## Supplementary materials

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# Theoretical investigation of inclusion complex of 2-methyl mercapto phenothiazine with hydroxy propyl β-cyclodextrin by DFT approaches

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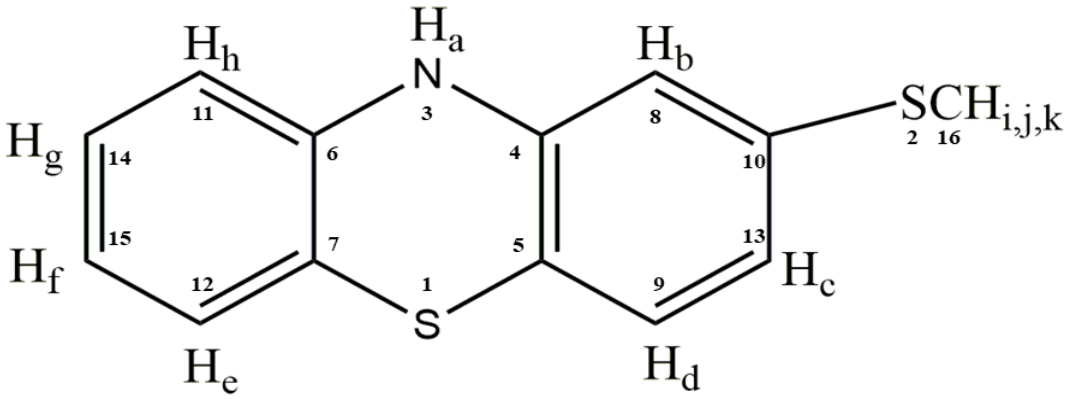


**Scheme S1**. Chemical structure of 2-Methyl Mercapto Phenothiazine. The numerals correspond to proton positions mentioned to in the 1HNMR analysis and the numerals correspond to other atoms positions mentioned to in the IR analysis.

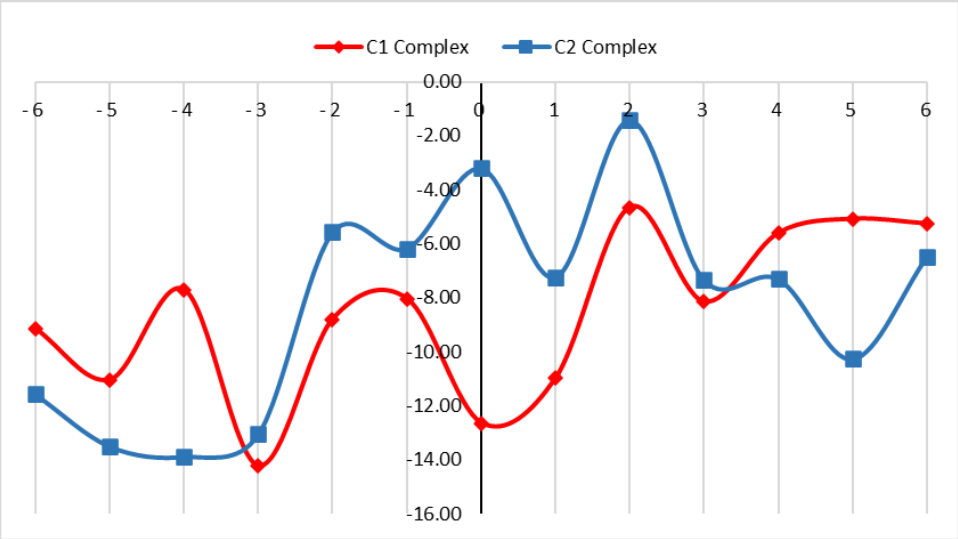


**Fig. 1S.** The variation of the binding energy for both complexes.

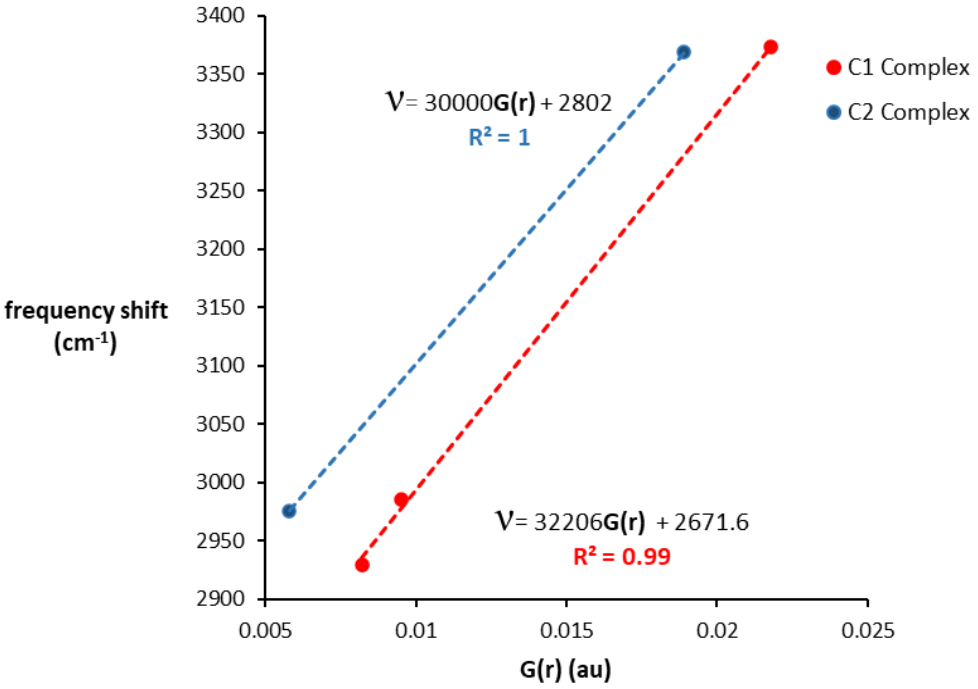


**Fig 2S.** The Frequency ($cm^{-1}$) shift as a function of kinetic energy density G(r) (au).

**Table 1S.** The optimized structures by B97-D3/6-31G(d,p) and BP86-D3/6-31G(d,p) methods in gas and in aqueous phases and intermolecular C-H…O distance for the both complexes.

| **B97-D3/6-31G(d,p) in gas phase for the two complexes** | | | |
|---|---|---|---|
| d(A°) | C1 | d(A°) | C2 |
| O(32) - H (237) | 2.4 | O(32) - H(234) | 2.6 |
| O(62) - H(238) | 2.4 | O(73) - H(236) | 2.6 |
| O(74) - H(234) | 2.4 | O(74) - H(237) | 2.7 |
| O(80) - H(236) | 2.8 | O(121) - H(234) | 2.1 |
| O(135) - H(244) | 2.6 | O(183) - H(244) | 2.2 |
| O(183) - H(240) | 2.6 | / | / |
| O(194) - H(241) | 2.8 | / | / |
| **BP86-D3/6-31G(d,p) in gas phase for the two complexes** | | | |
| d(A°) | C1 | d(A°) | C2 |
| O(32) - H(237) | 2.3 | O(73) - H(236) | 2.6 |
| O(62) - H(238) | 2.3 | O(74) - H(237) | 2.7 |
| O(74) - H(234) | 2.3 | O(96) - H(243) | 2.8 |
| O(80) - H(236) | 2.6 | O(106) - H(242) | 2.7 |
| O(135) - H(244) | 2.5 | O(121) - H(234) | 2.2 |
| O(183) - H(240) | 2.5 | / | / |
| O(194) - H(241) | 2.6 | / | / |
| **B97-D3/6-31G(d,p) in aqueous phase for the two complexes** | | | |
| d(A°) | C1 | d(A°) | C2 |
| O(62) - H(238) | 2.6 | O(32) - H(234) | 2.6 |
| O(22) - H(234) | 2.4 | O(73) - H(239) | 2.4 |
| O(80) - H(236) | 2.8 | O(121) - H(237) | 2.4 |
| O(133) - H(235) | 2.7 | / | / |
| O(135) - H(244) | 2.6 | / | / |
| O(183) - H(240) | 2.3 | / | / |
| O(194) - H(241) | 2.5 | / | / |
| **BP86-D3/6-31G(d,p) in aqueous phase for gas phase for the two complexes** | | | |
| d(A°) | C1 | d(A°) | C2 |
| O(22) - H(234) | 2.1 | O(32) - H(235) | 2.8 |
| O(80) - H(236) | 2.7 | O(73) - H(236) | 2.4 |
| O(85) - H(238) | 2.7 | O(74) - H(237) | 2.5 |
| O(96) - H(237) | 2.5 | O(115) - H(239) | 2.9 |
| O(133) - H(235) | 2.7 | O(121) - H(234) | 2.2 |
| O(135) - H(244) | 2.4 | | |
| O(183) - H(240) | 2.3 | / | / |
| O(194) - H(241) | 2.1 | / | / |

**Table 2S. a.** Condensed Fukui functions ($fk^+$, $f_k^-$) associated to the nucleophilic and electrophilic attacks, respectively for isoleted guest in aqueous phase.

| Atoms | $\rho_N(r)$ | $\rho_{N-1}(r)$ | $\rho_{N+1}(r)$ | $f^-(r)$ | $f^+(r)$ | $f°(r)$ | $\Delta f(r)$ |
|---|---|---|---|---|---|---|---|
| **S1** | **0.319** | **0.207** | **0.546** | **0.227** | **0.112** | **0.170** | **-0.115** |
| **S2** | **0.282** | **0.226** | **0.416** | **0.134** | **0.056** | **0.095** | **-0.078** |
| **N3** | **-0.590** | **-0.595** | **-0.493** | **0.097** | **0.005** | **0.051** | **-0.092** |
| **C4** | **0.159** | **0.086** | **0.179** | **0.020** | **0.073** | **0.047** | **0.053** |
| **C5** | **0.144** | **0.083** | **0.162** | **0.018** | **0.061** | **0.039** | **0.042** |
| **C6** | **-0.245** | **-0.310** | **-0.199** | **0.046** | **0.065** | **0.055** | **0.018** |
| **C7** | **-0.231** | **-0.307** | **-0.216** | **0.015** | **0.076** | **0.046** | **0.061** |
| **C8** | **-0.301** | **-0.314** | **-0.279** | **0.022** | **0.013** | **0.017** | **-0.009** |
| **C9** | **-0.242** | **-0.255** | **-0.230** | **0.012** | **0.013** | **0.012** | **0.001** |
| **C10** | **-0.197** | **-0.259** | **-0.181** | **0.016** | **0.062** | **0.039** | **0.046** |
| **C11** | **-0.276** | **-0.291** | **-0.248** | **0.029** | **0.014** | **0.022** | **-0.014** |
| **C12** | **-0.252** | **-0.269** | **-0.237** | **0.015** | **0.017** | **0.016** | **0.002** |
| **C13** | **-0.281** | **-0.359** | **-0.201** | **0.080** | **0.078** | **0.079** | **-0.003** |
| **C14** | **-0.246** | **-0.331** | **-0.213** | **0.033** | **0.085** | **0.059** | **0.053** |
| **C15** | **-0.269** | **-0.334** | **-0.217** | **0.052** | **0.065** | **0.059** | **0.014** |
| **C16** | **-0.873** | **-0.869** | **-0.881** | **-0.008** | **-0.004** | **0.006** | **0.004** |

**Table 2S. b.** Condensed Fukui functions ($fk^+$, $f_k^-$) associated to the nucleophilic and electrophilic attacks for guest in the two complexes C1/C2 in aqueous phase.

| Atoms | $\rho_N(r)$ C1/C2 | $\rho_{N-1}(r)$ C1/C2 | $\rho_{N+1}(r)$ C1/C2 | $f^-(r)$ C1/C2 | $f^+(r)$ C1/C2 | $f°(r)$ C1/C2 | $\Delta f(r)$ C1/C2 |
|---|---|---|---|---|---|---|---|
| **S1** | **0.332 / 0.331** | **0.227 / 0.248** | **0.563 / 0.564** | **0.232 / 0.233** | **0.105 / 0.083** | **0.168 / 0.158** | **-0.127 / -0.149** |
| **S2** | **0.211 / 0.269** | **0.135 / 0.203** | **0.313 / 0.375** | **0.103 / 0.107** | **0.075 / 0.066** | **0.089 / 0.086** | **-0.027 / -0.041** |
| **N3** | **-0.586 / -0.584** | **-0.592 / -0.586** | **-0.481 / -0.481** | **0.105 / 0.103** | **0.007 / 0.002** | **0.056 / 0.053** | **-0.098 / -0.101** |
| **C4** | **0.161 / 0.156** | **0.117 / 0.090** | **0.177 / 0.175** | **0.016 / 0.019** | **0.044 / 0.066** | **0.030 / 0.043** | **0.027 / 0.047** |
| **C5** | **0.141 / 0.142** | **0.087 / 0.077** | **0.164 / 0.162** | **0.023 / 0.020** | **0.054 / 0.066** | **0.038 / 0.043** | **0.031 / 0.046** |
| **C6** | **-0.238 / -0.238** | **-0.346 / -0.319** | **-0.204 / -0.201** | **0.034 / 0.038** | **0.108 / 0.081** | **0.071 / 0.059** | **0.074 / 0.043** |
| **C7** | **-0.234 / -0.229** | **-0.266 / -0.296** | **-0.212 / -0.211** | **0.021 / 0.018** | **0.033 / 0.068** | **0.027 / 0.043** | **0.011 / 0.050** |
| **C8** | **-0.280 / -0.295** | **-0.309 / -0.308** | **-0.248 / -0.268** | **0.032 / 0.027** | **0.029 / 0.014** | **0.031 / 0.020** | **-0.002 / -0.013** |
| **C9** | **-0.244 / -0.248** | **-0.280 / -0.263** | **-0.228 / -0.232** | **0.016 / 0.016** | **0.036 / 0.015** | **0.026 / 0.016** | **0.021 / -0.001** |
| **C10** | **-0.199 / -0.206** | **-0.296 / -0.284** | **-0.179 / -0.186** | **0.020 / 0.020** | **0.098 / 0.078** | **0.059 / 0.049** | **0.078 / 0.058** |
| **C11** | **-0.274 / -0.275** | **-0.290 / -0.289** | **-0.244 / -0.244** | **0.030 / 0.031** | **0.016 / 0.014** | **0.023 / 0.023** | **-0.014 / -0.018** |
| **C12** | **-0.250 / -0.256** | **-0.262 / -0.270** | **-0.236 / -0.238** | **0.015 / 0.018** | **0.012 / 0.014** | **0.013 / 0.016** | **-0.003 / -0.004** |
| **C13** | **-0.272 / -0.280** | **-0.328 / -0.355** | **-0.198 /-0.206** | **0.074 / 0.073** | **0.057 / 0.075** | **0.065 / 0.074** | **-0.017 / 0.002** |
| **C14** | **-0.246 / -0.249** | **-0.290 / -0.326** | **-0.210 / -0.214** | **0.035 / 0.036** | **0.045 / 0.077** | **0.040 / 0.056** | **0.010 / 0.042** |
| **C15** | **-0.267 / -0.269** | **-0.325 / -0.337** | **-0.209 / -0.215** | **0.058 / 0.054** | **0.058 / 0.069** | **0.058 / 0.061** | **0.000 / 0.015** |
| **C16** | **-0.848 / -0.869** | **-0.857 / -0.867** | **-0.851 / -0.873** | **-0.003 / -0.005** | **0.009 / -0.002** | **0.003 / 0.003** | **0.012 / 0.003** |

**Table 3S. a.** Condensed Fukui functions ($fk^+$, $f_k^-$) associated to the nucleophilic and electrophilic attacks, respectively for isoleted guest in gas phase

| Atoms | $\rho_N(r)$ | $\rho_{N-1}(r)$ | $\rho_{N+1}(r)$ | $f$-(r) | $f^+(r)$ | $f°(r)$ | $\Delta f(r)$ |
|---|---|---|---|---|---|---|---|
| S1 | 0.346 | 0.250 | 0.558 | 0.211 | 0.096 | 0.154 | -0.115 |
| S2 | 0.312 | 0.242 | 0.471 | 0.158 | 0.071 | 0.115 | -0.088 |
| N3 | -0.584 | -0.584 | -0.504 | 0.080 | 0.000 | 0.04 | -0.080 |
| C4 | 0.163 | 0.100 | 0.176 | 0.013 | 0.063 | 0.038 | 0.050 |
| C5 | 0.149 | 0.097 | 0.158 | 0.010 | 0.052 | 0.031 | 0.042 |
| C6 | -0.237 | -0.291 | -0.205 | 0.032 | 0.054 | 0.043 | 0.022 |
| C7 | -0.222 | -0.285 | -0.220 | 0.002 | 0.063 | 0.033 | 0.061 |
| C8 | -0.302 | -0.309 | -0.288 | 0.014 | 0.006 | 0.010 | -0.008 |
| C9 | -0.234 | -0.240 | -0.226 | 0.008 | 0.007 | 0.007 | -0.001 |
| C10 | -0.192 | -0.255 | -0.183 | 0.009 | 0.063 | 0.036 | 0.054 |
| C11 | -0.275 | -0.285 | -0.252 | 0.023 | 0.010 | 0.017 | -0.014 |
| C12 | -0.243 | -0.254 | -0.230 | 0.013 | 0.010 | 0.012 | -0.003 |
| C13 | -0.271 | -0.348 | -0.197 | 0.074 | 0.077 | 0.075 | 0.003 |
| C14 | -0.241 | -0.323 | -0.200 | 0.041 | 0.082 | 0.062 | 0.042 |
| C15 | -0.261 | -0.328 | -0.207 | 0.054 | 0.067 | 0.060 | 0.012 |
| C16 | -0.876 | -0.868 | -0.888 | -0.012 | -0.008 | 0.010 | 0.005 |

**Table 3S.b**. Condensed Fukui functions (fk+, fk−) associated to the nucleophilic and electrophilic attacks for guest in the two complexes C1/C2 in gas phase.

| Atoms | $\rho_N(r)$ | $\rho_{N-1}(r)$ | $\rho_{N+1}(r)$ | $f^-(r)$ | $f^+(r)$ | $f°(r)$ | $\Delta f(r)$ |
|---|---|---|---|---|---|---|---|
| S1 | **0.335 / 0.352** | **0.244 / 0.260** | **0.562 / 0.562** | **0.227 / 0.210** | **0.09 / 0.092** | **0.159 / 0.151** | **-0.137 / -0.118** |
| S2 | **0.256 / 0.286** | **0.163 / 0.204** | **0.427 / 0.427** | **0.169 / 0.142** | **0.096 / 0.082** | **0.132 / 0.112** | **-0.073 / -0.060** |
| N3 | **-0.604 / -0.578** | **-0.611 / -0.577** | **-0.497 / -0.497** | **0.107 / 0.081** | **0.007 / -0.001** | **0.057 / 0.040** | **-0.100 / -0.082** |
| C4 | **0.162 / 0.157** | **0.164 / 0.114** | **0.167 / 0.167** | **0.006 / 0.010** | **-0.002 / 0.043** | **0.002 / 0.027** | **-0.008 / 0.033** |
| C5 | **0.146 / 0.142** | **0.124 / 0.102** | **0.164 / 0.164** | **0.018 / 0.011** | **0.023 / 0.052** | **0.021 / 0.032** | **0.005 / 0.041** |
| C6 | **-0.230 / -0.227** | **-0.299 / -0.295** | **-0.203 / -0.203** | **0.026 / 0.024** | **0.069 / 0.068** | **0.048 / 0.046** | **0.043 / 0.044** |
| C7 | **-0.218 / -0.225** | **-0.211 / -0.279** | **-0.219 / -0.219** | **-0.001 / 0.007** | **-0.007 / 0.054** | **0.004 / 0.030** | **-0.006 / 0.047** |
| C8 | **-0.286 / -0.285** | **-0.349 / -0.295** | **-0.267 / -0.267** | **0.020 / 0.018** | **0.062 / 0.010** | **0.041 / 0.014** | **0.043 / -0.008** |
| C9 | **-0.233 / -0.239** | **-0.298 / -0.252** | **-0.228 / -0.228** | **0.005 / 0.012** | **0.065 / 0.012** | **0.035 / 0.012** | **0.06 / 0.001** |
| C10 | **-0.190 / -0.223** | **-0.266 / -0.279** | **-0.188 / -0.188** | **0.002 / 0.015** | **0.075 / 0.076** | **0.039 / 0.046** | **0.073 / 0.060** |
| C11 | **-0.267 / -0.278** | **-0.339 / -0.289** | **-0.250 / -0.250** | **0.017 / 0.038** | **0.073 / 0.011** | **0.045 / 0.020** | **0.056 / -0.017** |
| C12 | **-0.238 / -0.247** | **-0.309 / -0.257** | **-0.234 / -0.234** | **0.004 / 0.013** | **0.071 / 0.010** | **0.038 / 0.012** | **0.067 / -0.004** |
| C13 | **-0.265 / -0.265** | **-0.277 / -0.327** | **-0.198 /-0.198** | **0.068 / 0.068** | **0.011 / 0.061** | **0.040 / 0.067** | **-0.056 / -0.006** |
| C14 | **-0.240 / -0.242** | **-0.262 / -0.314** | **-0.202 / -0.202** | **0.038 / 0.040** | **0.022 / 0.072** | **0.030 / 0.056** | **-0.016 / 0.032** |
| C15 | **-0.257 / -0.263** | **-0.301 / -0.325** | **-0.203 / -0.203** | **0.054 / 0.060** | **0.044 / 0.062** | **0.049 / 0.061** | **-0.010 / 0.002** |
| C16 | **-0.855 / -0.865** | **-0.867 / -0.866** | **-0.872 / -0.872** | **-0.018 / -0.007** | **0.012 / 0.001** | **0.003 / 0.003** | **0.029 / 0.008** |

**Table 4S.** The calculated excitation energies, oscillator strength (*f*) and wavelength (λ) and configurations of excitations.

| | **λ(nm)** | **E(eV)** | ***f*** | **Configuration** |
|---|---|---|---|---|
| **C1 complex** | 492.51 | 2.9414 | 0.0078 | H - 1 → L (97.24%) |
| | 368.95 | 3.3605 | 0.0599 | H-3 → L (4.10%) |
| | | | | H → L+1 (97.24%) |
| **C2 complex** | 410.59 | 3.0196 | 0.0046 | H → L (96.97%) |
| | 387.30 | 3.2013 | 0.0721 | H-1 → L (7.47%) |
| | | | | H → L+1 (89.72%) |
| | 362.81 | 3.4174 | 0.0549 | H → L+1 (90.53%) |

**Table 5S**. Experimental and calculated of Wave numbers ($cm^{-1}$) and assignments for the bands observed in the FTIR spectra of 2MMPT, HPβ-CD and 2MMPT@HBCD inclusion complexes.

| Peak assignments | Wave numbers ($cm^{-1}$) | | | | | | |
|---|---|---|---|---|---|---|---|
| | **2MMPT calculated** | **2MMPT experimental** | **HPβ-CD calculated** | **HPβ-CD experimental** | **C1 calculated** | **C2 calculated** | **2MMPT@HPβCD experimental** |
| **Aromatic O-H stretching** | / | / | 3398 | 3404 | 3430 | 3435 | / |
| **Aromatic C-H stretching** | 2982 | 2925 | 2950 | 2931 | 2960 | 2952 | 2928 |
| **Aromatic C-O stretching** | / | / | 1120 | 1160 | 1121 | 1122 | / |
| **Aromatic C=C stretching** | 1453 | 1468 | / | / | 1457 | 1462 | 1466 |
| **Aromatic C-C stretching** | 1423 | 1425 | 1378 | 1370 | 1424 | 1424 | 1424 |
| **Aromatic C-H bending** | 900 | 802 | 921 | / | 920 | 920 | / |
| **Aromatic C-N stretching** | 1335 | 1309 | / | / | 1337 | 1333 | / |
| **Aromatic N-H stretching** | 3500 | 3384 | / | / | 3373 | 3369 | 3393 |
| **Aromatic N-H bending** | 1584 | 1590 | / | / | 1590 | 1570 | 1642 |
| **Aromatic C-S stretching** | 550 | 594 | / | / | 536 | 523 | / |
| **Aliphatic C-S-$CH_3$ stretching** | 690 | 615 | / | / | 665 | 706 | 615 |

**Table 6S.** The EDA analysis at functional BP86-D3/6-31G(d,p) for the both complexes.

| Å | $\Delta E_{Pauli}$ | $\Delta E_{Elstat}$ | $\Delta E_{Orb}$ | $\Delta E_{Disp}$ | $\Delta E_{Total\ Bonding}$ |
|---|---|---|---|---|---|
| **C1 Complex** | | | | | |
| **6** | 2459.37 | -26728.69 | -2115.08 | -298.83 | -26683.23 |
| **5** | 2454.28 | -26732.76 | -2278.46 | -300.54 | -26857.48 |
| **4** | 2450.91 | -26718.74 | -2270.58 | -292.88 | -26831.29 |
| **3** | 2448.68 | -26705.61 | -2273.07 | -294.69 | -26824.69 |
| **2** | 2474.15 | -26757.11 | -2215.30 | -315.71 | -26813.97 |
| **1** | 2470.94 | -26765.77 | -2167.82 | -313.71 | -26776.36 |
| **0** | 2468.60 | -26727.19 | -2179.23 | -309.82 | -26747.64 |
| **-1** | 2448.64 | -26700.56 | -2345.36 | -290.80 | -26888.08 |
| **-2** | 2468.31 | -26722.32 | -2172.67 | -307.49 | -26734.17 |
| **-3** | 2470.84 | -26731.38 | -2183.06 | -312.46 | -26756.06 |
| **-4** | 2475.48 | -26731.85 | -2165.12 | -312.21 | -26733.7 |
| **-5** | 2464.34 | -26734.20 | -2174.28 | -307.38 | -26751.52 |
| **-6** | 2463.42 | -26718.62 | -2207.64 | -304.49 | -26767.33 |
| **C2 Complex** | | | | | |
| **6** | 2439.21 | -26702.09 | -2347.90 | -284.76 | -26895.54 |
| **5** | 2438.63 | -26709.98 | -2307.15 | -287.38 | -26865.88 |
| **4** | 2426.62 | -26683.60 | -2425.12 | -277.32 | -26959.42 |
| **3** | 2447.55 | -26727.71 | -2320.42 | -292.21 | -26892.79 |
| **2** | 2461.39 | -26706.51 | -2313.99 | -299.74 | -26858.85 |
| **1** | 2462.01 | -26729.10 | -2263.70 | -306.23 | -26837.02 |
| **0** | 2474.42 | -26726.47 | -2148.36 | -313.60 | -26714.01 |
| **-1** | 2469.86 | -26719.15 | -2268.07 | -309.50 | -26826.86 |
| **-2** | 2460.83 | -26722.59 | -2259.02 | -303.85 | -26824.63 |
| **-3** | 2458.61 | -26721.30 | -2247.54 | -301.99 | -26812.22 |
| **-4** | 2461.62 | -26727.34 | -2221.97 | -304.79 | -26792.48 |
| **-5** | 2457.51 | -26722.57 | -2230.32 | -302.33 | -26797.71 |
| **-6** | 2471.13 | -26741.01 | -2182.99 | -310.91 | -26763.78 |