

Redox-Triggered Switching of Conformational State in Triple-Decker Lanthanide Phthalocyaninates

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ELECTRONIC SUPPORTING INFORMATION

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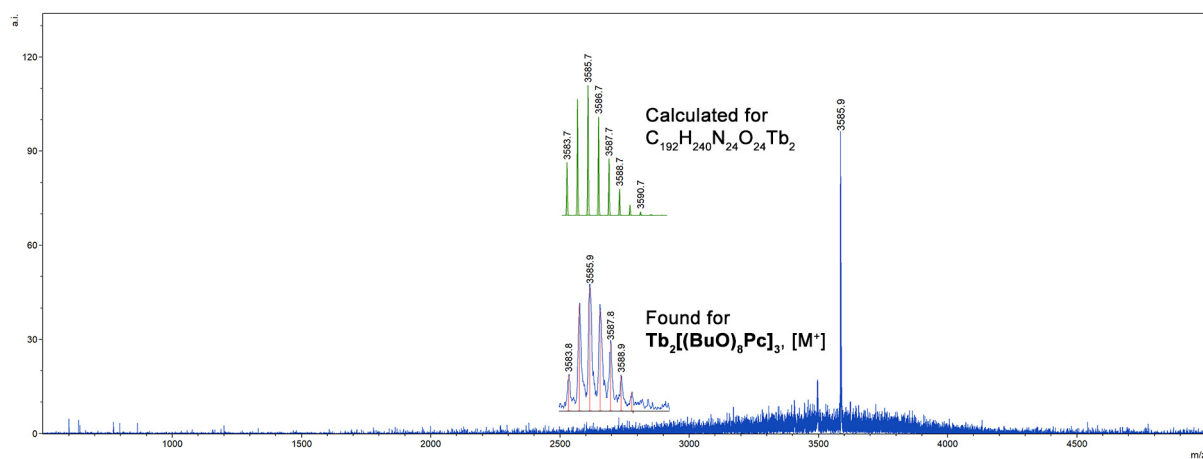


Figure S1. MALDI TOF mass-spectrum of $\text{Tb}_2[(\text{BuO})_8\text{Pc}]_3$.

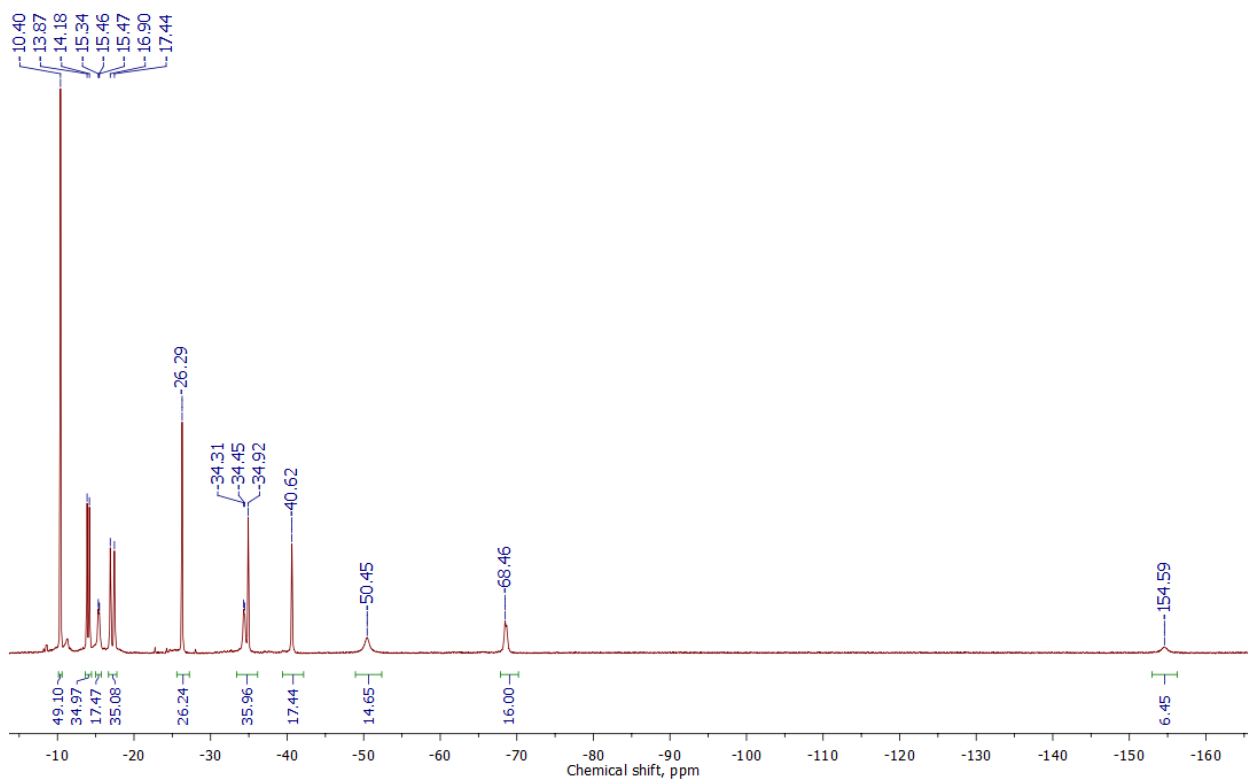


Figure S2. ^1H -NMR spectrum of $\text{Tb}_2[(\text{BuO})_8\text{Pc}]_3$ in CDCl_3 .

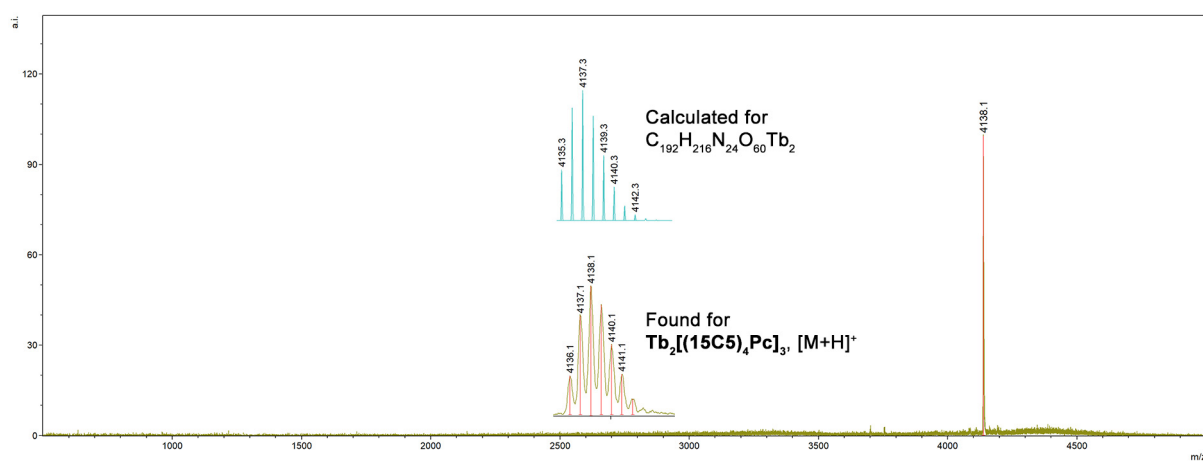


Figure S3. MALDI TOF mass-spectrum of $Tb_2[(15C5)_4Pc]_3$

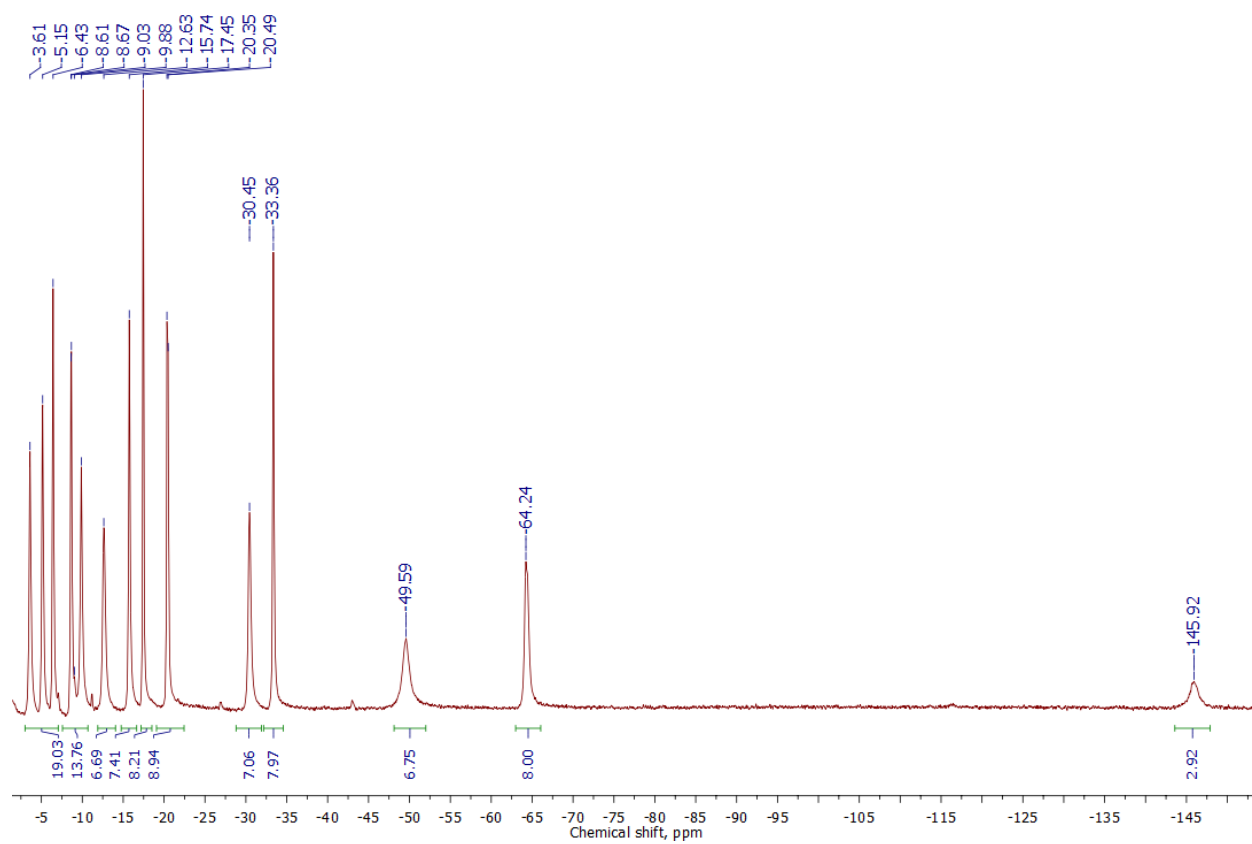


Figure S4. 1H -NMR spectrum of $Tb_2[(15C5)_4Pc]_3$ in $CDCl_3$.

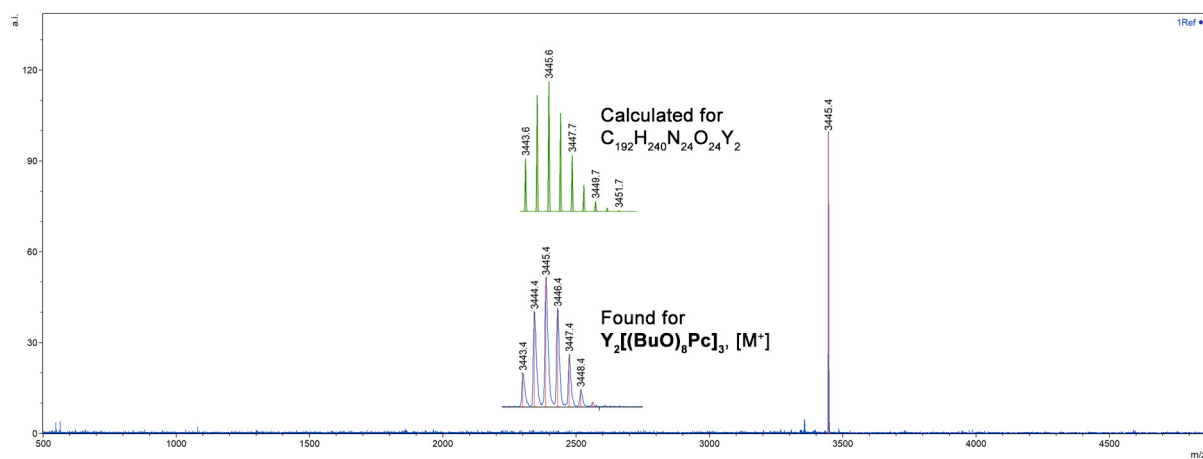


Figure S5. MALDI TOF mass-spectrum of $Y_2[(BuO)_8Pc]_3$.

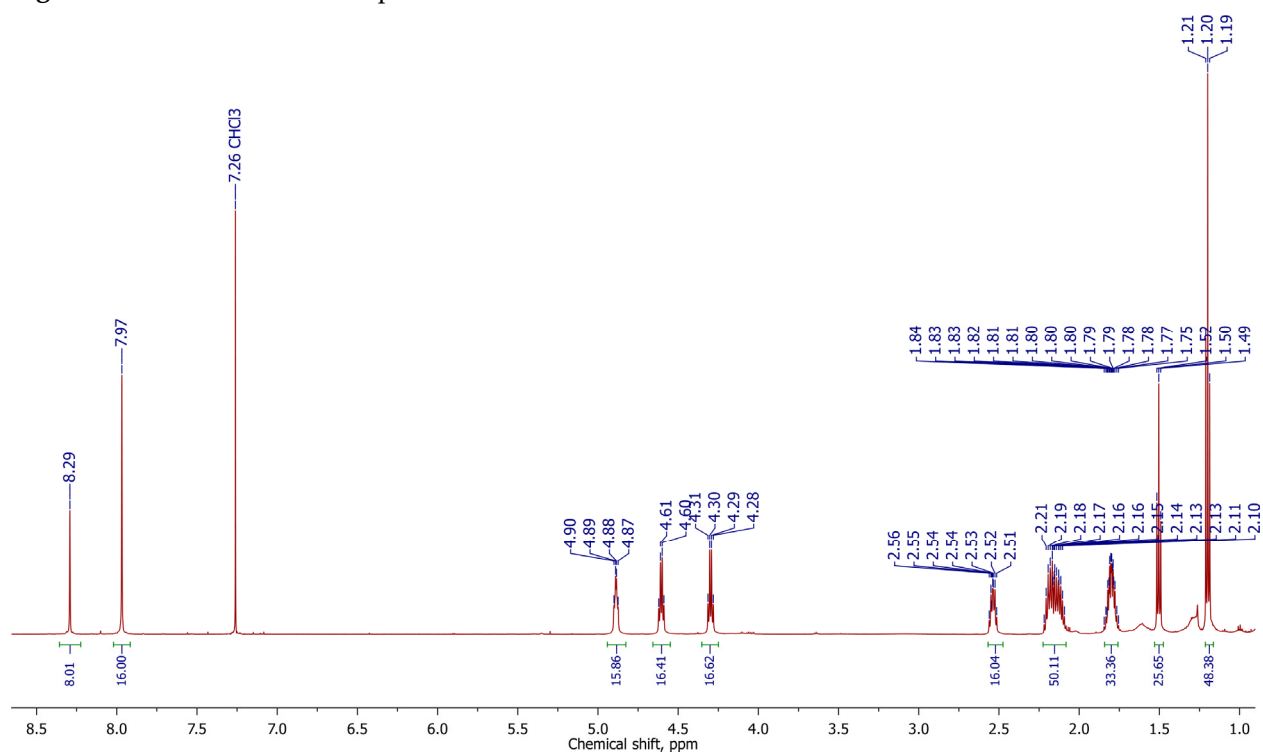


Figure S6. 1H -NMR spectrum of $Y_2[(BuO)_8Pc]_3$ in $CDCl_3$.

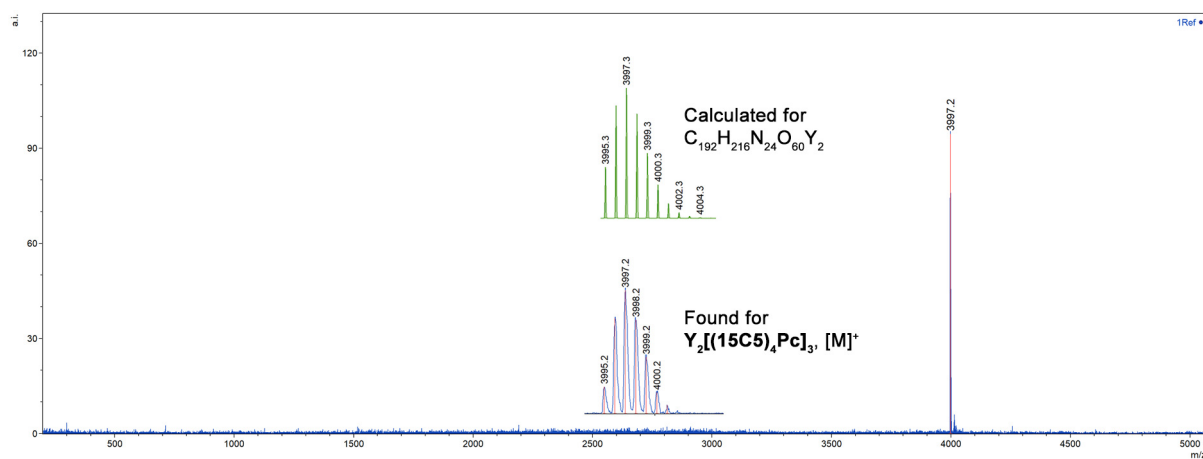


Figure S7. MALDI TOF mass-spectrum of $Y_2[(15C5)_4Pc]_3$.

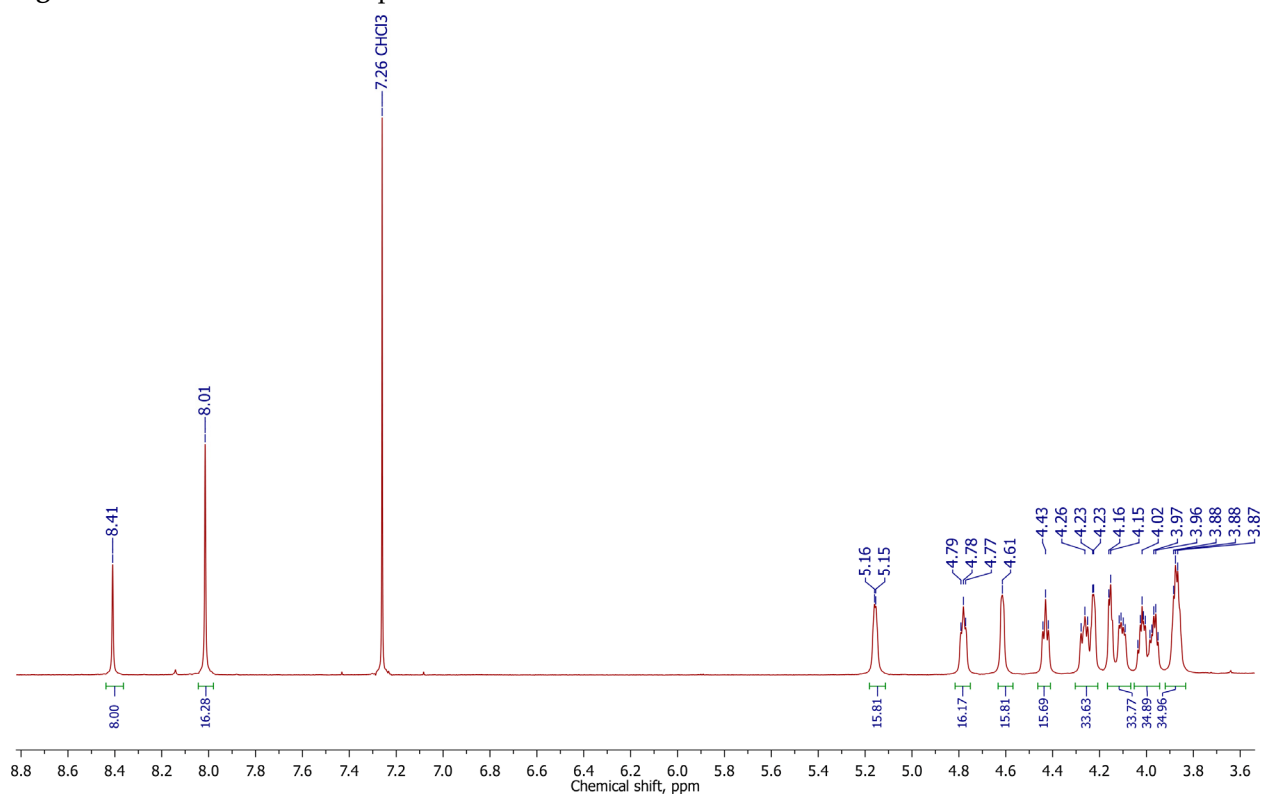


Figure S8. 1H -NMR spectrum of $Y_2[(15C5)_4Pc]_3$ in $CDCl_3$.

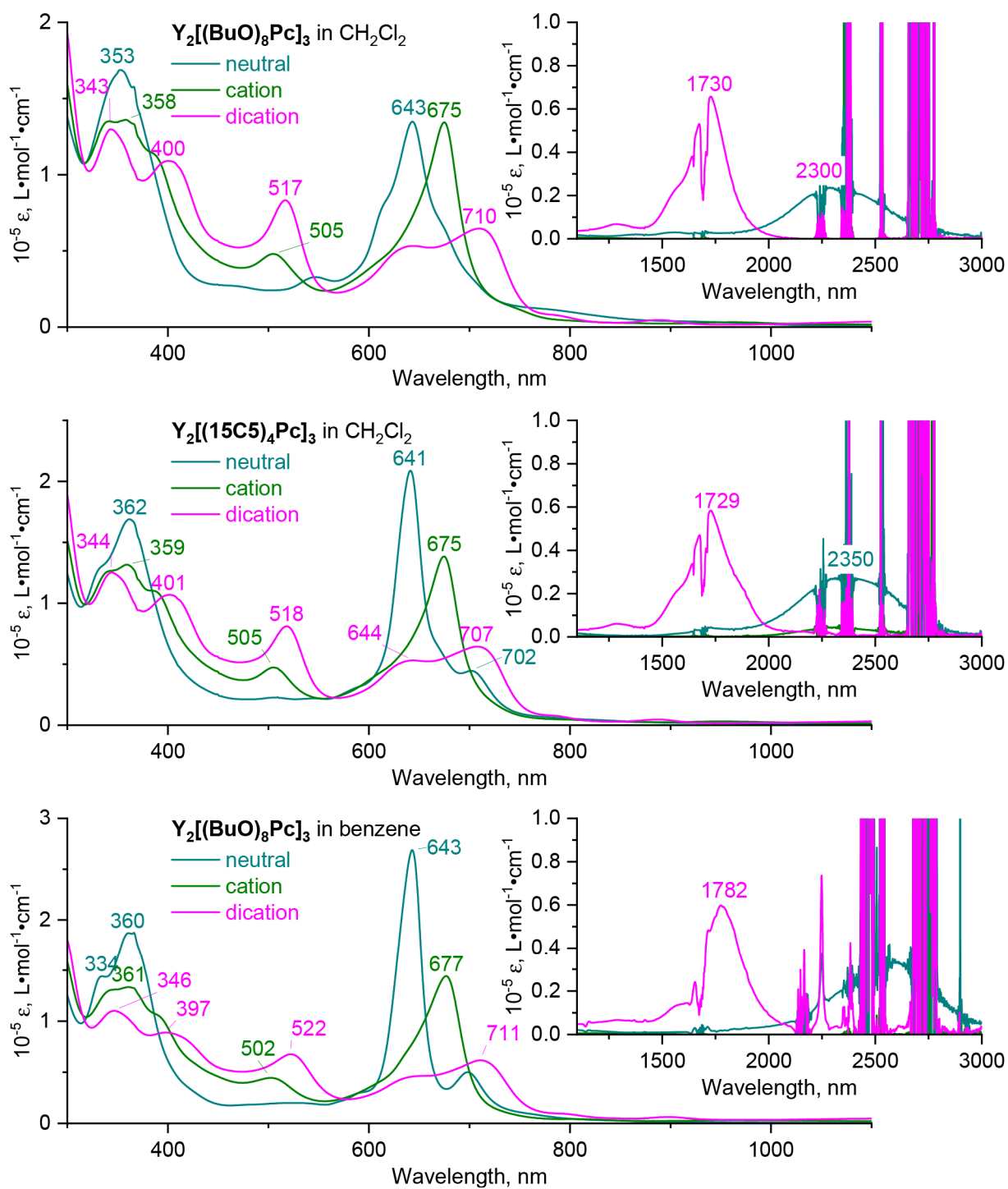


Figure S9. UV-vis-NIR spectra of neutral forms of $\text{Y}_2[(\text{BuO})_8\text{Pc}]_3$ and $\text{Y}_2[(15\text{C}5)_4\text{Pc}]_3$ and their mono- and dicationic forms, obtained by 1e- and 2e-oxidation with OxSbCl_6 .

Table S1. The calculated UV-vis-NIR absorption spectrum of **s-Y₂[(MeO)₈Pc]₃** for the BP86/def2-SVP geometry calculated by the sTDA method at the CAM-B3LYP/6-31G(d) level of theory.

| Wavelength, nm | Energy, eV | F _{osc.} ⁽¹⁾ | Wavefunction ^(2,3) |
|----------------|------------|----------------------------------|--|
| 932.4 | 1.33 | 0.06 | -0.83 H→L+5; 0.36 H-2→L; 0.32 H-2→L+1; ... |
| 932.4 | 1.33 | 0.06 | 0.83 H→L+4; -0.36 H-2→L+1; 0.32 H-2→L; ... |
| 654.0 | 1.90 | 0.01 | -0.67 H-1→L+2; -0.43 H-1→L+3; 0.4 H-2→L; ... |
| 654.0 | 1.90 | 0.01 | -0.67 H-1→L+3; 0.43 H-1→L+2; -0.4 H-2→L+1; ... |
| 579.5 | 2.14 | 1.35 | 0.49 H-2→L+1; -0.39 H-1→L+3; -0.37 H-1→L+2; ... |
| 579.5 | 2.14 | 1.35 | 0.49 H-2→L; 0.39 H-1→L+2; -0.37 H-1→L+3; ... |
| 527.0 | 2.35 | 0.12 | 0.9 H-3→L; 0.25 H-7→L; -0.21 H-17→L; ... |
| 526.9 | 2.35 | 0.12 | 0.9 H-3→L+1; 0.25 H-7→L+1; -0.21 H-17→L+1; ... |
| 473.3 | 2.62 | 0.03 | -0.77 H-8→L; -0.4 H-7→L; -0.35 H-8→L+1; ... |
| 473.3 | 2.62 | 0.03 | -0.77 H-8→L+1; 0.4 H-7→L+1; 0.35 H-8→L; ... |
| 457.3 | 2.71 | 0.01 | 0.55 H-11→L+1; 0.55 H-10→L; 0.42 H-10→L+1; ... |
| 447.9 | 2.77 | 0.06 | 0.93 H-12→L; 0.26 H-7→L; -0.17 H-7→L+1; ... |
| 447.9 | 2.77 | 0.06 | 0.93 H-12→L+1; -0.26 H-7→L+1; -0.17 H-7→L; ... |
| 427.3 | 2.90 | 0.01 | -0.96 H-2→L+5; -0.12 H-3→L+1; 0.08 H-27→L+1; ... |
| 427.3 | 2.90 | 0.01 | 0.96 H-2→L+4; -0.12 H-3→L; 0.08 H-27→L; ... |

⁽¹⁾ Excitations with oscillator strength, F_{osc.} above 0.01 are shown.

⁽²⁾ Only contributions of greater than 10% are consistently included.

⁽³⁾ H stands for HOMO, L stands for LUMO

Table S2. The calculated UV-vis-NIR absorption spectrum of $s\text{-Y}_2[(\text{MeO})_8\text{Pc}]_3^+$ for the BP86/def2-SVP geometry calculated by the sTDA method at the CAM-B3LYP/6-31G(d) level of theory.

| Wavelength, nm | Energy, eV | $F_{\text{osc.}}^{(1)}$ | Wavefunction ⁽²⁾ |
|----------------|------------|-------------------------|--|
| 2491.8 | 0.50 | 0.22 | -1 bH→bL; -0.02 aH-17→bL+6; -0.02 aH-18→bL+5; ... |
| 842.5 | 1.47 | 0.03 | -0.65 bH-2→bL; 0.52 bH-1→bL+1; 0.48 bH→bL+5; ... |
| 842.5 | 1.47 | 0.03 | 0.65 bH-2→bL+1; -0.52 bH-1→bL+2; -0.48 bH→bL+4; ... |
| 795.2 | 1.56 | 0.03 | -0.49 bH-1→bL+1; 0.49 bH→bL+3; 0.48 bH→bL+4; ... |
| 795.2 | 1.56 | 0.03 | 0.49 bH-1→bL+2; 0.49 bH→bL+4; -0.48 bH→bL+3; ... |
| 662.7 | 1.87 | 0.01 | -0.59 bH-1→bL+2; 0.48 bH-2→bL+1; 0.39 bH-3→bL; ... |
| 662.7 | 1.87 | 0.01 | 0.59 bH-1→bL+3; -0.48 bH-2→bL; 0.39 bH-3→bL+1; ... |
| 623.9 | 1.99 | 0.66 | -0.48 bH-1→bL+3; -0.36 aH-12→bL; -0.35 bH-2→bL; ... |
| 623.9 | 1.99 | 0.66 | -0.48 bH-1→bL+2; 0.36 aH-13→bL; -0.35 bH-2→bL+1; ... |
| 596.0 | 2.08 | 0.10 | 0.85 bH-5→bL; 0.19 bH-3→bL; 0.17 bH-3→bL+1; ... |
| 596.0 | 2.08 | 0.10 | -0.85 bH-4→bL; -0.19 bH-3→bL+1; 0.17 bH-3→bL; ... |
| 564.7 | 2.20 | 0.03 | 0.65 aH-9→bL; 0.48 bH-3→bL; -0.26 aH-8→bL+1; ... |
| 564.7 | 2.20 | 0.03 | 0.65 aH-9→bL+1; 0.48 bH-3→bL+1; -0.26 aH-8→bL; ... |
| 543.3 | 2.28 | 0.21 | -0.57 bH-2→bL+1; 0.44 aH-9→bL; 0.33 aH-11→bL+1; ... |
| 543.3 | 2.28 | 0.21 | 0.57 bH-2→bL+2; -0.44 aH-9→bL+1; -0.33 aH-11→bL+2; ... |
| 535.5 | 2.32 | 0.01 | 0.53 aH-11→bL; -0.52 aH-10→bL+1; -0.43 aH-11→bL+1; ... |
| 526.4 | 2.36 | 0.15 | -0.46 bH-2→bL+2; -0.44 aH-12→bL; -0.36 aH-13→bL; ... |
| 526.4 | 2.36 | 0.15 | -0.46 bH-2→bL+1; -0.44 aH-13→bL; 0.36 aH-12→bL; ... |
| 515.1 | 2.41 | 0.01 | 0.41 bH-7→bL+1; -0.41 aH-11→bL+2; 0.34 aH-14→bL+1; ... |
| 515.1 | 2.41 | 0.01 | 0.41 aH-11→bL+1; -0.41 bH-7→bL+2; 0.34 aH-14→bL; ... |
| 508.4 | 2.44 | 0.03 | 0.52 aH-14→bL+1; 0.43 aH-14→bL; -0.42 bH-7→bL+1; ... |
| 508.4 | 2.44 | 0.03 | 0.52 aH-14→bL; -0.43 aH-14→bL+1; 0.42 bH-7→bL+2; ... |
| 503.1 | 2.46 | 0.02 | -0.47 aH-11→bL+1; -0.45 bH-7→bL+2; -0.38 aH-11→bL+2; ... |
| 503.1 | 2.47 | 0.02 | 0.47 aH-11→bL+2; 0.45 bH-7→bL+1; -0.38 aH-11→bL+1; ... |
| 491.7 | 2.52 | 0.01 | -0.51 aH-10→bL+1; 0.51 aH-9→bL+2; 0.44 aH-10→bL+2; ... |
| 461.2 | 2.69 | 0.09 | -0.9 aH-14→bL+1; 0.3 aH-14→bL; -0.19 aH-13→bL; ... |
| 461.2 | 2.69 | 0.09 | 0.9 aH-14→bL+2; -0.3 aH-14→bL+1; -0.19 aH-12→bL; ... |
| 427.7 | 2.90 | 0.01 | 0.51 aH-16→bL; 0.49 aH-19→bL+1; -0.28 aH-22→bL+2; ... |
| 427.7 | 2.90 | 0.01 | -0.51 aH-15→bL; 0.49 aH-19→bL; -0.28 aH-22→bL+1; ... |
| 422.6 | 2.93 | 0.02 | -0.55 bH-4→bL+2; -0.31 bH-4→bL+3; 0.3 aH-8→bL+4; ... |
| 422.6 | 2.93 | 0.02 | 0.55 bH-4→bL+3; -0.31 bH-4→bL+2; -0.3 aH-8→bL+5; ... |
| 417.2 | 2.97 | 0.26 | 0.57 aH-16→bL; -0.5 aH-19→bL+1; 0.34 aH-15→bL; ... |
| 417.2 | 2.97 | 0.26 | -0.57 aH-15→bL; -0.5 aH-19→bL; 0.34 aH-16→bL; ... |
| 409.2 | 3.03 | 0.04 | -0.58 bH-2→bL+4; -0.52 bH-1→bL+5; 0.28 bH-3→bL+5; ... |

| | | | |
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| 409.2 | 3.03 | 0.04 | 0.58 bH-2→bL+5; 0.52 bH-1→bL+6; 0.28 bH-3→bL+4; ... |
| 402.4 | 3.08 | 0.13 | -0.33 bH-4→bL+3; -0.33 bH-7→bL+3; -0.32 bH-3→bL+5; ... |
| 402.4 | 3.08 | 0.13 | 0.33 bH-4→bL+2; -0.32 bH-7→bL+2; -0.32 bH-3→bL+4; ... |
| 401.2 | 3.09 | 0.01 | -0.52 bH-5→bL+2; -0.52 bH-6→bL+3; -0.24 bH-5→bL+3; ... |

⁽¹⁾ Excitations with oscillator strength, F_{osc} , above 0.01 are shown.

⁽²⁾ H stands for HOMO, L stands for LUMO

Table S3. The calculated UV-vis-NIR absorption spectrum of **s-Y₂[(MeO)₈Pc]₃²⁺** for the BP86/def2-SVP geometry calculated by the sTDA method at the CAM-B3LYP/6-31G(d) level of theory.

| Wavelength, nm | Energy, eV | F _{osc.} ⁽¹⁾ | Wavefunction ⁽²⁾ |
|----------------|------------|----------------------------------|---|
| 1616.0 | 0.77 | 0.74 | -0.99 H→L; 0.03 H-8→L+2; -0.03 H-9→L+1 |
| 748.1 | 1.66 | 0.01 | -0.56 H-1→L+1; -0.52 H→L+3; -0.48 H→L+4 |
| 748.1 | 1.66 | 0.01 | -0.56 H-1→L+2; -0.52 H→L+4; 0.48 H→L+3 |
| 701.8 | 1.77 | 0.42 | 0.58 H→L+4; -0.57 H-1→L+2; -0.33 H-12→L |
| 701.8 | 1.77 | 0.42 | 0.58 H→L+3; -0.57 H-1→L+1; -0.33 H-11→L |
| 691.4 | 1.79 | 0.01 | -0.94 H-6→L; 0.17 H-12→L; -0.11 H→L+3 |
| 603.9 | 2.05 | 0.03 | -0.87 H-2→L+1; 0.37 H-10→L+1; 0.2 H-1→L+2 |
| 603.9 | 2.05 | 0.03 | 0.87 H-2→L+2; -0.37 H-10→L+2; 0.2 H-1→L+1 |
| 579.7 | 2.14 | 0.02 | -0.67 H-7→L+1; -0.38 H-11→L; -0.37 H-10→L+1 |
| 579.7 | 2.14 | 0.02 | -0.67 H-7→L+2; 0.38 H-12→L; 0.37 H-10→L+2 |
| 570.2 | 2.17 | 0.42 | -0.49 H-10→L+2; -0.47 H-10→L+1; -0.33 H-7→L+2 |
| 570.2 | 2.17 | 0.42 | -0.49 H-10→L+1; 0.47 H-10→L+2; 0.33 H-7→L+1 |
| 568.3 | 2.18 | 0.21 | -0.64 H-11→L; 0.53 H-7→L+1; 0.25 H-10→L+2 |
| 568.3 | 2.18 | 0.21 | 0.64 H-12→L; 0.53 H-7→L+2; 0.25 H-10→L+1 |
| 558.5 | 2.22 | 0.02 | -0.58 H-9→L+1; 0.58 H-8→L+2; 0.39 H-9→L+2 |
| 501.5 | 2.47 | 0.10 | 0.95 H-13→L+2; -0.15 H-11→L; -0.13 H-13→L+1 |
| 501.5 | 2.47 | 0.10 | 0.95 H-13→L+1; -0.15 H-12→L; 0.13 H-13→L+2 |
| 445.5 | 2.78 | 0.45 | 0.8 H-15→L; -0.47 H-14→L; 0.12 H-21→L+2 |
| 445.5 | 2.78 | 0.45 | -0.8 H-14→L; -0.47 H-15→L; -0.12 H-21→L+1 |
| 404.8 | 3.06 | 0.01 | 0.76 H-4→L+3; 0.29 H-3→L+4; -0.27 H-7→L+6 |
| 404.8 | 3.06 | 0.01 | -0.76 H-4→L+4; -0.29 H-3→L+3; 0.27 H-7→L+5 |

⁽¹⁾ Excitations with oscillator strength, F_{osc.} above 0.01 are shown.

⁽²⁾ H stands for HOMO, L stands for LUMO

Table S4. The calculated UV-vis-NIR absorption spectrum of **g-Y₂[(MeO)₈Pc]₃** for the BP86/def2-SVP geometry calculated by the sTDA method at the CAM-B3LYP/6-31G(d) level of theory.

| Wavelength, nm | Energy, eV | F _{osc.} ⁽¹⁾ | Wavefunction ⁽²⁾ |
|----------------|------------|----------------------------------|---|
| 1613.3 | 0.77 | 0.02 | -0.97 H→L; -0.18 H→L+5; 0.06 H→L+4 |
| 1613.2 | 0.77 | 0.02 | -0.97 H→L+1; -0.18 H→L+4; -0.06 H→L+5 |
| 1052.5 | 1.18 | 0.03 | 0.87 H-2→L; -0.37 H-1→L; 0.15 H-1→L+5 |
| 1052.5 | 1.18 | 0.03 | 0.87 H-2→L+1; -0.37 H-1→L+1; 0.15 H-1→L+4 |
| 807.6 | 1.54 | 0.01 | 0.66 H-2→L+3; -0.63 H-1→L+3; 0.29 H→L+2 |
| 807.6 | 1.54 | 0.01 | -0.66 H-2→L+2; 0.63 H-1→L+2; 0.29 H→L+3 |
| 709.2 | 1.75 | 0.03 | -0.66 H→L+2; -0.61 H→L+3; -0.22 H-1→L+3 |
| 709.2 | 1.75 | 0.03 | -0.66 H→L+3; 0.61 H→L+2; 0.22 H-1→L+2 |
| 686.8 | 1.81 | 0.10 | -0.53 H→L+5; 0.49 H-2→L+4; -0.46 H-1→L+4 |
| 686.8 | 1.81 | 0.10 | 0.53 H→L+4; 0.49 H-2→L+5; -0.46 H-1→L+5 |
| 577.5 | 2.15 | 0.24 | 0.74 H-1→L+5; -0.3 H-1→L+4; 0.27 H-2→L+5 |
| 577.5 | 2.15 | 0.24 | -0.74 H-1→L+4; -0.3 H-1→L+5; -0.27 H-2→L+4 |
| 550.4 | 2.25 | 0.82 | 0.67 H-2→L+4; 0.3 H→L+5; 0.28 H-2→L+5 |
| 550.4 | 2.25 | 0.82 | -0.67 H-2→L+5; 0.3 H→L+4; 0.28 H-2→L+4 |
| 526.2 | 2.36 | 0.01 | -0.92 H-3→L+1; 0.21 H-6→L+1; -0.19 H-3→L |
| 526.2 | 2.36 | 0.01 | 0.92 H-3→L; 0.21 H-6→L; -0.19 H-3→L+1 |
| 496.3 | 2.50 | 0.05 | 0.81 H-6→L+1; -0.33 H-6→L; 0.22 H-3→L |
| 496.2 | 2.50 | 0.05 | -0.81 H-6→L; -0.33 H-6→L+1; -0.22 H-3→L+1 |
| 474.8 | 2.61 | 0.02 | -0.88 H-7→L+1; -0.32 H-7→L; -0.2 H-3→L+3 |
| 474.8 | 2.61 | 0.02 | 0.88 H-7→L; -0.32 H-7→L+1; -0.2 H-3→L+2 |
| 440.7 | 2.81 | 0.02 | -0.56 H-11→L; 0.55 H-15→L; -0.3 H-10→L+1 |
| 440.7 | 2.81 | 0.02 | -0.56 H-11→L+1; 0.55 H-15→L+1; 0.3 H-10→L |
| 436.3 | 2.84 | 0.09 | -0.81 H-10→L; -0.45 H-11→L+1; -0.17 H-6→L+2 |
| 436.3 | 2.84 | 0.09 | 0.81 H-10→L+1; -0.45 H-11→L; -0.17 H-6→L+3 |
| 413.9 | 3.00 | 0.02 | -0.78 H-12→L+1; -0.29 H-11→L+1; -0.23 H-7→L+3 |
| 413.9 | 3.00 | 0.02 | 0.78 H-12→L; -0.29 H-11→L; -0.23 H-7→L+2 |
| 407.1 | 3.05 | 0.01 | -0.64 H-13→L+1; -0.64 H-14→L; -0.21 H-13→L |

⁽¹⁾ Excitations with oscillator strength, F_{osc.} above 0.01 are shown.

⁽²⁾ H stands for HOMO, L stands for LUMO

Table S5. The calculated UV-vis-NIR absorption spectrum of $g\text{-Y}_2[(\text{MeO})_8\text{Pc}]_3^+$ for the BP86/def2-SVP geometry calculated by the sTDA method at the CAM-B3LYP/6-31G(d) level of theory.

| Wavelength, nm | Energy, eV | $F_{\text{osc.}}^{(1)}$ | Wavefunction ⁽²⁾ |
|----------------|------------|-------------------------|--|
| 1160.6 | 1.07 | 0.01 | -0.69 bH-1→bL+1; 0.52 bH-1→bL; 0.42 bH-1→bL+2 |
| 1093.9 | 1.13 | 0.01 | 0.8 bH-1→bL+2; 0.43 bH-1→bL+3; -0.36 bH-1→bL+1 |
| 896.6 | 1.38 | 0.02 | 0.68 bH-2→bL; -0.29 bH→bL+2; 0.29 bH-2→bL |
| 889.5 | 1.39 | 0.01 | -0.61 bH-2→bL+1; -0.39 bH-1→bL+2; 0.35 bH-4→bL |
| 875.4 | 1.42 | 0.01 | 0.59 bH-4→bL; 0.53 bH-2→bL+1; -0.42 aH-9→bL |
| 828.7 | 1.50 | 0.05 | -0.66 bH-1→bL+2; -0.36 bH-1→bL+1; -0.34 bH-4→bL |
| 827.6 | 1.50 | 0.01 | 0.76 bH-5→bL; -0.42 aH-10→bL; 0.24 bH-7→bL |
| 815.2 | 1.52 | 0.04 | -0.76 bH-1→bL+3; 0.38 bH-1→bL+2; 0.28 bH-3→bL |
| 739.4 | 1.68 | 0.06 | 0.63 bH→bL+4; -0.31 bH→bL+3; 0.28 bH→bL+6 |
| 738.4 | 1.68 | 0.06 | 0.61 bH→bL+3; 0.33 bH→bL+4; -0.28 bH→bL+5 |
| 718.4 | 1.73 | 0.04 | 0.46 bH-7→bL; -0.43 bH-3→bL; 0.33 bH→bL+3 |
| 717.9 | 1.73 | 0.04 | 0.47 aH-9→bL; 0.44 bH-4→bL; -0.29 bH→bL+4 |
| 680.7 | 1.82 | 0.02 | -0.87 bH-1→bL+3; 0.19 bH-1→bL+4; -0.16 bH-2→bL+2 |
| 673.0 | 1.84 | 0.01 | -0.74 bH-1→bL+4; -0.3 bH-5→bL; -0.28 aH-11→bL |
| 638.8 | 1.94 | 0.18 | -0.55 bH→bL+5; 0.47 bH→bL+4; -0.35 bH→bL+6 |
| 637.6 | 1.95 | 0.17 | 0.54 bH→bL+6; 0.47 bH→bL+5; -0.36 bH→bL+5 |
| 630.2 | 1.97 | 0.02 | -0.73 aH-11→bL; 0.49 aH-10→bL; -0.21 bH-7→bL |
| 620.6 | 2.00 | 0.02 | 0.49 bH-3→bL+1; -0.34 bH-5→bL+1; -0.32 bH-2→bL+2 |
| 618.5 | 2.01 | 0.03 | -0.65 bH-3→bL; -0.28 bH-2→bL+3; 0.27 bH-4→bL+1 |
| 613.2 | 2.02 | 0.03 | 0.75 bH-2→bL+2; 0.21 aH-13→bL; 0.18 bH-5→bL |
| 609.3 | 2.04 | 0.02 | 0.45 aH-12→bL; -0.44 bH-2→bL+3; 0.33 bH-5→bL |
| 606.7 | 2.04 | 0.01 | 0.5 aH-12→bL; -0.48 aH-14→bL; -0.38 bH-3→bL |
| 593.3 | 2.09 | 0.01 | 0.5 aH-13→bL; 0.3 bH-4→bL; 0.27 bH-2→bL+2 |
| 592.2 | 2.09 | 0.02 | 0.51 aH-14→bL; 0.39 bH-1→bL+5; 0.31 aH-12→bL |
| 585.5 | 2.12 | 0.03 | 0.51 bH-1→bL+5; 0.46 bH-1→bL+4; 0.38 aH-13→bL |
| 582.6 | 2.13 | 0.01 | 0.5 bH-2→bL+1; -0.33 bH-3→bL+2; -0.31 bH-1→bL+5 |
| 579.4 | 2.14 | 0.03 | 0.51 bH-1→bL+6; -0.47 bH-1→bL+5; -0.36 bH-2→bL+1 |
| 571.5 | 2.17 | 0.02 | 0.64 aH-15→bL; -0.34 bH-3→bL+1; -0.21 bH-6→bL |
| 569.3 | 2.18 | 0.02 | 0.51 bH-3→bL+1; 0.46 aH-15→bL; 0.28 bH-5→bL+1 |
| 549.1 | 2.26 | 0.01 | -0.46 bH-4→bL+1; 0.4 bH-6→bL+1; 0.38 bH-3→bL+1 |
| 531.3 | 2.33 | 0.04 | 0.47 bH-7→bL; 0.37 bH-2→bL+2; -0.27 bH-1→bL+5 |
| 530.6 | 2.34 | 0.14 | -0.49 bH-7→bL; 0.41 bH-1→bL+6; 0.29 bH-1→bL+5 |
| 529.8 | 2.34 | 0.16 | 0.39 bH-1→bL+5; -0.32 bH-1→bL+4; 0.29 bH-1→bL+6 |
| 528.4 | 2.35 | 0.02 | 0.42 bH-7→bL+1; -0.37 bH-4→bL+2; -0.35 aH-8→bL |

| | | | |
|-------|------|------|--|
| 524.7 | 2.36 | 0.09 | 0.36 bH-7→bL; -0.31 bH-3→bL+2; -0.28 bH-2→bL+2 |
| 520.2 | 2.38 | 0.11 | 0.4 bH-5→bL+1; 0.4 aH-9→bL+1; -0.34 aH-8→bL |
| 519.0 | 2.39 | 0.02 | 0.41 bH-4→bL+2; -0.4 aH-8→bL; -0.38 bH-5→bL+1 |
| 507.7 | 2.44 | 0.03 | -0.47 aH-8→bL+1; -0.42 aH-9→bL; -0.31 aH-8→bL |
| 504.7 | 2.46 | 0.02 | -0.4 aH-10→bL; -0.39 aH-9→bL+1; 0.32 aH-8→bL+1 |
| 502.9 | 2.47 | 0.01 | -0.62 bH-5→bL+2; 0.37 bH-3→bL+2; 0.24 aH-15→bL |
| 501.4 | 2.47 | 0.02 | 0.4 aH-20→bL; -0.39 aH-15→bL; -0.39 bH-5→bL+2 |
| 498.4 | 2.49 | 0.02 | -0.51 aH-10→bL; 0.35 aH-9→bL+1; -0.24 bH-6→bL |
| 484.8 | 2.56 | 0.02 | 0.6 bH-6→bL+2; -0.39 bH-7→bL+1; 0.24 aH-9→bL+2 |
| 480.9 | 2.58 | 0.01 | 0.5 bH-6→bL+1; -0.35 bH-7→bL+2; -0.32 aH-10→bL+1 |
| 479.2 | 2.59 | 0.02 | -0.52 aH-11→bL; -0.31 aH-22→bL; 0.28 aH-20→bL |
| 477.4 | 2.60 | 0.06 | -0.41 aH-19→bL; 0.36 aH-11→bL+1; -0.31 aH-17→bL |
| 471.5 | 2.63 | 0.01 | 0.61 aH-9→bL+1; -0.36 bH-6→bL+1; 0.22 aH-16→bL |
| 468.8 | 2.65 | 0.03 | 0.4 bH-3→bL+2; -0.29 aH-16→bL; -0.27 aH-11→bL |
| 468.0 | 2.65 | 0.01 | 0.34 bH-3→bL+2; 0.28 aH-12→bL+1; -0.27 bH-4→bL+2 |
| 467.3 | 2.65 | 0.01 | 0.49 bH-3→bL+3; -0.32 aH-17→bL; 0.29 aH-21→bL |
| 465.3 | 2.66 | 0.12 | 0.39 aH-10→bL+1; 0.28 aH-16→bL; 0.27 bH-3→bL+2 |
| 464.4 | 2.67 | 0.01 | -0.45 bH-3→bL+3; 0.31 aH-10→bL+1; -0.24 aH-11→bL+1 |
| 463.2 | 2.68 | 0.01 | 0.36 aH-17→bL; -0.3 bH-3→bL+2; 0.29 aH-10→bL+1 |
| 461.3 | 2.69 | 0.02 | -0.48 aH-18→bL; 0.32 aH-27→bL; -0.28 aH-23→bL |
| 461.2 | 2.69 | 0.02 | 0.33 aH-18→bL; -0.28 aH-27→bL; -0.27 aH-16→bL |
| 460.0 | 2.70 | 0.02 | -0.34 bH-4→bL+3; -0.3 aH-12→bL; -0.26 bH-4→bL+2 |
| 459.2 | 2.70 | 0.06 | 0.39 bH-5→bL+2; 0.26 aH-16→bL; 0.26 aH-18→bL |
| 458.6 | 2.70 | 0.06 | 0.31 aH-15→bL; -0.28 aH-26→bL; -0.28 aH-16→bL |
| 456.4 | 2.72 | 0.07 | -0.25 bH-7→bL+2; -0.25 aH-9→bL+1; 0.24 aH-12→bL |
| 454.8 | 2.73 | 0.01 | 0.48 bH-4→bL+3; -0.36 bH-5→bL+2; -0.29 bH-4→bL+2 |
| 454.4 | 2.73 | 0.05 | 0.36 bH-6→bL+1; 0.31 aH-9→bL+1; 0.3 bH-7→bL+1 |
| 451.2 | 2.75 | 0.05 | 0.31 aH-12→bL+1; 0.3 bH-4→bL+2; -0.26 bH-5→bL+2 |
| 450.6 | 2.75 | 0.01 | -0.41 bH→bL+7; -0.26 aH-10→bL+2; -0.24 bH→bL+8 |
| 448.5 | 2.76 | 0.09 | -0.29 aH-15→bL+1; -0.28 aH-11→bL; -0.25 bH→bL+6 |
| 447.5 | 2.77 | 0.04 | 0.35 aH-13→bL; 0.27 aH-15→bL+2; -0.26 aH-15→bL |
| 446.3 | 2.78 | 0.01 | 0.34 aH-13→bL; 0.27 aH-10→bL+2; -0.26 aH-15→bL+2 |
| 443.6 | 2.80 | 0.02 | 0.34 aH-10→bL+2; -0.34 aH-9→bL+2; -0.25 aH-15→bL+1 |
| 442.7 | 2.80 | 0.01 | -0.47 aH-9→bL+2; -0.35 bH→bL+6; -0.26 aH-14→bL |
| 442.3 | 2.80 | 0.01 | 0.41 bH-6→bL+2; 0.32 bH-6→bL+3; -0.28 aH-13→bL |
| 437.3 | 2.84 | 0.02 | 0.39 aH-21→bL; 0.38 aH-26→bL; 0.32 aH-17→bL |
| 437.2 | 2.84 | 0.01 | -0.42 bH→bL+6; -0.3 bH→bL+7; 0.26 aH-14→bL |

| | | | |
|-------|------|------|--|
| 436.8 | 2.84 | 0.03 | 0.48 aH-25→bL; 0.25 aH-16→bL; 0.25 bH-6→bL+3 |
| 434.8 | 2.85 | 0.02 | 0.34 aH-14→bL+1; 0.29 aH-14→bL; -0.23 aH-18→bL |
| 428.0 | 2.90 | 0.04 | 0.3 aH-15→bL+1; 0.24 aH-11→bL+1; 0.21 aH-15→bL |
| 420.2 | 2.95 | 0.01 | 0.35 bH-2→bL+3; 0.32 bH-2→bL+5; 0.28 bH-3→bL+4 |
| 417.9 | 2.97 | 0.01 | 0.32 bH-4→bL+5; 0.27 bH-4→bL+3; 0.27 aH-9→bL+2 |
| 412.3 | 3.01 | 0.05 | -0.5 aH-11→bL+1; 0.22 aH-19→bL; 0.21 bH-1→bL+6 |
| 411.1 | 3.02 | 0.01 | -0.43 aH-11→bL+2; -0.24 bH-7→bL+2; 0.23 aH-19→bL+1 |
| 410.5 | 3.02 | 0.02 | -0.45 aH-12→bL+1; 0.36 bH-7→bL+2; -0.33 bH-2→bL+4 |
| 408.4 | 3.04 | 0.03 | 0.33 bH-1→bL+6; -0.3 aH-12→bL+2; -0.23 aH-9→bL+3 |
| 407.6 | 3.04 | 0.02 | -0.43 bH-7→bL+3; -0.29 bH-2→bL+3; -0.21 aH-13→bL+1 |
| 406.3 | 3.05 | 0.09 | 0.27 bH-3→bL+3; -0.25 bH-4→bL+4; 0.25 aH-8→bL+3 |
| 405.4 | 3.06 | 0.01 | -0.31 aH-9→bL+2; -0.28 bH-5→bL+5; -0.26 bH-7→bL+2 |
| 404.3 | 3.07 | 0.04 | 0.27 bH-4→bL+5; 0.26 aH-8→bL+2; -0.26 bH-3→bL+3 |
| 403.8 | 3.07 | 0.05 | -0.36 bH-3→bL+4; 0.32 bH-5→bL+4; -0.25 aH-9→bL+3 |
| 403.4 | 3.07 | 0.14 | -0.43 bH-4→bL+4; 0.38 aH-14→bL+1; -0.24 bH-2→bL+4 |
| 401.6 | 3.09 | 0.07 | -0.55 bH-2→bL+4; 0.25 bH-3→bL+3; -0.23 aH-19→bL+1 |
| 400.9 | 3.09 | 0.03 | 0.35 aH-14→bL+1; -0.29 bH-2→bL+5; 0.27 bH-2→bL+4 |

⁽¹⁾ Excitations with oscillator strength, F_{osc} above 0.01 are shown.

⁽²⁾ H stands for HOMO, L stands for LUMO

Table S6. The calculated UV-vis-NIR absorption spectrum of **g-Y₂[(MeO)₈Pc]₃²⁺** for the BP86/def2-SVP geometry calculated by the sTDA method at the CAM-B3LYP/6-31G(d) level of theory.

| Wavelength, nm | Energy, eV | F _{osc.} ⁽¹⁾ | Wavefunction ⁽²⁾ |
|----------------|------------|----------------------------------|--|
| 3137.3 | 0.40 | 0.51 | 0.97 H→L; 0.18 H-1→L; 0.04 H-26→L |
| 1080.2 | 1.15 | 0.01 | -0.97 H-5→L; -0.09 H-14→L; 0.08 H-4→L+6 |
| 1072.0 | 1.16 | 0.08 | 0.71 H-1→L+1; 0.58 H-3→L; -0.19 H→L+4 |
| 1071.9 | 1.16 | 0.08 | -0.71 H-1→L+2; -0.58 H-4→L; -0.19 H→L+3 |
| 911.8 | 1.36 | 0.01 | -0.93 H-8→L; 0.21 H-7→L; 0.16 H→L+4 |
| 911.8 | 1.36 | 0.01 | -0.93 H-7→L; -0.21 H-8→L; 0.16 H→L+3 |
| 784.5 | 1.58 | 0.16 | -0.54 H→L+4; -0.5 H→L+3; 0.42 H-1→L+3 |
| 784.5 | 1.58 | 0.16 | 0.54 H→L+3; -0.5 H→L+4; 0.42 H-1→L+4 |
| 759.4 | 1.63 | 0.02 | -0.94 H-10→L; 0.25 H-14→L; -0.1 H-5→L |
| 750.7 | 1.65 | 0.08 | 0.77 H-1→L+3; 0.42 H→L+3; -0.27 H-12→L |
| 750.7 | 1.65 | 0.08 | 0.77 H-1→L+4; 0.42 H→L+4; 0.27 H-13→L |
| 696.6 | 1.78 | 0.11 | 0.88 H-12→L; 0.22 H→L+3; 0.17 H-1→L+5 |
| 696.6 | 1.78 | 0.11 | -0.88 H-13→L; 0.22 H→L+4; 0.17 H-1→L+6 |
| 631.8 | 1.96 | 0.01 | -0.92 H→L+6; -0.18 H-1→L+4; -0.15 H→L+1 |
| 631.8 | 1.96 | 0.01 | -0.92 H→L+5; -0.18 H-1→L+3; 0.15 H→L+2 |
| 595.2 | 2.08 | 0.03 | 0.83 H-2→L+1; 0.32 H-1→L+6; -0.28 H-5→L+2 |
| 595.2 | 2.08 | 0.03 | -0.83 H-2→L+2; -0.32 H-1→L+5; 0.28 H-5→L+1 |
| 590.5 | 2.10 | 0.01 | 0.62 H-4→L+2; 0.61 H-3→L+1; 0.31 H-4→L+1 |
| 586.6 | 2.11 | 0.09 | -0.75 H-1→L+5; 0.38 H-2→L+2; -0.3 H-15→L |
| 586.6 | 2.11 | 0.09 | -0.75 H-1→L+6; 0.38 H-2→L+1; 0.3 H-16→L |
| 554.4 | 2.24 | 0.03 | 0.87 H-5→L+1; 0.27 H-2→L+2; 0.2 H-5→L+2 |
| 554.4 | 2.24 | 0.03 | -0.87 H-5→L+2; -0.27 H-2→L+1; 0.2 H-5→L+1 |
| 525.5 | 2.36 | 0.11 | -0.61 H-16→L; 0.38 H-6→L+1; -0.31 H-19→L |
| 525.5 | 2.36 | 0.11 | 0.61 H-15→L; 0.37 H-6→L+2; 0.31 H-20→L |
| 518.6 | 2.39 | 0.03 | -0.83 H-6→L+2; 0.29 H-19→L; 0.21 H-23→L |
| 518.6 | 2.39 | 0.03 | 0.83 H-6→L+1; -0.29 H-20→L; 0.21 H-16→L |
| 508.6 | 2.44 | 0.41 | -0.54 H-15→L; 0.54 H-20→L; 0.3 H-19→L |
| 508.6 | 2.44 | 0.41 | 0.55 H-16→L; -0.54 H-19→L; 0.3 H-20→L |
| 501.1 | 2.47 | 0.01 | 0.66 H-8→L+2; 0.66 H-7→L+1; -0.16 H-21→L |
| 487.3 | 2.54 | 0.01 | -0.72 H-24→L; -0.44 H-20→L; 0.34 H-23→L |
| 487.3 | 2.54 | 0.01 | 0.72 H-23→L; -0.44 H-19→L; 0.34 H-24→L |
| 478.2 | 2.59 | 0.23 | 0.78 H-9→L+2; -0.42 H-10→L+1; -0.15 H-9→L+1 |
| 478.2 | 2.59 | 0.23 | -0.78 H-9→L+1; -0.42 H-10→L+2; -0.15 H-9→L+2 |
| 454.6 | 2.73 | 0.21 | 0.6 H-10→L+2; 0.5 H-11→L+1; -0.43 H-14→L+2 |

| | | | |
|-------|------|------|--|
| 454.6 | 2.73 | 0.21 | -0.6 H-10→L+1; -0.5 H-11→L+2; 0.43 H-14→L+1 |
| 444.4 | 2.79 | 0.01 | -0.53 H-12→L+2; -0.53 H-13→L+1; -0.42 H-12→L+1 |
| 440.2 | 2.82 | 0.18 | -0.63 H-11→L+2; -0.44 H-11→L+1; 0.39 H-10→L+2 |
| 440.2 | 2.82 | 0.18 | 0.62 H-11→L+1; -0.44 H-11→L+2; 0.39 H-10→L+1 |
| 432.0 | 2.87 | 0.05 | 0.78 H-2→L+4; 0.34 H-2→L+3; 0.24 H-5→L+4 |
| 432.0 | 2.87 | 0.05 | -0.78 H-2→L+3; 0.34 H-2→L+4; 0.24 H-5→L+3 |
| 430.9 | 2.88 | 0.01 | -0.39 H-13→L+2; 0.39 H-12→L+1; -0.36 H-4→L+3 |
| 430.4 | 2.88 | 0.04 | 0.55 H-4→L+3; -0.5 H-3→L+4; 0.31 H-12→L+1 |
| 412.9 | 3.00 | 0.23 | 0.61 H-5→L+3; 0.39 H-5→L+4; 0.29 H-2→L+6 |
| 412.9 | 3.00 | 0.23 | -0.61 H-5→L+4; 0.39 H-5→L+3; -0.29 H-2→L+5 |
| 407.3 | 3.04 | 0.06 | 0.44 H-14→L+2; -0.36 H-5→L+4; -0.34 H-6→L+3 |
| 407.3 | 3.04 | 0.07 | -0.44 H-14→L+1; 0.36 H-5→L+3; 0.34 H-6→L+4 |

⁽¹⁾ Excitations with oscillator strength, F_{osc} , above 0.01 are shown.

⁽²⁾ H stands for HOMO, L stands for LUMO

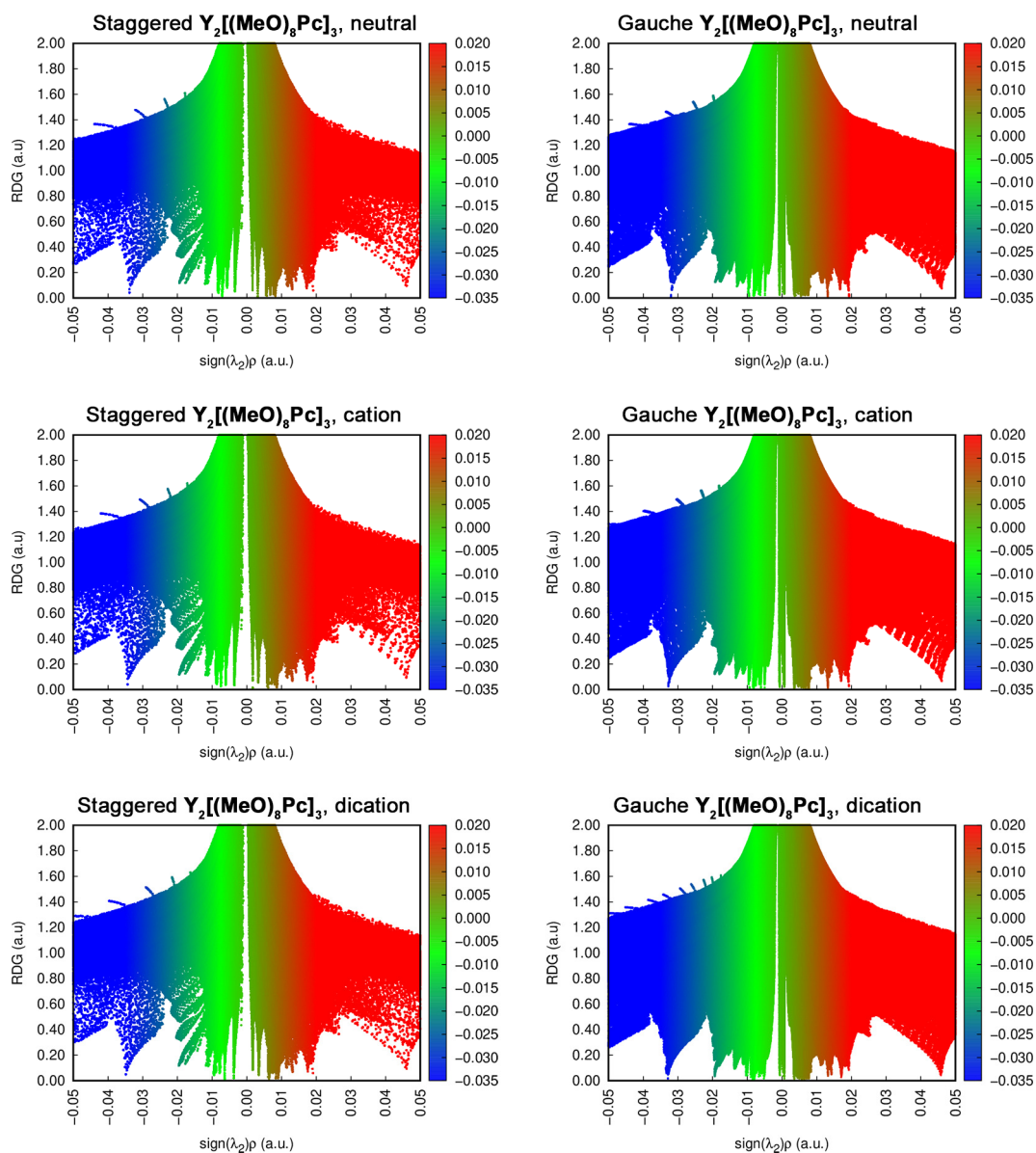


Figure S10. RDG vs. $\text{sign}(\lambda_2)\rho$ plots for staggered and gauche conformations of redox-forms of $\text{Y}_2[(\text{MeO})_8\text{Pc}]_3$.

Table S7. BP86/def2-SVP geometry of *s*-Y₂[(MeO)₈Pc]₃.

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|--------------------|-------------------|-------------------|
| C | -4.19022374357489 | -0.70694999595402 | 3.19212065920735 | C | 7.47219579611046 | -3.61357023921068 | -0.00056229788096 |
| C | -4.19024149117518 | 0.70697895597704 | 3.19207007614298 | C | 7.47218295846112 | 3.61365040996167 | -0.0002542791320 |
| C | -2.79408283831429 | 1.12459669558743 | 3.06073968948238 | C | 3.61355413194797 | 7.47220535537777 | 0.00065807984116 |
| C | -2.79406429273401 | -1.12455157324893 | 3.06080559154482 | C | -3.61358466932363 | 7.47220330278022 | -0.00007530652023 |
| C | 2.79385540487487 | 1.12458455790370 | 3.06089968289158 | C | -7.47219487859633 | 3.61363440472851 | -0.00050185142467 |
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| H | 7.32597777931353 | 2.89338652602945 | -4.72977601702448 | O | -7.82232033748144 | 1.30312685266012 | -3.45498406104800 |
| H | 7.43032014041129 | 3.32092738582186 | -2.98042403466382 | O | -7.82236641287235 | -1.30303926771526 | -3.45485041033560 |
| H | 2.94144102811312 | 8.93600624117716 | -3.89837757425214 | Y | -0.00006788028021 | 0.00001376858297 | 1.70131735226762 |
| H | 2.89364676458287 | 7.32629135592689 | -4.72929338268616 | Y | 0.00005688735274 | -0.00000350089957 | -1.70121407132855 |

Table S8. BP86/def2-SVP geometry of $s\text{-Y}_2[(\text{MeO})_8\text{Pc}]^{3+}$.

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|-------------------|-------------------|-------------------|
| C | -4.19205689394472 | -0.70670659425200 | 3.16067110350712 | C | 3.62172187639943 | -7.47752028133798 | 0.00034797607609 |
| C | -4.19205776308625 | 0.70664883869617 | 3.16066286307295 | C | 7.47752026890604 | -3.62165283952837 | 0.00031901852086 |
| C | -2.79478069757771 | 1.12433664975361 | 3.02842688030112 | C | 7.47749536128936 | 3.62172142686373 | 0.00025770681181 |
| C | -2.79478441295441 | -1.12439699407973 | 3.02840721332501 | C | 3.62159344772330 | 7.47750664227047 | 0.00027408597478 |
| C | 2.79428139908240 | 1.12434276429500 | 3.02877919550720 | C | -3.62163748915894 | 7.47749549790436 | 0.00036999133880 |
| C | 4.19157451163487 | 0.70665698351394 | 3.16083766626771 | C | -7.47750131168106 | 3.62167971396240 | 0.00086195250040 |
| C | 4.19155348923577 | -0.70669842549311 | 3.16108256970939 | C | -7.47753244029660 | -3.62161259037432 | 0.00062121466438 |
| C | 2.79429632724664 | -1.12439602162629 | 3.02870100093809 | C | -3.62177760098287 | -7.47751269763319 | 0.00008773038355 |
| C | -1.12461540673505 | -2.79456705381915 | 3.02853232484613 | C | -4.19155174002897 | -0.70667821954266 | -3.16099617350716 |
| C | 1.12412203029568 | -2.79456227398328 | 3.02869274430266 | C | -4.19154630926482 | 0.70667416755825 | -3.16097723772591 |
| C | 0.70642299821579 | -4.19183385013702 | 3.16093589114300 | C | -2.79427488629598 | 1.12436035650450 | -3.02873177798131 |
| C | -0.70693144547444 | -4.19183748845170 | 3.16082244732386 | C | -2.79428375419281 | -1.12437537698465 | -3.02874473460126 |
| C | -0.70693381015136 | 4.19180084860298 | 3.16056370381138 | C | 2.79476640475784 | 1.12435296774705 | -3.02853040366903 |
| C | 0.70642174110255 | 4.19181218044288 | 3.16060270487347 | C | 4.19204657916580 | 0.70668214056986 | -3.16071574041453 |
| C | 1.12412400413007 | 2.79452302531970 | 3.02853856780600 | C | 4.19204470619786 | -0.70667150734167 | -3.16094994010781 |
| C | -1.12461047353348 | 2.79451153118875 | 3.02844831609002 | C | 2.79480118785789 | -1.12437720262442 | -3.02843138874519 |
| C | -1.43684293241613 | -5.38480998332676 | 3.26723113873617 | C | -1.12411197130237 | -2.79453648826463 | -3.02876378184241 |
| C | -0.72243946558510 | -6.59144276158580 | 3.34977081641255 | C | 1.12462286357524 | -2.79453176134185 | -3.02864491345352 |
| C | 0.72190934590599 | -6.59144202076916 | 3.34986610178912 | C | 0.70694135440593 | -4.19178061306423 | -3.16114997230838 |
| C | 1.43632214626973 | -5.38480659007227 | 3.26743228107741 | C | -0.70641145337421 | -4.19179095766061 | -3.16116710595770 |
| C | -5.38501586403484 | 1.43655018349085 | 3.26733089650809 | C | -0.70641361657398 | 4.19180364573951 | -3.16087715471414 |
| C | -6.59163133264028 | 0.72213658120102 | 3.35004941648650 | C | 0.70693947537572 | 4.19179593008972 | -3.16079320096641 |
| C | -6.59163012762011 | -0.72221030774879 | 3.35003816005066 | C | 1.12461531149226 | 2.79452765373705 | -3.02850491180231 |
| C | -5.38501039156106 | -1.43661643683914 | 3.26731902963194 | C | -1.12411331551536 | 2.79453271188175 | -3.02863307293882 |
| C | 5.38454406502253 | -1.43660900628240 | 3.26724624164614 | C | -1.43630483658999 | -5.38474579037684 | -3.26791000299585 |
| C | 6.59117227606209 | -0.72220391964596 | 3.34983146841430 | C | -0.72188544466026 | -6.59136152646239 | -3.35057830357635 |
| C | 6.59114976492630 | 0.72213962961160 | 3.35015599097771 | C | 0.72246351428615 | -6.59135985438183 | -3.35041761913081 |
| C | 5.38452606471970 | 1.43655210277267 | 3.26755836016675 | C | 1.43686033350738 | -5.38473567088771 | -3.26770329582314 |
| C | 1.43630888285853 | 5.38479577774809 | 3.26703055322973 | C | -5.38450515747754 | 1.43658782739251 | -3.26747682947738 |
| C | 0.72188444722692 | 6.59142840799474 | 3.34942689581010 | C | -6.59114285190390 | 0.72218814871695 | -3.34999379342175 |
| C | -0.72245707329416 | 6.59141290823237 | 3.34939522363968 | C | -6.59115074367850 | -0.72215703255514 | -3.34999377470450 |
| C | -1.43685124733203 | 5.38476816392610 | 3.26695183678802 | C | -5.38452232286409 | -1.43657347395504 | -3.26749525380961 |
| C | -2.67934047279034 | -7.87003425106674 | 3.79180883026807 | C | 5.38503624516721 | -1.43655655389710 | -3.26733525137188 |
| C | 2.67876143915674 | -7.87004153400318 | 3.79209905461755 | C | 6.59162824551161 | -0.72212085296187 | -3.35021852413201 |
| C | 7.86978367907088 | -2.67917878624456 | 3.79147392093263 | C | 6.59157614432831 | 0.72222491075578 | -3.35057741761229 |
| C | 7.86983794555651 | 2.67902374885556 | 3.79201014055523 | C | 5.38495641582575 | 1.43661015710620 | -3.26769884718245 |
| C | 2.67873554874773 | 7.87011579030206 | 3.79143606493939 | C | 1.43686489852659 | 5.38474554855647 | -3.26732586001494 |
| C | -2.67933817595463 | 7.87004904762848 | 3.79141827871279 | C | 0.72247363800699 | 6.59137879952345 | -3.34996382063306 |
| C | -7.87023408527060 | 2.67899233282953 | 3.79228580463136 | C | -0.72186971901005 | 6.59139300943334 | -3.35004726505162 |
| C | -7.87022518942614 | -2.67909511439519 | 3.79216616463242 | C | -1.43629908509797 | 5.38477359054749 | -3.26748014323208 |
| C | -2.44912710170178 | -3.44688415082319 | 0.00007120581105 | C | -2.67874883855102 | -7.86993549965967 | -3.79284591690493 |
| C | -3.44686528999188 | -2.44912781889474 | 0.00006973367518 | C | 2.67937738673064 | -7.86986623538541 | -3.79265204850293 |
| C | -2.75887473678312 | -1.16912440532254 | -0.00003304604642 | C | 7.87021863270048 | -2.67903203985653 | -3.79219720902331 |
| C | -1.16911134084711 | -2.75890604156799 | 0.00001901938986 | C | 7.87015117859681 | 2.67910314716609 | -3.79278197449010 |
| C | 1.16911202142189 | 2.75885119540086 | 0.00025891019462 | C | 2.67935685557484 | 7.86994876601364 | -3.79214642343032 |
| C | 2.44911536339375 | 3.44684243437056 | 0.00041087366864 | C | -2.67869620954630 | 7.87003291882458 | -3.79227670364546 |
| C | 3.44687132987714 | 2.44910426908145 | 0.00046167435193 | C | -7.86977493955115 | 2.67912872880550 | -3.79173702589200 |
| C | 2.75889271740752 | 1.16908992835571 | 0.00036021058273 | C | -7.86979647825373 | -2.67906043212037 | -3.79186364665523 |
| C | 1.16910889841264 | -2.75890024014460 | 0.00021865614461 | H | -2.53374714459742 | -5.35236902890040 | 3.27637682067691 |
| C | 2.75887947900461 | -1.16912659115549 | 0.00034764877414 | H | 2.53322529748986 | -5.35236547401975 | 3.27669323792797 |
| C | 3.44686551523679 | -2.44913118151840 | 0.00045852106034 | H | -5.35256188380743 | 2.53345302410035 | 3.27680472710252 |
| C | 2.44912232351495 | -3.44688145324653 | 0.00039726049910 | H | -5.35254482550711 | -2.53351851281840 | 3.27678873874564 |
| C | -3.44685926102884 | 2.44910291180405 | 0.00015868222530 | H | 5.35205771560780 | -2.53350896260915 | 3.27691681069007 |
| C | -2.44910806814046 | 3.44684580066682 | 0.00017389288385 | H | 5.35201119017294 | 2.53344561411766 | 3.27785002088038 |
| C | -1.16910347349523 | 2.75885619276088 | 0.00007903386208 | H | 2.53321158887233 | 5.35235133465370 | 3.27650885522843 |
| C | -2.75887941705874 | 1.16909039451772 | 0.00000207721708 | H | -2.53375352220942 | 5.35229906911775 | 3.27639226183599 |
| C | 2.77379000069385 | -4.80959827465704 | 0.00042544210028 | H | -2.88504125025502 | -7.32309119799700 | 4.73815381698853 |
| C | 4.13359838258808 | -5.15778092675552 | 0.00050359982531 | H | -3.32428560288731 | -7.44491269345564 | 2.99108884333942 |
| C | 5.15778936039212 | -4.13357827951730 | 0.00055476958481 | H | -2.92722587639104 | -8.93927874262912 | 3.92148604664778 |
| C | 4.80958638471203 | -2.77377743959107 | 0.00053857406291 | H | 2.88437346849697 | -7.32311169306104 | 4.73847110844130 |
| C | -4.80958944456853 | -2.77375798226581 | 0.00015655692705 | H | 3.32378447060636 | -7.44491084929357 | 2.99144648052648 |
| C | -5.15780660354506 | -4.13355525889623 | 0.00022967956765 | H | 2.92663220007651 | -8.93928811812289 | 3.92178660858546 |
| C | -4.13362458349365 | -5.15776520726621 | 0.00018702184793 | H | 8.93904845756659 | -2.92711161237408 | 3.92089676248977 |
| C | -2.77381215760377 | -4.80959728820999 | 0.00011738794989 | H | 7.44452488394150 | -3.32405243867717 | 2.99076907560737 |
| C | 4.80958612208801 | 2.77377872346946 | 0.00047055992600 | H | 7.32296480797127 | -2.88494844358499 | 4.73787393172857 |
| C | 5.15775703240732 | 4.13359813142690 | 0.00040974605342 | H | 8.93911682234942 | 2.92689050195697 | 3.92145014379584 |
| C | 4.13354691478546 | 5.15778180244056 | 0.00038444003903 | H | 7.44458293803641 | 3.32410181817709 | 2.99146580674906 |
| C | 2.77374835732473 | 4.80956600517951 | 0.00039198293943 | H | 7.32305457247426 | 2.88459162163338 | 4.73847434022168 |
| C | -2.77375945163569 | 4.80956534665837 | 0.00027008413339 | H | 2.92659182418159 | 8.93939499786988 | 3.92089004794164 |
| C | -4.13356252318045 | 5.15776477451122 | 0.00038204839436 | H | 3.32385362790565 | 7.44486371809102 | 2.99092176784288 |
| C | -5.15776384699187 | 4.13357339854498 | 0.00041689114788 | H | 2.88426213879043 | 7.32333902421500 | 4.73791243504640 |
| C | -4.80957688020236 | 2.77376592159831 | 0.00029317188576 | H | -2.92722066047035 | 8.93932196723005 | 3.92087514961909 |

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|-------------------|-------------------|--------------------|
| H | -3.32447352931555 | 7.44477465924722 | 2.99093072182807 | H | 2.88483320022819 | 7.32291538596979 | -4.73848171136758 |
| H | -2.88480916200211 | 7.32327134506969 | 4.73790578867296 | H | 3.32447533601643 | 7.44495506998092 | -2.99149655227948 |
| H | -7.32313008335356 | 2.88461152889060 | 4.73855467874424 | H | -2.92653605239435 | 8.93927730018014 | -3.92205931157196 |
| H | -7.44530220238316 | 3.32405806799277 | 2.99156206954510 | H | -2.88419481702359 | 7.32300561636938 | -4.73861132392727 |
| H | -8.93946912207964 | 2.92680803892052 | 3.92218124657739 | H | -3.32383578225980 | 7.44506693750004 | -2.99162781768688 |
| H | -7.32316678889810 | -2.88477099791697 | 4.73844951701833 | H | -7.44452304658666 | 3.32405067114460 | -2.99106895795159 |
| H | -7.44523855806185 | -3.32409554651564 | 2.99141999713654 | H | -7.32296642242266 | 2.88482670815016 | -4.73816025720763 |
| H | -8.93946253713441 | -2.92693619031217 | 3.92199119156423 | H | -8.93903491525220 | 2.92703276759721 | -3.92125151260132 |
| H | 1.97381381387713 | -5.55929360536352 | 0.00034360855289 | H | -7.44460518720022 | -3.32404421596329 | -2.99121227856928 |
| H | 5.55927195034847 | -1.97379175854671 | 0.00055957534802 | H | -7.32293889299274 | -2.88470784894362 | -4.73826917261347 |
| H | -5.55926252802738 | -1.97376092799492 | 0.00018814920253 | H | -8.93905432630083 | -2.92693573187329 | -3.921452595993802 |
| H | -1.97384822547800 | -5.55930615594986 | 0.00012124007547 | N | -1.99786355791077 | -0.00003223271356 | 2.89652521564399 |
| H | 5.55929406933161 | 1.97382075651837 | 0.00050155762717 | N | 1.99736874981121 | -0.00003072591158 | 2.89687938224072 |
| H | 1.97375435400337 | 5.55924193763497 | 0.00034530935018 | N | -0.00024123855213 | -1.99765029626928 | 2.89669912580486 |
| H | -1.97377864771074 | 5.55925563767205 | 0.00028563679996 | N | -0.00023344954621 | 1.99758634106494 | 2.89669487463807 |
| H | -5.55927142760603 | 1.97378856620750 | 0.00033410321073 | N | -2.39957629277539 | -2.39935540584380 | 3.06032754971512 |
| H | 2.96996858952487 | -7.43582811757083 | 0.89966741083345 | N | -2.39957033196710 | 2.39929659791934 | 3.06028249049956 |
| H | 2.97017262028806 | -7.43576281058818 | -0.89911739044228 | N | 2.39907899354260 | 2.39930971098895 | 3.06051152850960 |
| H | 4.18739176551577 | -8.42651639353366 | 0.00037819693109 | N | 2.39908017716323 | -2.39935177756038 | 3.06062156076548 |
| H | 7.43585871079971 | -2.96986069137322 | 0.89960716975115 | N | -1.37538010221394 | -1.37540522023918 | -0.00002743906818 |
| H | 7.43571140177085 | -2.97014108429824 | -0.89916967372472 | N | 1.37539252347225 | 1.37535667719410 | 0.00027818556161 |
| H | 8.42652687180913 | -1.8730462025553 | 0.0003308168020 | N | 1.37538154309122 | -1.37540165016695 | 0.00023865783604 |
| H | 8.42649252526793 | 4.18739039121126 | 0.00023582011291 | N | -1.37538088377401 | 1.37535848832550 | 0.00000702967441 |
| H | 7.43574166439821 | 2.97010135251326 | -0.89915520091559 | N | -0.00000001929311 | -3.39431648780267 | 0.00015127311166 |
| H | 7.43580845271713 | 2.97005115288059 | 0.89963517864585 | N | -3.39429346246167 | -0.00001704520442 | 0.00000661792528 |
| H | 4.18723515841757 | 8.42651997129355 | 0.00030677303508 | N | 0.00000499759025 | 3.39426720746640 | 0.00021386605969 |
| H | 2.96996052260959 | 7.43579865637304 | -0.89912924682787 | N | 3.39429969238028 | -0.00002084131037 | 0.00043917775430 |
| H | 2.96993700037168 | 7.43573502158886 | 0.89965595783531 | N | -1.99736734251196 | -0.00001206900313 | -2.89679880262366 |
| H | -4.18729019237046 | 8.42650237343924 | 0.00053305263799 | N | 1.99787820989847 | -0.00001989495771 | -2.89647724676471 |
| H | -2.97014586321306 | 7.43583297962234 | -0.89913894471001 | N | 0.00024671903999 | -1.99764014786403 | -2.89664744356791 |
| H | -2.96983722209753 | 7.43569433242301 | 0.89964645789747 | N | 0.00024508490629 | 1.99761748065279 | -2.89662196469494 |
| H | -8.42650089687844 | 4.18734478766274 | 0.00115809253657 | N | -2.39906680773476 | -2.39932633699913 | -3.06070398508584 |
| H | -7.43607510276924 | 2.97003099445381 | -0.89854345646554 | N | -2.39906512491430 | 2.39931720751861 | -3.06060583229887 |
| H | -7.43547943699519 | 2.97003494686151 | 0.90024300386850 | N | 2.39956382679112 | 2.39930949767597 | -3.06040636462155 |
| H | -7.43552637659813 | -2.96997947117439 | 0.90001137787489 | N | 2.39958063507392 | -2.39932276144038 | -3.06047950325421 |
| H | -7.43605583976992 | -2.96994375920867 | -0.89876853258135 | O | -1.29978547153783 | -7.81730795009906 | 3.45526470131828 |
| H | -8.42654250575079 | -4.18725846608696 | 0.00087859289560 | O | 1.29924005368749 | -7.81730835765881 | 3.45542198701606 |
| H | -2.97002044289988 | -7.43581374861323 | 0.89940427479201 | O | 7.81705022197258 | -1.29957791930173 | 3.45510300894290 |
| H | -2.97022939316486 | -7.43578179269658 | -0.89937986359347 | O | 7.81704389932696 | 1.29950620150282 | 3.45531522060182 |
| H | -4.18746027259762 | -8.42650120821650 | 0.00013688424820 | O | 1.29923387650658 | 7.81732120545884 | 3.45467284502993 |
| H | -2.53320658689941 | -5.35229552194296 | -3.27732747893379 | O | -1.29984466242729 | 7.81729344535377 | 3.45460494417087 |
| H | 2.53376572520462 | -5.35229641753308 | -3.27670546599958 | O | -7.81749870774464 | 1.29947727763883 | 3.45557407339726 |
| H | -5.35203079656983 | 2.53348845348443 | -3.27695332118494 | O | -7.81749504192223 | -1.29955534464163 | 3.45555430923784 |
| H | -5.35206952244511 | -2.53347488714927 | -3.27695850397019 | O | 4.58998466282074 | -6.43502318105166 | 0.00049004645210 |
| H | 5.35259381939232 | -2.53345823235643 | -3.27700293577101 | O | 6.43503937937859 | -4.58993958020825 | 0.00053249305324 |
| H | 5.35241527435179 | 2.53350232406422 | -3.27803405658022 | O | 6.43499811819400 | 4.58998736049351 | 0.00032570990762 |
| H | 2.53376724231733 | 5.35228398700398 | -3.27669716205123 | O | 4.58989471695403 | 6.43503636319648 | 0.00026462387304 |
| H | -2.53320092739571 | 5.35233882461366 | -3.27701129610642 | O | -4.58992442172908 | 6.43501454814544 | 0.00045748360314 |
| H | -3.32372539798642 | -7.44497410415879 | -2.99206502084794 | O | -6.43500836271383 | 4.58995156314070 | 0.00054813907435 |
| H | -2.88444703977400 | -7.32283752759749 | -4.73910224966750 | O | -6.43505993536845 | -4.58990714857779 | 0.00031607540593 |
| H | -2.92659590332138 | -8.93916593992419 | -3.92271263903828 | O | -4.59002465127022 | -6.43500265437915 | 0.00021221295961 |
| H | 3.32430072627977 | -7.44493617631683 | -2.99181194119647 | O | -1.29920616529263 | -7.81722147189126 | -3.45625700156410 |
| H | 2.88510935253781 | -7.32270842902631 | -4.73886589912946 | O | 1.29981388824419 | -7.81720419799633 | -3.45613105212823 |
| H | 2.92725595129928 | -8.93908343579156 | -3.92256706325970 | O | 7.81750153377469 | -1.29945491477583 | -3.45572495469494 |
| H | 8.93943856102987 | -2.92687347582064 | -3.92217919670166 | O | 7.81744036344681 | 1.29960786843178 | -3.45596369437690 |
| H | 7.32296051313707 | -2.88481825433211 | -4.73833582921718 | O | 1.29986308854306 | 7.81724620424095 | -3.45530446097450 |
| H | 7.44547814528809 | -3.32396170213639 | -2.99125960824921 | O | -1.29921148844757 | 7.81727676745883 | -3.45542499816445 |
| H | 8.93938135714016 | 2.92695455289517 | -3.92266143830154 | O | -7.81702364196722 | 1.29956051133853 | -3.45522705250164 |
| H | 7.32302588875808 | 2.88461879119055 | -4.73905661873354 | O | -7.81703669375979 | -1.29951537064978 | -3.45525987077301 |
| H | 7.44526337565678 | 3.32421985450028 | -2.99207474044696 | Y | -0.00014144262179 | -0.00002242059127 | 1.69268191418957 |
| H | 2.92723837981268 | 8.93918396507128 | -3.92192501862389 | Y | 0.00014808277808 | -0.00001218747869 | -1.69258795229889 |

Table S9. BP86/def2-SVP geometry of $s\text{-Y}_2[(\text{MeO})_8\text{Pc}]_3^{2+}$.

| | | | | | | | |
|---|-------------------|-------------------|------------------|---|-------------------|-------------------|-------------------|
| C | -4.19274024229602 | -0.70657411062013 | 3.13806419680171 | C | 3.63240923672143 | -7.48437921043074 | 0.00022444778242 |
| C | -4.19274287070403 | 0.70649473709438 | 3.13805139918995 | C | 7.48438122189407 | -3.63233620986199 | 0.00049538874316 |
| C | -2.79507408698898 | 1.12406804478132 | 3.00123418444191 | C | 7.48435117199174 | 3.63239608321150 | 0.00038722697516 |
| C | -2.79507573635538 | -1.12414902607098 | 3.00121835740026 | C | 3.63228501979353 | 7.48436479138904 | 0.00014967362021 |
| C | 2.79498077092632 | 1.12406988122476 | 3.00138604433403 | C | -3.63232816209876 | 7.48435304338599 | 0.00012829619324 |
| C | 4.19265631438316 | 0.70650243598528 | 3.13814840672725 | C | -7.48435958316075 | 3.63235211277451 | 0.00014828481188 |
| C | 4.19263694725876 | -0.70656675947102 | 3.13836031904524 | C | -7.48438981668860 | -3.63229708549058 | 0.00005369938181 |
| C | 2.79499733584489 | -1.12414846499743 | 3.00128865999684 | C | -3.63245273868230 | -7.48437007914549 | 0.00008004335528 |
| C | -1.12415197478304 | -2.79507575963017 | 3.00127837392850 | C | -4.19263562726188 | -0.70652114283682 | -3.13828397389862 |
| C | 1.12406659001916 | -2.79506893607814 | 3.00133802063215 | C | -4.19263115200758 | 0.70654575720126 | -3.13825116689370 |
| C | 0.70649249600011 | -4.19272679415250 | 3.13823615122337 | C | -2.79497367823312 | 1.12411242151133 | -3.00133229442663 |
| C | -0.70657655239672 | -4.19273314154061 | 3.13819542336791 | C | -2.79498117613352 | -1.12410125814329 | -3.00136657132457 |
| C | -0.70657885072998 | 4.19267299411440 | 3.13799116878182 | C | 2.79506526487836 | 1.12411193533455 | -3.00132162743005 |
| C | 0.70648997516678 | 4.19267480683669 | 3.13799542842343 | C | 4.19274158091515 | 0.70655586834306 | -3.13807803704071 |
| C | 1.12406616961122 | 2.79500250984681 | 3.00123321248007 | C | 4.19273462061178 | -0.70651285182520 | -3.13831678296514 |
| C | -1.12414909866374 | 2.79499861799052 | 3.00121762151040 | C | 2.79509517902803 | -1.12410258022099 | -3.00126082461210 |
| C | -1.43770247845786 | -5.38270142876205 | 3.25832813988052 | C | -1.12405540232819 | -2.79502132230800 | -3.00142011223734 |
| C | -0.72292966004488 | -6.59028586362596 | 3.35560543927989 | C | 1.12416119513660 | -2.79501392176222 | -3.00141865787570 |
| C | 0.72286214731150 | -6.59027527777935 | 3.35567411501530 | C | 0.70659208282623 | -4.19266820348901 | -3.13837680590149 |
| C | 1.43762552677207 | -5.38268378555932 | 3.25843249032319 | C | -0.70647594752064 | -4.19266203949079 | -3.13848482459468 |
| C | -5.38270454291978 | 1.43761905915076 | 3.25825024810406 | C | -0.70648103334124 | 4.19270621566492 | -3.13809540423690 |
| C | -6.59029145854066 | 0.72284623845179 | 3.35549713532291 | C | 0.70658658510135 | 4.19270761813691 | -3.13805115017705 |
| C | -6.59028900486251 | -0.72294238849470 | 3.35549061948610 | C | 1.12415531577314 | 2.79504348201195 | -3.00120939092002 |
| C | -5.38269706965219 | -1.43770720053772 | 3.25824790911168 | C | -1.12405458152307 | 2.79504131965980 | -3.00125705762742 |
| C | 5.38261122306073 | -1.43770141007225 | 3.25834661525978 | C | -1.43760334197940 | -5.38263295578742 | -3.25858764842273 |
| C | 6.59018408522946 | -0.72293387234681 | 3.35578408924918 | C | -0.72283015490151 | -6.59021389069069 | -3.35591197926893 |
| C | 6.59016169656199 | 0.72285333690236 | 3.35603645457980 | C | 0.72296183822206 | -6.59018511032569 | -3.35616707974577 |
| C | 5.38258981793095 | 1.43762475979313 | 3.25861760190276 | C | 1.43772539141777 | -5.38260341629848 | -3.25878869905869 |
| C | 1.43761622806056 | 5.38264125734890 | 3.25810412390303 | C | -5.38257644213456 | 1.43768486648542 | -3.25850535992483 |
| C | 0.72284693718776 | 6.59023934564991 | 3.35523163958246 | C | -6.59016610239707 | 0.72292540256597 | -3.35582299497174 |
| C | -0.72293792545687 | 6.59023841902746 | 3.35522937307370 | C | -6.59017478890737 | -0.72286395171251 | -3.35582775241983 |
| C | -1.43770646434545 | 5.38263975714689 | 3.25809403858497 | C | -5.38259294623759 | -1.43764126218300 | -3.25854454661528 |
| C | -2.67773845431128 | -7.87101550309571 | 3.81622018506410 | C | 5.38272550892764 | -1.43762809515114 | -3.25827751464561 |
| C | 2.67765646315123 | -7.87100323956005 | 3.81635861433314 | C | 6.59028772158706 | -0.72283826180713 | -3.35571565395580 |
| C | 7.87097145515375 | -2.67782443036581 | 3.81590964566894 | C | 6.59024517223282 | 0.72294984975267 | -3.35596879531360 |
| C | 7.87089459460610 | 2.67762497184631 | 3.81682615223095 | C | 5.38266209821274 | 1.43770201592489 | -3.25853221433485 |
| C | 2.67762842316803 | 7.87104449980026 | 3.81578465593672 | C | 1.43772106967844 | 5.38266538991651 | -3.25821126926622 |
| C | -2.67771774670178 | 7.87103792603682 | 3.81580360755464 | C | 0.72295494910356 | 6.59025704832373 | -3.35546096641580 |
| C | -7.87107771656692 | 2.67763675302121 | 3.81604743723278 | C | -0.72283220471165 | 6.59025672653812 | -3.35551508872493 |
| C | -7.87106713465648 | -2.67775279583006 | 3.81595784446096 | C | -1.43760673745769 | 5.38266678016408 | -3.25829144005988 |
| C | -2.45060726531514 | -3.44849021362741 | 0.00007303573221 | C | -2.67763522115134 | -7.8708546096792 | -3.25878713814039 |
| C | -3.44847470768534 | -2.45060527147652 | 0.00008543339295 | C | 2.67778817732898 | -7.87095760944438 | -3.81659894856492 |
| C | -2.75938873946371 | -1.16976741185679 | 0.00003833608278 | C | 7.87110291188173 | -2.67769772583380 | -3.81584869168682 |
| C | -1.16975742793775 | -2.75941654359696 | 0.00003661488258 | C | 7.87095009564237 | 2.67775189607151 | -3.81666174604675 |
| C | 1.16975737057183 | 2.75936967421480 | 0.00011937581897 | C | 2.67773920803285 | 7.87100752215480 | -3.81611668779336 |
| C | 2.45059547891929 | 3.44845554819731 | 0.00019603374368 | C | -2.67759304780361 | 7.87103351602536 | -3.81620013867687 |
| C | 3.44847917340064 | 2.45058706397228 | 0.00021794999053 | C | -7.87092620748268 | 2.67776303664640 | -3.81624943354117 |
| C | 2.75940357017674 | 1.16973904990739 | 0.00014470992663 | C | -7.87094003021078 | -2.67766046803824 | -3.81641444425127 |
| C | 1.16975577375535 | -2.75941334030678 | 0.00009443055260 | H | -2.53447805727431 | -5.35108441396239 | 3.27549793856161 |
| C | 2.75939477291391 | -1.16977063457454 | 0.00013825520059 | H | 2.53439856322365 | -5.35104801081005 | 3.27571136469208 |
| C | 3.44847702458261 | -2.45061057796561 | 0.00027014217457 | H | -5.35106757178347 | 2.53439076556942 | 3.27567745308791 |
| C | 2.45060451482687 | -3.44849014418717 | 0.00018212269465 | H | -5.35104874670090 | -2.53447824349841 | 3.27567657284983 |
| C | -3.44846726203004 | 2.45058359793629 | 0.00012340822913 | H | 5.35093461671472 | -2.53446762450266 | 3.27604729672195 |
| C | -2.45058840601216 | 3.44845703067053 | 0.00011562464490 | H | 5.35088163542651 | 2.53438206710617 | 3.27682527084616 |
| C | -1.16974863930705 | 2.75937340509114 | 0.00007974522265 | H | 2.53438756451692 | 5.35099966364352 | 3.27553130121957 |
| C | -2.75939001990152 | 1.16973871597708 | 0.00005979517984 | H | -2.53447796689344 | 5.35099774898871 | 3.27553130559484 |
| C | 2.77316695581811 | -4.81084916789918 | 0.00033770185878 | H | -2.88581466563194 | -7.31486283686439 | 4.75579200913657 |
| C | 4.13477183779588 | -5.15978409882735 | 0.00044293658920 | H | -3.32296966769204 | -7.46179943780097 | 3.00801164400405 |
| C | 5.15979510938544 | -4.13474853440634 | 0.00032386620580 | H | -2.91447619064432 | -8.94052329554030 | 3.95917518853582 |
| C | 4.81083967506893 | -2.77315116809677 | 0.00026935025138 | H | 2.88565108707433 | -7.31484882310444 | 4.75597469768976 |
| C | -4.81084062290727 | -2.77313167323954 | 0.00009466231265 | H | 3.32294426326425 | -7.46173834585351 | 3.00822090989426 |
| C | -5.15980838118974 | -4.13472627268160 | 0.00008937183436 | H | 2.91439726500318 | -8.94051513170448 | 3.95927792436515 |
| C | -4.13479235334584 | -5.15976838083886 | 0.00006763252381 | H | 8.94051029707127 | -2.91459963500525 | 3.95857310083539 |
| C | -2.77318428234009 | -4.81084561305488 | 0.00007308420315 | H | 7.46159342879543 | -3.32298195439150 | 3.00772490206474 |
| C | 4.81083652132408 | 2.77315970903324 | 0.00025777307351 | H | 7.31498443479414 | 2.885982799718296 | 4.7555949049007 |
| C | 5.15976215512392 | 4.13476749271856 | 0.00025285763609 | H | 8.94041271480085 | 2.91434144364930 | 3.95974704271525 |
| C | 4.13472142382990 | 5.15978515389354 | 0.00022581763678 | H | 7.46167031646650 | 3.32305357702340 | 3.00877727798072 |
| C | 2.77312612221450 | 4.81082016617808 | 0.00020493262061 | H | 7.31474329364418 | 2.88548185955234 | 4.75644519239384 |
| C | -2.77313691305956 | 4.81081838720708 | 0.00012016090743 | H | 2.91436648861118 | 8.94059322965764 | 3.95843745110742 |
| C | -4.13473732171347 | 5.15976739823375 | 0.00011214308932 | H | 3.32304808227323 | 7.46160012648318 | 3.00784077503730 |
| C | -5.15976954140033 | 4.13474112286103 | 0.00013609216726 | H | 2.88547175983954 | 7.31513172194995 | 4.75554754540825 |
| C | -4.81082740932718 | 2.77313820237918 | 0.00014296453088 | H | -2.91445380187578 | 8.94058468145779 | 3.95847544497701 |

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|-------------------|-------------------|-------------------|
| H | -3.32314244551387 | 7.46160854504101 | 3.00785577209405 | H | 2.88561859304797 | 7.31483375464384 | -4.75571375167410 |
| H | -2.88555699978334 | 7.31511014758825 | 4.75555852958778 | H | 3.32313240228701 | 7.46186661640271 | -3.00799837713878 |
| H | -7.31498914421563 | 2.88560764155410 | 4.75568015817869 | H | -2.91430495384585 | 8.94054842517254 | -3.95916061480824 |
| H | -7.46182188132457 | 3.32296847400792 | 3.00793988059691 | H | -2.88544485107748 | 7.31488614047885 | -4.75581920554508 |
| H | -8.94059887528695 | 2.91434500062112 | 3.95895599363812 | H | -3.32301799197494 | 7.46187696093631 | -3.00811515335999 |
| H | -7.31502311742867 | -2.88576587914566 | 4.75560887585287 | H | -7.46160212193363 | 3.32301161347232 | -3.00811224967779 |
| H | -7.46175690754027 | -3.32303963112207 | 3.00783947181834 | H | -7.31488469055773 | 2.88579408480918 | -4.75589689430262 |
| H | -8.94059138206646 | -2.91448975137571 | 3.95880126104788 | H | -8.94044826567236 | 2.91451194150534 | -3.95907982203571 |
| H | 1.97473541490790 | -5.56215890125267 | 0.00052625178803 | H | -7.46168720500803 | -3.32297234268049 | -3.00829058847238 |
| H | 5.56213895843994 | -1.97470956534264 | 0.00003504967328 | H | -7.31483644500121 | -2.88563864052900 | -4.75603671994987 |
| H | -5.56212994552250 | -1.97468084188915 | 0.00012116032902 | H | -8.94045668616272 | -2.91437975847819 | -3.95933560554346 |
| H | -1.97476353155911 | -5.56216712105586 | 0.00004838375292 | N | -1.99654292584872 | -0.00004114282213 | 2.87250365621322 |
| H | 5.56215674173343 | 1.97473703905146 | 0.00027944624422 | N | 1.99646375373103 | -0.00004232883955 | 2.87257782295736 |
| H | 1.97467828375016 | 5.56211226084160 | 0.00017183211045 | N | -0.00004334096163 | -1.99654957758419 | 2.87252739290041 |
| H | -1.97470158604172 | 5.56212435026660 | 0.00010554091598 | N | -0.00003803211583 | 1.99646387309345 | 2.87254096115331 |
| H | -5.56213474268658 | 1.97470416323262 | 0.00018927141894 | N | -2.39935807297652 | -2.39935409077452 | 3.03309374998353 |
| H | 2.98263353564111 | -7.44687672091211 | 0.90069951707894 | N | -2.39935563185658 | 2.39927628213862 | 3.03304877626443 |
| H | 2.98278114210074 | -7.44677768653634 | -0.90035421053791 | N | -2.39926726505911 | 2.39928001132534 | 3.03313758801274 |
| H | 4.20795617750242 | -8.42685434121222 | 0.00021813397996 | N | 2.39927156251082 | -2.39934815478502 | 3.03320043444352 |
| H | 7.44667002008174 | -2.98248597872795 | 0.90090297523781 | N | -1.37492895312808 | -1.37495151710319 | 0.00003359555139 |
| H | 7.44696613703195 | -2.98278246173807 | -0.90014288970233 | N | 1.37493959411636 | 1.37490967650788 | 0.00011434999550 |
| H | 8.42686744102263 | -4.20786461804312 | 0.00074087006912 | N | 1.37493184846510 | -1.37494997286988 | 0.00008498542187 |
| H | 8.42682999670017 | 4.20793812986203 | 0.00049953261485 | N | -1.37492751794424 | 1.37491068621513 | 0.00006914091912 |
| H | 7.44691734366025 | 2.98269759578275 | -0.90014687604829 | N | -0.00000034998577 | -3.39499480166046 | 0.00008633775781 |
| H | 7.44668363468014 | 2.98270569739568 | 0.90091498385455 | N | -3.39497180132886 | -0.00001432131003 | 0.00007192134841 |
| H | 4.20780513658047 | 8.42685689162891 | 0.00017119838986 | N | 0.00000513671705 | 3.39495168624526 | 0.00012323049337 |
| H | 2.98261663149264 | 7.44680702286812 | -0.90039782333422 | N | 3.39497927796393 | -0.00001833893592 | 0.00019117363874 |
| H | 2.98256401481076 | 7.44679059787643 | 0.90065685041717 | N | -1.99645624352789 | 0.00000102902398 | -2.87254079842668 |
| H | -4.20785915893508 | 8.42683857373982 | 0.00016749627122 | N | 1.99655678415191 | -0.00000440378238 | -2.87248995777867 |
| H | -2.98263782172580 | 7.44683272554057 | -0.90040552309537 | N | 0.00004893590652 | -1.99650789518020 | -2.87254167093737 |
| H | -2.98262721421555 | 7.44675734513200 | 0.90064956759342 | N | 0.00004987221195 | 1.99651193247582 | -2.87247773522094 |
| H | -8.42684026473463 | -4.20789122452744 | 0.00011379897871 | N | -2.39925816000848 | -2.39930023399070 | -3.0330336414471 |
| H | -7.44681429164469 | 2.98259390817174 | -0.90033455763555 | N | -2.39925613956399 | 2.39931787556424 | -3.03315463027928 |
| H | -7.44679900984965 | 2.98271785752088 | 0.90072102043121 | N | 2.39935274886652 | 2.39931964686486 | -3.03310455816095 |
| H | -7.44682096614228 | -2.98260625884144 | 0.90058525149408 | N | 2.39936700675512 | -2.39929740756585 | -3.03324478946961 |
| H | -7.44681976826908 | -2.98258559644223 | -0.90046317936652 | O | -1.29566603904968 | -7.81035326871900 | 3.47910603118366 |
| H | -8.42687966732984 | -4.20781955713288 | 0.00004705521852 | O | 1.29560767374605 | -7.81034296411791 | 3.47914289676050 |
| H | -2.98273570098541 | -7.44680567727340 | 0.90059479224991 | O | 7.81027376704673 | -1.29570282673610 | 3.47898436806105 |
| H | -2.98276430638378 | -7.44684655192603 | -0.90045790733003 | O | 7.81023640860383 | 1.29561758559471 | 3.47943159473999 |
| H | -4.20801034860629 | -8.42683879377448 | 0.00010964009656 | O | 1.29561661606455 | 7.81033471107767 | 3.47840592756687 |
| H | -2.53438497500011 | -5.35104290898657 | -3.27542735337691 | O | -1.29570872963540 | 7.81033197717938 | 3.47841521440049 |
| H | 2.53449270594020 | -5.35093488463292 | -3.27639143653861 | O | -7.81037828361530 | 1.29559817382851 | 3.47878484339333 |
| H | -5.35091877150160 | 2.53445517397528 | -3.27594791782455 | O | -7.81037308506092 | -1.29570071357226 | 3.47876782413042 |
| H | -5.35095664117783 | -2.53441263338618 | -3.27597783195385 | O | 4.59212245729767 | -6.43102278200245 | 0.00035906551446 |
| H | 5.35108505115846 | -2.53439581518290 | -3.27596829579226 | O | 6.43104123722074 | -4.59207381903697 | 0.00047190246769 |
| H | 5.35094117944848 | 2.53445885610091 | -3.27674051719096 | O | 6.43100068296763 | 4.59211767150716 | 0.00025994688609 |
| H | 2.53449387876867 | 5.35103534830790 | -3.27556073956884 | O | 4.59203590037283 | 6.43103515993815 | 0.00017732745645 |
| H | -2.53437799007096 | 5.35103584654537 | -3.27575638214785 | O | -4.59206526438838 | 6.43101294669230 | 0.00009900163649 |
| H | -3.32287154559770 | -7.46179942140802 | -3.00850036675506 | O | -6.43101173482908 | 4.59207940704565 | 0.00009098818928 |
| H | -2.88570370908495 | -7.31451699882834 | -4.75625060357484 | O | -6.43105807593207 | -4.59204274202094 | 0.00004686005474 |
| H | -2.91437042318369 | -8.94033419533081 | -3.95995619779273 | O | -4.59215356239365 | -6.43100301098325 | 0.00007095254797 |
| H | 3.32300401819619 | -7.46169939496548 | -3.00839955502959 | O | -1.2956581778915 | -7.81025802567202 | -3.47964604379793 |
| H | 2.88588822207740 | -7.31486324813056 | -4.75620037238041 | O | 1.29570818030117 | -7.81026329587548 | -3.47952139751910 |
| H | 2.91451907422099 | -8.94047633294330 | -3.95948309523872 | O | 7.81038783137311 | -1.29558490867109 | -3.4788808541237 |
| H | 8.94061678549610 | -2.91442029628296 | -3.95879929713771 | O | 7.81031488282590 | 1.29573294724898 | -3.47929821710476 |
| H | 7.31490161421193 | -2.88588994964701 | -4.75536068316168 | O | 1.29572405825148 | 7.81033941053327 | -3.47873441415200 |
| H | 7.46202234948665 | -3.32286480965406 | -3.00751880948947 | O | -1.29559130975576 | 7.81034547931093 | -3.47877095043166 |
| H | 8.94044469612594 | 2.91447738508184 | -3.95975243943691 | O | -7.81024637680391 | 1.29569277976849 | -3.47910628261064 |
| H | 7.31467042783383 | 2.88564972762419 | -4.75619260223066 | O | -7.81025755716835 | -1.29561451192284 | -3.47917288179743 |
| H | 7.46190140299345 | 3.32313129101218 | -3.00848506919485 | Y | -0.00002256067097 | -0.00003246314088 | 1.68285369501251 |
| H | 2.91446433153764 | 8.94051678082056 | -3.95909738850620 | Y | 0.00003113520926 | -0.0000882073099 | -1.68281519035637 |

Table S10. BP86/def2-SVP geometry of $g\text{-Y}_2(\text{MeO})_8\text{Pc}_3$.

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|--------------------|-------------------|--------------------|
| C | -3.60744293632975 | -2.26305974432049 | 3.17522424730590 | C | 7.49461741589391 | -3.67287685631480 | 0.11554363639980 |
| C | -4.14990830812512 | -0.95740959749504 | 3.14338827681462 | C | 7.49384375624533 | 3.67493585251528 | -0.09257610954966 |
| C | -3.01818504355876 | -0.03220598406284 | 3.07607116097097 | C | 3.67291646288044 | 7.49469248352171 | 0.10302512515491 |
| C | -2.15253995025151 | -2.10911124327839 | 3.09352491008598 | C | -3.67476632923649 | 7.49361255031147 | -0.11242088843417 |
| C | 2.14154492240307 | 2.11348709534417 | 3.09794921702676 | C | -7.494656674529235 | 3.67307372875101 | 0.08769380725521 |
| C | 3.59617106221398 | 2.26755516720427 | 3.18401954182850 | C | -7.49342157115818 | -3.67523969648729 | -0.11136311457017 |
| C | 4.13873271462155 | 0.96185014471998 | 3.15603648848911 | C | -3.67304048374969 | -7.49460277646098 | 0.10146569030777 |
| C | 3.00724056978851 | 0.03653260958700 | 3.08655697312491 | C | -4.13910346893754 | 0.95608967632968 | -3.15707467021656 |
| C | 0.02887172851346 | -3.01053251016558 | 3.08366701128986 | C | -3.59693576177179 | 2.26191084463877 | -3.18703397241790 |
| C | 2.10578643791450 | -2.14486353208050 | 3.10110311703609 | C | -2.14225493090760 | 2.10840045591249 | -3.10092091761669 |
| C | 2.25963455792550 | -3.59957280876591 | 3.18620806840788 | C | -3.00731800254501 | 0.03121341669822 | -3.08645516340287 |
| C | 0.95400604850681 | -4.14209875981719 | 3.15437044392255 | C | 3.01813572568409 | -0.03562175392827 | -3.07635224062813 |
| C | -2.27095739765722 | 3.60402046288679 | 3.17328262917137 | C | 4.15012250661053 | -0.96057982712876 | -3.14261210474892 |
| C | -0.96523731153763 | 4.14653591724510 | 3.14521821651439 | C | 3.60804707893948 | -2.26644103365116 | -3.17258269434634 |
| C | -0.03984356253984 | 3.01489844362552 | 3.07907521880551 | C | 2.15311284486136 | -2.11282429480181 | -3.09080224553395 |
| C | -2.11678893581042 | 2.14920707552992 | 3.09044670431600 | C | -2.10519482801848 | -2.14990385717862 | -3.09790644287605 |
| C | 0.74213289633329 | -5.52854862604682 | 3.10698983504624 | C | -0.02802728375368 | -3.01491274839466 | -3.07942370057915 |
| C | 1.86730806534280 | -6.36393889256641 | 3.08305594459555 | C | -0.95282237303405 | -4.14686045089159 | -3.14859934012414 |
| C | 3.19841878409343 | -5.81476104628385 | 3.15181058160138 | C | -2.25861338060475 | -3.60477011947202 | -3.18107624405634 |
| C | 3.39409089445561 | -4.42682500224453 | 3.20944580387428 | C | 0.96386583180856 | 4.14238116933698 | -3.15082245626142 |
| C | -5.53625543669878 | -0.74550711314272 | 3.09310417815998 | C | 2.26976946579743 | 3.60026191082457 | -3.17807649873109 |
| C | -6.37158890738731 | -1.87066246716420 | 3.06646757439634 | C | 2.11606792227124 | 2.14549898454678 | -3.09357792926176 |
| C | -5.82256666794515 | -3.20182353231916 | 3.13546849211593 | C | 0.03884076010644 | 3.01052924986001 | -3.08333344641057 |
| C | -4.43475124489619 | -3.39753145625342 | 3.19588072896320 | C | -3.39280871277046 | -4.43240886169890 | -3.20337670369298 |
| C | 5.52523589464981 | 0.74989794646812 | 3.11034384405636 | C | -3.19671836465943 | -5.82021141011388 | -3.14394052909208 |
| C | 6.36061083474182 | 1.87504311778277 | 3.08451650489268 | C | -1.86544640154888 | -6.36889439803731 | -3.07437276320157 |
| C | 5.81135917708264 | 3.20630580800593 | 3.14975579624437 | C | -0.74052892713958 | -5.53318034906792 | -3.09930426661993 |
| C | 4.42336760315142 | 3.40208465783614 | 3.20551593947496 | C | -4.42448311198648 | 3.39615625835345 | -3.21000117391587 |
| C | -0.75325326122402 | 5.53294813479575 | 3.09689854968853 | C | -5.81240587594311 | 3.20003878815835 | -3.15360970909329 |
| C | -1.87837621991934 | 6.36826520311046 | 3.06846138193063 | C | -6.36124938782039 | 1.86870679186163 | -3.08640811533488 |
| C | -3.20968776230267 | 5.81914478104406 | 3.13378049667483 | C | -5.52552951642678 | 0.74378113264917 | -3.11083490258889 |
| C | -3.40550303796993 | 4.43126701834683 | 3.19220897839422 | C | 4.43570128203793 | -3.40068308421040 | -3.19189962497560 |
| C | 0.53689771697418 | -8.32467217999285 | 2.88151638519370 | C | 5.82346869142437 | -3.20446789049264 | -3.13209086544572 |
| C | 5.53833849602270 | -6.28116185684185 | 3.15497265678446 | C | 6.37209668668274 | -1.87305025785841 | -3.06495140750945 |
| C | 8.32161647399069 | 0.54427528020331 | 2.88788697559906 | C | 5.53641670900755 | -0.74818557821651 | -3.09290142043595 |
| C | 6.27787793186631 | 5.54622596072381 | 3.14945836829984 | C | 3.40404192316341 | 4.42786211828102 | -3.19767409819095 |
| C | -0.54745553999548 | 8.32893383767962 | 2.86952658137185 | C | 3.20774967447346 | 5.81573885200555 | -3.14081497032953 |
| C | -5.54960619849302 | 6.28563859980108 | 3.13057295528530 | C | 1.87624591086596 | 6.36449693625506 | -3.07640590620951 |
| C | -8.33195635784360 | -0.54008870712446 | 2.86244663800473 | C | 0.75140619196879 | 5.52877311010330 | -3.10410191167949 |
| C | -6.28900378682993 | -5.54174007081431 | 3.13633279115898 | C | -5.53649198840585 | -6.28738534135869 | -3.14820164827258 |
| C | -2.44867111211622 | -3.44851459306094 | 0.01629296362171 | C | -0.53443423875275 | -8.32891407665959 | -2.86993479050231 |
| C | -3.44772581978986 | -2.44971503014241 | -0.02266590315401 | C | 6.29058341073983 | -5.54424107974218 | -3.12942472359742 |
| C | -2.75787989851278 | -1.16989533169470 | -0.01536478404105 | C | 8.33209034954302 | -0.54164357593708 | -2.86273383069361 |
| C | -1.16904796143839 | -2.75830226748058 | 0.01095207956397 | C | 5.54751168557326 | 6.28301528433659 | -3.13771747309976 |
| C | 1.16913293926075 | 2.75823061545832 | 0.01147941365688 | C | 0.54464065882569 | 8.32488727785566 | -2.87931788688089 |
| C | 2.44873118619887 | 3.44845023553731 | 0.02022575264638 | C | -6.27962778871523 | 5.53982521001267 | -3.15713407610283 |
| C | 3.44789962847890 | 2.44958721914474 | -0.01407883290031 | C | -8.32176429575795 | -0.54164357593708 | -2.887538114141668 |
| C | 2.75802642433498 | 1.16978627692418 | -0.00725557792083 | H | -0.28334216772287 | -5.91509909606704 | 3.05303667073715 |
| C | 1.16992036368073 | -2.75800951291190 | -0.00726162836484 | H | 4.39583232397732 | -3.97944362021908 | 3.21512591259471 |
| C | 2.75829551725042 | -1.16912211652483 | 0.01694730670584 | H | -5.92267480150377 | 0.28000301396903 | 3.03883780041707 |
| C | 3.44851586396851 | -2.44871721227585 | 0.02591490315899 | H | -3.98741523128499 | -4.39928826303825 | 3.20202056229132 |
| C | 2.44975630282510 | -3.44785615160702 | -0.01192078539075 | H | 5.91185688882302 | -0.27568489370277 | 3.05901371180659 |
| C | -3.44843726511626 | 2.44869389432838 | 0.01066144301337 | H | 3.97596545790279 | 4.40382797286962 | 3.20864299295893 |
| C | -2.44953040400994 | 3.44777582544347 | -0.02491525523152 | H | 0.27237077918704 | 5.91945745167790 | 3.04551097333111 |
| C | -1.16975368554970 | 2.75790059899588 | -0.01536363868106 | H | -4.40726037702670 | 3.98390324161970 | 3.19549383372619 |
| C | -2.75823598270947 | 1.16905805449925 | 0.005492616686836 | H | -0.06681891447888 | -8.12605477619758 | 3.79502057542117 |
| C | 2.77804808718953 | -4.81117551126281 | -0.05176290624969 | H | -0.03469854655043 | -7.96302738655577 | 1.99619525846438 |
| C | 4.13541241970153 | -5.15278128664795 | -0.03005992911561 | H | 0.70543939223670 | -9.41351279139977 | 2.78730068196641 |
| C | 5.15395899373187 | -4.13375472524477 | 0.05043395418432 | H | 5.72606422085218 | -5.65458559814133 | 4.05480924215948 |
| C | 4.81187125769827 | -2.77646315110456 | 0.06896825380401 | H | 5.80688293202785 | -5.71366056927270 | 2.23918972616640 |
| C | -4.81097269328090 | -2.7779378283695 | -0.06557173168765 | H | 6.16862682424170 | -7.18803832848772 | 3.20784525482475 |
| C | -5.15263761611994 | -4.13531757403145 | -0.04553344359856 | H | 9.41053200656278 | 0.71268854537870 | 2.79429275496924 |
| C | -4.13379228517846 | -5.15393011775067 | 0.03641650248736 | H | 7.96087423852508 | -0.02938849316232 | 2.00352604942528 |
| C | -2.77653861339178 | -4.81188679925260 | 0.05784816708503 | H | 8.12221853205799 | -0.05740581482948 | 3.80256868747044 |
| C | 4.81126311095130 | 2.7776002624628 | -0.05320938410277 | H | 7.18474591999290 | 6.17654233775681 | 3.20214167781743 |
| C | 5.15288868036826 | 4.13515794108227 | -0.03419683185110 | H | 5.71131227326550 | 5.81323883073856 | 2.23265566185729 |
| C | 4.13380171061048 | 5.15389860212830 | 0.04302125949444 | H | 5.65042994409507 | 5.73555406722501 | 4.04835365798377 |
| C | 2.77648190626600 | 4.81187938420127 | 0.06071756157200 | H | -0.71579430471592 | 9.41768284612888 | 2.77388236370583 |
| C | -2.77761682830755 | 4.81107376379857 | -0.06706016199972 | H | 0.02703513940909 | 7.96666788994875 | 1.98632734681655 |
| C | -4.13502346068486 | 5.15276629397367 | -0.04972793322620 | H | 0.05336679008954 | 8.13112726570668 | 3.78511634131066 |
| C | -5.15384047467352 | 4.13386092299526 | 0.0284382408298 | H | -6.17999427061049 | 7.199276170427658 | 3.18039653560232 |
| C | -4.81188177729022 | 2.77657386407475 | 0.04948522397986 | H | -5.81561934822430 | 5.71686266447459 | 2.21484850690450 |
| C | 3.67533951680076 | -7.49367676499395 | -0.09146734385287 | H | -5.73991235471519 | 5.66035619298163 | 4.03077753937836 |

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|-------------------|-------------------|-------------------|
| H | -8.13500570182055 | 0.06279491410782 | 3.77686034064516 | H | 0.71260877609012 | 9.41377199361056 | -2.78455933574289 |
| H | -7.96870453889316 | 0.03230930255802 | 1.97830319983006 | H | -0.05608955972628 | 8.12614840847220 | -3.79476798469296 |
| H | -9.42062148136164 | -0.70855435018333 | 2.76609069657613 | H | -0.02975230883977 | 7.96315591874607 | -1.99583536977686 |
| H | -5.66464741750356 | -5.73021195952950 | 4.03756198804963 | H | -5.71299379012755 | 5.80858700206370 | -2.24088431850997 |
| H | -5.71925903285952 | -5.80955383533971 | 2.22173415739636 | H | -5.65238050322933 | 5.72779845058961 | -4.05645168697486 |
| H | -7.19601071509533 | -6.17206256534087 | 3.18647606740286 | H | -7.18669360815801 | 6.16977744283735 | -3.21075236528130 |
| H | 1.98121506667491 | -5.56369102642844 | -0.07751158670036 | H | -7.96058222675113 | -0.03469670385357 | -2.00245636563374 |
| H | 5.56406300653881 | -1.97931162383529 | 0.09451629683277 | H | -8.12237540151979 | -0.06533133284949 | -3.80141801217830 |
| H | -5.56340001139285 | -1.98105287683325 | -0.09250546897141 | H | -9.41071604332954 | 0.70573561112321 | -2.79393072304176 |
| H | -1.97946885497504 | -5.56411448323696 | 0.08474515453863 | N | -1.84626967897210 | -0.76277704543803 | 2.98014841028192 |
| H | 5.56379029302699 | 1.98086841524106 | -0.07672906803552 | N | 1.83564831077388 | 0.76696918638837 | 2.98577223986336 |
| H | 1.97935138044708 | 5.56416089578380 | 0.08409350512847 | N | 0.75955116800564 | -1.83885583276342 | 2.98579645856941 |
| H | -1.98066206855183 | 5.56351301910307 | -0.09146147590929 | N | -0.77017249860352 | 1.84306821626102 | 2.98015532408101 |
| H | -5.56420968986680 | 1.97952575189502 | 0.07404788806234 | N | -1.29982624230252 | -3.13648090877586 | 3.11610890158052 |
| H | 3.10052898973764 | -7.53622843347810 | 0.85696766542484 | N | -3.14420497170030 | 1.29645365838590 | 3.10959072380298 |
| H | 2.97734522570919 | -7.41123023055588 | -0.95449354165632 | N | 1.28873923803107 | 3.14088479546550 | 3.11601871161556 |
| H | 4.26868523033789 | -8.42091129463879 | -0.19210783567509 | N | 3.13314116511004 | -1.29209058466777 | 3.12251497349021 |
| H | 7.41032464544508 | -2.97494577955644 | 0.97722714072827 | N | -1.37612150304746 | -1.37658591589130 | -0.00167777537918 |
| H | 7.53883132379302 | -3.09965342644585 | -0.83376684476648 | N | 1.37623306054012 | 1.37650301631235 | 0.00157127570756 |
| H | 8.42182952296085 | -4.26578131584704 | 0.21894464515807 | N | 1.37659383303459 | -1.37622255686743 | 0.00367041765456 |
| H | 8.42115711371711 | 4.26805322122980 | -0.19383117800486 | N | -1.37649449735655 | 1.37613377494201 | -0.00376415080646 |
| H | 7.41211073002263 | -5.56416089578380 | -0.95405185159738 | N | 0.00052028116305 | -3.39208601835545 | 0.00223326034614 |
| H | 7.53561632136012 | 3.10233424885658 | 0.85722354784710 | N | -3.39198645556181 | -0.00050862589236 | -0.00601110818283 |
| H | 4.26571907235808 | 8.42207674476752 | 0.20546328565503 | N | -0.00039525048966 | 3.39198835873487 | -0.00234728268343 |
| H | 3.10097452204614 | 7.53711445056703 | -0.84713998888557 | N | 3.39208492255350 | 0.00041480348221 | 0.00592617121664 |
| H | 2.97234616746833 | 7.41205729267567 | 0.96393997255643 | N | -1.83593188310115 | 0.76213017331524 | -2.98687870068702 |
| H | -4.26782314571570 | 8.42072641008314 | -0.21582566820038 | N | 1.84646277912281 | -0.76643050871506 | -2.97920547018085 |
| H | -2.97425218705345 | 7.41021712790616 | -0.97330936709745 | N | -0.75904848194276 | -1.84331980531801 | -2.98309748682709 |
| H | -3.10272734728001 | 7.53723911835675 | 0.83762933626990 | N | 0.76954753235097 | 1.83906883437614 | -2.98294806381795 |
| H | -8.42214504983176 | 4.26605209688941 | 0.18816771271251 | N | -3.13282299452691 | -1.29749266473735 | -3.12044806619362 |
| H | -7.53623096068431 | 3.09926858488988 | -0.86139046869453 | N | -1.28978375081600 | 3.13604685915083 | -3.12042285400800 |
| H | -7.41274070652725 | 2.97419597142308 | 0.95005332973434 | N | 3.14374458275673 | 1.29303451110461 | -3.11168064064064 |
| H | -7.53787979139722 | -3.10096965273856 | 0.83730414429317 | N | 1.30070458109902 | -3.14048979487210 | -3.11184785044562 |
| H | -7.40927101292216 | -2.97674384281532 | -0.97381605919740 | O | 1.81721037645711 | -7.72506061072075 | 2.96029713613910 |
| H | -8.42044495478559 | -4.26853971523689 | -0.21418509518338 | O | 4.19363229760968 | -6.74056231982744 | 3.11450015309149 |
| H | -2.97533417152098 | 7.41064985364090 | 0.96457728059647 | O | 7.72185279741570 | 1.82471206753106 | 2.96318802681290 |
| H | -3.09793172212194 | -7.53841569928952 | -0.84672354153620 | O | 6.73723657801392 | 4.20142097335472 | 3.11177033662910 |
| H | -4.26614052229244 | -8.42186266167479 | 0.20331078404053 | O | -1.82795398246866 | 7.72928087123498 | 2.94466551646137 |
| H | -4.39469365414564 | -3.98536145086784 | -3.20972043762719 | O | -4.20477314731812 | 6.74494542132720 | 3.09322776521534 |
| H | 0.28506561041029 | -5.91932273584945 | -3.04468186528597 | O | -7.73247417590192 | -1.82046779482365 | 2.94115248285123 |
| H | -3.97737376969281 | 4.39802514511538 | -3.21438250819961 | O | -6.74830940404123 | -4.19700137507928 | 3.09580664024516 |
| H | -5.91181277542408 | -0.28184645003072 | -3.05788613201291 | O | 4.61557421973147 | -6.42622257648818 | -0.08110775991330 |
| H | 3.98869262926198 | -4.40259287887218 | -3.19673560484286 | O | 6.42745250337927 | -4.61343143271069 | 0.10475793186591 |
| H | 5.92252710827028 | 0.27752232954464 | -3.04021067841122 | O | 6.42637863628235 | 4.61518813634305 | -0.08527332749105 |
| H | 4.40594771292485 | 3.98082467704309 | -3.20019395803941 | O | 4.61345191345180 | 6.42747910734210 | 0.09550480592111 |
| H | -0.27436254376962 | 5.91498822603178 | -3.05342091032781 | O | -4.61501148989919 | 6.42615821426106 | -0.10363098294218 |
| H | -5.80573857075116 | -5.71876984603301 | -2.23331851196679 | O | -6.42746164148646 | 4.61361872388575 | 0.07923252481047 |
| H | -5.72392906388105 | -5.66205968529441 | -4.04897062190860 | O | -6.42597256797859 | -4.61545437564220 | -0.09943580289391 |
| H | -6.16645456102464 | -7.19453582769340 | -3.20023272410876 | O | -4.61358537225284 | -6.42744305123746 | 0.08923030717245 |
| H | 0.03693173250471 | -7.96581948034450 | -1.98506177434865 | O | -4.19165731079373 | -6.74630524485376 | -3.10637411875685 |
| H | 0.06931750320257 | -8.13138117449194 | -3.78365035044014 | O | -1.81493516191535 | -7.72982747722355 | -2.94970793204591 |
| H | -0.70263240612023 | -9.41767452405288 | -2.77419927625090 | O | 6.74950899993789 | -4.19931037469216 | -3.09105715802978 |
| H | 7.19777156040276 | -6.17437781527505 | -3.17861134563955 | O | 7.73298118049711 | -1.82228923614581 | -2.93984386460190 |
| H | 5.66623752265010 | -5.73432153135183 | -4.03032678580230 | O | 4.20252255238351 | 6.74190960333148 | -3.10102874192581 |
| H | 5.72096985217258 | -5.81077644180463 | -2.21436891502321 | O | 1.82534808360768 | 7.72561517137358 | -2.9532652819392 |
| H | 9.42081109968258 | -0.70968056111761 | -2.76624445895239 | O | -6.73857533817535 | 4.19494426945885 | -3.11707186067489 |
| H | 8.13491157780596 | 0.06009200404237 | -3.77785589283025 | O | -7.72245671805149 | 1.81810802334652 | -2.96480799114129 |
| H | 7.96876233771512 | 0.03171773011103 | -1.97924268845576 | Y | -0.00294594562809 | 0.00119133918453 | 1.74298612141875 |
| H | 6.17759584083969 | 7.19014374229096 | -3.18865356660443 | Y | 0.00300112892160 | -0.00119750019603 | -1.74302466013243 |
| H | 5.73806622382979 | 5.65665481484888 | -4.03711594386867 | | | | |
| H | 5.81366841633340 | 5.71549583016725 | -2.22125724688767 | | | | |

Table S11. BP86/def2-SVP geometry of $g\text{-Y}_2(\text{MeO})_8\text{Pc}]^{\text{+}}$.

| | | | | | | | |
|---|-------------------|--------------------|-------------------|---|-------------------|-------------------|-------------------|
| C | -3.58984201430422 | -2.29044092418638 | 3.16779630366956 | C | 3.68187020385483 | -7.49901048002115 | -0.07115519188720 |
| C | -4.14191007688467 | -0.98971270771584 | 3.14169157825650 | C | 7.50004535035740 | -3.67913016318999 | 0.09685281611885 |
| C | -3.01650147634995 | -0.05653268860412 | 3.06649993107939 | C | 7.49899061944419 | 3.68258822401704 | -0.06956282340251 |
| C | -2.13442484805709 | -2.12443900750367 | 3.08102892596446 | C | 3.67838792405454 | 7.50064104268926 | 0.08429550542102 |
| C | 2.12450628741335 | 2.12858459478776 | 3.08514022808060 | C | -3.68129414057813 | 7.49938491337328 | -0.09000156290161 |
| C | 3.57968209587042 | 2.29467859734414 | 3.17567865123845 | C | -7.50035723804260 | 3.67986870706177 | 0.06456156296899 |
| C | 4.13178529094208 | 0.99389488508706 | 3.15326429966334 | C | -7.49931283279359 | -3.68084834202920 | -0.09101745550322 |
| C | 3.00658617600162 | 0.06065007012898 | 3.07594831531282 | C | -3.68034682734681 | -7.49982617512616 | 0.07744572635791 |
| C | 0.05362835088109 | -3.00951841486533 | 3.07292402012990 | C | -4.13210834117181 | 0.98811313800741 | -3.15489145244199 |
| C | 2.12148746867873 | -2.12739330209202 | 3.08772849990951 | C | -3.58041315054769 | 2.28904289488052 | -3.17914977731451 |
| C | 2.28743399421941 | -3.58264277725080 | 3.17725723263636 | C | -2.12519010836537 | 2.12354489422456 | -3.08827076113146 |
| C | 0.98674228919356 | -4.13477853836050 | 3.15108115323114 | C | -3.00661942705664 | 0.05532204618958 | -3.07629446413431 |
| C | -2.29767368930497 | 3.58689924262498 | 3.16610317465922 | C | 3.01655786730019 | -0.05998554005963 | -3.06620221617225 |
| C | -0.99688579646184 | 4.13900176869297 | 3.14352492778537 | C | 4.14227349300704 | -0.99292839182676 | -3.13972725980729 |
| C | -0.06353127406489 | 3.01367463921999 | 3.06932696063430 | C | 3.59058728697334 | -2.29384656913160 | -3.16412868209369 |
| C | -2.13146770186838 | 2.13156245760032 | 3.07837828690582 | C | 2.13510343192777 | -2.12813110086109 | -3.07796439513581 |
| C | 0.78361940203435 | -5.52227145506372 | 3.12300556791611 | C | -2.12084030843383 | -2.13247001246023 | -3.08487650874991 |
| C | 1.91583611046742 | -6.35072844032425 | 3.10692292080950 | C | -0.05267072936015 | -3.0138406392791 | -3.06910819083028 |
| C | 3.24374565154589 | -5.78992925320888 | 3.16174084511869 | C | -0.98536414081572 | -4.13952080395101 | -3.14580758838498 |
| C | 3.42864007718598 | -4.39735989659842 | 3.20597097346950 | C | -2.28627378738296 | -3.58792209658716 | -3.17248436170731 |
| C | -5.52934283068958 | -0.78651198957383 | 3.11132158665784 | C | 0.99567474107591 | 4.13482217071128 | -3.14948120612364 |
| C | -6.35779849143355 | -1.91868110433780 | 3.09252845941589 | C | 2.29657484745598 | 3.58297127372113 | -3.17177014353047 |
| C | -5.79713409564099 | -3.24665491806167 | 3.14710762198474 | C | 2.13076631517527 | 2.12776053662131 | -3.08172051013327 |
| C | -4.40466046888857 | -3.43163807664275 | 3.19377038637841 | C | 0.06258826289456 | 3.00935111805516 | -3.07369011910447 |
| C | 5.51930878468805 | 0.79064087095456 | 3.12743321121124 | C | -3.42714820116500 | -4.40318452359154 | -3.19909697555092 |
| C | 6.34782512195339 | 1.92277648893885 | 3.10938859024268 | C | -3.24161478438220 | -5.79563303572335 | -3.15326142224983 |
| C | 5.78702253458268 | 3.25085073121868 | 3.16004839681520 | C | -1.91342925769410 | -6.35583255854711 | -3.09909601575401 |
| C | 4.39441591624169 | 3.43592331463725 | 3.20225477968565 | C | -0.78160822325840 | -5.52689504847387 | -3.11673775841047 |
| C | -0.79364759295734 | 5.52648035998486 | 3.11521348192690 | C | -4.39551986538804 | 3.42998624266491 | -3.20699704867497 |
| C | -1.92579893177127 | 6.35491182513460 | 3.09446716894545 | C | -5.78806831792542 | 3.24451577163673 | -3.16450111779912 |
| C | -3.25389468630329 | 5.79417507465410 | 3.14523828097813 | C | -6.34844813428637 | 1.91632591962342 | -3.11225513086596 |
| C | -3.43895374340741 | 4.40165624090703 | 3.19013006277444 | C | -5.51956452449591 | 0.78443950338478 | -3.12897497731403 |
| C | 0.60559601710808 | -8.33517063978513 | 2.98781462076541 | C | 4.40571906029647 | -3.43484976324942 | -3.18862559262491 |
| C | 5.58818625207754 | -6.24393661990837 | 3.17768867882545 | C | 5.79812872381615 | -3.24942558969852 | -3.14182043583890 |
| C | 8.33248349125020 | 0.61222488837977 | 2.99706739801900 | C | 6.35839735356928 | -1.92123350686869 | -3.08851766207784 |
| C | 6.24102380944664 | 5.59529746561251 | 3.16800993707916 | C | 5.52964267229248 | -0.78930685684958 | -3.10900641980823 |
| C | -0.61517737677872 | 8.33935215682721 | 2.97958662320904 | C | 3.43769011731110 | 4.39787560841307 | -3.19765757859287 |
| C | -5.59838337510082 | 6.24802143531769 | 3.14964789683605 | C | 3.25241311671112 | 5.79040839753573 | -3.15465190250045 |
| C | -8.34189904385241 | -0.60821160443649 | 2.97079281339738 | C | 1.92424598678001 | 6.35096584948844 | -3.10368921640754 |
| C | -6.25100146971402 | -5.59112573736801 | 3.15694143604551 | C | 0.79221203551359 | 5.52230728634781 | -3.12274350383573 |
| C | -2.44806959259621 | -2.758472125186566 | 0.01439809618929 | C | -5.58587583869979 | -6.25051572360184 | -3.16477701269470 |
| C | -3.44840613174493 | -3.44848742102552 | -0.02120717606412 | C | -0.60214164064358 | -8.33948773992515 | -2.97891708462534 |
| C | -2.75836232704569 | -1.17011558277334 | -0.01434441816788 | C | 6.25283852780805 | -5.59376525536724 | -3.15137229865417 |
| C | -1.16975097446474 | -2.75843280814470 | 0.01012332722327 | C | 8.34217170920178 | -0.61012420212481 | -2.96820439545711 |
| C | 1.16941984695805 | 2.75879937890121 | 0.01049512096949 | C | 5.59683849778836 | 6.24460794478256 | -3.16137475039280 |
| C | 2.44755829850351 | 3.44923407630746 | 0.01874672540295 | C | 0.61342394530309 | 8.33532786936859 | -2.98946038083739 |
| C | 3.44817029820317 | 2.44912267217720 | -0.01227484795249 | C | -6.24272680198879 | 5.58882490504359 | -3.17458182665224 |
| C | 2.75824513070687 | 1.17060369971656 | -0.00664954366936 | C | -8.33261541072743 | 0.60517998783119 | -2.99858807687852 |
| C | 1.17026581856882 | -2.75811972772512 | -0.00624416035556 | H | -0.23812245957512 | -5.91980203191545 | 3.08177661597532 |
| C | 2.75851446410043 | -1.16935059404718 | 0.01576638108933 | H | 4.42723176234824 | -3.94330096144026 | 3.21330597172163 |
| C | 3.44885713010288 | -2.44757675014358 | 0.02428212233259 | H | -5.92672638547000 | 0.235300797550496 | 3.07042724341752 |
| C | 2.44873414490265 | -3.44808654176794 | -0.00990992996544 | H | -3.95069493635433 | -4.43027176681032 | 3.20091723067508 |
| C | -3.44906778039671 | 2.44806938240598 | 0.00880143168717 | H | 5.91686821616571 | -0.23122487270944 | 3.08966622821295 |
| C | -2.44881869971720 | 3.44847738099930 | -0.02390018522012 | H | 3.94039937053811 | 4.43455365393373 | 3.20662062291129 |
| C | -1.17042926155501 | 2.75845689540716 | -0.01471368328362 | H | 0.22823649384201 | 5.92395480293121 | 3.07700323307574 |
| C | -2.75872322134153 | 1.16980924231232 | 0.00464180031185 | H | -4.43758522667836 | 3.94765365049598 | 3.19446412976773 |
| C | 2.77590201054988 | -4.81179517151367 | -0.04349758199752 | H | 0.02834525677932 | -8.11620431666669 | 3.91280442590210 |
| C | 4.13363089639762 | -5.15386593538388 | -0.02225048630606 | H | 0.00345011638271 | -8.01547157617602 | 2.10780217119502 |
| C | 5.15516892787553 | -4.13183933468338 | 0.04417520804513 | H | 0.79433557821466 | -9.42238738638155 | 2.92576974124724 |
| C | 4.81259348565360 | -2.77418627538934 | 0.06172666854613 | H | 5.76749210091215 | -5.60817211838524 | 4.07170223978047 |
| C | -4.81202270461700 | -2.77545359999530 | -0.05975975599745 | H | 5.85815327199425 | -5.68824289687904 | 2.25546250481680 |
| C | -5.15431612583686 | -4.13314646296001 | -0.04068028660764 | H | 6.21675120312504 | -7.15021180347913 | 3.24517047662011 |
| C | -4.13265848300031 | -5.15479575433595 | 0.02941520066502 | H | 9.41978309059706 | 0.80082754309106 | 2.93609419251301 |
| C | -2.77498306915365 | -4.81242825353131 | 0.05063370435397 | H | 8.01424377111864 | 0.00748496402010 | 2.11757194755339 |
| C | 4.81183469525784 | 2.77643274882417 | -0.04649529586892 | H | 8.11202633940432 | 0.03759097294131 | 3.92333144208465 |
| C | 5.15373353999497 | 4.13426070744546 | -0.02727709380651 | H | 7.14725048924514 | 6.22412016419820 | 3.23373724968752 |
| C | 4.13162706711176 | 5.15571054311843 | 0.03904137528520 | H | 5.68584133136486 | 5.86194199760144 | 2.24451368957059 |
| C | 2.77401584456291 | 4.81300220582106 | 0.05578032875460 | H | 5.60473208738728 | 5.77778021243347 | 4.06100670500749 |
| C | -2.77580906892844 | 4.81211297996332 | -0.06163550017719 | H | -0.80369754529409 | 9.42653146786106 | 2.91625780820521 |
| C | -4.13357508097791 | 5.15430178666614 | -0.04498592108841 | H | -0.00963369908994 | 8.01930783477635 | 2.10130130891933 |
| C | -5.15528125990769 | 4.13251677138230 | 0.02226925722859 | H | -0.04142988826617 | 8.12072681309436 | 3.90683060240213 |
| C | -4.81285199867107 | 2.77486238859907 | 0.04269744244570 | H | -6.22734683220059 | 7.15434582730277 | 3.21259664055449 |

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|-------------------|-------------------|-------------------|
| H | -5.86380412636274 | 5.69082078151925 | 2.22699669111890 | H | 5.86313250236014 | 5.68881451706872 | -2.23811973335002 |
| H | -5.78199239705689 | 5.61366456419412 | 4.04379425203563 | H | 0.80188876471907 | 9.42259212204537 | -2.92732362802212 |
| H | -8.12472660119481 | -0.03183165207996 | 3.89674552841500 | H | 0.03890406072239 | 8.11586431608647 | -3.91602520179818 |
| H | -8.02032977204965 | -0.00531499160181 | 2.09125399598687 | H | 0.00873291322720 | 8.01614280142929 | -2.11027746054356 |
| H | -9.42900729752119 | -0.79677930863385 | 2.90637937351832 | H | -5.68767004941778 | 5.85649707179049 | -2.25129273730639 |
| H | -5.61733060889525 | -5.77245609081077 | 4.05203656558040 | H | -5.60643814625566 | 5.77064055915203 | -4.06771574939725 |
| H | -5.69309814837425 | -5.85889474917827 | 2.23539079146033 | H | -7.14912356735839 | 6.21733181513420 | -3.24097682402508 |
| H | -7.15737448996884 | -6.21992558500557 | 3.22082425679948 | H | -8.01412932037958 | 0.00163892053174 | -2.11836746519898 |
| H | 1.98014588357510 | -5.56556026563162 | -0.06283776634459 | H | -8.11198563112466 | 0.02955883349056 | -3.92419855496154 |
| H | 5.56603093297909 | -1.97811337035074 | 0.08105755409448 | H | -9.41999736172209 | 0.79343427268214 | -2.93796240493479 |
| H | -5.56557932865709 | -1.97959733410751 | -0.08320729346259 | N | -1.83751354171408 | -0.77585940619115 | 2.96713432450560 |
| H | -1.97910063060697 | -5.56595207460810 | 0.07425149338539 | N | 1.82791488702997 | 0.77986394245617 | 2.97215187991449 |
| H | 5.56568792984983 | 1.98077788771272 | -0.06705923657693 | N | 0.77300844556361 | -1.83070559505062 | 2.97203576184419 |
| H | 1.97789103538206 | 5.56634947246109 | 0.07682104304441 | N | -0.78264709271692 | 1.83479347173076 | 2.96713749074573 |
| H | -1.97997484988122 | 5.56574684508069 | -0.08343637380237 | N | -1.27493836867075 | -3.14575171363266 | 3.10496326931634 |
| H | -5.56637611447356 | 1.97892581628123 | 0.06438116384576 | N | -3.15279623461623 | 1.27200995689813 | 3.09947088228673 |
| H | 3.11084244789093 | -7.54171086245198 | 0.87919634598165 | N | 1.26494135397597 | 3.14991835765504 | 3.10533352830380 |
| H | 2.98329646329998 | -7.42310208864933 | -0.93351198531045 | N | 3.14276430352912 | -1.26785090812467 | 3.11095474039338 |
| H | 4.28340121080122 | -8.42047946046866 | -0.16956148660304 | N | -1.37584284000393 | -1.37594105177884 | -0.00155454270169 |
| H | 7.42221093854590 | -2.97889775466749 | 0.95768736485575 | N | 1.37567080152732 | 1.37631495397376 | 0.00137377246920 |
| H | 7.54436425121999 | -3.10993817945464 | -0.85452770549013 | N | 1.37603879667863 | -1.37556388604953 | 0.00344810485980 |
| H | 8.42154496466552 | -4.28012179535895 | 0.19822074462350 | N | -1.37621570817725 | 1.37592539457156 | -0.00369188976261 |
| H | 8.42070852104025 | 4.28406284769458 | -0.16597759333218 | N | 0.00033756145162 | -3.39190284621035 | 0.00238505178709 |
| H | 7.42539010110518 | 2.98333491876620 | -0.93157094814053 | N | -3.39216113956360 | -0.00023341681412 | -0.00591353108094 |
| H | 7.53911653262740 | 3.11228983097128 | 0.88134307246871 | N | -0.00059347853811 | 3.39224004937595 | -0.00257887560739 |
| H | 4.27916109799164 | 8.42257865413243 | 0.18296813518356 | N | 3.39200258142485 | 0.00071163575340 | 0.00561907719589 |
| H | 3.10930614706532 | 7.54197326118224 | -0.86729484255190 | N | -1.82818026092002 | 0.77505436183444 | -2.97348272088104 |
| H | 2.97806922389928 | 7.42524001664225 | 0.94528262970246 | N | 1.83776723615217 | -0.77948791050237 | -2.96601373975870 |
| H | -4.28243505568869 | 8.42111340918532 | -0.18837633895466 | N | -0.77246203273588 | -1.83516590004530 | -2.96959934633274 |
| H | -2.98108064438676 | 7.42441933611860 | -0.95111738091698 | N | 0.78201307483352 | 1.83080049381709 | -2.96988283381346 |
| H | -3.11205038764457 | 7.54070169087590 | 0.86149384391385 | N | -3.14239008727848 | -1.27328678255032 | -3.10935846676809 |
| H | -8.42234827758529 | -4.28104824527704 | 0.16023441277368 | N | -1.26594366582212 | 3.14513355569869 | -3.10987516326578 |
| H | -7.54011378943229 | 3.10862506486357 | -0.88579347615239 | N | 3.15239413651251 | 1.26853807967622 | -3.10131363020619 |
| H | -7.42661075876960 | 2.98150438302812 | 0.92728350164230 | N | 1.27593677106507 | -3.14971491157861 | -3.10072582865632 |
| H | -7.54243367931874 | -3.10971535810840 | 0.85925767283217 | O | 1.87827379566249 | -7.70868543400219 | 3.00844380073608 |
| H | -7.42269941579921 | -2.98235492238269 | -0.95338054214876 | O | 4.24129869455656 | -6.70491818001335 | 3.13309853572508 |
| H | -8.42087551823079 | -4.28215534942682 | -0.18993499477913 | O | 7.70591931391707 | 1.88492161598083 | 3.01298584685341 |
| H | -2.98284402076287 | -7.42422121667768 | 0.94069589947337 | O | 6.70204517494829 | 4.24827636920609 | 3.12850032244140 |
| H | -3.10814022974792 | -7.54178140208977 | -0.87222920526242 | O | -1.88789759770024 | 7.71282966686124 | 2.99556101773970 |
| H | -4.28173845675213 | -8.42152572674344 | 0.17456455182044 | O | -4.25133935929243 | 6.70907102216685 | 3.11089202018374 |
| H | -4.42595318944148 | -3.94958718204723 | -3.20576205195663 | O | -7.71556869880999 | -1.88096816580915 | 2.99152897187643 |
| H | 0.24035983711599 | -5.92391194825531 | -3.07623544510280 | O | -6.71201020400223 | -4.24417982253110 | 3.11439631895198 |
| H | -3.94181883421353 | 4.42875359738303 | -3.21239615099111 | O | 4.61466015110945 | -6.42196321720468 | -0.06558009463733 |
| H | -5.91677087896672 | -0.23750022211135 | -3.08953935204964 | O | 6.42334603158082 | -4.61232390979788 | 0.09107022320704 |
| H | 3.95203999167046 | -4.43361918987415 | -3.19460987287553 | O | 6.42190763584168 | 4.61533829002798 | -0.06764337588478 |
| H | 5.92672181829989 | 0.23265791188358 | -3.06894435864206 | O | 4.61183386092625 | 6.42413446486957 | 0.08191394895710 |
| H | 4.43639460285296 | 3.94402989376394 | -3.20207288771158 | O | -4.61430730696374 | 6.42252546359183 | -0.08768291373242 |
| H | -0.22971499414857 | 5.91967933652546 | -3.08460392459476 | O | -6.42367072196838 | 4.61308562383837 | 0.06189162366253 |
| H | -5.85442418482038 | -5.69351893679052 | -2.24291691730951 | O | -6.42249112880592 | -4.61389740762860 | -0.08477195589124 |
| H | -5.76694304411466 | -5.61615045808776 | -4.05942510105167 | O | -4.61341439366557 | -6.42303646634689 | 0.07140252597503 |
| H | -6.21424508420189 | -7.15710650266346 | -3.22980071654405 | O | -4.23876167150913 | -6.71096318266614 | -3.12180162556985 |
| H | 0.00045059640749 | -8.01843770208554 | -2.09898226444060 | O | -1.87516244892051 | -7.71367984842567 | -2.99935257641107 |
| H | -0.02567380152953 | -8.12125746160904 | -3.90456753772481 | O | 6.71334334885639 | -4.24663916414244 | -3.10892901555586 |
| H | -0.79026181050761 | -9.42673190716959 | -2.91550010758877 | O | 7.71614818879579 | -1.88305050054864 | -2.98741326206011 |
| H | 7.15946486795214 | -6.22223786059244 | -3.21486048787652 | O | 0.24974219978191 | 6.70550295116139 | -3.12218308922421 |
| H | 5.61951075088484 | -5.77548787028553 | -4.04663120108202 | O | 1.88621337732488 | 7.70896544581347 | -3.00596743338309 |
| H | 5.69478530841072 | -5.86160144308770 | -2.22995122996711 | O | -6.70337404763072 | 4.24170809088065 | -3.13382295829828 |
| H | 9.42931102658952 | -0.79837293870582 | -2.90331687014941 | O | -7.70655111407756 | 1.87810847316566 | -3.01606437520897 |
| H | 8.12501255428390 | -0.03492240462846 | -3.89488652231329 | Y | -0.00273682023057 | 0.00126554023734 | 1.72939651195519 |
| H | 8.02043625760984 | -0.00626314127221 | -2.08938795361247 | Y | 0.00268504273743 | -0.00111223810846 | -1.72954043135653 |
| H | 6.22560467722805 | 7.15093880364704 | -3.22617741282064 | | | | |
| H | 5.77979396234424 | 5.60898596337030 | -4.05475479398838 | | | | |

Table S12. BP86/def2-SVP geometry of $g\text{-Y}_2(\text{MeO})_8\text{Pc}]_3^{2+}$.

| | | | | | | | |
|---|-------------------|-------------------|-------------------|---|-------------------|-------------------|-------------------|
| C | -3.56750422018571 | -2.32670458191115 | 3.15690162275630 | C | 3.65654155238401 | -7.52755640529150 | -0.05233839753208 |
| C | -4.13142151561971 | -1.03124934224620 | 3.13712945301336 | C | 7.48390847978582 | -3.71771498500887 | 0.07615230009563 |
| C | -3.01584378577745 | -0.08793771969421 | 3.05346553797831 | C | 7.52742192153147 | 3.65671205604012 | -0.05093774546840 |
| C | -2.11253363656363 | -2.14576152575021 | 3.06502649661235 | C | 3.71715917437818 | 7.48426383133310 | 0.06193821863629 |
| C | 2.10310104640010 | 2.14937081432531 | 3.06854968522292 | C | -3.65686014803047 | 7.52742208064878 | -0.07006053966794 |
| C | 3.55780058911380 | 2.33044651638627 | 3.16439547179509 | C | -7.48444764375666 | 3.71738442597561 | 0.04597251840833 |
| C | 4.12170401569190 | 1.03493932868932 | 3.14865953972204 | C | -7.52758473237880 | -3.65650252013376 | -0.07277802024289 |
| C | 3.00634617099992 | 0.09155038977363 | 3.06306709607326 | C | -3.71810578401865 | -7.48405497187007 | 0.06000040011091 |
| C | 0.08504041864219 | -3.00930165641712 | 3.06066150272095 | C | -4.12941231428714 | 1.00333438743256 | -3.15299425673622 |
| C | 2.14281901771002 | -2.10598352032161 | 3.07180475873534 | C | -3.57248987173221 | 2.30206067228600 | -3.17238733253888 |
| C | 2.32370760234787 | -3.56071966478365 | 3.16717543203042 | C | -2.11592823699065 | 2.13089803946802 | -3.08068052215194 |
| C | 1.02828004761436 | -4.12469333555218 | 3.14775980578879 | C | -3.00752448604377 | 0.06827035432966 | -3.07117517209013 |
| C | -2.33345434567758 | 3.56465346901223 | 3.15356135828064 | C | 3.01709972319321 | -0.07206335248537 | -3.06126155278594 |
| C | -1.03787543013148 | 4.12841757143931 | 3.13805325219536 | C | 4.13925008053560 | -1.00722350122013 | -3.13806502147575 |
| C | -0.09446495559293 | 3.01283960818546 | 3.05607436816599 | C | 3.58242580252094 | -2.30599544262349 | -3.15741882148334 |
| C | -2.15236648408186 | 2.10968616185635 | 3.06139954857245 | C | 2.12555143272188 | -2.13472500082135 | -3.07064665997395 |
| C | 0.83507349562700 | -5.51334265847123 | 3.14293831245233 | C | -2.12797758522579 | -2.12262713389802 | -3.07771364850670 |
| C | 1.97436846302283 | -6.33422132535432 | 3.13782481904013 | C | -0.06537836195564 | -3.01422499918566 | -3.06416899137487 |
| C | 3.29867464086150 | -5.76075695196475 | 3.17598812854838 | C | -1.00038381422450 | -4.13629735746027 | -3.14418548368567 |
| C | 3.47212961532843 | -4.36351504103949 | 3.20312096895908 | C | -2.29908098138442 | -3.57940658197898 | -3.16615083582710 |
| C | -5.52004477904839 | -0.83798367622873 | 3.12919042923762 | C | 1.01017536551010 | 4.13240447762386 | -3.14658183014375 |
| C | -6.34093727437525 | -1.97723919629018 | 3.12123403437533 | C | 2.30896388522316 | 3.57553443719196 | -3.16339720862609 |
| C | -5.76759778983109 | -3.30159449564219 | 3.15970299271894 | C | 2.13760517461923 | 2.11885728210290 | -3.07359895808141 |
| C | -4.37043149560101 | -3.47512267402327 | 3.19000978816028 | C | 0.07494377318240 | 3.01043748053258 | -3.06812041640762 |
| C | 5.51033662426422 | 0.84161159552616 | 3.14558256795506 | C | -3.44380026726685 | -4.38518873775063 | -3.19709508579390 |
| C | 6.33130488198793 | 1.98081836963007 | 3.13817471941384 | C | -3.26527081695286 | -5.78198220382070 | -3.15980721654606 |
| C | 5.75792216269701 | 3.30526986479875 | 3.17227272557436 | C | -1.93850148424725 | -6.35028357044234 | -3.11362160696756 |
| C | 4.36066283127069 | 3.47890847032090 | 3.19779040117292 | C | -0.80261806223822 | -5.52528391554570 | -3.12773932079172 |
| C | -0.84436347868363 | 5.51700706089584 | 3.13201939379195 | C | -4.37817967236089 | 3.44682185441346 | -3.20394780211684 |
| C | -1.98344041354086 | 6.33808445957986 | 3.12130580867938 | C | -5.77505772177440 | 3.26826705007478 | -3.17014297848844 |
| C | -3.30800501294293 | 5.76492927865019 | 3.15503180878351 | C | -6.34346313119128 | 1.94144137380680 | -3.12687808582622 |
| C | -3.48185791970441 | 4.36774704384986 | 3.18357635430145 | C | -5.51843634507350 | 0.80556818898409 | -3.14023321556067 |
| C | 0.68601341256576 | -8.33991960673640 | 3.10134997418342 | C | 4.38829205414965 | -3.45074432210062 | -3.18479782644487 |
| C | 5.64760068504067 | -6.20264039658629 | 3.19407830301016 | C | 5.78504401968317 | -3.27205106823700 | -3.14677323397426 |
| C | 8.33689073727663 | 0.69215394590475 | 3.10749835182279 | C | 6.35324750902125 | -1.94513949309406 | -3.10347961263001 |
| C | 6.20007096170344 | 5.65418417478949 | 3.18451598385368 | C | 5.52821215640452 | -0.80934661959005 | -3.12104139812504 |
| C | -0.69443405858242 | 8.34339337584697 | 3.08811376435423 | C | 3.45375999567603 | 4.38130741943733 | -3.19143742921783 |
| C | -5.65686854836864 | 6.20740870943969 | 3.16337478458131 | C | 3.27506257680771 | 5.77814455852900 | -3.15665935956488 |
| C | -8.34649122925048 | -0.68878043122488 | 3.08122682939849 | C | 1.94811204505136 | 6.34645277754094 | -3.11593712395031 |
| C | -6.20959366806797 | -5.65052225821373 | 3.17497218243794 | C | 0.81231754681654 | 5.52140489670741 | -3.13283678780417 |
| C | -4.6904318682496 | -3.43305029471991 | 0.00681486974848 | C | -5.61375073493996 | -6.22789884831239 | -3.19864270819569 |
| C | -3.46578803361306 | -2.42602710693274 | -0.02449477071178 | C | -0.64448697567046 | -8.35137738914378 | -3.05618109916885 |
| C | -2.76690379736825 | -1.15400384033026 | -0.01914852728705 | C | 6.23110058090643 | -5.62059138827241 | -3.17949311949582 |
| C | -1.18671743879522 | -2.74989189913662 | 0.00295675561723 | C | 8.35417812825843 | -0.65085403378374 | -3.04686922272317 |
| C | 1.18645253004952 | 2.74994411386856 | 0.00405355318307 | C | 5.62364862350771 | 6.22409505573897 | -3.18749214591284 |
| C | 2.46872895871927 | 3.433122994192290 | 0.01172253179703 | C | 0.65377721882282 | 8.34750919471819 | -3.06525539255140 |
| C | 3.46560993164500 | 2.42611020620258 | -0.01557507622663 | C | -6.22082361234428 | 5.61680319814025 | -3.20669127387538 |
| C | 2.76676157700268 | 1.15403947031823 | -0.01136320243222 | C | -8.34466548381318 | 0.64733724077881 | -3.07553793525350 |
| C | 1.15392267427993 | -2.76682800515392 | -0.01179301881221 | H | -0.18265499075290 | -5.92215968880067 | 3.11668023464421 |
| C | 2.74981571387895 | -1.18657766355821 | 0.00870779515508 | H | 4.46761626721019 | -3.90279365304923 | 3.21216844133785 |
| C | 3.43296160761473 | -2.46888767951359 | 0.01631813804148 | H | -5.92872402528828 | 0.17979695924674 | 3.10277480556587 |
| C | 2.42597132705139 | -3.46570455845555 | -0.01413250622914 | H | -3.90980456831235 | -4.47064913921071 | 3.19937947256554 |
| C | -3.43322412125201 | 2.46885723504578 | 0.00239827496387 | H | 5.91911797749267 | -0.17620778422127 | 3.12241324988443 |
| C | -2.42618571129099 | 3.46569038792851 | -0.02554450731944 | H | 3.90001324821209 | 4.47445243829325 | 3.20385017353117 |
| C | -1.15412495589877 | 2.76684025153986 | -0.01861655227740 | H | 0.17355205626637 | 5.92556733894801 | 3.10912135488518 |
| C | -2.75001659712810 | 1.18658123343450 | -0.00157197307950 | H | -4.47748385660733 | 3.90727386932255 | 3.18954422303991 |
| C | 2.74805258369398 | -4.83148187109782 | -0.04631027095646 | H | 0.13160237403528 | -8.09833038729374 | 4.03377445993038 |
| C | 4.10500525111404 | -5.17904956073832 | -0.02947015207380 | H | 0.05898096344767 | -8.06211999130143 | 2.24442221322730 |
| C | 5.13327575777224 | -4.1754306846154 | 0.02708521770560 | H | 0.89534505492459 | -9.42424555714942 | 3.07227839047385 |
| C | 4.79451743617696 | -2.59749771990847 | 0.0486055905460 | H | 5.82518723413617 | -5.55654862651291 | 4.08009569277303 |
| C | -4.83151315050823 | -2.74802487207436 | -0.05953986256499 | H | 5.91189170689485 | -5.65977438318363 | 2.26296972434027 |
| C | -5.17913147290639 | -4.10498842374503 | -0.04492795875794 | H | 6.27547411014568 | -7.10788255054822 | 3.27259967300404 |
| C | -4.15772593743274 | -5.13335637815410 | 0.01182739710301 | H | 9.42127292797718 | 0.90126632003749 | 3.07896350950795 |
| C | -2.79772099897415 | -4.79465243415985 | 0.03650872828249 | H | 8.05986550165388 | 0.06286291999961 | 2.23194713782092 |
| C | 4.83142099365337 | 2.74818581417467 | -0.04623742121504 | H | 8.09428491931119 | 0.14023804507581 | 4.041139225807255 |
| C | 5.17891684403108 | 4.10519490929054 | -0.03219393859391 | H | 7.10533461105043 | 6.28215241593207 | 3.26203335637361 |
| C | 4.15727750888007 | 5.13356191736871 | 0.01994439412170 | H | 5.65790244167412 | 5.91609072778770 | 2.25234143202814 |
| C | 2.79723706917523 | 4.79477634903320 | 0.04071624078885 | H | 5.55338038195848 | 5.83417858972239 | 4.06961147433543 |
| C | -2.74823050707091 | 4.83144308731293 | -0.05918542546002 | H | -0.90332362590887 | 9.42774470614450 | 3.05688556793448 |
| C | -4.10526641798240 | 5.17894198347431 | -0.04725230193897 | H | -0.06392649500858 | 8.06433355841140 | 2.21407708568987 |
| C | -5.13367944868157 | 4.15738616232486 | 0.00564413892172 | H | -0.14389339587204 | 8.10276107399793 | 4.02307762819529 |
| C | -4.79490742460785 | 2.79739498779771 | 0.02937338356302 | H | -6.28481965857852 | 7.11294022592133 | 3.23783220704504 |

| | | | | | | | |
|---|-------------------|-------------------|--------------------|---|-------------------|-------------------|-------------------|
| H | -5.91764178661600 | 5.66296350692233 | 2.23221674099818 | H | 5.89843894670119 | 5.66981041852149 | -2.26624189362182 |
| H | -5.83809195746171 | 5.56293373107643 | 4.04983622347951 | H | 0.85905184606732 | 9.43221572991393 | -3.02395704464407 |
| H | -8.10710294621230 | -0.13524343891371 | 4.01473899745966 | H | 0.10357810504929 | 8.11381308527166 | -4.00223437513151 |
| H | -8.06656958191715 | -0.06094306687643 | 2.20554769337035 | H | 0.02410121629136 | 8.05839511936746 | -2.19378226580451 |
| H | -9.43075486465725 | -0.89803223855870 | 3.04937007586694 | H | -5.66745656287633 | 5.89362494660936 | -2.28549519451829 |
| H | -5.56566366880200 | -5.82884549476788 | 4.06241648598509 | H | -5.58551716928203 | 5.78405936019426 | -4.10227928605408 |
| H | -5.66447755878534 | -5.91409479955955 | 2.24497523031326 | H | -7.12843283044875 | 6.24153217403731 | -3.28210660649024 |
| H | -7.11504528401712 | -6.27842472244994 | 3.25079108778500 | H | -8.05667845573126 | 0.01964915599116 | -2.20226359770184 |
| H | 1.95147433046799 | -5.58440551544038 | -0.06423605192406 | H | -8.10986032456520 | 0.09494986098923 | -4.01095080841549 |
| H | 5.55121028947631 | -2.00444404821988 | 0.06796928931609 | H | -9.42940585375429 | 0.85279045150701 | -3.03606684235108 |
| H | -5.58439513459770 | -1.95140276652727 | -0.07713708729114 | N | -1.82774819664953 | -0.79529629369947 | 2.95019781622378 |
| H | -2.00469864267191 | -5.55138414775870 | 0.05552623417782 | N | 1.81859799873533 | 0.79875379053187 | 2.95499952227760 |
| H | 5.58441116257180 | 1.95160205368247 | -0.06079390093698 | N | 0.79246292710729 | -1.82145800347373 | 2.95514303674090 |
| H | 2.00413101395466 | 5.55149742444306 | 0.05640109582209 | N | -0.80162020004047 | 1.82487072706874 | 2.95005024268804 |
| H | -1.95163555684501 | 5.58441328175193 | -0.07416532767846 | N | -1.24202546027389 | -3.15884138055444 | 3.09090721694828 |
| H | -5.55162630228582 | 2.00430154752536 | 0.04580386034854 | N | -3.16548755060638 | 1.23912945507074 | 3.08417203803432 |
| H | 3.09625494543322 | -7.56341874153410 | 0.90442023874191 | N | 1.23250070539151 | 3.16244595431982 | 3.09024837950245 |
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