.83×10^{-8} | 0.10 | 57 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 331 | 133 | -1.83 | -5.00 | 2.70 | 165.4 | 15.1 | 127.0 | -2.7 | -1.6 | 9.4 | 7.9 | 5.75×10^{-8} | 0.36 | 124 |
| 332 | 304 | 2.53 | 3.89 | 2.02 | 165.3 | 2.9 | 115.9 | 17.8 | 9.1 | 11.9 | 0.5 | 5.51×10^{-8} | 0.29 | 61 |
| 333 | 80 | 1.86 | 1.92 | 2.84 | 168.0 | 7.8 | 177.9 | 3.2 | 8.2 | 25.5 | 14.1 | 5.35×10^{-8} | 0.27 | 65 |
| 334 | 96 | 6.53 | -1.11 | 2.91 | 179.1 | 0.3 | 117.9 | -14.4 | 3.3 | 8.7 | 5.8 | 5.18×10^{-8} | 0.58 | 110 |
| 335 | 68 | -2.46 | 3.97 | 2.02 | 16.2 | 2.6 | 65.0 | 19.4 | 11.3 | 10.6 | 3.7 | 5.09×10^{-8} | 0.31 | 42 |
| 336 | 499 | -6.42 | -1.51 | 3.01 | 176.7 | 2.3 | 115.3 | -10.1 | 7.4 | 3.3 | 0.9 | 5.02×10^{-8} | 0.38 | 67 |
| 337 | 464 | -6.40 | 1.29 | 3.18 | 175.9 | 3.5 | 117.5 | -10.6 | 6.8 | 7.1 | 1.1 | 4.99×10^{-8} | 0.34 | 58 |
| 338 | 311 | -6.38 | 1.51 | 3.14 | 174.6 | 3.5 | 115.5 | -11.2 | 8.7 | 4.1 | 1.3 | 4.97×10^{-8} | 0.37 | 72 |
| 339 | 101 | -6.38 | 1.31 | -3.27 | 175.0 | 4.5 | 116.3 | 10.4 | -9.1 | 9.2 | 1.9 | 4.94×10^{-8} | 0.37 | 152 |
| 340 | 226 | -6.49 | -1.35 | 2.96 | 7.3 | 2.0 | 61.4 | -14.1 | 3.2 | 0.4 | 6.4 | 4.93×10^{-8} | 0.61 | 40 |
| 341 | 152 | -6.45 | -1.40 | 3.01 | 178.6 | 2.2 | 115.9 | -10.5 | 7.5 | 6.9 | 0.5 | 4.92×10^{-8} | 0.34 | 50 |
| 342 | 466 | -6.33 | 1.31 | 3.30 | 177.5 | 3.9 | 115.7 | -12.4 | 7.7 | 10.7 | 0.7 | 4.89×10^{-8} | 0.37 | 53 |
| 343 | 407 | -6.51 | -1.24 | 2.95 | 4.2 | 1.2 | 61.4 | -13.3 | 2.3 | 4.3 | 7.7 | 4.87×10^{-8} | 0.61 | 64 |
| 344 | 164 | 6.46 | -1.30 | 2.98 | 4.3 | 0.6 | 64.3 | -11.2 | 7.6 | 10.9 | 2.8 | 4.86×10^{-8} | 0.30 | 66 |
| 345 | 190 | -6.55 | 1.43 | 2.89 | 7.0 | 1.1 | 61.0 | -15.6 | 3.2 | 0.9 | 6.3 | 4.85×10^{-8} | 0.61 | 53 |
| 346 | 277 | -6.51 | -1.27 | -2.98 | 176.8 | 1.0 | 116.2 | 13.0 | -7.3 | 10.4 | 1.2 | 4.83×10^{-8} | 0.33 | 71 |
| 347 | 198 | -6.29 | 1.42 | 3.29 | 175.0 | 4.4 | 114.3 | -9.9 | 8.8 | 9.1 | 1.0 | 4.80×10^{-8} | 0.36 | 97 |
| 348 | 450 | -6.41 | 1.34 | 3.12 | 4.9 | 3.0 | 62.3 | -12.5 | 3.5 | 8.5 | 7.2 | 4.73×10^{-8} | 0.70 | 155 |
| 349 | 443 | -6.37 | 1.18 | -3.23 | 5.1 | 3.8 | 63.3 | 13.9 | -4.5 | 10.4 | 2.3 | 4.59×10^{-8} | 0.60 | 67 |
| 350 | 264 | 5.34 | 2.49 | 2.80 | 172.6 | 3.1 | 117.1 | -3.4 | 8.0 | 6.2 | 9.6 | 3.93×10^{-8} | 0.21 | 218 |
| 351 | 382 | 5.32 | 2.67 | 2.62 | 176.4 | 2.9 | 118.1 | 1.1 | 6.0 | 11.6 | 11.0 | 3.91×10^{-8} | 0.21 | 121 |
| 352 | 181 | -5.39 | 2.56 | 2.70 | 3.8 | 3.6 | 64.0 | -2.0 | 2.7 | 7.5 | 7.5 | 3.87×10^{-8} | 0.31 | 152 |
| 353 | 294 | 5.28 | 2.22 | 3.09 | 165.2 | 4.8 | 116.2 | -4.5 | 4.1 | 3.4 | 8.1 | 3.86×10^{-8} | 0.21 | 157 |
| 354 | 497 | -5.34 | -2.08 | 3.09 | 15.8 | 3.3 | 62.9 | -3.7 | 4.6 | 9.3 | 10.0 | 3.85×10^{-8} | 0.28 | 60 |
| 355 | 0 | 7.68 | 0.14 | -2.40 | 0.4 | 5.6 | 1.1 | 22.8 | -2.6 | 7.8 | 8.8 | 3.84×10^{-8} | 0.37 | 93 |
| 356 | 394 | -5.23 | 2.10 | 3.27 | 17.8 | 5.0 | 63.2 | -3.7 | 6.1 | 8.8 | 8.9 | 3.83×10^{-8} | 0.27 | 46 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|-----|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 357 | 169 | 5.36 | 2.56 | 2.76 | 178.7 | 2.0 | 118.4 | -3.7 | 5.5 | 6.1 | 9.0 | 3.80×10^{-8} | 0.25 | 205 |
| 358 | 391 | -7.65 | -0.04 | 2.54 | 178.5 | 5.3 | 179.6 | -22.7 | 2.9 | 0.1 | 3.6 | 3.80×10^{-8} | 0.44 | 184 |
| 359 | 369 | -7.66 | -0.14 | 2.53 | 174.9 | 4.7 | 177.9 | -22.4 | 2.8 | 1.1 | 11.0 | 3.80×10^{-8} | 0.44 | 81 |
| 360 | 97 | -7.65 | 0.03 | 2.54 | 177.2 | 5.1 | 179.7 | -22.7 | 2.8 | 0.3 | 5.4 | 3.79×10^{-8} | 0.44 | 236 |
| 361 | 306 | -7.65 | 0.03 | 2.55 | 176.6 | 4.9 | 179.5 | -22.6 | 2.7 | 0.7 | 6.5 | 3.79×10^{-8} | 0.44 | 118 |
| 362 | 134 | -5.25 | -2.59 | 2.90 | 8.7 | 5.1 | 63.2 | -1.2 | 5.5 | 9.4 | 8.8 | 3.78×10^{-8} | 0.26 | 128 |
| 363 | 292 | -5.26 | -2.58 | 2.90 | 8.6 | 5.2 | 63.7 | -1.3 | 6.4 | 9.2 | 8.2 | 3.76×10^{-8} | 0.26 | 96 |
| 364 | 303 | 5.40 | 2.60 | -2.62 | 178.8 | 2.9 | 115.9 | 2.0 | -1.9 | 10.0 | 8.3 | 3.75×10^{-8} | 0.24 | 300 |
| 365 | 79 | -5.41 | 2.66 | 2.57 | 2.1 | 1.9 | 63.2 | -1.2 | 3.0 | 10.8 | 8.4 | 3.73×10^{-8} | 0.30 | 136 |
| 366 | 485 | -5.37 | 2.44 | 2.84 | 3.5 | 1.0 | 62.6 | -5.4 | 5.5 | 4.7 | 9.8 | 3.73×10^{-8} | 0.26 | 68 |
| 367 | 419 | -5.40 | 2.55 | -2.71 | 4.2 | 2.2 | 63.5 | 6.3 | -4.9 | 7.4 | 10.5 | 3.69×10^{-8} | 0.25 | 171 |
| 368 | 267 | -5.35 | 2.51 | -2.76 | 0.9 | 0.5 | 62.6 | 4.6 | -7.5 | 7.1 | 10.4 | 3.66×10^{-8} | 0.25 | 114 |
| 369 | 227 | -5.31 | 2.23 | 3.09 | 9.9 | 3.3 | 63.8 | -5.5 | 3.3 | 4.5 | 7.3 | 3.66×10^{-8} | 0.30 | 80 |
| 370 | 47 | 5.32 | 2.72 | 2.58 | 175.0 | 3.9 | 117.8 | 4.7 | 3.1 | 12.8 | 11.7 | 3.65×10^{-8} | 0.19 | 123 |
| 371 | 465 | 7.64 | 0.10 | 2.58 | 5.1 | 7.1 | 2.6 | -23.2 | 2.7 | 1.6 | 11.3 | 3.60×10^{-8} | 0.35 | 195 |
| 372 | 66 | -5.32 | 2.68 | 2.77 | 176.6 | 4.8 | 120.2 | -3.7 | 13.2 | 8.7 | 2.8 | 3.54×10^{-8} | 0.30 | 150 |
| 373 | 300 | 5.31 | 2.64 | 2.72 | 172.2 | 4.0 | 118.7 | -0.7 | 3.6 | 8.9 | 12.6 | 3.53×10^{-8} | 0.18 | 127 |
| 374 | 478 | -5.32 | 2.64 | -2.75 | 1.9 | 1.5 | 60.6 | 0.3 | -8.6 | 8.1 | 8.8 | 3.52×10^{-8} | 0.24 | 88 |
| 375 | 170 | -5.39 | 2.64 | 2.66 | 0.2 | 0.6 | 61.6 | -3.4 | 7.4 | 10.1 | 9.3 | 3.50×10^{-8} | 0.24 | 82 |
| 376 | 335 | 5.32 | 2.66 | 2.77 | 3.3 | 5.1 | 60.7 | -3.4 | 13.3 | 8.3 | 2.5 | 3.46×10^{-8} | 0.23 | 118 |
| 377 | 290 | -5.25 | 2.44 | -3.06 | 168.8 | 7.6 | 116.8 | 1.9 | -13.2 | 0.3 | 0.8 | 3.41×10^{-8} | 0.29 | 203 |
| 378 | 115 | 5.30 | 2.55 | 2.88 | 6.3 | 6.1 | 62.6 | -3.5 | 13.7 | 5.6 | 0.9 | 3.38×10^{-8} | 0.23 | 117 |
| 379 | 182 | -5.30 | 2.77 | -2.74 | 179.0 | 5.1 | 120.7 | -1.2 | -13.1 | 9.0 | 0.6 | 3.31×10^{-8} | 0.28 | 63 |
| 380 | 88 | -6.64 | 3.92 | -2.20 | 4.9 | 5.1 | 4.4 | 6.4 | -2.4 | 9.4 | 3.6 | 3.30×10^{-8} | 0.65 | 180 |
| 381 | 325 | -5.26 | 2.52 | 2.97 | 169.8 | 8.0 | 116.1 | -1.1 | 13.2 | 3.3 | 2.5 | 3.29×10^{-8} | 0.28 | 55 |
| 382 | 254 | 6.60 | 3.66 | 2.59 | 178.9 | 3.5 | 174.0 | -6.0 | 3.7 | 1.9 | 1.6 | 3.27×10^{-8} | 0.62 | 98 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|-----|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 383 | 14 | -5.25 | 2.76 | 2.77 | 175.8 | 6.3 | 119.7 | 1.7 | 11.5 | 8.2 | 3.6 | 3.24×10^{-8} | 0.27 | 63 |
| 384 | 136 | -6.65 | 3.30 | 2.98 | 2.7 | 0.4 | 10.2 | -4.5 | 2.9 | 4.5 | 9.8 | 3.21×10^{-8} | 0.64 | 55 |
| 385 | 231 | -6.56 | -3.79 | 2.57 | 174.4 | 2.7 | 171.8 | -4.3 | 5.5 | 14.0 | 9.3 | 3.18×10^{-8} | 0.35 | 82 |
| 386 | 127 | -6.68 | -3.28 | 2.90 | 4.7 | 2.0 | 8.9 | -6.6 | 5.9 | 8.6 | 7.7 | 3.17×10^{-8} | 0.65 | 95 |
| 387 | 30 | -6.67 | 3.52 | 2.65 | 0.1 | 4.4 | 7.3 | -7.6 | 3.3 | 0.8 | 1.7 | 3.17×10^{-8} | 0.64 | 79 |
| 388 | 459 | -6.47 | 4.07 | 2.31 | 174.1 | 2.2 | 178.3 | -2.1 | 5.6 | 9.2 | 4.0 | 3.17×10^{-8} | 0.36 | 85 |
| 389 | 280 | -6.79 | 3.82 | -1.89 | 169.8 | 5.1 | 171.0 | 6.7 | -6.4 | 17.4 | 8.7 | 3.15×10^{-8} | 0.36 | 121 |
| 390 | 408 | 6.62 | 3.87 | -2.25 | 3.7 | 2.6 | 5.0 | 5.6 | -3.9 | 10.9 | 5.4 | 3.10×10^{-8} | 0.28 | 98 |
| 391 | 286 | -6.66 | 3.94 | 2.06 | 171.1 | 4.1 | 174.5 | -4.8 | 5.7 | 12.8 | 1.7 | 3.10×10^{-8} | 0.35 | 88 |
| 392 | 189 | 6.57 | 3.99 | 2.22 | 5.6 | 3.5 | 3.4 | -3.5 | 4.7 | 11.6 | 5.2 | 3.08×10^{-8} | 0.31 | 84 |
| 393 | 285 | -6.52 | 3.47 | 2.95 | 4.3 | 2.8 | 5.3 | -5.2 | 0.7 | 5.5 | 0.2 | 3.06×10^{-8} | 0.54 | 97 |
| 394 | 61 | -6.63 | -3.69 | 2.56 | 3.2 | 0.0 | 8.4 | -7.4 | 1.9 | 12.4 | 8.0 | 3.03×10^{-8} | 0.55 | 176 |
| 395 | 205 | 6.55 | 3.49 | 2.87 | 177.1 | 4.7 | 175.3 | -9.4 | -2.2 | 5.5 | 1.5 | 3.03×10^{-8} | 0.51 | 98 |
| 396 | 331 | -6.51 | 4.19 | -2.06 | 175.1 | 3.0 | 179.2 | 4.2 | -5.1 | 14.0 | 8.3 | 3.02×10^{-8} | 0.31 | 52 |
| 397 | 307 | -6.66 | 3.89 | 2.23 | 4.2 | 2.7 | 6.1 | -8.0 | 2.5 | 9.5 | 6.5 | 3.02×10^{-8} | 0.53 | 295 |
| 398 | 242 | -6.56 | -3.75 | 2.55 | 176.4 | 1.5 | 172.9 | -4.0 | 0.8 | 13.6 | 8.2 | 2.98×10^{-8} | 0.36 | 153 |
| 399 | 85 | -6.62 | 4.00 | -2.15 | 4.5 | 3.5 | 4.3 | 4.5 | -2.7 | 11.9 | 6.4 | 2.96×10^{-8} | 0.53 | 59 |
| 400 | 249 | -6.46 | 4.16 | 2.29 | 177.0 | 3.9 | 179.7 | -3.0 | 3.9 | 9.7 | 6.5 | 2.96×10^{-8} | 0.34 | 79 |
| 401 | 185 | -6.50 | 4.15 | 2.13 | 175.6 | 2.9 | 179.2 | -3.2 | 3.8 | 12.2 | 7.7 | 2.96×10^{-8} | 0.31 | 54 |
| 402 | 58 | -6.56 | 4.01 | 2.15 | 174.9 | 4.5 | 177.2 | -4.1 | 1.1 | 11.9 | 2.3 | 2.96×10^{-8} | 0.31 | 37 |
| 403 | 98 | -6.45 | 4.33 | -2.10 | 175.7 | 5.1 | 178.1 | 1.8 | -4.6 | 13.3 | 5.5 | 2.96×10^{-8} | 0.34 | 135 |
| 404 | 28 | -6.64 | 3.99 | 2.09 | 172.4 | 3.4 | 174.7 | -2.2 | 5.6 | 13.3 | 4.6 | 2.95×10^{-8} | 0.34 | 51 |
| 405 | 236 | -7.65 | 0.50 | 2.48 | 2.2 | 6.8 | 3.5 | -22.2 | 0.1 | 1.2 | 11.0 | 2.88×10^{-8} | 0.84 | 82 |
| 406 | 318 | -7.66 | 0.61 | 2.37 | 0.9 | 7.3 | 2.8 | -22.3 | -0.7 | 4.7 | 13.0 | 2.87×10^{-8} | 0.84 | 79 |
| 407 | 354 | 5.26 | 2.68 | 2.83 | 6.3 | 1.7 | 61.0 | -3.2 | 15.2 | 4.2 | 7.6 | 2.87×10^{-8} | 0.27 | 106 |
| 408 | 352 | 5.25 | -2.63 | 2.94 | 4.6 | 2.5 | 62.5 | -4.3 | 15.3 | 3.1 | 6.4 | 2.80×10^{-8} | 0.26 | 139 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|-------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 409 | 218 | -5.31 | 2.89 | 2.63 | 169.7 | 1.3 | 120.7 | -0.5 | 13.9 | 9.1 | 9.7 | 2.77×10^{-8} | 0.29 | 107 |
| 410 | 209 | -6.23 | 5.26 | -1.45 | 165.9 | 1.5 | 131.3 | 2.9 | 0.0 | 13.0 | 13.4 | 2.77×10^{-8} | 0.37 | 215 |
| 411 | 139 | -6.11 | 5.49 | 1.13 | 166.7 | 5.1 | 128.5 | -3.1 | 0.2 | 18.3 | 12.7 | 2.73×10^{-8} | 0.36 | 45 |
| 412 | 384 | -5.27 | 2.88 | 2.69 | 170.9 | 1.9 | 120.6 | -0.6 | 15.0 | 7.6 | 9.7 | 2.71×10^{-8} | 0.28 | 76 |
| 413 | 78 | -6.20 | 5.33 | 1.34 | 166.1 | 2.1 | 130.3 | -2.6 | -0.5 | 15.0 | 13.3 | 2.68×10^{-8} | 0.36 | 90 |
| 414 | 452 | -5.28 | 2.89 | 2.68 | 170.1 | 1.7 | 120.4 | -0.5 | 14.1 | 8.5 | 9.6 | 2.65×10^{-8} | 0.28 | 70 |
| 415 | 449 | -6.30 | 1.72 | 2.60 | 174.7 | 3.3 | 175.9 | 2.0 | 13.4 | 22.7 | 16.9 | 2.62×10^{-8} | 0.20 | 63 |
| 416 | 370 | -6.08 | -1.73 | 3.16 | 176.6 | 6.3 | 176.6 | -0.5 | 12.1 | 21.5 | 19.2 | 2.52×10^{-8} | 0.16 | 55 |
| 417 | 435 | 6.41 | 1.90 | 2.29 | 171.4 | 3.7 | 177.6 | -6.0 | 8.6 | 25.6 | 19.5 | 2.35×10^{-8} | 0.41 | 62 |
| 418 | 401 | -6.39 | -1.14 | 3.13 | 16.4 | 5.3 | 63.7 | -3.9 | 13.6 | 7.8 | 11.0 | 2.32×10^{-8} | 0.39 | 84 |
| 419 | 155 | 7.54 | 0.06 | 2.58 | 173.8 | 8.4 | 174.4 | -18.5 | -2.8 | 1.5 | 0.8 | 2.30×10^{-8} | 0.71 | 75 |
| 420 | 12 | 6.37 | 1.80 | -2.38 | 170.7 | 2.8 | 176.0 | 3.7 | -10.2 | 24.8 | 17.8 | 2.29×10^{-8} | 0.40 | 160 |
| 421 | 463 | -6.31 | 1.78 | 2.48 | 7.9 | 1.4 | 4.2 | -2.4 | 11.4 | 24.0 | 19.6 | 2.28×10^{-8} | 0.45 | 80 |
| 422 | 184 | -6.26 | 1.10 | 3.21 | 18.8 | 5.8 | 67.7 | -1.4 | 12.7 | 1.8 | 12.7 | 2.27×10^{-8} | 0.31 | 51 |
| 423 | 206 | -3.87 | 5.67 | 1.90 | 2.9 | 3.1 | 58.8 | 0.8 | -2.9 | 11.6 | 3.9 | 2.26×10^{-8} | 0.23 | 98 |
| 424 | 37 | -4.02 | 5.63 | 1.92 | 1.3 | 5.5 | 62.5 | 1.6 | -0.8 | 9.9 | 3.6 | 2.25×10^{-8} | 0.27 | 65 |
| 425 | 161 | -6.24 | 1.00 | -3.32 | 22.9 | 6.5 | 65.8 | 1.5 | -9.7 | 7.2 | 12.3 | 2.24×10^{-8} | 0.31 | 117 |
| 426 | 193 | -3.65 | 5.65 | 2.04 | 2.6 | 3.8 | 55.8 | 2.5 | -3.3 | 7.1 | 0.2 | 2.23×10^{-8} | 0.22 | 82 |
| 427 | 279 | -6.25 | 0.99 | 3.30 | 19.8 | 6.6 | 67.6 | -3.7 | 11.7 | 7.2 | 11.6 | 2.23×10^{-8} | 0.36 | 89 |
| 428 | 475 | -7.39 | -0.24 | 2.76 | 12.1 | 9.5 | 10.4 | -15.7 | -0.3 | 5.9 | 9.9 | 2.21×10^{-8} | 0.76 | 111 |
| 429 | 291 | -3.93 | 5.68 | 2.00 | 4.1 | 6.5 | 60.5 | 2.9 | 1.0 | 10.1 | 8.8 | 2.20×10^{-8} | 0.26 | 86 |
| 430 | 248 | -6.36 | 1.83 | -2.37 | 10.1 | 3.5 | 3.7 | 4.3 | -9.5 | 25.0 | 16.2 | 2.19×10^{-8} | 0.44 | 40 |
| 431 | 368 | -6.38 | 1.91 | -2.35 | 8.8 | 2.9 | 2.8 | 2.9 | -9.8 | 26.7 | 19.1 | 2.18×10^{-8} | 0.44 | 141 |
| 432 | 414 | -7.50 | 0.00 | 2.63 | 7.3 | 8.5 | 7.4 | -16.8 | -2.5 | 1.6 | 1.9 | 2.17×10^{-8} | 0.74 | 72 |
| 433 | 348 | -7.51 | 0.04 | 2.54 | 13.8 | 9.2 | 8.5 | -16.9 | -2.9 | 3.6 | 5.9 | 2.16×10^{-8} | 0.73 | 45 |
| 434 | 49 | -7.40 | -0.15 | 2.69 | 14.6 | 10.6 | 10.8 | -15.1 | -1.6 | 2.3 | 9.3 | 2.16×10^{-8} | 0.75 | 91 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|------|-------|------|-----------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 435 | 223 | -7.53 | 0.08 | 2.56 | 9.5 | 9.0 | 7.0 | -17.4 | -3.0 | 1.6 | 0.3 | 2.15×10^{-8} | 0.73 | 105 |
| 436 | 334 | -6.24 | 1.24 | 3.36 | 155.4 | 10.6 | 117.5 | -1.9 | 13.0 | 5.1 | 6.6 | 2.14×10^{-8} | 0.25 | 72 |
| 437 | 110 | -3.77 | 5.44 | 2.54 | 4.8 | 5.2 | 59.1 | 1.9 | -3.6 | 1.2 | 0.3 | 2.14×10^{-8} | 0.25 | 83 |
| 438 | 460 | -6.26 | -1.53 | 3.28 | 157.9 | 12.1 | 119.3 | -2.4 | 11.6 | 1.6 | 1.2 | 2.10×10^{-8} | 0.26 | 85 |
| 439 | 327 | 6.39 | 1.85 | -2.36 | 170.4 | 7.9 | 175.8 | 3.4 | -9.8 | 24.9 | 19.1 | 2.06×10^{-8} | 0.42 | 85 |
| 440 | 362 | -7.45 | -0.05 | -2.66 | 8.9 | 8.7 | 8.9 | 16.2 | 3.1 | 1.5 | 1.1 | 2.05×10^{-8} | 0.72 | 72 |
| 441 | 240 | -3.76 | 5.64 | 2.15 | 0.1 | 3.4 | 57.6 | 2.4 | -2.3 | 7.6 | 5.9 | 2.02×10^{-8} | 0.19 | 44 |
| 442 | 23 | -6.32 | 1.66 | 3.04 | 162.4 | 11.6 | 116.7 | 1.9 | 10.8 | 8.9 | 8.9 | 2.00×10^{-8} | 0.31 | 127 |
| 443 | 405 | -6.12 | -1.92 | -3.00 | 9.0 | 2.2 | 2.9 | 3.5 | -7.6 | 25.7 | 19.2 | 1.98×10^{-8} | 0.47 | 95 |
| 444 | 116 | -4.24 | 4.25 | -3.42 | 25.1 | 14.9 | 56.2 | -2.1 | -6.4 | 9.8 | 6.2 | 1.96×10^{-8} | 0.34 | 300 |
| 445 | 208 | -6.33 | -4.90 | 1.67 | 32.2 | 2.3 | 35.8 | -8.3 | 1.3 | 15.8 | 13.1 | 1.93×10^{-8} | 0.63 | 285 |
| 446 | 467 | -6.35 | 1.91 | 2.39 | 9.6 | 7.8 | 3.9 | -2.0 | 7.1 | 23.6 | 20.3 | 1.93×10^{-8} | 0.44 | 39 |
| 447 | 469 | -6.35 | 1.98 | 2.32 | 10.5 | 8.8 | 3.4 | -3.6 | 5.2 | 24.1 | 20.7 | 1.85×10^{-8} | 0.43 | 81 |
| 448 | 389 | -6.32 | 1.91 | 2.39 | 10.8 | 8.1 | 4.5 | -2.2 | 6.3 | 24.0 | 20.4 | 1.77×10^{-8} | 0.41 | 87 |
| 449 | 360 | -6.50 | 4.56 | 1.80 | 27.4 | 2.9 | 33.0 | -10.6 | 2.8 | 11.5 | 11.0 | 1.59×10^{-8} | 0.56 | 300 |
| 450 | 106 | -5.35 | -3.92 | 3.09 | 149.6 | 9.1 | 106.4 | 1.1 | 10.8 | 11.4 | 9.0 | 1.58×10^{-8} | 0.52 | 300 |
| 451 | 447 | -7.83 | 1.86 | 2.67 | 33.4 | 11.9 | 64.6 | 3.4 | 4.8 | 11.0 | 9.0 | 4.47×10^{-9} | 0.71 | 73 |
| 452 | 125 | -7.73 | -1.79 | 3.03 | 33.8 | 13.5 | 65.2 | 3.8 | 4.3 | 7.5 | 12.1 | 4.41×10^{-9} | 0.70 | 69 |
| 453 | 117 | -7.86 | 1.67 | 2.76 | 153.6 | 10.2 | 117.9 | 4.2 | 4.8 | 7.9 | 10.3 | 4.34×10^{-9} | 0.40 | 49 |
| 454 | 422 | -7.83 | 1.50 | 3.00 | 151.8 | 12.9 | 118.0 | 4.8 | 5.7 | 1.8 | 14.2 | 4.32×10^{-9} | 0.40 | 95 |
| 455 | 147 | -7.80 | -1.51 | 2.99 | 155.6 | 10.8 | 117.3 | 4.5 | 4.3 | 1.2 | 7.8 | 4.30×10^{-9} | 0.40 | 131 |
| 456 | 197 | 7.84 | -1.32 | 2.94 | 16.8 | 8.9 | 62.6 | 5.6 | 4.1 | 6.7 | 5.9 | 4.26×10^{-9} | 0.35 | 111 |
| 457 | 412 | -7.82 | -1.49 | 3.01 | 27.6 | 12.8 | 65.3 | 1.7 | 7.7 | 4.9 | 10.8 | 4.13×10^{-9} | 0.69 | 230 |
| 458 | 288 | -7.84 | -1.45 | 2.98 | 158.2 | 11.1 | 117.3 | 4.0 | 3.0 | 0.7 | 8.3 | 4.13×10^{-9} | 0.37 | 285 |
| 459 | 410 | -7.75 | -1.48 | -3.10 | 29.0 | 14.9 | 65.3 | -5.3 | -5.3 | 3.5 | 10.8 | 4.12×10^{-9} | 0.59 | 246 |
| 460 | 160 | -8.92 | -0.03 | 2.69 | 176.3 | 0.5 | 180.0 | -1.2 | 1.5 | 2.9 | 5.4 | 3.08×10^{-9} | 0.42 | 71 |

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Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|------|-------|------|------------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 461 | 234 | -8.97 | 0.20 | 2.53 | 179.5 | 1.3 | 179.0 | 0.2 | 2.4 | 5.5 | 5.8 | 3.07×10^{-9} | 0.42 | 49 |
| 462 | 180 | -9.12 | 0.29 | -2.14 | 5.6 | 7.5 | 1.2 | 1.9 | -2.8 | 12.3 | 9.1 | 3.01×10^{-9} | 0.82 | 300 |
| 463 | 196 | -9.04 | 0.22 | 2.36 | 2.3 | 3.5 | 0.2 | -0.3 | 1.6 | 5.7 | 8.8 | 3.00×10^{-9} | 0.82 | 245 |
| 464 | 144 | -8.97 | 0.20 | -2.43 | 179.3 | 3.1 | 178.8 | -0.8 | 3.2 | 5.1 | 4.6 | 2.98×10^{-9} | 0.41 | 139 |
| 465 | 268 | -9.06 | 0.15 | -2.32 | 1.3 | 6.5 | 2.1 | 2.5 | -0.7 | 2.0 | 8.1 | 2.96×10^{-9} | 0.82 | 187 |
| 466 | 137 | -9.07 | 0.01 | 2.36 | 4.4 | 4.8 | 2.2 | -1.3 | 1.8 | 2.0 | 4.1 | 2.89×10^{-9} | 0.81 | 77 |
| 467 | 484 | -8.86 | -0.27 | 2.89 | 171.7 | 1.5 | 179.7 | -0.4 | 1.4 | 9.9 | 5.4 | 2.88×10^{-9} | 0.40 | 88 |
| 468 | 445 | -8.98 | -0.05 | 2.61 | 178.8 | 2.2 | 179.0 | -1.0 | 1.8 | 0.3 | 3.9 | 2.86×10^{-9} | 0.40 | 87 |
| 469 | 324 | -9.10 | -0.02 | 2.33 | 6.1 | 5.9 | 4.1 | -2.4 | 4.6 | 7.8 | 6.7 | 2.70×10^{-9} | 0.79 | 118 |
| 470 | 393 | 0.76 | 3.21 | 3.82 | 17.8 | 17.9 | 15.0 | -2.6 | -2.5 | 0.9 | 1.0 | 9.87×10^{-10} | 0.55 | 300 |
| 471 | 398 | -1.18 | 6.01 | 2.29 | 43.0 | 76.7 | 8.5 | 6.4 | 17.4 | 5.4 | 3.7 | 2.03×10^{-10} | 0.82 | 300 |
| 472 | 355 | -8.24 | 3.21 | -3.35 | 59.0 | 28.3 | 66.9 | -5.2 | 4.4 | 8.5 | 13.6 | 1.88×10^{-10} | 0.74 | 300 |
| 473 | 19 | -9.67 | 1.91 | 3.32 | 3.7 | 8.5 | 26.6 | 7.4 | -3.3 | 5.5 | 6.9 | 8.50×10^{-11} | 0.71 | 122 |
| 474 | 153 | -9.62 | 1.77 | 3.34 | 178.5 | 8.5 | 152.0 | 7.6 | -3.5 | 3.3 | 3.8 | 8.29×10^{-11} | 0.51 | 51 |
| 475 | 299 | -9.74 | -1.55 | 3.05 | 177.3 | 5.3 | 152.2 | 7.1 | -3.3 | 12.5 | 11.5 | 8.29×10^{-11} | 0.53 | 83 |
| 476 | 76 | -9.81 | -1.87 | 2.86 | 173.9 | 3.8 | 154.1 | 7.6 | -4.9 | 4.8 | 11.6 | 8.22×10^{-11} | 0.52 | 160 |
| 477 | 281 | 1.18 | 7.83 | 4.86 | 102.4 | 79.8 | 97.4 | 22.9 | -4.0 | 5.0 | 2.5 | 8.04×10^{-11} | 0.62 | 139 |
| 478 | 34 | -9.11 | 5.28 | 1.67 | 149.2 | 8.2 | 132.2 | 8.2 | -4.0 | 8.5 | 10.1 | 7.72×10^{-11} | 0.55 | 225 |
| 479 | 43 | -9.26 | 4.96 | 1.99 | 152.4 | 7.1 | 134.6 | 7.2 | -4.5 | 1.0 | 8.5 | 7.65×10^{-11} | 0.55 | 162 |
| 480 | 377 | -9.30 | 4.90 | -2.09 | 149.2 | 8.8 | 135.9 | -6.7 | 5.5 | 1.0 | 2.4 | 7.24×10^{-11} | 0.54 | 213 |
| 481 | 359 | -9.71 | 1.81 | 3.30 | 177.0 | 9.1 | 151.7 | 4.3 | -3.5 | 1.8 | 1.4 | 7.05×10^{-11} | 0.46 | 113 |
| 482 | 6 | -8.62 | 5.00 | 3.87 | 31.1 | 20.1 | 51.2 | 8.5 | -1.8 | 16.2 | 8.6 | 6.87×10^{-11} | 0.74 | 150 |
| 483 | 458 | -5.74 | 8.43 | -2.19 | 9.0 | 5.4 | 37.6 | -5.5 | 3.3 | 10.8 | 15.1 | 3.69×10^{-11} | 0.59 | 44 |
| 484 | 433 | -9.28 | 2.45 | 1.17 | 142.6 | 21.4 | 121.7 | 7.7 | 1.8 | 6.7 | 11.9 | 3.50×10^{-11} | 0.61 | 75 |
| 485 | 425 | -9.27 | 2.74 | -0.95 | 145.1 | 19.4 | 125.9 | -5.9 | -1.9 | 0.5 | 5.6 | 3.41×10^{-11} | 0.60 | 207 |
| 486 | 366 | -5.39 | 8.33 | 2.86 | 161.9 | 3.9 | 142.2 | 9.2 | -4.7 | 4.1 | 2.9 | 3.32×10^{-11} | 0.43 | 92 |

Continued on next page

Table 1 – Continued from previous page

| rank | id | translation | | | rotation | | | curvature | | twist | | rate | ΔE | steps |
|------|-----|-------------|-------|-------|----------|------|-------|-----------|------|-------|------|------------------------|------------|-------|
| | | x | y | z | x | y | z | A | B | A | B | | | |
| 487 | 282 | -5.31 | 8.41 | 2.75 | 157.0 | 9.5 | 139.0 | 7.0 | -3.8 | 6.6 | 3.4 | 3.31×10^{-11} | 0.43 | 82 |
| 488 | 54 | -7.18 | 7.38 | 1.73 | 155.1 | 7.3 | 116.1 | 14.3 | -2.6 | 9.1 | 2.6 | 3.17×10^{-11} | 0.63 | 225 |
| 489 | 39 | -5.39 | 8.44 | 2.50 | 163.3 | 6.0 | 140.0 | 7.0 | -3.1 | 9.8 | 10.8 | 3.16×10^{-11} | 0.41 | 56 |
| 490 | 430 | -5.67 | 8.12 | 3.09 | 162.3 | 1.2 | 145.2 | 4.9 | -3.3 | 5.6 | 4.2 | 3.16×10^{-11} | 0.41 | 158 |
| 491 | 104 | -5.51 | 8.47 | 2.38 | 17.4 | 7.6 | 39.6 | 3.8 | -4.0 | 10.2 | 10.7 | 3.13×10^{-11} | 0.57 | 56 |
| 492 | 295 | -5.51 | 8.45 | 2.34 | 161.0 | 8.8 | 140.3 | 2.6 | -3.0 | 12.0 | 7.9 | 3.03×10^{-11} | 0.40 | 79 |
| 493 | 471 | -10.04 | 0.30 | 5.07 | 154.2 | 33.2 | 139.4 | 7.8 | -4.5 | 1.3 | 5.6 | 1.46×10^{-11} | 0.80 | 107 |
| 494 | 403 | -5.86 | 6.36 | 1.92 | 25.2 | 20.6 | 42.6 | 9.0 | 0.6 | 5.8 | 16.0 | 1.21×10^{-11} | 0.74 | 300 |
| 495 | 225 | -5.66 | 7.81 | 1.78 | 115.8 | 38.8 | 98.4 | 8.2 | -2.6 | 4.9 | 8.3 | 1.18×10^{-11} | 0.83 | 224 |
| 496 | 371 | -5.41 | 7.90 | 1.69 | 61.4 | 38.3 | 79.2 | 6.8 | -1.4 | 6.7 | 9.5 | 1.14×10^{-11} | 0.65 | 142 |
| 497 | 276 | -6.70 | -0.83 | 3.86 | 37.6 | 34.2 | 11.8 | 2.6 | -1.3 | 1.1 | 8.5 | 4.60×10^{-12} | 1.02 | 300 |
| 498 | 90 | 2.46 | 9.64 | 2.95 | 154.1 | 3.4 | 141.4 | 1.0 | -8.3 | 7.2 | 1.2 | 1.00×10^{-13} | 1.00 | 300 |
| 499 | 183 | -2.75 | 5.23 | 3.66 | 90.7 | 52.5 | 13.7 | -0.7 | -0.1 | 0.4 | 0.2 | 4.88×10^{-15} | -0.14 | 300 |
| 500 | 245 | 1.36 | 10.91 | -1.16 | 50.0 | 27.5 | 72.9 | -0.8 | -0.3 | 0.6 | 0.2 | 2.69×10^{-17} | 0.10 | 300 |

3 Determining an Optimal Value for ω

In our optimization process, the objective function $L(\mathbf{x}) = E(\mathbf{x}) - \omega \log(T_{RP}(\mathbf{x})^2)$, where $E(\mathbf{x})$ represents the energy and $|T_{RP}(\mathbf{x})|^2$ signifies the effective SF coupling for the nuclear configuration \mathbf{x} , necessitates the careful selection of the free parameter ω to achieve a balance between optimizing energy and effective SF coupling. To this end, we adjust ω in increments of 0.1, ranging from 0.1 to 1.0. This adjustment is performed across the same set of 20 randomly translated and rotated ethene and PBI dimers, each optimized to minimize $L(\mathbf{x})$.

3.1 Model system: ethene

The average and standard deviation of the convergent steps, along with the effective SF coupling (SFC) and energy for each ω , are depicted in Figure 2. The graphical representation in Figure 2b illustrates a strong positive correlation between effective SF coupling and energy, complicating the choice of an ideal ω . Since our goal is to minimize energy while maximizing effective SF coupling, we select the value of ω that maximizes the hysteresis between these two parameters as optimal. Consequently, $\omega = 0.3$ has been identified as the preferred choice. Moreover, values exceeding this threshold tend to exhibit greater instability in terms of convergence steps and energy, as indicated by their standard deviations.

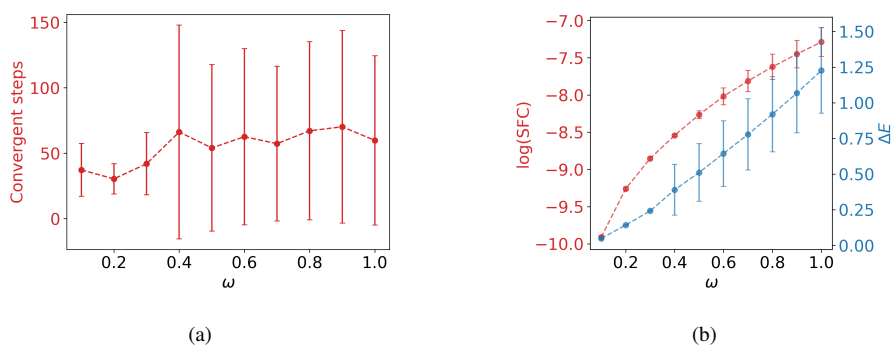


Figure 2: Optimization procedure with varying ω from 0.1 to 1.0 in steps of 0.1 for the same set of 20 randomly chosen ethylene dimers.

3.2 Actual system: PBI

Repeating this ω scan considering the PBI dimer gives very similar results (see Figure 3). The only notable difference can be found around $\omega > 0.5$. In this region some traceries failed due to convergence errors in the SCF cycle. This happens when some atoms get too close in distance during the optimization. The selected value of $\omega = 0.3$ has been identified as a "good" value also for the PBI system and is therefore employed in our study.

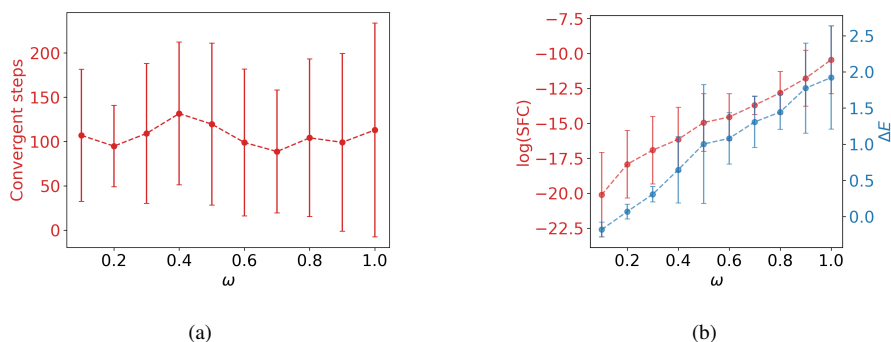


Figure 3: Optimization procedure with varying ω from 0.1 to 1.0 in steps of 0.1 for the same set of 20 randomly chosen PBI dimers.

4 Stability of PCA and K-Means Clustering Outcomes Under Variable Parameters

To explore the impact of varying input parameters on the results of PCA and k-means clustering, we conducted additional analyses modifying the number of PCA dimensions and cluster counts, and selectively excluding the least significant PCA dimensions. This approach was intended to rigorously test the robustness of our findings. Importantly, despite these variations, each analysis consistently identified distinct clusters that correspond to the specific structural motifs of "twisting," "curvature", and "planarity". These results are detailed in the following tables and affirm the reliability of our dimension reduction and clustering strategy. The consistent attribution of these motifs to particular clusters across different parameter settings underscores the stability and validity of the analytical framework used in our study.

Table 2: PCA results with the following settings: dimensions used: 3; clusters used: 4; z-translation ignored: True; x-rotation ignored: True; y-rotation ignored: True; only positive translations and degrees: True; Dimension 1: 33% of the variance. Dimension 2: 22% of the variance. Dimension 3: 13% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|------|------|----------|-----|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | 3.07 | 0.70 | 3.00 | 0.0 | 0.0 | -7.1 | -18.9 | 19.4 | 7.2 | 7.9 | 2.15×10^{-7} |
| 2 | 1.45 | 1.35 | 3.00 | 0.0 | 0.0 | -25.8 | 3.8 | 4.6 | 21.7 | 14.5 | 2.99×10^{-7} |
| 3 | 1.45 | 3.75 | 3.00 | 0.0 | 0.0 | 43.2 | -1.3 | 5.7 | 8.6 | 7.3 | 1.68×10^{-7} |
| 4 | 1.46 | 3.30 | 3.00 | 0.0 | 0.0 | -49.3 | 3.8 | 1.6 | 10.0 | 5.4 | 1.47×10^{-7} |

Table 3: PCA results with the following settings: dimensions used: 3; clusters used: 4; z-translation ignored: True; x-rotation ignored: True; y-rotation ignored: True; only positive translations and degrees: False; Dimension 1: 26% of the variance. Dimension 2: 19% of the variance. Dimension 3: 16% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|-------|------|----------|-----|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | -2.20 | -0.02 | 3.00 | 0.0 | 0.0 | 120.6 | -9.6 | 13.6 | 6.6 | 5.9 | 2.10×10^{-7} |
| 2 | -0.25 | -0.14 | 3.00 | 0.0 | 0.0 | 81.5 | 4.9 | 2.5 | 20.0 | 13.1 | 2.72×10^{-7} |
| 3 | 0.69 | 4.29 | 3.00 | 0.0 | 0.0 | 79.7 | 2.0 | 2.0 | 7.6 | 6.0 | 1.43×10^{-7} |
| 4 | 2.22 | 0.94 | 3.00 | 0.0 | 0.0 | 80.3 | -20.6 | 21.2 | 9.7 | 10.1 | 1.83×10^{-7} |

Table 4: PCA results with the following settings: dimensions used: 3; clusters used: 4; z-translation ignored: True; x-rotation ignored: True; y-rotation ignored: False; only positive translations and degrees: False; Dimension 1: 24% of the variance. Dimension 2: 18% of the variance. Dimension 3: 15% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|-------|------|----------|------|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | -1.79 | 0.74 | 3.00 | 0.0 | 3.9 | 101.3 | -5.9 | 10.4 | 5.5 | 4.7 | 2.03×10^{-7} |
| 2 | -0.09 | -0.21 | 3.00 | 0.0 | 5.4 | 72.8 | 5.0 | 2.5 | 19.5 | 12.7 | 2.69×10^{-7} |
| 3 | 0.76 | 4.77 | 3.00 | 0.0 | 10.7 | 94.6 | 1.8 | 1.3 | 9.4 | 7.4 | 1.28×10^{-7} |
| 4 | 1.58 | 0.87 | 3.00 | 0.0 | 5.6 | 97.7 | -19.7 | 20.9 | 9.7 | 9.9 | 1.91×10^{-7} |

Table 5: PCA results with the following settings: dimensions used: 3; clusters used: 4; z-translation ignored: True; x-rotation ignored: False; y-rotation ignored: False; only positive translations and degrees: False; Dimension 1: 23% of the variance. Dimension 2: 20% of the variance. Dimension 3: 16% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|-------|------|----------|-----|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | 0.12 | -0.21 | 3.00 | 92.1 | 6.0 | 89.5 | 4.5 | 3.4 | 20.7 | 13.7 | 2.79×10^{-7} |
| 2 | -0.51 | 0.94 | 3.00 | 175.9 | 5.3 | 148.1 | -11.8 | 16.0 | 7.3 | 6.9 | 2.03×10^{-7} |
| 3 | 0.10 | 4.35 | 3.00 | 79.0 | 9.6 | 79.8 | 3.6 | -0.2 | 8.6 | 6.4 | 1.27×10^{-7} |
| 4 | -0.05 | 0.46 | 3.00 | 3.4 | 3.5 | 34.2 | -12.4 | 13.9 | 7.4 | 7.1 | 1.97×10^{-7} |

Table 6: PCA results with the following settings: dimensions used: 3; clusters used: 4; z-translation ignored: False; x-rotation ignored: False; y-rotation ignored: False; only positive translations and degrees: False; Dimension 1: 23% of the variance. Dimension 2: 19% of the variance. Dimension 3: 15% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|-------|------|----------|-----|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | 0.02 | 4.01 | 0.83 | 83.8 | 9.1 | 82.3 | 4.7 | -1.8 | 8.5 | 6.4 | 1.31×10^{-7} |
| 2 | 0.22 | -0.06 | 2.81 | 89.2 | 6.3 | 87.8 | 3.8 | 4.2 | 20.9 | 13.8 | 2.75×10^{-7} |
| 3 | -0.50 | 1.15 | 3.12 | 174.7 | 5.6 | 147.3 | -11.4 | 15.9 | 7.3 | 6.8 | 2.02×10^{-7} |
| 4 | -0.06 | 0.64 | 2.97 | 5.6 | 3.8 | 35.7 | -12.1 | 13.8 | 7.3 | 7.0 | 1.95×10^{-7} |

Table 7: PCA results with the following settings: dimensions used: 5; clusters used: 4; z-translation ignored: True; x-rotation ignored: True; y-rotation ignored: True; only positive translations and degrees: True; Dimension 1: 33% of the variance. Dimension 2: 22% of the variance. Dimension 3: 13% of the variance. Dimension 4: 11% of the variance. Dimension 5: 9% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|------|------|----------|-----|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | 1.75 | 2.04 | 3.00 | 0.0 | 0.0 | 1.6 | -18.9 | 26.8 | 12.1 | 10.3 | 1.93×10^{-7} |
| 2 | 1.53 | 1.34 | 3.00 | 0.0 | 0.0 | -13.5 | 5.0 | 2.9 | 21.8 | 12.1 | 2.75×10^{-7} |
| 3 | 3.37 | 0.75 | 3.00 | 0.0 | 0.0 | -12.9 | -13.8 | 11.3 | 4.6 | 6.6 | 2.01×10^{-7} |
| 4 | 1.25 | 4.31 | 3.00 | 0.0 | 0.0 | 22.1 | 0.7 | 4.0 | 7.0 | 6.7 | 1.57×10^{-7} |

Table 8: PCA results with the following settings: dimensions used: 3; clusters used: 3; z-translation ignored: True; x-rotation ignored: True; y-rotation ignored: True; only positive translations and degrees: True; Dimension 1: 33% of the variance. Dimension 2: 22% of the variance. Dimension 3: 13% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|------|------|----------|-----|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | 1.36 | 3.91 | 3.00 | 0.0 | 0.0 | 23.7 | 0.9 | 3.8 | 8.5 | 6.4 | 1.58×10^{-7} |
| 2 | 2.93 | 0.95 | 3.00 | 0.0 | 0.0 | -9.5 | -17.0 | 17.9 | 7.3 | 7.7 | 2.08×10^{-7} |
| 3 | 1.44 | 1.55 | 3.00 | 0.0 | 0.0 | -23.7 | 3.7 | 4.4 | 20.7 | 13.8 | 2.81×10^{-7} |

Table 9: PCA results with the following settings: dimensions used: 10; clusters used: 3; z-translation ignored: True; x-rotation ignored: True; y-rotation ignored: True; only positive translations and degrees: True; Dimension 1: 33% of the variance. Dimension 2: 22% of the variance. Dimension 3: 13% of the variance. Dimension 4: 11% of the variance. Dimension 5: 9% of the variance. Dimension 6: 7% of the variance. Dimension 7: 5% of the variance. Dimension 8: 0% of the variance. Dimension 9: 0% of the variance. Dimension 10: 0% of the variance. The mean parameters for each cluster are given.

| cluster | translation | | | rotation | | | concavity | | twist | | coupling |
|---------|-------------|------|------|----------|-----|-------|-----------|------|-------|------|-----------------------|
| | x | y | z | x | y | z | A | B | A | B | |
| 1 | 1.48 | 1.28 | 3.00 | 0.0 | 0.0 | -10.9 | 5.3 | 0.6 | 20.6 | 11.6 | 2.70×10^{-7} |
| 2 | 2.89 | 0.88 | 3.00 | 0.0 | 0.0 | -8.3 | -16.4 | 17.3 | 6.9 | 8.0 | 2.05×10^{-7} |
| 3 | 1.31 | 4.48 | 3.00 | 0.0 | 0.0 | 19.9 | -0.4 | 6.5 | 7.6 | 6.9 | 1.53×10^{-7} |

5 Influence of Twisting on Effective SF Coupling

The results obtained by the functionality optimization procedure indicate, that monomer twisting in the PBI might be beneficial for the strength of the effective singlet fission coupling. To gain a deeper understanding of the interplay between twisting and coupling strength, we carried out further calculations, systematically scanning the effective SF coupling as a function of both molecular twisting angles in two chosen dimer configurations from our optimizations. The first structural motif (id = 316) bears comparatively large twisting angles for both monomers (A: 28.2° , B: 17.1°). The second one (id = 252) exhibits only subtle twisting angles below 10° and comparatively pronounced curvatures. For configuration 316, the highest effective SF coupling (see Figure 5a) is found for two planar monomers, however, a large twisting angle of 30° in monomer A is also favorable for the effective SF coupling. In contrast, for the ground state energy (see Figure 5b), a twist of about 20° in both monomers corresponds to a minimum, which is directly reflected in the scan of the objective function (see Figure 5c).

For configuration 252, the effective SF coupling is highest when monomer A exhibits strong twisting (30°), while monomer B is planar (see Figure 6a). Again the ground state energy (see Figure 6b) prefers a twist of about 15° in both monomers, which also corresponds to the minimum in the scan of the objective function (see Figure 6c). Therefore, according to our applied model for the description of effective SF couplings SF, twisting of one monomer seems to have a beneficial effect on the strength of the coupling, however, these conformations are mainly suppressed in the functionality optimization due to the energy constraint in the objective function.

In order to elucidate the effect of twisting on the energy condition required for efficient singlet fission, we further scanned the energy of the E_{S_1} and E_{T_1} of the monomer PBI as a function of the twisting angle. Energy calculations were performed using CASPT2 with the cc-pVDZ basis set and an active space of 4 electrons in 4 orbitals within the Bagel software package. The plot in Figure 7 illustrates the variations of E_{S_1} , E_{T_1} , and $2E_{T_1} - E_{S_1}$ with respect to the twist angle. The calculation reveals that as the twist angle increases, the energy of the singlet excited state, E_{S_1} , decreases, while simultaneously, the energy of the triplet excited state, E_{T_1} , increases. Consequently, the energy difference $2E_{T_1} - E_{S_1}$ increases, indicating that twisting is an unfavorable structural change for singlet fission.

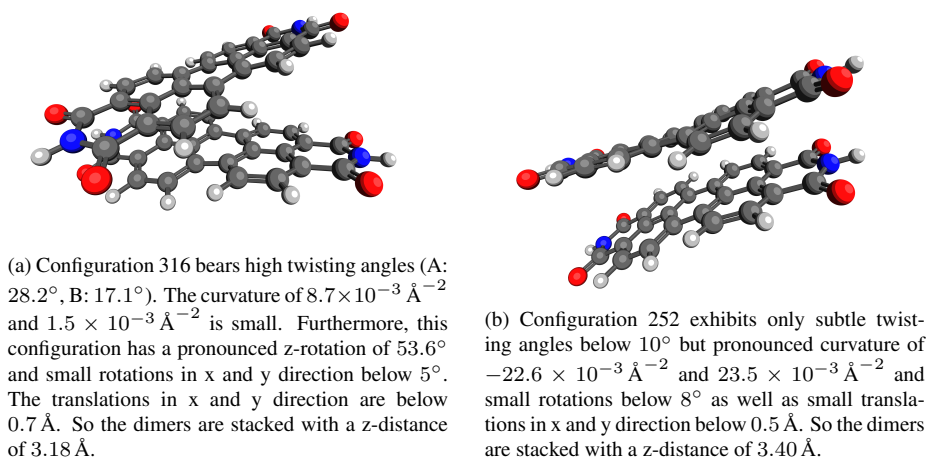


Figure 4: Two chosen exemplary configurations obtained by the functionality optimization procedure that are considered for the twisting mode scans.

6 Davydov splitting

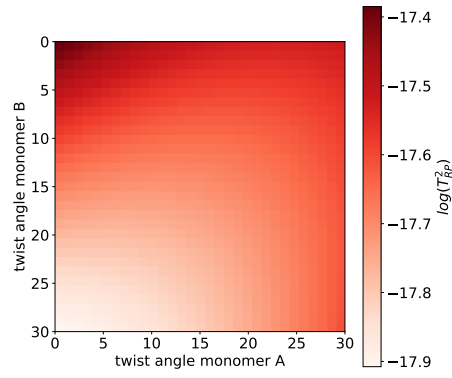
The Davydov splitting values calculated for the mean structures using equation,

$$\Delta E_{DS} = 4 \left| \langle h_A l_A | h_B l_B \rangle + \langle l_A | \hat{\mathbf{F}} | l_B \rangle \langle h_A | \hat{\mathbf{F}} | h_B \rangle \right| \quad (1)$$

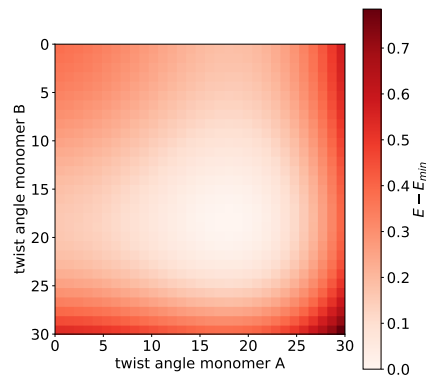
are shown in Table 10. **PBI-C2** has the highest ΔE_{DS} , **PBI-C1** has the second highest ΔE_{DS} , **PBI-C3** has the third highest ΔE_{DS} , and **PBI-C4** has the lowest ΔE_{DS} . Thus **PBI-C2** has the highest effective SF coupling and the highest ΔE_{DS} . The Davydov interaction becomes particularly relevant when the singlet fission (SF) process is sufficiently endoergic. In the cases of **PBI-C1_A**, **PBI-C1_B**, **PBI-C2_A**, **PBI-C2_B**, and **PBI-C4_A**, we observe that $2E_{T_1} - E_{S_1}$ is negative, indicating that singlet fission is exoergic. Thus, we assume that the Davydov splitting is not significantly influential.

| Structure | ΔE_{DS} |
|---------------|-----------------|
| PBI-C1 | 0.4165 eV |
| PBI-C2 | 0.5628 eV |
| PBI-C3 | 0.3447 eV |
| PBI-C4 | 0.2798 eV |

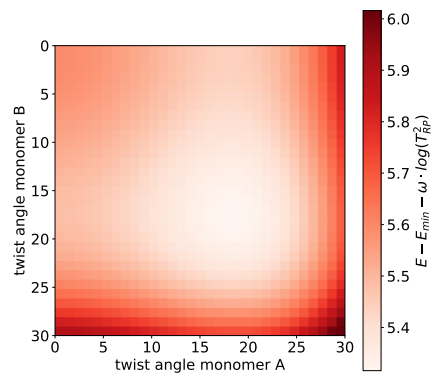
Table 10: Davydov splitting



(a) Effective SF coupling scan.

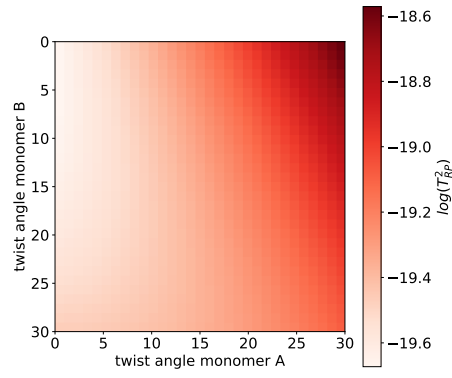


(b) AM1+D groundstate energy scan.

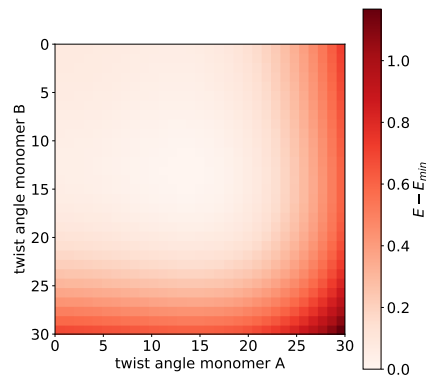


(c) Objective function scan.

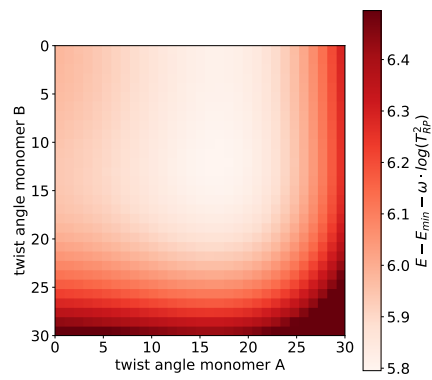
Figure 5: Scans for configuration 316.



(a) Effective SF coupling scan.



(b) AM1+D groundstate energy scan.



(c) Objective function scan.

Figure 6: Scans for configuration 252).

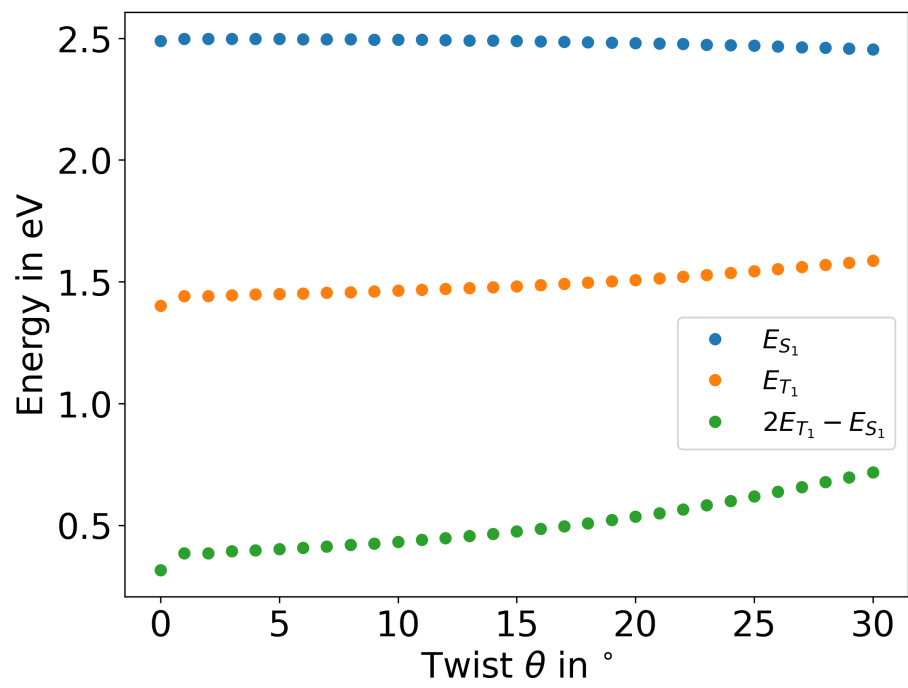


Figure 7: E_{S_1} and E_{T_1} energy scan (CASPT2) along the twisting mode.