Supporting Information

Water-Involved Hydrogen Bonds in Dimeric Supramolecular Structures of Magnesium and Zinc Phthalocyaninato Complexes.

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Figure S6. Hirshfeld surface of (ZnPc(H$_2$O)$\cdot$4-methylmorpholine)$_2$ dimer plotted overs (a) $d_i$, (b) $d_e$, (c) shape index and (d) curvedness.
$\Delta E(\text{HOMO}/\text{LUMO}) = 2.0154 \text{ eV (615 nm)}$

$\Delta E(\text{HOMO}/\text{LUMO}) = 2.0251 \text{ eV (612 nm)}$

$\Delta E(\text{HOMO}/\text{LUMO}) = 2.0857 \text{ eV (594 nm)}$

$\Delta E(\text{HOMO}/\text{LUMO}) = 2.0568 \text{ eV (603 nm)}$

**Figure S7.** HOMO and LUMO frontiers orbitals and the calculated absorption spectra for the MgPc, MgPc(H$_2$O), ZnPc and ZnPc(H$_2$O) complexes.
Table S1. DFT optimised geometrical parameters (Å,°) for MgPc(H$_2$O).

Deviation of Mg1 from N$_4$-plane = 0.372; Optimized MgPc(H$_2$O) molecule exhibits C$_{2v}$ symmetry

| Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) |
|------|------------|------|------------|------|------------|------|------------|
| Mg1-O1 | 2.146      | Mg1-N2 | 2.040      | Mg1-N4 | 2.043      | Mg1-N6 | 2.040      |
| Mg1-N8 | 2.043      | N1-C1 | 1.334      | C1-N2 | 1.372      | C1-C2 | 1.464      |
| C2-C7 | 1.413      | C2-C3 | 1.397      | C3-C4 | 1.396      | C4-C5 | 1.409      |
| C5-C6 | 1.396      | C6-C7 | 1.397      | C7-C8 | 1.464      | C8-N2 | 1.372      |
| C8-N3 | 1.334      | N3-C9 | 1.335      | C9-C10| 1.465      | C9-N4 | 1.370      |
| C10-C15| 1.413     | C10-C11| 1.396    | C11-C12| 1.396    | C12-C13| 1.409     |
| C13-C14| 1.396     | C14-C15| 1.396    | C15-C16| 1.465    | C16-N4 | 1.370      |
| C16-N5 | 1.335      | N5-C17| 1.335      | C17-N6| 1.372      | C17-C18| 1.464      |
| C18-C23| 1.413     | C18-C19| 1.397    | C19-C20| 1.396    | C20-C21| 1.409      |
| C21-C22| 1.396     | C22-C23| 1.397    | C23-C24| 1.464    | C24-N7 | 1.334      |
| C7-C8 | 1.087      | N2-Mg1-N4 | 88.10  | N2-Mg1-N8 | 88.10  | N4-Mg1-N6 | 88.10  |
| C24-C25| 1.396     | C25-C8 | 1.370     | C25-C26| 1.465     | C26-C31| 1.413      |
| C26-C27| 1.396     | C27-C28| 1.396    | C28-C29| 1.409     | C29-C30| 1.396      |
| C30-C31| 1.396     | C31-C32| 1.465    | C32-N1 | 1.335     | O1-H(x2)| 0.970      |
| C24-N8 | 109.60     | N6-C32-N1 | 127.50  | C24-N7 | 124.90    | N7-C25 | 124.90     |
| C13-C14 | 117.90    | C14-C15| 112.60   | C15-C16| 112.60    | C16-N5 | 112.60     |
| C16-N5 | 109.60     | C17-N6 | 124.90   | C17-N6 | 124.90    | C17-N6 | 124.90     |
| C24-N8 | 109.60     | C9-N4 | 124.90   | C24-N7 | 124.90    | C24-N7 | 124.90     |
| C25-N8 | 109.60     | N6-C24-N7 | 124.90  | N6-C24-N7 | 124.90 | N6-C24-N7 | 124.90 |
| C24-N8 | 109.60     | H-O1-H | 108.0    | H-O1-H | 108.0     | N2-Mg1-O1-H2O1 | 180.00  |
Table S2. DFT optimized geometrical parameters (Å, °) for ZnPc(H$_2$O).

Deviation of Zn1 from N$_4$-plane = 0.255; Optimized MgPc(H$_2$O) molecule exhibits $C_{2v}$ symmetry

| Bond                  | Length  | Angle   |
|-----------------------|---------|---------|
| Zn1—O1                | 2.309 Å |         |
| Zn1—N8                | 2.017 Å |         |
| C2—C3                 | 1.397 Å |         |
| C6—C7                 | 1.397 Å |         |
| C8—N3                 | 1.333 Å |         |
| C10—C11               | 1.397 Å |         |
| C14—C15               | 1.397 Å |         |
| C17—N5                | 1.332 Å |         |
| C19—C20               | 1.397 Å |         |
| C23—C18               | 1.412 Å |         |
| C25—N7                | 1.332 Å |         |
| C27—C28               | 1.397 Å |         |
| C31—C26               | 1.402 Å |         |
| N2—Zn1—N4             | 89.0°   |         |
| N6—Zn1—N8             | 89.4°   |         |
| O1—Zn1—N2             | 98.6°   |         |
| N2—C1—C2              | 108.7°  |         |
| C4—C5—C6              | 121.1°  |         |
| C7—C8—N2              | 108.6°  |         |
| N3—C9—N4              | 127.5°  |         |
| C10—C11—C12           | 117.9°  |         |
| C13—C14—C15           | 117.9°  |         |
| C15—C16—N5            | 123.8°  |         |
| N5—C17—C18            | 123.8°  |         |
| C19—C20—C21           | 121.1°  |         |
| C22—C23—C24           | 132.5°  |         |
| C25—C26—C27           | 124.9°  |         |
| C27—C28—C29           | 106.5°  |         |

N2—Zn1—O1—H1O1 -100.60° N2—Zn1—O1—H2O1 -105.0°
Table S3. DFT optimised geometrical parameters (Å,°) for (MgPcH₂O)₂ dimer.

View of the optimized (MgPcH₂O)₂ dimer

| Item                    | Value     | Threshold  | Converged? |
|-------------------------|-----------|------------|------------|
| Maximum Force           | 0.000405  | 0.000450   | YES        |
| RMS Force               | 0.000072  | 0.000300   | YES        |
| Maximum Displacement    | 0.001504  | 0.001800   | YES        |
| RMS Displacement        | 0.000260  | 0.001200   | YES        |

Predicted change in Energy=-1.846660D-07
Optimization completed. (for (MgPcH₂O)₂ dimer)

Optimized Parameters

(Angstroms and Degrees)

| ! Name | Definition | Value   | Derivative Info. |
|--------|------------|---------|------------------|
| ! R1   | R(1,2)     | 2.0336  | -DE/DX = -0.0003 |
| ! R2   | R(1,6)     | 2.0533  | -DE/DX = 0.0    |
| ! R3   | R(1,8)     | 2.0625  | -DE/DX = 0.0    |
| ! R4   | R(1,10)    | 2.0615  | -DE/DX = 0.0    |
| ! R5   | R(1,12)    | 2.0521  | -DE/DX = 0.0001 |
| ! R6   | R(2,3)     | 0.9812  | -DE/DX = 0.0002 |
| ! R7   | R(2,4)     | 1.115   | -DE/DX = -0.0002 |
| ! R8   | R(4,65)    | 1.4089  | -DE/DX = -0.0002 |
| ! R9   | R(5,13)    | 1.3499  | -DE/DX = -0.0001 |
| ! R10  | R(5,60)    | 1.3498  | -DE/DX = 0.0001 |
| ! R11  | R(5,64)    | 1.4078  | -DE/DX = -0.0002 |
| ! R12  | R(6,13)    | 1.3776  | -DE/DX = -0.0001 |
| ! R13  | R(6,24)    | 1.3919  | -DE/DX = -0.0001 |
| ! R14  | R(7,24)    | 1.3348  | -DE/DX = 0.0001 |
| ! R15  | R(7,25)    | 1.3379  | -DE/DX = 0.0    |
| ! R16  | R(8,25)    | 1.383   | -DE/DX = -0.0001 |
| ! R17  | R(8,36)    | 1.3854  | -DE/DX = -0.0001 |
| ! R18  | R(9,36)    | 1.3389  | -DE/DX = 0.0    |
| ! R19  | R(9,37)    | 1.3388  | -DE/DX = 0.0001 |
| ! R20  | R(10,37)   | 1.3851  | -DE/DX = 0.0    |
| ! R21  | R(10,48)   | 1.3828  | -DE/DX = 0.0    |
| ! R22  | R(11,48)   | 1.3377  | -DE/DX = 0.0001 |
| ! R23  | R(11,49)   | 1.3344  | -DE/DX = 0.0002 |
| ! R24  | R(12,49)   | 1.3924  | -DE/DX = -0.0002 |
| ! R25  | R(12,60)   | 1.3773  | -DE/DX = 0.0    |
| ! R26  | R(13,14)   | 1.4694  | -DE/DX = 0.0    |
| ! R27  | R(14,15)   | 1.3982  | -DE/DX = 0.0001 |
| R   | R(14,23) | 1.4164 | -DE/DX = -0.0001 |
| R28 |         |        |                  |
| R29 | R(15,16) | 1.0822 | -DE/DX = 0.0001  |
| R30 | R(15,17) | 1.3984 | -DE/DX = 0.0     |
| R31 | R(17,18) | 1.0859 | -DE/DX = 0.0001  |
| R32 | R(17,19) | 1.4093 | -DE/DX = 0.0001  |
| R33 | R(19,20) | 1.0856 | -DE/DX = 0.0001  |
| R34 | R(19,21) | 1.3983 | -DE/DX = 0.0     |
| R35 | R(21,22) | 1.0848 | -DE/DX = 0.0001  |
| R36 | R(21,23) | 1.3935 | -DE/DX = 0.0     |
| R37 | R(23,24) | 1.0859 | -DE/DX = 0.0001  |
| R38 | R(25,26) | 1.4605 | -DE/DX = -0.0001 |
| R39 | R(26,27) | 1.3940 | -DE/DX = 0.0     |
| R40 | R(26,35) | 1.0845 | -DE/DX = 0.0001  |
| R41 | R(27,28) | 1.0846 | -DE/DX = 0.0001  |
| R42 | R(29,30) | 1.0852 | -DE/DX = 0.0001  |
| R43 | R(29,31) | 1.4096 | -DE/DX = 0.0001  |
| R44 | R(31,32) | 1.0852 | -DE/DX = 0.0001  |
| R45 | R(31,33) | 1.4000 | -DE/DX = 0.0     |
| R46 | R(33,34) | 1.0844 | -DE/DX = 0.0001  |
| R47 | R(33,35) | 1.3935 | -DE/DX = 0.0001  |
| R48 | R(35,36) | 1.4663 | -DE/DX = 0.0001  |
| R49 | R(37,38) | 1.4666 | -DE/DX = 0.0     |
| R50 | R(38,39) | 1.3936 | -DE/DX = 0.0     |
| R51 | R(38,47) | 1.4160 | -DE/DX = 0.0     |
| R52 | R(39,40) | 1.0844 | -DE/DX = 0.0001  |
| R53 | R(39,41) | 1.4000 | -DE/DX = 0.0     |
| R54 | R(41,42) | 1.0852 | -DE/DX = 0.0001  |
| R55 | R(41,43) | 1.4096 | -DE/DX = 0.0     |
| R56 | R(43,44) | 1.0852 | -DE/DX = 0.0001  |
| R57 | R(43,45) | 1.3999 | -DE/DX = 0.0     |
| R58 | R(45,46) | 1.0845 | -DE/DX = 0.0001  |
| R59 | R(45,47) | 1.3940 | -DE/DX = 0.0     |
| R60 | R(47,48) | 1.4646 | -DE/DX = 0.0     |
| R61 | R(49,50) | 1.4600 | -DE/DX = 0.0001  |
| R62 | R(50,51) | 1.3937 | -DE/DX = 0.0     |
| R63 | R(50,59) | 1.4163 | -DE/DX = 0.0     |
| R64 | R(51,52) | 1.0847 | -DE/DX = 0.0001  |
| R65 | R(51,53) | 1.3981 | -DE/DX = 0.0001  |
| R66 | R(53,54) | 1.0856 | -DE/DX = 0.0001  |
| R67 | R(53,55) | 1.4093 | -DE/DX = 0.0001  |
| R68 | R(55,56) | 1.0859 | -DE/DX = 0.0001  |
| R69 | R(55,57) | 1.3983 | -DE/DX = 0.0     |
| R70 | R(57,58) | 1.0819 | -DE/DX = 0.0001  |
| R71 | R(57,59) | 1.3982 | -DE/DX = 0.0001  |
| R72 | R(59,60) | 1.4692 | -DE/DX = 0.0001  |
| R73 | R(61,62) | 2.0336 | -DE/DX = -0.0003 |
| R74 | R(61,66) | 2.0535 | -DE/DX = 0.0001  |
| R75 | R(61,68) | 2.0621 | -DE/DX = 0.0001  |
| R76 | R(61,70) | 2.0620 | -DE/DX = 0.0     |
| R77 | R(61,72) | 2.0520 | -DE/DX = 0.0001  |
| R78 | R(62,63) | 0.9811 | -DE/DX = 0.0004  |
| R79 | R(62,64) | 1.1160 | -DE/DX = -0.0004 |
| R80 | R(65,73) | 1.3497 | -DE/DX = 0.0002  |
| R81 | R(65,120) | 1.3499 | -DE/DX = -0.0001 |
| R82 | R(66,73) | 1.3777 | -DE/DX = 0.0     |
| R83 | R(66,84) | 1.3919 | -DE/DX = -0.0001 |
| R84 | R(67,84) | 1.3348 | -DE/DX = 0.0001  |
| R85 | R(67,85) | 1.3378 | -DE/DX = 0.0     |
| R86 | R(68,85) | 1.3831 | -DE/DX = -0.0001 |
| R    | R(71,72) | 1.0833 | DE/DX = 0.0 |
| R    | R(71,73) | 1.0841 | DE/DX = 0.0 |
| R    | R(71,74) | 1.0845 | DE/DX = 0.0 |
| R    | R(71,75) | 1.0850 | DE/DX = 0.0 |
| R    | R(71,76) | 1.0853 | DE/DX = 0.0 |
| R    | R(71,77) | 1.0855 | DE/DX = 0.0 |
| R    | R(71,78) | 1.0859 | DE/DX = 0.0 |
| R    | R(71,79) | 1.0862 | DE/DX = 0.0 |
| R    | R(71,80) | 1.0866 | DE/DX = 0.0 |
| R    | R(71,81) | 1.0868 | DE/DX = 0.0 |
| R    | R(71,82) | 1.0870 | DE/DX = 0.0 |
| R    | R(71,83) | 1.0872 | DE/DX = 0.0 |
| R    | R(71,84) | 1.0874 | DE/DX = 0.0 |
| R    | R(71,85) | 1.0876 | DE/DX = 0.0 |
| R    | R(71,86) | 1.0878 | DE/DX = 0.0 |
| R    | R(71,87) | 1.0880 | DE/DX = 0.0 |
| R    | R(71,88) | 1.0882 | DE/DX = 0.0 |
| R    | R(71,89) | 1.0884 | DE/DX = 0.0 |
| R    | R(71,90) | 1.0886 | DE/DX = 0.0 |
| R    | R(71,91) | 1.0888 | DE/DX = 0.0 |
| R    | R(71,92) | 1.0890 | DE/DX = 0.0 |
| R    | R(71,93) | 1.0892 | DE/DX = 0.0 |
| R    | R(71,94) | 1.0894 | DE/DX = 0.0 |
| R    | R(71,95) | 1.0896 | DE/DX = 0.0 |
| R    | R(71,96) | 1.0898 | DE/DX = 0.0 |
| R    | R(71,97) | 1.0900 | DE/DX = 0.0 |
| R    | R(71,98) | 1.0902 | DE/DX = 0.0 |
| R    | R(71,99) | 1.0904 | DE/DX = 0.0 |
| R    | R(71,100) | 1.0906 | DE/DX = 0.0 |
| R    | R(71,101) | 1.0908 | DE/DX = 0.0 |
| R    | R(71,102) | 1.0910 | DE/DX = 0.0 |
| R    | R(71,103) | 1.0912 | DE/DX = 0.0 |
| R    | R(71,104) | 1.0914 | DE/DX = 0.0 |
| R    | R(71,105) | 1.0916 | DE/DX = 0.0 |
| R    | R(71,106) | 1.0918 | DE/DX = 0.0 |
| R    | R(71,107) | 1.0920 | DE/DX = 0.0 |
| R    | R(71,108) | 1.0922 | DE/DX = 0.0 |
| R    | R(71,109) | 1.0924 | DE/DX = 0.0 |
| R    | R(71,110) | 1.0926 | DE/DX = 0.0 |
| R    | R(71,111) | 1.0928 | DE/DX = 0.0 |
| R    | R(71,112) | 1.0930 | DE/DX = 0.0 |
| R    | R(71,113) | 1.0932 | DE/DX = 0.0 |
| R    | R(71,114) | 1.0934 | DE/DX = 0.0 |
| R    | R(71,115) | 1.0936 | DE/DX = 0.0 |
| R    | R(71,116) | 1.0938 | DE/DX = 0.0 |
| R    | R(71,117) | 1.0940 | DE/DX = 0.0 |
| R    | R(71,118) | 1.0942 | DE/DX = 0.0 |
| R    | R(71,119) | 1.0944 | DE/DX = 0.0 |
| R    | R(71,120) | 1.0946 | DE/DX = 0.0 |
| A    | A(2,1,6) | 106.4074 | DE/DX = 0.0 |
| A    | A(2,1,8) | 97.4975 | DE/DX = 0.0003 |
| A    | A(2,1,10) | 98.0417 | DE/DX = 0.0002 |
| index | A        | value        | DE/DX       |
|-------|----------|--------------|-------------|
| A4    | A(2,1,12)| 106.9554     | -0.0001     |
| A5    | A(6,1,8 )| 88.0132      | -0.0001     |
| A6    | A(6,1,10)| 155.4802     | -0.0001     |
| A7    | A(6,1,12)| 86.6125      | 0.0         |
| A8    | A(8,1,10)| 86.9772      | 0.0         |
| A9    | A(8,1,12)| 155.4968     | -0.0001     |
| A10   | A(10,1,12)| 88.0663     | 0.0         |
| A11   | A(1,2,3 )| 127.7485     | 0.0003      |
| A12   | A(1,2,4 )| 113.742      | 0.0         |
| A13   | A(3,2,4 )| 118.3188     | -0.0001     |
| A14   | A(13,5,60)| 126.2074    | -0.0001     |
| A15   | A(13,5,64)| 116.1813    | -0.0001     |
| A16   | A(60,5,64)| 116.03      | 0.0002      |
| A17   | A(1,6,13)| 127.2141     | 0.0         |
| A18   | A(1,6,24)| 123.8956     | 0.0         |
| A19   | A(13,6,24)| 108.664     | 0.0         |
| A20   | A(24,7,25)| 125.3267    | -0.0001     |
| A21   | A(1,8,25)| 125.271      | 0.0         |
| A22   | A(1,8,36)| 125.4122     | 0.0         |
| A23   | A(25,8,36)| 108.907     | 0.0         |
| A24   | A(36,9,37)| 124.9419    | -0.0001     |
| A25   | A(1,10,37)| 125.4237    | 0.0         |
| A26   | A(1,10,48)| 125.1602    | 0.0         |
| A27   | A(37,10,48)| 108.9062   | 0.0         |
| A28   | A(48,11,49)| 125.3386   | -0.0001     |
| A29   | A(1,12,49)| 123.8558    | 0.0         |
| A30   | A(1,12,60)| 127.2895    | -0.0001     |
| A31   | A(49,12,60)| 108.6601   | 0.0         |
| A32   | A(5,13,6 )| 125.3947     | 0.0001      |
| A33   | A(5,13,14)| 125.0401     | -0.0001     |
| A34   | A(6,13,14)| 109.5139     | 0.0001      |
| A35   | A(13,14,15)| 133.4613    | 0.0         |
| A36   | A(13,14,23)| 105.9025    | -0.0001     |
| A37   | A(15,14,23)| 120.4987    | 0.0001      |
| A38   | A(14,15,16)| 121.4122    | 0.0         |
| A39   | A(14,15,17)| 118.0855    | -0.0001     |
| A40   | A(16,15,17)| 120.4858    | 0.0001      |
| A41   | A(15,17,18)| 119.5015    | 0.0         |
| A42   | A(15,17,19)| 121.1844    | 0.0         |
| A43   | A(18,17,19)| 119.3126    | 0.0         |
| A44   | A(17,19,20)| 119.3205    | 0.0         |
| A45   | A(17,19,21)| 120.8864    | 0.0         |
| A46   | A(20,19,21)| 119.7931    | 0.0         |
| A47   | A(19,21,22)| 121.6749    | 0.0         |
| A48   | A(19,21,23)| 117.9732    | 0.0         |
| A49   | A(22,21,23)| 120.3507    | 0.0         |
| A50   | A(14,23,21)| 121.3577    | 0.0         |
| A51   | A(14,23,24)| 107.155     | 0.0         |
| A52   | A(21,23,24)| 131.4103    | 0.0         |
| A53   | A(6,24,7 )| 128.1039     | 0.0001      |
| A54   | A(6,24,23)| 108.7419     | 0.0         |
| A55   | A(7,24,23)| 122.9108     | -0.0001     |
| A56   | A(7,25,8 )| 126.6641     | 0.0001      |
| A57   | A(7,25,26)| 124.2304     | -0.0001     |
| A58   | A(8,25,26)| 109.0935     | 0.0         |
| A59   | A(25,26,27)| 132.3442    | -0.0001     |
| A60   | A(25,26,35)| 106.4946    | 0.0         |
| A61   | A(27,26,35)| 121.1608    | 0.0         |
| A62   | A(26,27,28)| 120.6569    | 0.0         |
| A63   | A(26,27,29)| 117.7968    | 0.0         |
|    | A(28,27,29) | 121.5462 | -DE/DX = 0.0 |
|----|-------------|----------|--------------|
| A64| A(27,29,30) | 119.6942 | -DE/DX = 0.0 |
| A65| A(27,29,31) | 121.0637 | -DE/DX = 0.0 |
| A66| A(30,29,31) | 119.2415 | -DE/DX = 0.0 |
| A67| A(29,31,30) | 119.2412 | -DE/DX = 0.0 |
| A68| A(29,31,31) | 119.6534 | -DE/DX = 0.0 |
| A69| A(29,31,32) | 121.0637 | -DE/DX = 0.0 |
| A70| A(30,29,31) | 119.2415 | -DE/DX = 0.0 |
| A71| A(30,29,32) | 106.6609 | -DE/DX = 0.0 |
| A72| A(30,29,33) | 117.8669 | -DE/DX = 0.0 |
| A73| A(30,29,34) | 119.2415 | -DE/DX = 0.0 |
| A74| A(30,29,35) | 119.2412 | -DE/DX = 0.0 |
| A75| A(30,29,36) | 119.6534 | -DE/DX = 0.0 |
| A76| A(30,29,37) | 121.0637 | -DE/DX = 0.0 |
| A77| A(30,29,38) | 119.6534 | -DE/DX = 0.0 |
| A78| A(30,29,39) | 121.0637 | -DE/DX = 0.0 |
| A79| A(30,29,40) | 119.6534 | -DE/DX = 0.0 |
| A80| A(30,29,41) | 121.0637 | -DE/DX = 0.0 |
| A81| A(30,29,42) | 119.6534 | -DE/DX = 0.0 |
| A82| A(30,29,43) | 121.0637 | -DE/DX = 0.0 |
| A83| A(30,29,44) | 119.6534 | -DE/DX = 0.0 |
| A84| A(30,29,45) | 121.0637 | -DE/DX = 0.0 |
| A85| A(30,29,46) | 119.6534 | -DE/DX = 0.0 |
| A86| A(30,29,47) | 121.0637 | -DE/DX = 0.0 |
| A87| A(30,29,48) | 119.6534 | -DE/DX = 0.0 |
| A88| A(30,29,49) | 121.0637 | -DE/DX = 0.0 |
| A89| A(30,29,50) | 119.6534 | -DE/DX = 0.0 |
| A90| A(30,29,51) | 121.0637 | -DE/DX = 0.0 |
| A91| A(30,29,52) | 119.6534 | -DE/DX = 0.0 |
| A92| A(30,29,53) | 121.0637 | -DE/DX = 0.0 |
| A93| A(30,29,54) | 119.6534 | -DE/DX = 0.0 |
| A94| A(30,29,55) | 121.0637 | -DE/DX = 0.0 |
| A95| A(30,29,56) | 119.6534 | -DE/DX = 0.0 |
| A96| A(30,29,57) | 121.0637 | -DE/DX = 0.0 |
| A97| A(30,29,58) | 119.6534 | -DE/DX = 0.0 |
| A98| A(30,29,59) | 121.0637 | -DE/DX = 0.0 |
| A99| A(30,29,60) | 119.6534 | -DE/DX = 0.0 |
| A100| A(30,29,61) | 121.0637 | -DE/DX = 0.0 |
| A101| A(30,29,62) | 119.6534 | -DE/DX = 0.0 |
| A102| A(30,29,63) | 121.0637 | -DE/DX = 0.0 |
| A103| A(30,29,64) | 119.6534 | -DE/DX = 0.0 |
| A104| A(30,29,65) | 121.0637 | -DE/DX = 0.0 |
| A105| A(30,29,66) | 119.6534 | -DE/DX = 0.0 |
| A106| A(30,29,67) | 121.0637 | -DE/DX = 0.0 |
| A107| A(30,29,68) | 119.6534 | -DE/DX = 0.0 |
| A108| A(30,29,69) | 121.0637 | -DE/DX = 0.0 |
| A109| A(30,29,70) | 119.6534 | -DE/DX = 0.0 |
| A110| A(30,29,71) | 121.0637 | -DE/DX = 0.0 |
| A111| A(30,29,72) | 119.6534 | -DE/DX = 0.0 |
| A112| A(30,29,73) | 121.0637 | -DE/DX = 0.0 |
| A113| A(30,29,74) | 119.6534 | -DE/DX = 0.0 |
| A114| A(30,29,75) | 121.0637 | -DE/DX = 0.0 |
| A115| A(30,29,76) | 119.6534 | -DE/DX = 0.0 |
| A116| A(30,29,77) | 121.0637 | -DE/DX = 0.0 |
| A117| A(30,29,78) | 119.6534 | -DE/DX = 0.0 |
| A118| A(30,29,79) | 121.0637 | -DE/DX = 0.0 |
| A119| A(30,29,80) | 119.6534 | -DE/DX = 0.0 |
| A120| A(30,29,81) | 121.0637 | -DE/DX = 0.0 |
| A121| A(30,29,82) | 119.6534 | -DE/DX = 0.0 |
| A122| A(30,29,83) | 121.0637 | -DE/DX = 0.0 |
| A123| A(30,29,84) | 119.6534 | -DE/DX = 0.0 |
| A184 | A(67,85,86) | 124.2154 | -DE/DX = 0.0 |
| A185 | A(68,85,86) | 109.094  | -DE/DX = 0.0 |
| A186 | A(68,85,86) | 132.3398 | -DE/DX = -0.0001 |
| A187 | A(85,86,87) | 106.4965 | -DE/DX = 0.0 |
| A188 | A(85,86,95) | 121.1631 | -DE/DX = 0.0 |
| A189 | A(86,87,88) | 120.6577 | -DE/DX = 0.0 |
| A190 | A(86,87,89) | 117.795  | -DE/DX = 0.0 |
| A191 | A(88,87,89) | 121.5472 | -DE/DX = 0.0 |
| A192 | A(87,86,95) | 121.1631 | -DE/DX = 0.0 |
| A193 | A(87,86,95) | 120.6577 | -DE/DX = 0.0 |
| A194 | A(86,87,88) | 117.795  | -DE/DX = 0.0 |
| A195 | A(86,87,89) | 121.1631 | -DE/DX = 0.0 |
| A196 | A(87,89,90) | 119.6942 | -DE/DX = 0.0 |
| A197 | A(89,90,91) | 117.8664 | -DE/DX = 0.0 |
| A198 | A(90,91,92) | 120.6436 | -DE/DX = 0.0 |
| A199 | A(90,91,92) | 120.6436 | -DE/DX = 0.0 |
| A200 | A(91,92,93) | 117.8664 | -DE/DX = 0.0 |
| A201 | A(92,93,94) | 108.8365 | -DE/DX = 0.0 |
| A202 | A(93,94,95) | 108.8365 | -DE/DX = 0.0 |
| A203 | A(94,95,96) | 132.3331 | -DE/DX = 0.0 |
| A204 | A(68,96,69) | 127.157  | -DE/DX = 0.0001 |
| A205 | A(68,96,95) | 108.8365 | -DE/DX = 0.0 |
| A206 | A(69,95,96) | 123.9501 | -DE/DX = 0.0 |
| A207 | A(69,97,70) | 127.133  | -DE/DX = 0.0 |
| A208 | A(70,97,71) | 123.9707 | -DE/DX = 0.0 |
| A209 | A(70,97,71) | 108.8364 | -DE/DX = 0.0 |
| A210 | A(97,98,99) | 132.3532 | -DE/DX = 0.0 |
| A211 | A(97,98,100)| 106.6477 | -DE/DX = 0.0 |
| A212 | A(98,99,100)| 120.9924 | -DE/DX = 0.0 |
| A213 | A(98,99,100)| 120.6491 | -DE/DX = 0.0 |
| A214 | A(98,99,101)| 117.8669 | -DE/DX = 0.0 |
| A215 | A(100,99,101)| 121.4822 | -DE/DX = 0.0 |
| A216 | A(99,100,101)| 119.6523 | -DE/DX = 0.0 |
| A217 | A(99,100,101)| 121.1049 | -DE/DX = 0.0 |
| A218 | A(100,101,102)| 119.2419 | -DE/DX = 0.0 |
| A219 | A(101,102,103)| 119.2451 | -DE/DX = 0.0 |
| A220 | A(101,102,103)| 121.0628 | -DE/DX = 0.0 |
| A221 | A(102,103,104)| 119.6917 | -DE/DX = 0.0 |
| A222 | A(103,104,105)| 121.5445 | -DE/DX = 0.0 |
| A223 | A(104,105,106)| 117.7865 | -DE/DX = 0.0 |
| A224 | A(105,106,107)| 120.6688 | -DE/DX = 0.0 |
| A225 | A(98,107,108)| 121.1759 | -DE/DX = 0.0 |
| A226 | A(98,107,108)| 106.4953 | -DE/DX = 0.0 |
| A227 | A(105,107,108)| 132.3282 | -DE/DX = 0.0 |
| A228 | A(70,108,71)| 126.642  | -DE/DX = 0.0001 |
| A229 | A(70,108,71)| 109.0939 | -DE/DX = 0.0 |
| A230 | A(71,108,71)| 124.2159 | -DE/DX = -0.0001 |
| A231 | A(71,109,72)| 128.1327 | -DE/DX = 0.0 |
| A232 | A(71,109,72)| 122.9082 | -DE/DX = 0.0 |
| A233 | A(72,109,10)| 108.7312 | -DE/DX = 0.0 |
| A234 | A(109,110,11)| 131.3839 | -DE/DX = 0.0 |
| A235 | A(109,110,11)| 107.1678 | -DE/DX = 0.0 |
| A236 | A(110,110,11)| 121.3699 | -DE/DX = 0.0 |
| A237 | A(110,111,12)| 120.3281 | -DE/DX = 0.0 |
| A238 | A(110,111,12)| 117.9955 | -DE/DX = 0.0 |
| A239 | A(112,111,13)| 121.6753 | -DE/DX = 0.0 |
| A240 | A(111,113,14)| 119.8065 | -DE/DX = 0.0 |
| A241 | A(111,113,15)| 120.8737 | -DE/DX = 0.0 |
| A242 | A(114,113,15)| 119.3193 | -DE/DX = 0.0 |
| A243 | A(113,115,16)| 119.3197 | -DE/DX = 0.0 |
| D46 | D(60,5,13,14) | 175.3915 | -DE/DX = 0.0 |
| D47 | D(64,5,13,6)  | 163.2875 | -DE/DX = 0.0001 |
| D48 | D(64,5,13,14) | -19.5952 | -DE/DX = 0.0001 |
| D49 | D(13,5,60,12) | 2.1546  | -DE/DX = 0.0 |
| D50 | D(13,5,60,59) | -175.3845 | -DE/DX = -0.0001 |
| D51 | D(64,5,60,12) | -162.8786 | -DE/DX = -0.0001 |
| D52 | D(64,5,60,59) | 19.5823  | -DE/DX = -0.0001 |
| D53 | D(13,5,62,61) | -78.7367 | -DE/DX = -0.0002 |
| D54 | D(13,5,62,63) | 106.1496 | -DE/DX = -0.0002 |
| D55 | D(60,5,62,61) | 79.0335  | -DE/DX = -0.0001 |
| D56 | D(60,5,62,63) | -96.0801 | -DE/DX = -0.0001 |
| D57 | D(1,6,13,5)   | -9.363  | -DE/DX = 0.0 |
| D58 | D(1,6,13,14)  | 173.1408 | -DE/DX = 0.0 |
| D59 | D(24,6,13,5)  | 175.9768 | -DE/DX = 0.0 |
| D60 | D(24,6,13,14) | -1.5194  | -DE/DX = 0.0 |
| D61 | D(1,6,24,7)   | 11.6995 | -DE/DX = 0.0001 |
| D62 | D(1,6,24,23)  | -173.9047 | -DE/DX = 0.0 |
| D63 | D(13,6,24,7)  | -173.423 | -DE/DX = 0.0001 |
| D64 | D(13,6,24,23) | 0.9727  | -DE/DX = 0.0 |
| D65 | D(25,7,24,6)  | 1.7249  | -DE/DX = 0.0001 |
| D66 | D(25,7,24,23) | -171.9508 | -DE/DX = 0.0 |
| D67 | D(24,7,25,8)  | -3.1084  | -DE/DX = -0.0001 |
| D68 | D(24,7,25,26) | 175.4871 | -DE/DX = -0.0001 |
| D69 | D(1,8,25,7)   | -9.2672  | -DE/DX = 0.0 |
| D70 | D(1,8,25,26)  | 171.9616 | -DE/DX = 0.0 |
| D71 | D(36,8,25,7)  | 177.7672 | -DE/DX = 0.0 |
| D72 | D(36,8,25,26) | -1.004  | -DE/DX = 0.0 |
| D73 | D(1,8,36,9)   | 10.8267 | -DE/DX = 0.0 |
| D74 | D(1,8,36,35)  | -171.9881 | -DE/DX = 0.0 |
| D75 | D(25,8,36,9)  | -176.2201 | -DE/DX = 0.0 |
| D76 | D(25,8,36,35) | 0.9651  | -DE/DX = 0.0 |
| D77 | D(37,9,36,8)  | 2.5099  | -DE/DX = 0.0 |
| D78 | D(37,9,36,35) | -174.2781 | -DE/DX = 0.0001 |
| D79 | D(36,9,37,10) | -2.1777  | -DE/DX = -0.0001 |
| D80 | D(36,9,37,38) | 174.8292 | -DE/DX = 0.0 |
| D81 | D(1,10,37,9)  | -11.4506 | -DE/DX = 0.0 |
| D82 | D(1,10,37,38) | 171.1719 | -DE/DX = 0.0 |
| D83 | D(48,10,37,9) | 176.4142 | -DE/DX = 0.0 |
| D84 | D(48,10,37,38) | -0.9633 | -DE/DX = 0.0 |
| D85 | D(1,10,48,11) | 10.2011 | -DE/DX = 0.0 |
| D86 | D(1,10,48,47) | -171.0927 | -DE/DX = 0.0 |
| D87 | D(37,10,48,11) | -177.638 | -DE/DX = 0.0 |
| D88 | D(37,10,48,47) | 1.0682  | -DE/DX = 0.0 |
| D89 | D(49,11,48,10) | 2.8184  | -DE/DX = 0.0001 |
| D90 | D(49,11,48,47) | -175.7026 | -DE/DX = 0.0001 |
| D91 | D(48,11,49,12) | -2.3068 | -DE/DX = 0.0 |
| D92 | D(48,11,49,50) | 171.7166 | -DE/DX = 0.0 |
| D93 | D(1,12,49,11) | -11.0492 | -DE/DX = -0.0001 |
| D94 | D(1,12,49,50) | 174.2448 | -DE/DX = -0.0001 |
| D95 | D(60,12,49,11) | 173.6982 | -DE/DX = -0.0001 |
| D96 | D(60,12,49,50) | -1.0077 | -DE/DX = -0.0001 |
| D97 | D(1,12,60,5)  | 8.5622  | -DE/DX = 0.0 |
| D98 | D(1,12,60,59) | -173.5755 | -DE/DX = 0.0001 |
| D99 | D(49,12,60,5) | -176.3938 | -DE/DX = 0.0 |
| D100 | D(49,12,60,59) | 1.4685 | -DE/DX = 0.0001 |
| D101 | D(5,13,14,15) | -0.444 | -DE/DX = 0.0 |
| D102 | D(5,13,14,23) | -176.0341 | -DE/DX = 0.0 |
| D103 | D(6,13,14,15) | 177.0632 | -DE/DX = 0.0 |
| D104 | D(6,13,14,23) | 1.4731 | -DE/DX = 0.0 |
| D105 | D(13,14,15,16) | 5.3783 | -DE/DX = 0.0 |
| D106  | D(13,14,15,17) | -176.0945 | -DE/DX = 0.0 |
| D107  | D(23,14,15,16) | -179.545  | -DE/DX = 0.0 |
| D108  | D(13,14,15,17) | -1.0178   | -DE/DX = 0.0 |
| D109  | D(13,14,23,21) | 176.3082  | -DE/DX = 0.0 |
| D110  | D(13,14,23,24) | -0.8432   | -DE/DX = 0.0 |
| D111  | D(15,14,23,21) | 0.022     | -DE/DX = 0.0 |
| D112  | D(15,14,23,24) | -177.1295 | -DE/DX = 0.0 |
| D113  | D(14,15,17,18) | 1.388     | -DE/DX = 0.0 |
| D114  | D(14,15,17,19) | 179.9295  | -DE/DX = 0.0 |
| D115  | D(15,17,19,20) | -0.5203   | -DE/DX = 0.0 |
| D116  | D(15,17,19,21) | 0.022     | -DE/DX = 0.0 |
| D117  | D(15,19,21,22) | -179.0617 | -DE/DX = 0.0 |
| D118  | D(15,19,21,23) | 1.388     | -DE/DX = 0.0 |
| D119  | D(16,15,17,18) | -0.5203   | -DE/DX = 0.0 |
| D120  | D(16,15,17,19) | 179.9295  | -DE/DX = 0.0 |
| D121  | D(16,15,17,20) | 0.022     | -DE/DX = 0.0 |
| D122  | D(16,15,17,21) | -177.1295 | -DE/DX = 0.0 |
| D123  | D(17,19,21,22) | -179.346  | -DE/DX = 0.0 |
| D124  | D(17,19,21,23) | -0.2519   | -DE/DX = 0.0 |
| D125  | D(19,21,23,14) | 0.6175    | -DE/DX = 0.0 |
| D126  | D(19,21,23,24) | 176.9875  | -DE/DX = 0.0 |
| D127  | D(22,21,23,14) | -178.9859 | -DE/DX = 0.0 |
| D128  | D(22,21,23,24) | -2.616    | -DE/DX = 0.0 |
| D129  | D(23,24,14)    | -0.0362   | -DE/DX = 0.0 |
| D130  | D(23,24,17)    | 174.7119  | -DE/DX = 0.0 |
| D131  | D(23,24,21)    | -176.7925 | -DE/DX = 0.0 |
| D132  | D(23,24,24)    | -2.0444   | -DE/DX = 0.0 |
| D133  | D(25,26,27)    | 1.5876    | -DE/DX = 0.0 |
| D134  | D(25,26,27)    | -178.1615 | -DE/DX = 0.0 |
| D135  | D(25,26,29)    | -179.6046 | -DE/DX = 0.0 |
| D136  | D(25,26,35)    | 0.6463    | -DE/DX = 0.0 |
| D137  | D(25,26,27,28) | 0.0321    | -DE/DX = 0.0 |
| D138  | D(25,26,27,29) | -179.8393 | -DE/DX = 0.0 |
| D139  | D(25,26,27,28) | -179.751  | -DE/DX = 0.0 |
| D140  | D(25,26,27,29) | -0.1204   | -DE/DX = 0.0 |
| D141  | D(25,26,35,33) | 178.9523  | -DE/DX = 0.0 |
| D142  | D(25,26,35,36) | -0.0571   | -DE/DX = 0.0 |
| D143  | D(27,26,35,33) | -0.8309   | -DE/DX = 0.0 |
| D144  | D(27,26,35,36) | -179.8404 | -DE/DX = 0.0 |
| D145  | D(26,27,29,30) | -179.7238 | -DE/DX = 0.0 |
| D146  | D(26,27,29,31) | 0.5393    | -DE/DX = 0.0 |
| D147  | D(26,27,29,30) | 0.406     | -DE/DX = 0.0 |
| D148  | D(27,29,31,32) | -179.3309 | -DE/DX = 0.0 |
| D149  | D(27,29,31,32) | 179.6135  | -DE/DX = 0.0 |
| D150  | D(27,29,31,33) | -0.266    | -DE/DX = 0.0 |
| D151  | D(30,29,31,32) | -0.1246   | -DE/DX = 0.0 |
| D152  | D(30,29,31,33) | -179.7647 | -DE/DX = 0.0 |
| D153  | D(29,31,33,34) | 179.5906  | -DE/DX = 0.0 |
| D154  | D(29,31,33,35) | -0.9008   | -DE/DX = 0.0 |
| D155  | D(32,31,33,34) | -0.048    | -DE/DX = 0.0 |
| D156  | D(32,31,33,35) | 179.4605  | -DE/DX = 0.0 |
| D157  | D(31,33,35,26) | 1.3184    | -DE/DX = 0.0 |
| D158  | D(31,33,35,36) | -179.9654 | -DE/DX = 0.0 |
| D159  | D(34,33,35,26) | 179.1687  | -DE/DX = 0.0 |
| D160  | D(34,33,35,36) | -0.4525   | -DE/DX = 0.0 |
| D161  | D(26,35,36,8)  | -0.548    | -DE/DX = 0.0 |
| D162  | D(26,35,36,9)  | 176.7476  | -DE/DX = 0.0 |
| D163  | D(33,35,36,8)  | -179.3993 | -DE/DX = 0.0 |
| D164  | D(33,35,36,9)  | -2.1038   | -DE/DX = 0.0 |
| D165  | D(9,37,38,39)  | 2.0975    | -DE/DX = 0.0 |
| D226 | D(50,59,60,12) | -1.3554 | -DE/DX = 0.0 |
| D227 | D(57,59,60,5)  | 0.8858  | -DE/DX = 0.0 |
| D228 | D(57,59,60,12) | -176.9865 | -DE/DX = 0.0 |
| D229 | D(66,61,62,63) | 129.8223 | -DE/DX = 0.0 |
| D230 | D(66,61,62,64) | -45.1186 | -DE/DX = 0.0 |
| D231 | D(68,61,62,63) | 39.5494  | -DE/DX = 0.0 |
| D232 | D(68,61,62,64) | -135.3915 | -DE/DX = 0.0001 |
| D233 | D(70,61,62,63) | -48.4422 | -DE/DX = 0.0 |
| D234 | D(70,61,62,64) | 136.6169 | -DE/DX = 0.0 |
| D235 | D(72,61,62,63) | -138.7282 | -DE/DX = 0.0 |
| D236 | D(72,61,62,64) | 46.3309  | -DE/DX = 0.0 |
| D237 | D(66,61,63,67) | 92.8625  | -DE/DX = 0.0 |
| D238 | D(66,61,63,68) | -81.2547 | -DE/DX = 0.0 |
| D239 | D(68,61,63,67) | -169.5452 | -DE/DX = 0.0001 |
| D240 | D(68,61,63,68) | 16.3377  | -DE/DX = 0.0001 |
| D241 | D(70,61,63,67) | -91.2908 | -DE/DX = 0.0001 |
| D242 | D(70,61,63,68) | 94.592   | -DE/DX = 0.0 |
| D243 | D(72,61,63,67) | -13.5448 | -DE/DX = 0.0 |
| D244 | D(72,61,63,68) | 172.338  | -DE/DX = 0.0 |
| D245 | D(66,61,68,65) | 90.9167  | -DE/DX = -0.0002 |
| D246 | D(66,61,68,66) | -80.8714 | -DE/DX = -0.0002 |
| D247 | D(66,61,68,67) | -15.6546 | -DE/DX = -0.0001 |
| D248 | D(66,61,68,68) | 172.5573 | -DE/DX = -0.0001 |
| D249 | D(70,61,68,65) | -171.6846 | -DE/DX = 0.0001 |
| D250 | D(70,61,68,66) | 16.5273  | -DE/DX = 0.0001 |
| D251 | D(72,61,68,65) | -93.0516 | -DE/DX = 0.0001 |
| D252 | D(72,61,68,66) | 95.1603  | -DE/DX = 0.0001 |
| D253 | D(66,61,69,67) | 80.6016  | -DE/DX = 0.0001 |
| D254 | D(66,61,69,68) | -90.3285 | -DE/DX = 0.0001 |
| D255 | D(68,61,69,67) | -95.3837 | -DE/DX = 0.0 |
| D256 | D(68,61,69,68) | 93.6862  | -DE/DX = 0.0 |
| D257 | D(70,61,69,67) | -16.9086 | -DE/DX = 0.0 |
| D258 | D(70,61,69,68) | 172.1613 | -DE/DX = 0.0 |
| D259 | D(72,61,69,67) | -172.8221 | -DE/DX = 0.0001 |
| D260 | D(72,61,69,68) | 16.2478  | -DE/DX = 0.0001 |
| D261 | D(66,61,70,67) | 81.0049  | -DE/DX = 0.0002 |
| D262 | D(66,61,70,68) | -93.0987 | -DE/DX = 0.0001 |
| D263 | D(66,61,70,69) | -172.5877 | -DE/DX = 0.0 |
| D264 | D(66,61,70,70) | 13.3087  | -DE/DX = 0.0 |
| D265 | D(66,61,70,71) | -94.8909 | -DE/DX = 0.0 |
| D266 | D(66,61,70,72) | 91.0054  | -DE/DX = 0.0 |
| D267 | D(70,61,70,67) | -16.4889 | -DE/DX = -0.0001 |
| D268 | D(70,61,70,68) | 169.4075 | -DE/DX = -0.0001 |
| D269 | D(4,65,73,66)  | -163.0813 | -DE/DX = -0.0001 |
| D270 | D(4,65,73,74)  | 19.7667  | -DE/DX = -0.0001 |
| D271 | D(4,65,73,76)  | 1.7852   | -DE/DX = 0.0 |
| D272 | D(4,65,73,74)  | -175.3668 | -DE/DX = -0.0001 |
| D273 | D(4,65,73,72)  | 162.795  | -DE/DX = 0.0002 |
| D274 | D(4,65,73,71)  | -19.6898 | -DE/DX = 0.0002 |
| D275 | D(73,65,70,72) | -2.0644  | -DE/DX = 0.0 |
| D276 | D(73,65,70,71) | 175.4508 | -DE/DX = 0.0 |
| D277 | D(61,66,73,65) | 9.2159   | -DE/DX = 0.0 |
| D278 | D(61,66,73,74) | -173.2582 | -DE/DX = 0.0 |
| D279 | D(84,66,73,65) | -175.9346 | -DE/DX = 0.0 |
| D280 | D(84,66,73,74) | 1.5913   | -DE/DX = 0.0001 |
| D281 | D(61,66,84,67) | -11.5121 | -DE/DX = -0.0001 |
| D282 | D(61,66,84,83) | 174.0045 | -DE/DX = 0.0 |
| D283 | D(73,66,84,67) | 173.4291 | -DE/DX = -0.0001 |
| D284 | D(73,66,84,83) | -1.0543  | -DE/DX = -0.0001 |
| D285 | D(85,67,84,66) | -1.9086  | -DE/DX = 0.0 |
| D2| D(85,67,84,83) | 171.8644 | -DE/DX = -0.0001 |
| D287| D(84,67,84,85) | 3.132 | -DE/DX = 0.0001 |
| D288| D(84,67,84,86) | -175.3779 | -DE/DX = 0.0001 |
| D289| D(61,68,84,67) | 9.3713 | -DE/DX = 0.0 |
| D290| D(61,68,84,68) | -191.9326 | -DE/DX = 0.0 |
| D291| D(96,68,84,67) | -175.3849 | -DE/DX = 0.0 |
| D292| D(96,68,84,86) | 1.0013 | -DE/DX = 0.0 |
| D293| D(61,68,96,69) | -10.6966 | -DE/DX = 0.0 |
| D294| D(61,68,96,95) | 171.9713 | -DE/DX = 0.0 |
| D295| D(85,68,96,69) | 176.3849 | -DE/DX = 0.0 |
| D296| D(85,68,96,86) | -0.9472 | -DE/DX = 0.0 |
| D297| D(97,69,96,68) | -2.5728 | -DE/DX = 0.0 |
| D298| D(97,69,96,95) | 174.3829 | -DE/DX = -0.0001 |
| D299| D(96,69,97,68) | 2.1114 | -DE/DX = 0.0001 |
| D300| D(96,69,97,98) | -174.7548 | -DE/DX = 0.0 |
| D301| D(61,70,97,69) | 11.5506 | -DE/DX = 0.0 |
| D302| D(61,70,97,98) | -171.951 | -DE/DX = 0.0 |
| D303| D(108,70,97,69) | -176.2791 | -DE/DX = 0.0 |
| D304| D(108,70,97,98) | 0.9753 | -DE/DX = 0.0 |
| D305| D(61,70,97,98) | -10.1241 | -DE/DX = 0.0 |
| D306| D(61,70,98,71) | 171.1128 | -DE/DX = 0.0 |
| D307| D(97,70,98,71) | -177.6812 | -DE/DX = 0.0 |
| D308| D(97,70,98,107) | -1.0819 | -DE/DX = 0.0 |
| D309| D(109,71,108,70) | -2.8489 | -DE/DX = 0.0 |
| D310| D(109,71,108,107) | 175.7369 | -DE/DX = -0.0001 |
| D311| D(108,71,109,72) | 2.1585 | -DE/DX = 0.0 |
| D312| D(108,71,109,97) | -171.7207 | -DE/DX = 0.0 |
| D313| D(61,72,109,71) | 11.2977 | -DE/DX = 0.0 |
| D314| D(61,72,109,98) | -174.1261 | -DE/DX = 0.0 |
| D315| D(61,72,109,110) | -173.8515 | -DE/DX = 0.0001 |
| D316| D(61,72,109,110) | 0.9246 | -DE/DX = 0.0001 |
| D317| D(61,72,120,65) | -176.4582 | -DE/DX = 0.0 |
| D318| D(61,72,120,110) | 2.1585 | -DE/DX = 0.0 |
| D319| D(61,72,120,107) | -179.1172 | -DE/DX = 0.0 |
| D320| D(61,72,120,97) | -179.5401 | -DE/DX = 0.0 |
| D321| D(65,73,74,75) | -10.6966 | -DE/DX = 0.0 |
| D322| D(65,73,74,75) | 176.0305 | -DE/DX = 0.0 |
| D323| D(66,73,74,75) | -177.1747 | -DE/DX = 0.0 |
| D324| D(66,73,74,83) | -1.5066 | -DE/DX = 0.0 |
| D325| D(73,74,75,76) | -177.1747 | -DE/DX = 0.0 |
| D326| D(73,74,75,77) | -176.1752 | -DE/DX = 0.0 |
| D327| D(83,74,75,76) | 179.5401 | -DE/DX = 0.0 |
| D328| D(83,74,75,77) | 1.0119 | -DE/DX = 0.0 |
| D329| D(83,74,75,77) | -176.3356 | -DE/DX = 0.0 |
| D330| D(83,74,75,78) | 0.827 | -DE/DX = 0.0 |
| D331| D(75,74,75,81) | 0.0156 | -DE/DX = 0.0 |
| D332| D(75,74,75,83) | 177.1783 | -DE/DX = 0.0 |
| D333| D(74,75,77,78) | 179.0284 | -DE/DX = 0.0 |
| D334| D(74,75,77,79) | -14108 | -DE/DX = 0.0 |
| D335| D(76,75,77,78) | 0.4861 | -DE/DX = 0.0 |
| D336| D(76,75,77,79) | -179.953 | -DE/DX = 0.0 |
| D337| D(75,77,79,80) | -179.1172 | -DE/DX = 0.0 |
| D338| D(75,77,79,81) | 0.7891 | -DE/DX = 0.0001 |
| D339| D(78,77,79,80) | 0.4444 | -DE/DX = 0.0 |
| D340| D(78,77,79,81) | -179.6493 | -DE/DX = 0.0 |
| D341| D(77,79,81,82) | -179.3452 | -DE/DX = 0.0 |
| D342| D(77,79,81,83) | 0.2622 | -DE/DX = 0.0001 |
| D343| D(80,79,81,82) | 0.5607 | -DE/DX = 0.0 |
| D344| D(80,79,81,83) | -179.832 | -DE/DX = 0.0 |
| D345| D(79,81,83,74) | -0.6566 | -DE/DX = 0.0 |
| D346 | D(79,81,83,84) | -177.0407 | -DE/DX = 0.0 |
|------|----------------|-----------|--------------|
| D347 | D(82,81,83,84) | 178.9562  | -DE/DX = 0.0 |
| D348 | D(82,81,83,84) | 2.5721    | -DE/DX = 0.0 |
| D349 | D(74,83,84,66) | -174.731  | -DE/DX = 0.0 |
| D350 | D(74,83,84,67) | 178.8651  | -DE/DX = 0.0 |
| D351 | D(81,83,84,66) | 2.0378    | -DE/DX = 0.0 |
| D352 | D(81,83,84,67) | -1.6469   | -DE/DX = 0.0 |
| D353 | D(85,86,87,88) | 179.6177  | -DE/DX = 0.0 |
| D354 | D(85,86,87,88) | 0.2398    | -DE/DX = 0.0 |
| D355 | D(86,87,89,90) | -179.7277 | -DE/DX = 0.0 |
| D356 | D(86,87,89,91) | 179.5168  | -DE/DX = 0.0 |
| D357 | D(86,87,89,92) | 2.0378    | -DE/DX = 0.0 |
| D358 | D(86,87,89,93) | -1.6469   | -DE/DX = 0.0 |
| D359 | D(86,87,89,94) | 178.8651  | -DE/DX = 0.0 |
| D360 | D(86,87,89,95) | 2.0378    | -DE/DX = 0.0 |
| D361 | D(86,87,89,96) | -1.6469   | -DE/DX = 0.0 |
| D362 | D(86,87,89,97) | 178.8651  | -DE/DX = 0.0 |
| D363 | D(86,87,89,98) | 2.0378    | -DE/DX = 0.0 |
| D364 | D(86,87,89,99) | -1.6469   | -DE/DX = 0.0 |
| D365 | D(86,87,90,91) | 179.6177  | -DE/DX = 0.0 |
| D366 | D(86,87,90,92) | 2.0378    | -DE/DX = 0.0 |
| D367 | D(86,87,90,93) | -1.6469   | -DE/DX = 0.0 |
| D368 | D(86,87,90,94) | 178.8651  | -DE/DX = 0.0 |
| D369 | D(86,87,90,95) | 2.0378    | -DE/DX = 0.0 |
| D370 | D(86,87,90,96) | -1.6469   | -DE/DX = 0.0 |
| D371 | D(86,87,90,97) | 178.8651  | -DE/DX = 0.0 |
| D372 | D(86,87,90,98) | 2.0378    | -DE/DX = 0.0 |
| D373 | D(86,87,90,99) | -1.6469   | -DE/DX = 0.0 |
| D374 | D(86,87,90,100)| 178.8651  | -DE/DX = 0.0 |
| D375 | D(86,87,90,101)| 2.0378    | -DE/DX = 0.0 |
| D376 | D(86,87,90,102)| -1.6469   | -DE/DX = 0.0 |
| D377 | D(86,87,90,103)| 178.8651  | -DE/DX = 0.0 |
| D378 | D(86,87,90,104)| 2.0378    | -DE/DX = 0.0 |
| D379 | D(86,87,90,105)| -1.6469   | -DE/DX = 0.0 |
| D380 | D(86,87,90,106)| 178.8651  | -DE/DX = 0.0 |
| D381 | D(86,87,90,107)| 2.0378    | -DE/DX = 0.0 |
| D382 | D(86,87,90,108)| -1.6469   | -DE/DX = 0.0 |
| D383 | D(86,87,90,109)| 178.8651  | -DE/DX = 0.0 |
| D384 | D(86,87,90,110)| 2.0378    | -DE/DX = 0.0 |
| D385 | D(86,87,90,111)| -1.6469   | -DE/DX = 0.0 |
| D386 | D(86,87,90,112)| 178.8651  | -DE/DX = 0.0 |
| D387 | D(86,87,90,113)| 2.0378    | -DE/DX = 0.0 |
| D388 | D(86,87,90,114)| -1.6469   | -DE/DX = 0.0 |
| D389 | D(86,87,90,115)| 178.8651  | -DE/DX = 0.0 |
| D390 | D(86,87,90,116)| 2.0378    | -DE/DX = 0.0 |
| D391 | D(86,87,90,117)| -1.6469   | -DE/DX = 0.0 |
| D392 | D(86,87,90,118)| 178.8651  | -DE/DX = 0.0 |
| D393 | D(86,87,90,119)| 2.0378    | -DE/DX = 0.0 |
| D394 | D(86,87,90,120)| -1.6469   | -DE/DX = 0.0 |
| D395 | D(86,87,90,121)| 178.8651  | -DE/DX = 0.0 |
| D396 | D(86,87,90,122)| 2.0378    | -DE/DX = 0.0 |
| D397 | D(86,87,90,123)| -1.6469   | -DE/DX = 0.0 |
| D398 | D(86,87,90,124)| 178.8651  | -DE/DX = 0.0 |
| D399 | D(86,87,90,125)| 2.0378    | -DE/DX = 0.0 |
| D400 | D(86,87,90,126)| -1.6469   | -DE/DX = 0.0 |
| D401 | D(86,87,90,127)| 178.8651  | -DE/DX = 0.0 |
| D402 | D(86,87,90,128)| 2.0378    | -DE/DX = 0.0 |
| D403 | D(86,87,90,129)| -1.6469   | -DE/DX = 0.0 |
| D404 | D(86,87,90,130)| 178.8651  | -DE/DX = 0.0 |
| D405 | D(86,87,90,131)| 2.0378    | -DE/DX = 0.0 |
Standard orientation (optimized): for (MgPcH₂O)₂ dimer

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
| 1             | 12            | Mg          | -2.950673 0.000112 0.321666 |
| 2             | 8             | O           | -2.635637 0.008571 -1.687337 |
| 3             | 1             | H           | -3.306265 0.077345 -2.400216 |
| 4             | 1             | H           | -1.557811 0.014957 -1.972697 |
| 5             | 7             | N           | 0.157486 0.000336 1.819049 |
| 6             | 7             | N           | -1.684111 1.409100 1.113292 |
| 7             | 7             | N           | -3.100226 3.391985 0.840157 |
| 8             | 7             | N           | -4.444118 1.421958 0.365878 |
| 9             | 7             | N           | -6.382914 0.003809 -0.061361 |
| 10  | 7  | N   | -4.447735 | -1.416233 | 0.372864 |
| 11  | 7  | N   | -3.106774 | -3.387873 | 1.606622 |
| 12  | 6  | C   | -0.414235 | 1.204586  | 1.606622 |
| 13  | 6  | C   | 0.203590  | 2.499509  | 1.923715 |
| 14  | 6  | C   | 1.428976  | 2.868239  | 2.487075 |
| 15  | 1  | H   | 2.189943  | 2.132697  | 2.713180 |
| 16  | 7  | N   | 1.662150  | 4.226382  | 2.724870 |
| 17  | 6  | C   | -0.549675 | 8.30456   | 1.883786 |
| 18  | 1  | H   | -1.316924 | 5.56417   | 1.665046 |
| 19  | 6  | C   | -0.774977 | 3.479494  | 1.626743 |
| 20  | 1  | H   | 0.203590  | 2.499509  | 1.923715 |
| 21  | 6  | C   | 1.428976  | 2.868239  | 2.487075 |
| 22  | 1  | H   | 2.189943  | 2.132697  | 2.713180 |
| 23  | 6  | C   | -0.549675 | 8.30456   | 1.883786 |
| 24  | 6  | C   | -1.950191 | 2.75269   | 1.120745 |
| 25  | 6  | C   | -4.247577 | 2.781959  | 0.521881 |
| 26  | 6  | C   | -5.519239 | 3.477151  | 0.310543 |
| 27  | 6  | C   | -5.868438 | 4.826325  | 0.342570 |
| 28  | 1  | H   | -5.123872 | 5.583331  | 0.556438 |
| 29  | 6  | C   | -7.204717 | 5.160960  | 0.932666 |
| 30  | 1  | H   | -7.50528 | 6.202334  | 0.106077 |
| 31  | 6  | C   | -8.16935 | 4.165008  | -0.169869 |
| 32  | 1  | H   | -9.195890 | 4.457237  | -0.35264 |
| 33  | 6  | C   | -7.817635 | 2.809415  | -0.91009 |
| 34  | 1  | H   | -8.554040 | 2.037757  | -0.386279 |
| 35  | 6  | C   | -6.483828 | 2.476827  | 0.037550 |
| 36  | 6  | C   | -5.781159 | 1.90758   | 0.086361 |
| 37  | 6  | C   | -5.782958 | 1.83802   | 0.086993 |
| 38  | 6  | C   | -6.485331 | 2.469879  | 0.027424 |
| 39  | 6  | C   | -7.817115 | 2.801985  | -0.213566 |
| 40  | 1  | H   | -8.552632 | 2.029703  | -0.409799 |
| 41  | 6  | C   | -8.165727 | 4.157860  | -0.202647 |
| 42  | 1  | H   | -9.193247 | 4.449576  | -0.394362 |
| 43  | 6  | C   | -7.204660 | 5.154785  | 0.060970 |
| 44  | 1  | H   | -7.508812 | 6.196488  | 0.065233 |
| 45  | 6  | C   | -5.870152 | 4.820962  | 0.320724 |
| 46  | 1  | H   | -5.126447 | 5.580840  | 0.534543 |
| 47  | 6  | C   | -5.521864 | 3.471311  | 0.299061 |
| 48  | 6  | C   | -4.251890 | 2.776853  | 0.522807 |
| 49  | 6  | C   | -1.958143 | 2.772555  | 1.134466 |
| 50  | 6  | C   | -0.787912 | 3.476615  | 1.650697 |
| 51  | 6  | C   | -0.567452 | 4.827062  | 1.913532 |
| 52  | 1  | H   | -1.335285 | 5.560918  | 1.694983 |
| 53  | 6  | C   | 0.660036  | 5.194296  | 2.47810 |
| 54  | 1  | H   | 0.863971  | 6.238546  | 2.690414 |
| 55  | 6  | C   | 1.639581  | 4.224790  | 2.769269 |
| 56  | 1  | H   | 2.585212  | 4.538413  | 3.201290 |
| 57  | 6  | C   | 1.411304  | 2.867450  | 2.522876 |
| 58  | 1  | H   | 2.170894  | 2.133523  | 2.757242 |
| 59  | 6  | C   | 0.191260  | 2.497622  | 1.948650 |
| 60  | 6  | C   | -0.420175 | 1.203079  | 1.618562 |
| 61  | 12 | Mg  | 2.950587  | -0.001544 | -0.320962 |
| 62  | 8  | O   | 2.635255  | 0.002008  | 1.688026 |
| 63  | 1  | H   | 3.305947  | 0.006038  | 2.401321 |
| 64  | 1  | H   | 1.556652  | 0.004227  | 1.974575 |
| 65  | 7  | N   | -0.157278 | 0.008977  | -1.819663 |
| 66  | 7  | N   | 1.679859  | -1.405900 | -1.114723 |
| 67  | 7  | N   | 3.090990  | -3.392702 | -0.845859 |
| 68  | 7  | N   | 4.440270  | -1.426584 | -0.369407 |
| 69  | 7  | N   | 6.383091  | -0.014596 | 0.060409 |
| N | C | H |
|---|---|---|
| 70 | 7 | N | 4.451424, 1.411565, -0.368806 |
| 71 | 7 | N | 3.115254, 3.387218, -0.838472 |
| 72 | 7 | N | 1.691868, 1.409870, -1.117364 |
| 73 | 6 | C | 0.411187, -1.196998, -1.609559 |
| 74 | 6 | C | -0.209612, -2.489343, -1.930469 |
| 75 | 6 | C | -1.435952, -2.853397, -2.494704 |
| 76 | 1 | H | -2.194754, -2.115159, -2.719585 |
| 77 | 6 | C | -1.672939, -4.210426, -2.735020 |
| 78 | 1 | H | -2.623944, -4.520378, -3.157872 |
| 79 | 6 | C | -0.695703, -5.184167, -2.44982 |
| 80 | 6 | C | 0.537245, -4.822390, -0.317829 |
| 81 | 6 | C | 0.855359, -4.834948, -0.352148 |
| 82 | 1 | H | 5.108481, -5.591625, -0.566187 |
| 83 | 6 | C | 7.190948, -5.173497, -0.104611 |
| 84 | 1 | H | 7.492922, -6.215736, -0.119205 |
| 85 | 6 | C | 8.156138, -4.180598, 0.159027 |
| 86 | 1 | H | 9.184416, -4.475923, 0.340956 |
| 87 | 6 | C | 7.810603, -2.824084, 0.182286 |
| 88 | 1 | H | 8.549293, -2.054711, 0.377953 |
| 89 | 6 | C | 6.477573, -2.487489, -0.045078 |
| 90 | 6 | C | 5.778382, -1.99488, -0.091101 |
| 91 | 6 | C | 5.785879, 1.175031, -0.083393 |
| 92 | 6 | C | 6.491683, 2.459194, -0.021301 |
| 93 | 6 | C | 7.824489, 2.787256, 0.219400 |
| 94 | 1 | H | 8.558036, 2.012642, 0.413796 |
| 95 | 6 | C | 8.176655, 4.142246, 0.211261 |
| 96 | 1 | H | 9.205032, 4.430850, 0.403091 |
| 97 | 6 | C | 7.218121, 5.142210, -0.099224 |
| 98 | 1 | H | 7.524955, 6.183130, -0.052040 |
| 99 | 6 | C | 5.882650, 4.812394, -0.309978 |
| 100 | 1 | H | 5.140918, 5.574664, -0.522129 |
| 101 | 6 | C | 5.530842, 3.463644, -0.291144 |
| 102 | 1 | H | 4.259064, 2.772835, -0.516396 |
| 103 | 6 | C | 1.964998, 2.774925, -1.126825 |
| 104 | 1 | H | 0.796394, 3.483362, -1.640939 |
| 105 | 6 | C | 0.597477, 4.835091, -1.901864 |
| 106 | 1 | H | 1.348776, 5.566438, -1.678284 |
| 107 | 6 | C | 1.646242, 5.286845, -2.462167 |
| 108 | 1 | H | -0.847246, 6.252176, -2.675347 |
| 109 | 6 | C | -1.627498, 4.240525, -2.761099 |
| 110 | 1 | H | -2.571329, 4.557542, -3.194584 |
| 111 | 6 | C | -1.402993, 2.882021, -2.517733 |
| 112 | 1 | H | -2.163813, 2.150647, -2.755785 |
| 113 | 6 | C | -0.184904, 2.507549, -1.942342 |
| 114 | 6 | C | 0.423429, 1.210486, -1.616059 |
Table S4. DFT optimised geometrical parameters (Å,°) for (ZnPcH₂O)₂ dimer.

![View of the optimized (ZnPcH₂O)₂ dimer](image)

| Item                  | Value     | Threshold  | Converged? |
|-----------------------|-----------|------------|------------|
| Maximum Force         | 0.000069  | 0.000450   | YES        |
| RMS Force             | 0.000005  | 0.000300   | YES        |
| Maximum Displacement  | 0.001262  | 0.001800   | YES        |
| RMS Displacement      | 0.000214  | 0.001200   | YES        |

Predicted change in Energy=-5.625132D-08
Optimization completed. (for (ZnPcH₂O)₂ dimer)

| ! Name Definition | Value | Derivative Info. | ! |
|-------------------|-------|------------------|---|
| ! R1 R(1,2)       | 2.1296| -DE/DX = 0.0     | |
| ! R2 R(1,6)       | 2.0506| -DE/DX = 0.0     | |
| ! R3 R(1,8)       | 2.0504| -DE/DX = 0.0     | |
| ! R4 R(1,10)      | 2.05  | -DE/DX = 0.0     | |
| ! R5 R(1,12)      | 2.048 | -DE/DX = 0.0     | |
| ! R6 R(2,3)       | 0.971 | -DE/DX = 0.0     | |
| ! R7 R(2,4)       | 1.0266| -DE/DX = 0.0001  | |
| ! R8 R(4,65)      | 1.6559| -DE/DX = 0.0     | |
| ! R9 R(5,13)      | 1.3485| -DE/DX = 0.0     | |
| ! R10 R(5,60)     | 1.3487| -DE/DX = 0.0     | |
| ! R11 R(5,64)     | 1.6559| -DE/DX = 0.0     | |
| ! R12 R(6,13)     | 1.3762| -DE/DX = 0.0     | |
| ! R13 R(6,24)     | 1.3852| -DE/DX = 0.0     | |
| ! R14 R(7,24)     | 1.3349| -DE/DX = 0.0     | |
| ! R15 R(7,25)     | 1.3369| -DE/DX = 0.0     | |
| ! R16 R(8,25)     | 1.3807| -DE/DX = 0.0     | |
| ! R17 R(8,36)     | 1.3823| -DE/DX = 0.0     | |
| ! R18 R(9,36)     | 1.3376| -DE/DX = 0.0     | |
| ! R19 R(9,37)     | 1.3379| -DE/DX = 0.0     | |
| ! R20 R(10,37)    | 1.3816| -DE/DX = 0.0     | |
| ! R21 R(10,48)    | 1.3804| -DE/DX = 0.0     | |
| ! R22 R(11,48)    | 1.3368| -DE/DX = 0.0     | |
| ! R23 R(11,49)    | 1.3347| -DE/DX = 0.0     | |
| ! R24 R(12,49)    | 1.3855| -DE/DX = 0.0     | |
| ! R25 R(12,60)    | 1.3759| -DE/DX = 0.0     | |
| ! R26 R(13,14)    | 1.4699| -DE/DX = 0.0     | |
! R27  R(14,15)     1.3992  -DE/DX =  0.0  !
! R28  R(14,23)     1.4186  -DE/DX =  0.0  !
! R29  R(15,16)     1.083   -DE/DX =  0.0  !
! R30  R(15,17)     1.4007  -DE/DX =  0.0  !
! R31  R(17,18)     1.0856  -DE/DX =  0.0  !
! R32  R(17,19)     1.41   -DE/DX =  0.0  !
! R33  R(19,20)     1.0856  -DE/DX =  0.0  !
! R34  R(19,21)     1.4001  -DE/DX =  0.0  !
! R35  R(21,22)     1.0845  -DE/DX =  0.0  !
! R36  R(21,23)     1.3965  -DE/DX =  0.0  !
! R37  R(23,24)     1.4615  -DE/DX =  0.0  !
! R38  R(25,26)     1.4648  -DE/DX =  0.0  !
! R39  R(26,27)     1.3972  -DE/DX =  0.0  !
! R40  R(26,35)     1.4179  -DE/DX =  0.0  !
! R41  R(27,28)     1.0847  -DE/DX =  0.0  !
! R42  R(27,29)     1.4013  -DE/DX =  0.0  !
! R43  R(29,30)     1.0857  -DE/DX =  0.0  !
! R44  R(29,31)     1.4114  -DE/DX =  0.0  !
! R45  R(31,32)     1.0857  -DE/DX =  0.0  !
! R46  R(31,33)     1.4013  -DE/DX =  0.0  !
! R47  R(33,34)     1.0847  -DE/DX =  0.0  !
! R48  R(33,35)     1.3972  -DE/DX =  0.0  !
! R49  R(35,36)     1.4652  -DE/DX =  0.0  !
! R50  R(37,38)     1.4652  -DE/DX =  0.0  !
! R51  R(38,39)     1.3971  -DE/DX =  0.0  !
! R52  R(38,47)     1.4179  -DE/DX =  0.0  !
! R53  R(39,40)     1.0847  -DE/DX =  0.0  !
! R54  R(39,41)     1.4014  -DE/DX =  0.0  !
! R55  R(41,42)     1.0857  -DE/DX =  0.0  !
! R56  R(41,43)     1.4113  -DE/DX =  0.0  !
! R57  R(43,44)     1.0857  -DE/DX =  0.0  !
! R58  R(43,45)     1.4013  -DE/DX =  0.0  !
! R59  R(45,46)     1.0847  -DE/DX =  0.0  !
! R60  R(45,47)     1.3972  -DE/DX =  0.0  !
! R61  R(47,48)     1.4648  -DE/DX =  0.0  !
! R62  R(49,50)     1.4614  -DE/DX =  0.0  !
! R63  R(50,51)     1.3966  -DE/DX =  0.0  !
! R64  R(50,59)     1.4186  -DE/DX =  0.0  !
! R65  R(51,52)     1.0845  -DE/DX =  0.0  !
! R66  R(51,53)     1.4001  -DE/DX =  0.0  !
! R67  R(53,54)     1.0856  -DE/DX =  0.0  !
! R68  R(53,55)     1.4101  -DE/DX =  0.0  !
! R69  R(55,56)     1.0856  -DE/DX =  0.0  !
! R70  R(55,57)     1.4004  -DE/DX =  0.0  !
! R71  R(57,58)     1.0832  -DE/DX =  0.0  !
! R72  R(57,59)     1.3992  -DE/DX =  0.0  !
! R73  R(59,60)     1.4694  -DE/DX =  0.0  !
! R74  R(61,62)     2.1295  -DE/DX =  0.0  !
! R75  R(61,66)     2.0506  -DE/DX =  0.0  !
! R76  R(61,68)     2.0504  -DE/DX =  0.0  !
! R77  R(61,70)     2.05  -DE/DX =  0.0  !
! R78  R(61,72)     2.048  -DE/DX =  0.0  !
! R79  R(62,63)     0.9709  -DE/DX =  0.0  !
! R80  R(62,64)     1.0266  -DE/DX =  0.0001  !
! R81  R(65,73)     1.3485  -DE/DX =  0.0  !
! R82  R(65,120)    1.3487  -DE/DX =  0.0  !
! R83  R(66,73)     1.3762  -DE/DX =  0.0  !
! R84  R(66,84)     1.3852  -DE/DX =  0.0  !
! R85  R(67,84)     1.3349  -DE/DX =  0.0  !
! R86  R(67,85)     1.3369  -DE/DX =  0.0  !
| R     | (x,y,z) | DE/DX |  
|-------|--------|-------|  
| R87   | R(68,85) | 1.3807 | -DE/DX = 0.0  
| R88   | R(68,86) | 1.3823 | -DE/DX = 0.0  
| R89   | R(69,87) | 1.3376 | -DE/DX = 0.0  
| R90   | R(69,88) | 1.3379 | -DE/DX = 0.0  
| R91   | R(70,89) | 1.3816 | -DE/DX = 0.0  
| R92   | R(70,90) | 1.3804 | -DE/DX = 0.0  
| R93   | R(71,91) | 1.3368 | -DE/DX = 0.0  
| R94   | R(71,92) | 1.3347 | -DE/DX = 0.0  
| R95   | R(72,93) | 1.3855 | -DE/DX = 0.0  
| R96   | R(72,94) | 1.3759 | -DE/DX = 0.0  
| R97   | R(73,95) | 1.4699 | -DE/DX = 0.0  
| R98   | R(74,96) | 1.3992 | -DE/DX = 0.0  
| R99   | R(74,97) | 1.4186 | -DE/DX = 0.0  
| R100  | R(75,98) | 1.083  | -DE/DX = 0.0  
| R101  | R(75,99) | 1.4007 | -DE/DX = 0.0  
| R102  | R(77,80) | 1.0856 | -DE/DX = 0.0  
| R103  | R(77,81) | 1.4100 | -DE/DX = 0.0  
| R104  | R(79,82) | 1.0856 | -DE/DX = 0.0  
| R105  | R(79,83) | 1.4001 | -DE/DX = 0.0  
| R106  | R(81,84) | 1.0845 | -DE/DX = 0.0  
| R107  | R(81,85) | 1.3965 | -DE/DX = 0.0  
| R108  | R(83,84) | 1.4615 | -DE/DX = 0.0  
| R109  | R(85,86) | 1.4648 | -DE/DX = 0.0  
| R110  | R(86,87) | 1.3972 | -DE/DX = 0.0  
| R111  | R(86,88) | 1.4179 | -DE/DX = 0.0  
| R112  | R(87,89) | 1.0847 | -DE/DX = 0.0  
| R113  | R(87,90) | 1.4013 | -DE/DX = 0.0  
| R114  | R(89,91) | 1.4114 | -DE/DX = 0.0  
| R115  | R(91,92) | 1.0857 | -DE/DX = 0.0  
| R116  | R(91,93) | 1.4013 | -DE/DX = 0.0  
| R117  | R(93,94) | 1.0847 | -DE/DX = 0.0  
| R118  | R(93,95) | 1.3972 | -DE/DX = 0.0  
| R119  | R(95,96) | 1.4652 | -DE/DX = 0.0  
| R120  | R(97,98) | 1.4652 | -DE/DX = 0.0  
| R121  | R(98,99) | 1.3971 | -DE/DX = 0.0  
| R122  | R(98,100)| 1.4179 | -DE/DX = 0.0  
| R123  | R(99,101)| 1.0847 | -DE/DX = 0.0  
| R124  | R(99,102)| 1.4014 | -DE/DX = 0.0  
| R125  | R(101,102)| 1.0857 | -DE/DX = 0.0  
| R126  | R(101,103)| 1.4113 | -DE/DX = 0.0  
| R127  | R(103,104)| 1.0857 | -DE/DX = 0.0  
| R128  | R(103,105)| 1.4013 | -DE/DX = 0.0  
| R129  | R(105,106)| 1.0847 | -DE/DX = 0.0  
| R130  | R(105,107)| 1.3972 | -DE/DX = 0.0  
| R131  | R(107,108)| 1.4648 | -DE/DX = 0.0  
| R132  | R(109,110)| 1.4614 | -DE/DX = 0.0  
| R133  | R(110,111)| 1.3966 | -DE/DX = 0.0  
| R134  | R(110,112)| 1.4186 | -DE/DX = 0.0  
| R135  | R(111,112)| 1.0845 | -DE/DX = 0.0  
| R136  | R(111,113)| 1.4001 | -DE/DX = 0.0  
| R137  | R(113,114)| 1.0856 | -DE/DX = 0.0  
| R138  | R(113,115)| 1.4101 | -DE/DX = 0.0  
| R139  | R(115,116)| 1.0856 | -DE/DX = 0.0  
| R140  | R(115,117)| 1.4004 | -DE/DX = 0.0  
| R141  | R(117,118)| 1.0832 | -DE/DX = 0.0  
| R142  | R(117,119)| 1.3992 | -DE/DX = 0.0  
| R143  | R(119,120)| 1.4694 | -DE/DX = 0.0  

| A1    | A(2,1,6) | 101.5115 | -DE/DX = 0.0  
| A2    | A(2,1,8) | 99.3909  | -DE/DX = 0.0  

S29
| # | A (i,j,k) | Value  | \(-\Delta E/\Delta x\) |
|---|----------|--------|-------------------------|
| 1 | A(2,1,10) | 99.7926 | 0.0                     |
| 2 | A(2,1,12) | 101.7281 | 0.0                     |
| 3 | A(6,1,8)  | 88.6249 | 0.0                     |
| 4 | A(6,1,10) | 158.6918 | 0.0                     |
| 5 | A(6,1,12) | 87.4097 | 0.0                     |
| 6 | A(8,1,10) | 87.5055 | 0.0                     |
| 7 | A(8,1,12) | 158.8798 | 0.0                     |
| 8 | A(10,1,12) | 88.6928 | 0.0                     |
| 9 | A(1,2,3)  | 120.454 | 0.0                     |
| 10| A(1,2,4)  | 125.3863 | 0.0                     |
| 11| A(3,2,4)  | 113.4918 | 0.0                     |
| 12| A(13,5,60) | 125.5117 | 0.0                     |
| 13| A(13,5,64) | 114.8216 | 0.0                     |
| 14| A(1,6,13) | 125.9759 | 0.0                     |
| 15| A(1,6,24) | 124.4204 | 0.0                     |
| 16| A(13,6,24) | 109.2253 | 0.0                     |
| 17| A(1,8,25) | 125.8695 | 0.0                     |
| 18| A(1,8,36) | 124.9297 | 0.0                     |
| 19| A(60,5,64) | 114.9503 | 0.0                     |
| 20| A(1,10,37) | 125.9759 | 0.0                     |
| 21| A(1,10,48) | 124.4204 | 0.0                     |
| 22| A(1,12,49) | 125.8695 | 0.0                     |
| 23| A(1,12,60) | 125.9759 | 0.0                     |
| 24| A(5,13,6)  | 126.137 | 0.0                     |
| 25| A(5,13,14) | 124.7928 | 0.0                     |
| 26| A(6,13,14) | 125.0566 | 0.0                     |
| 27| A(25,8,36) | 109.2402 | 0.0                     |
| 28| A(36,9,37) | 125.2211 | 0.0                     |
| 29| A(1,10,37) | 125.4944 | 0.0                     |
| 30| A(10,10,48) | 124.8415 | 0.0                     |
| 31| A(10,10,64) | 125.8695 | 0.0                     |
| 32| A(10,10,37) | 125.9759 | 0.0                     |
| 33| A(10,10,48) | 124.4204 | 0.0                     |
| 34| A(1,12,60) | 126.073 | 0.0                     |
| 35| A(1,12,60) | 126.073 | 0.0                     |
| 36| A(1,12,60) | 126.073 | 0.0                     |
| 37| A(1,12,60) | 126.073 | 0.0                     |
| 38| A(1,12,60) | 126.073 | 0.0                     |
| 39| A(1,12,60) | 126.073 | 0.0                     |
| 40| A(1,12,60) | 126.073 | 0.0                     |
| 41| A(1,12,60) | 126.073 | 0.0                     |
| 42| A(1,12,60) | 126.073 | 0.0                     |
| 43| A(1,12,60) | 126.073 | 0.0                     |
| 44| A(1,12,60) | 126.073 | 0.0                     |
| 45| A(1,12,60) | 126.073 | 0.0                     |
| 46| A(1,12,60) | 126.073 | 0.0                     |
| 47| A(1,12,60) | 126.073 | 0.0                     |
| 48| A(1,12,60) | 126.073 | 0.0                     |
| 49| A(1,12,60) | 126.073 | 0.0                     |
| 50| A(1,12,60) | 126.073 | 0.0                     |
| 51| A(1,12,60) | 126.073 | 0.0                     |
| 52| A(1,12,60) | 126.073 | 0.0                     |
| 53| A(1,12,60) | 126.073 | 0.0                     |
| 54| A(1,12,60) | 126.073 | 0.0                     |
| 55| A(1,12,60) | 126.073 | 0.0                     |
| 56| A(1,12,60) | 126.073 | 0.0                     |
| 57| A(1,12,60) | 126.073 | 0.0                     |
| 58| A(1,12,60) | 126.073 | 0.0                     |
| 59| A(1,12,60) | 126.073 | 0.0                     |
| 60| A(1,12,60) | 126.073 | 0.0                     |
| 61| A(1,12,60) | 126.073 | 0.0                     |
| 62| A(1,12,60) | 126.073 | 0.0                     |
| A63   | A(26,27,29) | 117.9256 | -DE/DX = 0.0 |
| A64   | A(28,27,29) | 121.4302 | -DE/DX = 0.0 |
| A65   | A(27,29,30) | 119.6299 | -DE/DX = 0.0 |
| A66   | A(27,29,31) | 121.0623 | -DE/DX = 0.0 |
| A67   | A(29,31,30) | 119.3076 | -DE/DX = 0.0 |
| A68   | A(27,29,31) | 121.0623 | -DE/DX = 0.0 |
| A69   | A(30,29,31) | 119.3093 | -DE/DX = 0.0 |
| A70   | A(29,31,32) | 119.3093 | -DE/DX = 0.0 |
| A71   | A(29,31,33) | 121.0701 | -DE/DX = 0.0 |
| A72   | A(32,31,33) | 119.6203 | -DE/DX = 0.0 |
| A73   | A(31,33,34) | 121.4137 | -DE/DX = 0.0 |
| A74   | A(31,33,35) | 117.9207 | -DE/DX = 0.0 |
| A75   | A(34,33,35) | 120.6655 | -DE/DX = 0.0 |
| A76   | A(26,35,33) | 121.0102 | -DE/DX = 0.0 |
| A77   | A(33,35,36) | 132.4285 | -DE/DX = 0.0 |
| A78   | A(33,35,36) | 126.9591 | -DE/DX = 0.0 |
| A79   | A(8,36,35)  | 108.7844 | -DE/DX = 0.0 |
| A80   | A(8,36,35)  | 124.2295 | -DE/DX = 0.0 |
| A81   | A(9,37,10)  | 126.9506 | -DE/DX = 0.0 |
| A82   | A(9,37,10)  | 124.217  | -DE/DX = 0.0 |
| A83   | A(10,37,38) | 108.8044 | -DE/DX = 0.0 |
| A84   | A(37,38,39) | 132.4404 | -DE/DX = 0.0 |
| A85   | A(37,38,47) | 120.692  | -DE/DX = 0.0 |
| A86   | A(38,39,40) | 117.921  | -DE/DX = 0.0 |
| A87   | A(38,39,41) | 121.4098 | -DE/DX = 0.0 |
| A88   | A(39,41,42) | 119.6213 | -DE/DX = 0.0 |
| A89   | A(39,41,43) | 121.0675 | -DE/DX = 0.0 |
| A90   | A(41,43,44) | 119.311  | -DE/DX = 0.0 |
| A91   | A(41,43,44) | 119.3087 | -DE/DX = 0.0 |
| A92   | A(41,43,45) | 121.0619 | -DE/DX = 0.0 |
| A93   | A(41,43,45) | 119.6292 | -DE/DX = 0.0 |
| A94   | A(43,45,46) | 121.4239 | -DE/DX = 0.0 |
| A95   | A(43,45,47) | 117.9264 | -DE/DX = 0.0 |
| A96   | A(46,45,47) | 120.6496 | -DE/DX = 0.0 |
| A97   | A(43,45,46) | 121.0086 | -DE/DX = 0.0 |
| A98   | A(38,47,45) | 121.0086 | -DE/DX = 0.0 |
| A99   | A(38,47,48) | 106.5344 | -DE/DX = 0.0 |
| A100  | A(45,47,48) | 132.4537 | -DE/DX = 0.0 |
| A101  | A(10,48,11) | 126.8788 | -DE/DX = 0.0 |
| A102  | A(10,48,47) | 108.8637 | -DE/DX = 0.0 |
| A103  | A(11,48,47) | 124.2275 | -DE/DX = 0.0 |
| A104  | A(11,49,50) | 127.457  | -DE/DX = 0.0 |
| A105  | A(11,49,50) | 123.812  | -DE/DX = 0.0 |
| A106  | A(12,49,50) | 108.7105 | -DE/DX = 0.0 |
| A107  | A(49,50,51) | 131.7514 | -DE/DX = 0.0 |
| A108  | A(49,50,59) | 106.8418 | -DE/DX = 0.0 |
| A109  | A(51,50,59) | 121.3836 | -DE/DX = 0.0 |
| A110  | A(50,51,52) | 120.411  | -DE/DX = 0.0 |
| A111  | A(50,51,53) | 118.044  | -DE/DX = 0.0 |
| A112  | A(52,51,53) | 121.5444 | -DE/DX = 0.0 |
| A113  | A(51,53,54) | 119.7782 | -DE/DX = 0.0 |
| A114  | A(51,53,55) | 120.8359 | -DE/DX = 0.0 |
| A115  | A(54,53,55) | 119.3853 | -DE/DX = 0.0 |
| A116  | A(53,55,56) | 119.3945 | -DE/DX = 0.0 |
| A117  | A(53,55,57) | 121.039  | -DE/DX = 0.0 |
| A118  | A(56,55,57) | 119.5016 | -DE/DX = 0.0 |
| A119  | A(55,57,58) | 120.2687 | -DE/DX = 0.0 |
| A120  | A(55,57,59) | 118.3615 | -DE/DX = 0.0 |
| A121  | A(58,57,59) | 121.3697 | -DE/DX = 0.0 |
| A122  | A(50,59,57) | 120.2623 | -DE/DX = 0.0 |
| A | Code | Value 1 | Value 2 | Column 3 |
|---|------|---------|---------|----------|
| A123 | A(50,59,60) | 106.1814 | -DE/DX = 0.0 |
| A124 | A(57,59,60) | 133.5058 | -DE/DX = 0.0 |
| A125 | A(5,60,12) | 126.238 | -DE/DX = 0.0 |
| A126 | A(5,60,59) | 124.7245 | -DE/DX = 0.0 |
| A127 | A(12,60,59) | 109.0146 | -DE/DX = 0.0 |
| A128 | A(62,61,66) | 101.5122 | -DE/DX = 0.0 |
| A129 | A(62,61,68) | 99.385 | -DE/DX = 0.0 |
| A130 | A(62,61,70) | 99.7934 | -DE/DX = 0.0 |
| A131 | A(62,61,72) | 101.7314 | -DE/DX = 0.0 |
| A132 | A(66,61,68) | 88.6248 | -DE/DX = 0.0 |
| A133 | A(66,61,70) | 158.6903 | -DE/DX = 0.0 |
| A134 | A(66,61,72) | 87.4102 | -DE/DX = 0.0 |
| A135 | A(68,61,70) | 87.5051 | -DE/DX = 0.0 |
| A136 | A(68,61,72) | 158.8824 | -DE/DX = 0.0 |
| A137 | A(70,61,72) | 88.6931 | -DE/DX = 0.0 |
| A138 | A(61,62,63) | 120.442 | -DE/DX = 0.0 |
| A139 | A(61,62,64) | 125.3829 | -DE/DX = 0.0 |
| A140 | A(63,62,64) | 113.4979 | -DE/DX = 0.0 |
| A141 | A(4,65,73) | 114.8245 | -DE/DX = 0.0 |
| A142 | A(4,65,120) | 114.9476 | -DE/DX = 0.0 |
| A143 | A(73,65,120) | 125.5119 | -DE/DX = 0.0 |
| A144 | A(61,66,73) | 125.975 | -DE/DX = 0.0 |
| A145 | A(61,66,84) | 124.4206 | -DE/DX = 0.0 |
| A146 | A(73,66,84) | 109.2255 | -DE/DX = 0.0 |
| A147 | A(84,67,85) | 125.698 | -DE/DX = 0.0 |
| A148 | A(61,68,85) | 124.9299 | -DE/DX = 0.0 |
| A149 | A(61,68,96) | 125.5067 | -DE/DX = 0.0 |
| A150 | A(85,68,96) | 109.2403 | -DE/DX = 0.0 |
| A151 | A(96,69,97) | 125.2214 | -DE/DX = 0.0 |
| A152 | A(61,70,97) | 125.4944 | -DE/DX = 0.0 |
| A153 | A(61,70,108) | 124.8413 | -DE/DX = 0.0 |
| A154 | A(97,70,108) | 109.2413 | -DE/DX = 0.0 |
| A155 | A(108,71,109) | 125.8569 | -DE/DX = 0.0 |
| A156 | A(61,72,109) | 124.4293 | -DE/DX = 0.0 |
| A157 | A(61,72,120) | 126.0724 | -DE/DX = 0.0 |
| A158 | A(109,72,120) | 109.2517 | -DE/DX = 0.0 |
| A159 | A(65,73,66) | 126.137 | -DE/DX = 0.0 |
| A160 | A(65,73,74) | 124.7927 | -DE/DX = 0.0 |
| A161 | A(66,73,74) | 109.0374 | -DE/DX = 0.0 |
| A162 | A(73,74,75) | 133.4843 | -DE/DX = 0.0 |
| A163 | A(73,74,83) | 106.1468 | -DE/DX = 0.0 |
| A164 | A(75,74,83) | 120.3336 | -DE/DX = 0.0 |
| A165 | A(74,75,76) | 121.333 | -DE/DX = 0.0 |
| A166 | A(74,75,77) | 118.2653 | -DE/DX = 0.0 |
| A167 | A(76,75,77) | 120.3985 | -DE/DX = 0.0 |
| A168 | A(75,77,78) | 119.4517 | -DE/DX = 0.0 |
| A169 | A(75,77,79) | 121.1594 | -DE/DX = 0.0 |
| A170 | A(78,77,79) | 119.3887 | -DE/DX = 0.0 |
| A171 | A(77,79,80) | 119.3942 | -DE/DX = 0.0 |
| A172 | A(77,79,81) | 120.8418 | -DE/DX = 0.0 |
| A173 | A(80,79,81) | 119.764 | -DE/DX = 0.0 |
| A174 | A(79,81,82) | 121.5532 | -DE/DX = 0.0 |
| A175 | A(79,81,83) | 118.0168 | -DE/DX = 0.0 |
| A176 | A(82,81,83) | 120.4297 | -DE/DX = 0.0 |
| A177 | A(74,83,81) | 121.3805 | -DE/DX = 0.0 |
| A178 | A(74,83,84) | 106.8534 | -DE/DX = 0.0 |
| A179 | A(81,83,84) | 131.7309 | -DE/DX = 0.0 |
| A180 | A(66,84,67) | 127.4248 | -DE/DX = 0.0 |
| A181 | A(66,84,83) | 108.7356 | -DE/DX = 0.0 |
| A182 | A(67,84,83) | 123.824 | -DE/DX = 0.0 |
| A243 | A(113,115,116) | 119.3944 | -DE/DX = 0.0 |
| A244 | A(113,115,117) | 121.104   | -DE/DX = 0.0 |
| A245 | A(115,117,118) | 120.2686  | -DE/DX = 0.0 |
| A246 | A(115,117,119) | 118.3614  | -DE/DX = 0.0 |
| A247 | A(118,117,119) | 121.3699  | -DE/DX = 0.0 |
| A248 | A(110,119,117) | 120.2624  | -DE/DX = 0.0 |
| A249 | A(110,119,120) | 106.1812  | -DE/DX = 0.0 |
| A250 | A(117,119,120) | 133.506   | -DE/DX = 0.0 |
| A251 | A(65,120,72)   | 126.2378  | -DE/DX = 0.0 |
| A252 | A(65,120,119)  | 124.725   | -DE/DX = 0.0 |
| A253 | A(72,120,119)  | 109.0142  | -DE/DX = 0.0 |
| A254 | L(2,4,65,6,-1) | 170.4417  | -DE/DX = 0.0 |
| A255 | L(2,4,65,6,-2) | 174.5004  | -DE/DX = 0.0 |
| A256 | D(6,1,2,3)     | -125.6583 | -DE/DX = 0.0 |
| A257 | D(6,1,2,4)     | 44.3474   | -DE/DX = 0.0 |
| A258 | D(8,1,2,3)     | -35.1507  | -DE/DX = 0.0 |
| A259 | D(8,1,2,4)     | 134.855   | -DE/DX = 0.0 |
| A260 | D(10,1,2,3)    | 53.9198   | -DE/DX = 0.0 |
| A261 | D(10,1,2,4)    | -136.0744 | -DE/DX = 0.0 |
| A262 | D(12,1,2,3)    | 144.6181  | -DE/DX = 0.0 |
| A263 | D(12,1,2,4)    | -45.3762  | -DE/DX = 0.0 |
| A264 | D(2,1,6,13)    | -85.7558  | -DE/DX = 0.0 |
| A265 | D(2,1,6,24)    | 86.4101   | -DE/DX = 0.0 |
| A266 | D(8,1,6,13)    | 174.9399  | -DE/DX = 0.0 |
| A267 | D(8,1,6,24)    | -12.8942  | -DE/DX = 0.0 |
| A268 | D(10,1,6,13)   | 95.3883   | -DE/DX = 0.0 |
| A269 | D(10,1,6,24)   | -92.4458  | -DE/DX = 0.0 |
| A270 | D(12,1,6,13)   | 15.6898   | -DE/DX = 0.0 |
| A271 | D(12,1,6,24)   | -172.1442 | -DE/DX = 0.0 |
| A272 | D(2,1,8,25)    | 88.0308   | -DE/DX = 0.0 |
| A273 | D(2,1,8,36)    | 84.7262   | -DE/DX = 0.0 |
| A274 | D(6,1,8,25)    | 13.4105   | -DE/DX = 0.0 |
| A275 | D(6,1,8,36)    | -173.8325 | -DE/DX = 0.0 |
| A276 | D(8,1,8,25)    | 172.4516  | -DE/DX = 0.0 |
| A277 | D(8,1,8,36)    | -14.7914  | -DE/DX = 0.0 |
| A278 | D(10,1,8,25)   | 92.5975   | -DE/DX = 0.0 |
| A279 | D(10,1,8,36)   | -94.6455  | -DE/DX = 0.0 |
| A280 | D(12,1,8,25)   | -83.9253  | -DE/DX = 0.0 |
| A281 | D(12,1,8,36)   | 87.7987   | -DE/DX = 0.0 |
| A282 | D(2,1,10,37)   | 94.937    | -DE/DX = 0.0 |
| A283 | D(2,1,10,48)   | -173.0977 | -DE/DX = 0.0 |
| A284 | D(6,1,10,37)   | 171.5011  | -DE/DX = 0.0 |
| A285 | D(6,1,10,48)   | -93.3389  | -DE/DX = 0.0 |
| A286 | D(8,1,10,37)   | 15.1783   | -DE/DX = 0.0 |
| A287 | D(8,1,10,48)   | -173.977  | -DE/DX = 0.0 |
| A288 | D(12,1,10,37)  | 174.3981  | -DE/DX = 0.0 |
| A289 | D(12,1,10,48)  | -13.8779  | -DE/DX = 0.0 |
| A290 | D(2,1,12,49)   | 87.2755   | -DE/DX = 0.0 |
| A291 | D(2,1,12,60)   | 86.3991   | -DE/DX = 0.0 |
| A292 | D(6,1,12,49)   | 171.5011  | -DE/DX = 0.0 |
| A293 | D(6,1,12,60)   | -14.8243  | -DE/DX = 0.0 |
| A294 | D(8,1,12,49)   | 92.0915   | -DE/DX = 0.0 |
| A295 | D(8,1,12,60)   | -94.2339  | -DE/DX = 0.0 |
| A296 | D(10,1,12,49)  | 12.4551   | -DE/DX = 0.0 |
| A297 | D(10,1,12,60)  | -173.8703 | -DE/DX = 0.0 |
| A298 | D(1,2,65,73)   | 76.3056   | -DE/DX = 0.0 |
| A299 | D(1,2,65,120)  | -77.0836  | -DE/DX = 0.0 |
| A300 | D(3,2,65,73)   | -113.557  | -DE/DX = 0.0 |
| A301 | D(3,2,65,120)  | 93.4551   | -DE/DX = 0.0 |

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| D45 | D(60,5,13,6) | -5.6765 | -DE/DX = 0.0 |
| D46 | D(60,5,13,14) | 172.0048 | -DE/DX = 0.0 |
| D47 | D(64,5,13,6) | 148.6166 | -DE/DX = 0.0 |
| D48 | D(64,5,13,14) | -33.7021 | -DE/DX = 0.0 |
| D49 | D(13,5,60,12) | 6.7126 | -DE/DX = 0.0 |
| D50 | D(13,5,60,59) | -171.3512 | -DE/DX = 0.0 |
| D51 | D(64,5,60,12) | 148.6166 | -DE/DX = 0.0 |
| D52 | D(64,5,60,59) | 34.3845 | -DE/DX = 0.0 |
| D53 | D(13,5,62,61) | -76.3003 | -DE/DX = 0.0 |
| D54 | D(13,5,62,63) | 113.228 | -DE/DX = 0.0 |
| D55 | D(60,5,62,61) | 77.089 | -DE/DX = 0.0 |
| D56 | D(60,5,62,63) | -93.3828 | -DE/DX = 0.0 |
| D57 | D(1,6,13,5) | -9.1897 | -DE/DX = 0.0 |
| D58 | D(1,6,13,14) | 172.8245 | -DE/DX = 0.0 |
| D59 | D(24,6,13,5) | 177.6493 | -DE/DX = 0.0 |
| D60 | D(24,6,13,14) | -0.3365 | -DE/DX = 0.0 |
| D61 | D(1,6,24,7) | 8.2927 | -DE/DX = 0.0 |
| D62 | D(1,6,24,23) | -173.1078 | -DE/DX = 0.0 |
| D63 | D(13,6,24,7) | -178.4159 | -DE/DX = 0.0 |
| D64 | D(13,6,24,23) | 0.1835 | -DE/DX = 0.0 |
| D65 | D(25,7,24,6) | 1.841 | -DE/DX = 0.0 |
| D66 | D(25,7,24,23) | -176.5624 | -DE/DX = 0.0 |
| D67 | D(24,7,25,8) | -1.3268 | -DE/DX = 0.0 |
| D68 | D(24,7,25,26) | 176.6064 | -DE/DX = 0.0 |
| D69 | D(1,8,25,7) | -9.2818 | -DE/DX = 0.0 |
| D70 | D(1,8,25,26) | 172.5241 | -DE/DX = 0.0 |
| D71 | D(36,8,25,7) | 176.9588 | -DE/DX = 0.0 |
| D72 | D(36,8,25,26) | -1.2353 | -DE/DX = 0.0 |
| D73 | D(1,8,36,9) | 9.439 | -DE/DX = 0.0 |
| D74 | D(1,8,36,35) | -172.4031 | -DE/DX = 0.0 |
| D75 | D(25,8,36,9) | -176.8464 | -DE/DX = 0.0 |
| D76 | D(25,8,36,35) | 1.3116 | -DE/DX = 0.0 |
| D77 | D(37,9,36,8) | 2.4763 | -DE/DX = 0.0 |
| D78 | D(37,9,36,35) | -175.4143 | -DE/DX = 0.0 |
| D79 | D(36,9,37,10) | -2.0099 | -DE/DX = 0.0 |
| D80 | D(36,9,37,38) | 175.8464 | -DE/DX = 0.0 |
| D81 | D(1,10,37,9) | -10.3053 | -DE/DX = 0.0 |
| D82 | D(1,10,37,12) | 171.5673 | -DE/DX = 0.0 |
| D83 | D(48,10,37,9) | 176.8828 | -DE/DX = 0.0 |
| D84 | D(48,10,37,38) | -1.2446 | -DE/DX = 0.0 |
| D85 | D(1,10,48,11) | 10.2468 | -DE/DX = 0.0 |
| D86 | D(1,10,48,47) | -171.6925 | -DE/DX = 0.0 |
| D87 | D(37,10,48,11) | -176.8835 | -DE/DX = 0.0 |
| D88 | D(37,10,48,47) | 1.1772 | -DE/DX = 0.0 |
| D89 | D(49,11,48,10) | 0.8936 | -DE/DX = 0.0 |
| D90 | D(49,11,48,47) | -176.8867 | -DE/DX = 0.0 |
| D91 | D(48,11,49,12) | -2.5426 | -DE/DX = 0.0 |
| D92 | D(48,11,49,50) | 175.621 | -DE/DX = 0.0 |
| D93 | D(1,12,49,11) | -7.2102 | -DE/DX = 0.0 |
| D94 | D(1,12,49,50) | 174.4007 | -DE/DX = 0.0 |
| D95 | D(60,12,49,11) | 178.2023 | -DE/DX = 0.0 |
| D96 | D(60,12,49,50) | -0.1868 | -DE/DX = 0.0 |
| D97 | D(1,12,60,5) | 7.2889 | -DE/DX = 0.0 |
| D98 | D(1,12,60,59) | -174.3943 | -DE/DX = 0.0 |
| D99 | D(49,12,60,5) | -178.2348 | -DE/DX = 0.0 |
| D100 | D(49,12,60,59) | 0.082 | -DE/DX = 0.0 |
| D101 | D(5,13,14,15) | 0.1018 | -DE/DX = 0.0 |
| D102 | D(5,13,14,23) | -177.6606 | -DE/DX = 0.0 |
| D103 | D(6,13,14,15) | 178.121 | -DE/DX = 0.0 |
| D104 | D(6,13,14,23) | 0.3586 | -DE/DX = 0.0 |
| D105 | D(13,14,15,16) | 2.5428 | -DE/DX = 0.0 |
| D106 | D(13,14,15,17) | -178.0947 | -DE/DX = 0.0 |
| D107 | D(23,14,15,16) | -179.9476 | -DE/DX = 0.0 |
| D108 | D(23,14,15,17) | -0.5851 | -DE/DX = 0.0 |
| D109 | D(13,14,23,21) | 178.5019 | -DE/DX = 0.0 |
| D110 | D(13,14,23,24) | -0.2388 | -DE/DX = 0.0 |
| D111 | D(15,14,23,21) | 0.3829 | -DE/DX = 0.0 |
| D112 | D(15,14,23,24) | -178.3579 | -DE/DX = 0.0 |
| D113 | D(14,15,17,18) | -0.368 | -DE/DX = 0.0 |
| D114 | D(14,15,17,19) | -179.9476 | -DE/DX = 0.0 |
| D115 | D(16,15,17,18) | -0.0756 | -DE/DX = 0.0 |
| D116 | D(16,15,17,19) | 179.7367 | -DE/DX = 0.0 |
| D117 | D(15,17,19,20) | 0.0669 | -DE/DX = 0.0 |
| D118 | D(15,17,19,21) | -0.1993 | -DE/DX = 0.0 |
| D119 | D(18,17,19,20) | 179.8793 | -DE/DX = 0.0 |
| D120 | D(18,17,19,21) | 179.508 | -DE/DX = 0.0 |
| D121 | D(17,19,21,22) | -0.2783 | -DE/DX = 0.0 |
| D122 | D(17,19,21,23) | 178.5132 | -DE/DX = 0.0 |
| D123 | D(20,19,21,22) | 0.148 | -DE/DX = 0.0 |
| D124 | D(20,19,21,23) | 178.5005 | -DE/DX = 0.0 |
| D125 | D(19,21,23,14) | 0.0567 | -DE/DX = 0.0 |
| D126 | D(19,21,23,24) | 178.4412 | -DE/DX = 0.0 |
| D127 | D(22,21,23,14) | -179.7321 | -DE/DX = 0.0 |
| D128 | D(22,21,23,24) | -1.3476 | -DE/DX = 0.0 |
| D129 | D(14,23,24,6) | 0.0457 | -DE/DX = 0.0 |
| D130 | D(14,23,24,7) | 178.7069 | -DE/DX = 0.0 |
| D131 | D(21,23,24,6) | 0.148 | -DE/DX = 0.0 |
| D132 | D(21,23,24,7) | 178.5132 | -DE/DX = 0.0 |
| D133 | D(7,25,26,27) | 1.7197 | -DE/DX = 0.0 |
| D134 | D(7,25,26,28) | -177.586 | -DE/DX = 0.0 |
| D135 | D(8,25,26,27) | 179.9737 | -DE/DX = 0.0 |
| D136 | D(8,25,26,28) | 0.668 | -DE/DX = 0.0 |
| D137 | D(25,26,27,28) | 0.4057 | -DE/DX = 0.0 |
| D138 | D(25,26,27,29) | 179.501 | -DE/DX = 0.0 |
| D139 | D(35,26,27,28) | 179.6292 | -DE/DX = 0.0 |
| D140 | D(35,26,27,29) | -0.2774 | -DE/DX = 0.0 |
| D141 | D(25,26,35,33) | 179.3855 | -DE/DX = 0.0 |
| D142 | D(25,26,35,36) | 0.1207 | -DE/DX = 0.0 |
| D143 | D(27,26,35,33) | -0.0167 | -DE/DX = 0.0 |
| D144 | D(27,26,35,36) | -179.2815 | -DE/DX = 0.0 |
| D145 | D(26,27,29,30) | -179.8953 | -DE/DX = 0.0 |
| D146 | D(26,27,29,31) | 0.2795 | -DE/DX = 0.0 |
| D147 | D(28,27,29,30) | 0.1988 | -DE/DX = 0.0 |
| D148 | D(28,27,29,31) | -179.6264 | -DE/DX = 0.0 |
| D149 | D(27,29,31,32) | 179.8259 | -DE/DX = 0.0 |
| D150 | D(27,29,31,33) | 0.0128 | -DE/DX = 0.0 |
| D151 | D(30,29,31,32) | 0.0 | -DE/DX = 0.0 |
| D152 | D(30,29,31,33) | -179.813 | -DE/DX = 0.0 |
| D153 | D(29,31,33,34) | 179.5872 | -DE/DX = 0.0 |
| D154 | D(29,31,33,35) | -0.3062 | -DE/DX = 0.0 |
| D155 | D(32,31,33,34) | -0.2253 | -DE/DX = 0.0 |
| D156 | D(32,31,33,35) | 179.8813 | -DE/DX = 0.0 |
| D157 | D(31,33,35,26) | 0.3079 | -DE/DX = 0.0 |
| D158 | D(31,33,35,36) | 179.3531 | -DE/DX = 0.0 |
| D159 | D(34,33,35,26) | -179.5863 | -DE/DX = 0.0 |
| D160 | D(34,33,35,36) | -0.5411 | -DE/DX = 0.0 |
| D161 | D(26,35,36,8) | -0.8703 | -DE/DX = 0.0 |
| D162 | D(26,35,36,9) | 177.3495 | -DE/DX = 0.0 |
| D163 | D(33,35,36,8) | 179.9834 | -DE/DX = 0.0 |
| D164 | D(33,35,36,9) | -1.7968 | -DE/DX = 0.0 |
| D165 | D(9,37,38,39) | 1.8244 | -DE/DX = 0.0 |
| D166 | D(9,37,38,47) | -177.3695 | -DE/DX = 0.0 |
| D167 | D(10,37,38,39) | 0.8208 | -DE/DX = 0.0 |
| D168 | D(10,37,38,47) | 0.514 | -DE/DX = 0.0 |
| D169 | D(37,38,39,40) | 179.6123 | -DE/DX = 0.0 |
| D170 | D(37,38,39,41) | -179.3869 | -DE/DX = 0.0 |
| D171 | D(47,38,39,40) | 178.8805 | -DE/DX = 0.0 |
| D172 | D(47,38,39,41) | -0.2885 | -DE/DX = 0.0 |
| D173 | D(37,38,47,45) | 179.3135 | -DE/DX = 0.0 |
| D174 | D(37,38,47,48) | -0.1067 | -DE/DX = 0.0 |
| D175 | D(39,38,47,45) | 0.0076 | -DE/DX = 0.0 |
| D176 | D(39,38,47,48) | -179.4126 | -DE/DX = 0.0 |
| D177 | D(38,39,41,42) | 178.4354 | -DE/DX = 0.0 |
| D178 | D(38,39,41,43) | 0.2891 | -DE/DX = 0.0 |
| D179 | D(40,39,41,42) | 0.2194 | -DE/DX = 0.0 |
| D180 | D(40,39,41,43) | -179.611 | -DE/DX = 0.0 |
| D181 | D(39,41,43,44) | 179.8236 | -DE/DX = 0.0 |
| D182 | D(39,41,43,45) | -0.0085 | -DE/DX = 0.0 |
| D183 | D(42,41,43,44) | -0.0073 | -DE/DX = 0.0 |
| D184 | D(42,41,43,45) | -179.394 | -DE/DX = 0.0 |
| D185 | D(41,43,45,46) | 179.6484 | -DE/DX = 0.0 |
| D186 | D(41,43,45,47) | -0.2731 | -DE/DX = 0.0 |
| D187 | D(44,43,45,46) | -0.1832 | -DE/DX = 0.0 |
| D188 | D(44,43,45,47) | 179.8953 | -DE/DX = 0.0 |
| D189 | D(43,45,47,38) | 0.2734 | -DE/DX = 0.0 |
| D190 | D(43,45,47,48) | 179.5201 | -DE/DX = 0.0 |
| D191 | D(46,45,47,38) | -179.6488 | -DE/DX = 0.0 |
| D192 | D(46,45,47,48) | 0.4021 | -DE/DX = 0.0 |
| D193 | D(38,47,48,10) | 0.6418 | -DE/DX = 0.0 |
| D194 | D(38,47,48,11) | 177.482 | -DE/DX = 0.0 |
| D195 | D(45,47,48,10) | 179.9683 | -DE/DX = 0.0 |
| D196 | D(45,47,48,11) | -1.8445 | -DE/DX = 0.0 |
| D197 | D(11,49,50,51) | -0.0255 | -DE/DX = 0.0 |
| D198 | D(11,49,50,59) | 0.5164 | -DE/DX = 0.0 |
| D199 | D(12,49,50,51) | 178.4354 | -DE/DX = 0.0 |
| D200 | D(12,49,50,59) | 0.22 | -DE/DX = 0.0 |
| D201 | D(49,50,51,52) | 1.7632 | -DE/DX = 0.0 |
| D202 | D(49,50,51,53) | -177.9516 | -DE/DX = 0.0 |
| D203 | D(50,59,51,52) | 179.7624 | -DE/DX = 0.0 |
| D204 | D(50,59,51,53) | 0.4777 | -DE/DX = 0.0 |
| D205 | D(49,50,59,57) | 177.3686 | -DE/DX = 0.0 |
| D206 | D(49,50,59,60) | -0.1645 | -DE/DX = 0.0 |
| D207 | D(51,50,59,57) | -178.6051 | -DE/DX = 0.0 |
| D208 | D(51,50,59,60) | 178.7773 | -DE/DX = 0.0 |
| D209 | D(50,51,53,54) | 0.5164 | -DE/DX = 0.0 |
| D210 | D(50,51,53,55) | 0.5113 | -DE/DX = 0.0 |
| D211 | D(52,51,53,54) | 0.5113 | -DE/DX = 0.0 |
| D212 | D(52,51,53,55) | -179.1949 | -DE/DX = 0.0 |
| D213 | D(51,53,55,56) | 179.6923 | -DE/DX = 0.0 |
| D214 | D(51,53,55,57) | -0.2903 | -DE/DX = 0.0 |
| D215 | D(54,53,55,56) | -0.0151 | -DE/DX = 0.0 |
| D216 | D(54,53,55,57) | -179.9977 | -DE/DX = 0.0 |
| D217 | D(53,55,57,58) | 179.39 | -DE/DX = 0.0 |
| D218 | D(53,55,57,59) | -0.5930 | -DE/DX = 0.0 |
| D219 | D(56,55,57,58) | -0.5926 | -DE/DX = 0.0 |
| D220 | D(56,55,57,59) | 179.5082 | -DE/DX = 0.0 |
| D221 | D(55,57,59,50) | 1.0638 | -DE/DX = 0.0 |
| D222 | D(55,57,59,60) | 178.0857 | -DE/DX = 0.0 |
| D223 | D(58,57,59,50) | -178.8342 | -DE/DX = 0.0 |
| D224 | D(58,57,59,60) | -1.8123 | -DE/DX = 0.0 |
|   |   |   |   |   |
|---|---|---|---|---|
| D225 | D(50,59,60,5) | 178.4051 | -DE/DX = 0.0 |
| D226 | D(50,59,60,12) | 0.0569 | -DE/DX = 0.0 |
| D227 | D(57,59,60,5) | 1.0832 | -DE/DX = 0.0 |
| D228 | D(57,59,60,12) | -177.265 | -DE/DX = 0.0 |
| D229 | D(66,61,62,63) | 125.5868 | -DE/DX = 0.0 |
| D230 | D(66,61,62,64) | -44.3515 | -DE/DX = 0.0 |
| D231 | D(68,61,62,63) | 35.0803 | -DE/DX = 0.0 |
| D232 | D(68,61,62,64) | -134.858 | -DE/DX = 0.0 |
| D233 | D(70,61,62,63) | -53.9889 | -DE/DX = 0.0 |
| D234 | D(70,61,62,64) | 136.0728 | -DE/DX = 0.0 |
| D235 | D(72,61,62,63) | -144.6883 | -DE/DX = 0.0 |
| D236 | D(72,61,62,64) | 45.3734 | -DE/DX = 0.0 |
| D237 | D(62,61,66,73) | 85.7572 | -DE/DX = 0.0 |
| D238 | D(62,61,66,84) | -86.4052 | -DE/DX = 0.0 |
| D239 | D(68,61,66,73) | -174.9446 | -DE/DX = 0.0 |
| D240 | D(68,61,66,84) | 12.8931 | -DE/DX = 0.0 |
| D241 | D(70,61,66,73) | -95.3935 | -DE/DX = 0.0 |
| D242 | D(70,61,66,84) | 92.4442 | -DE/DX = 0.0 |
| D243 | D(72,61,66,73) | 15.692 | -DE/DX = 0.0 |
| D244 | D(72,61,66,84) | 172.1457 | -DE/DX = 0.0 |
| D245 | D(62,61,68,85) | 88.0348 | -DE/DX = 0.0 |
| D246 | D(62,61,68,96) | -84.7272 | -DE/DX = 0.0 |
| D247 | D(66,61,68,85) | -13.4071 | -DE/DX = 0.0 |
| D248 | D(66,61,68,96) | 173.8309 | -DE/DX = 0.0 |
| D249 | D(70,61,68,85) | -172.4467 | -DE/DX = 0.0 |
| D250 | D(70,61,68,96) | 14.7913 | -DE/DX = 0.0 |
| D251 | D(72,61,68,85) | -92.594 | -DE/DX = 0.0 |
| D252 | D(72,61,68,96) | 94.644 | -DE/DX = 0.0 |
| D253 | D(62,61,70,97) | 83.9182 | -DE/DX = 0.0 |
| D254 | D(62,61,70,108) | -87.8045 | -DE/DX = 0.0 |
| D255 | D(66,61,70,97) | -94.9377 | -DE/DX = 0.0 |
| D256 | D(66,61,70,108) | 93.3397 | -DE/DX = 0.0 |
| D257 | D(68,61,70,97) | -15.1793 | -DE/DX = 0.0 |
| D258 | D(68,61,70,108) | 173.0981 | -DE/DX = 0.0 |
| D259 | D(70,61,70,97) | -174.4018 | -DE/DX = 0.0 |
| D260 | D(70,61,70,108) | 13.8756 | -DE/DX = 0.0 |
| D261 | D(62,61,72,109) | 87.2772 | -DE/DX = 0.0 |
| D262 | D(62,61,72,120) | -86.3955 | -DE/DX = 0.0 |
| D263 | D(66,61,72,109) | -171.4985 | -DE/DX = 0.0 |
| D264 | D(66,61,72,120) | 14.8287 | -DE/DX = 0.0 |
| D265 | D(68,61,72,109) | -92.0891 | -DE/DX = 0.0 |
| D266 | D(68,61,72,120) | 94.2381 | -DE/DX = 0.0 |
| D267 | D(70,61,72,109) | -12.4543 | -DE/DX = 0.0 |
| D268 | D(70,61,72,120) | 173.8729 | -DE/DX = 0.0 |
| D269 | D(4,65,73,66) | -148.6172 | -DE/DX = 0.0 |
| D270 | D(4,65,73,74) | 33.7 | -DE/DX = 0.0 |
| D271 | D(4,65,73,66) | 5.6768 | -DE/DX = 0.0 |
| D272 | D(4,65,73,74) | -172.006 | -DE/DX = 0.0 |
| D273 | D(4,65,120,72) | 147.5561 | -DE/DX = 0.0 |
| D274 | D(4,65,120,119) | -34.3818 | -DE/DX = 0.0 |
| D275 | D(73,65,120,72) | -6.7104 | -DE/DX = 0.0 |
| D276 | D(73,65,120,119) | 171.3517 | -DE/DX = 0.0 |
| D277 | D(61,66,73,65) | 9.19 | -DE/DX = 0.0 |
| D278 | D(61,66,73,74) | -172.8229 | -DE/DX = 0.0 |
| D279 | D(84,66,73,65) | 0.3349 | -DE/DX = 0.0 |
| D280 | D(84,66,73,74) | -177.6521 | -DE/DX = 0.0 |
| D281 | D(84,66,84,67) | -8.2945 | -DE/DX = 0.0 |
| D282 | D(61,66,84,67) | 173.1082 | -DE/DX = 0.0 |
| D283 | D(73,66,84,67) | 178.4174 | -DE/DX = 0.0 |
| D284 | D(73,66,84,83) | -0.1799 | -DE/DX = 0.0 |
| D285 | D(85,67,84,66) | -1.8381 | -DE/DX = 0.0 |
| D286 | D(85,67,84,83) | 176.5629 | -DE/DX = 0.0 |
| D287 | D(84,67,85,68) | 1.3268  | -DE/DX = 0.0 |
| D288 | D(84,67,85,86) | -176.6061 | -DE/DX = 0.0 |
| D289 | D(61,68,85,67) | 9.2783  | -DE/DX = 0.0 |
| D290 | D(61,68,85,86) | -172.528 | -DE/DX = 0.0 |
| D291 | D(96,68,85,67) | -176.958 | -DE/DX = 0.0 |
| D292 | D(96,68,85,86) | 1.2357  | -DE/DX = 0.0 |
| D293 | D(61,68,96,69) | -9.4375 | -DE/DX = 0.0 |
| D294 | D(61,68,96,95) | 172.4066 | -DE/DX = 0.0 |
| D295 | D(85,68,96,69) | 176.8435 | -DE/DX = 0.0 |
| D296 | D(85,68,96,95) | -1.3124 | -DE/DX = 0.0 |
| D297 | D(96,69,96,68) | -2.4781 | -DE/DX = 0.0 |
| D298 | D(96,69,96,95) | 175.4101 | -DE/DX = 0.0 |
| D299 | D(96,69,97,70) | 2.0102  | -DE/DX = 0.0 |
| D300 | D(96,69,97,98) | -175.8443 | -DE/DX = 0.0 |
| D301 | D(61,70,97,69) | 10.3065 | -DE/DX = 0.0 |
| D302 | D(61,70,97,98) | -171.567 | -DE/DX = 0.0 |
| D303 | D(108,70,97,69) | -176.8829 | -DE/DX = 0.0 |
| D304 | D(108,70,97,98) | 1.2431 | -DE/DX = 0.0 |
| D305 | D(108,70,107,71) | -10.2449 | -DE/DX = 0.0 |
| D306 | D(108,70,107,97) | 171.693 | -DE/DX = 0.0 |
| D307 | D(97,70,107,71) | 176.8866 | -DE/DX = 0.0 |
| D308 | D(97,70,107,97) | -1.1755 | -DE/DX = 0.0 |
| D309 | D(109,71,108,70) | -0.8925 | -DE/DX = 0.0 |
| D310 | D(109,71,108,107) | 176.8894 | -DE/DX = 0.0 |
| D311 | D(109,71,108,72) | 2.5398 | -DE/DX = 0.0 |
| D312 | D(109,71,108,107) | -175.626 | -DE/DX = 0.0 |
| D313 | D(109,71,108,97) | 7.2116 | -DE/DX = 0.0 |
| D314 | D(109,71,108,98) | -174.3974 | -DE/DX = 0.0 |
| D315 | D(109,71,108,107) | -178.2025 | -DE/DX = 0.0 |
| D316 | D(109,71,108,110) | 0.1885 | -DE/DX = 0.0 |
| D317 | D(109,71,108,72) | -176.8894 | -DE/DX = 0.0 |
| D318 | D(109,71,108,107) | 176.8894 | -DE/DX = 0.0 |
| D319 | D(109,71,108,72) | -175.626 | -DE/DX = 0.0 |
| D320 | D(109,71,108,107) | 2.5398 | -DE/DX = 0.0 |
| D321 | D(61,72,73,65) | -0.0997 | -DE/DX = 0.0 |
| D322 | D(61,72,73,74) | 177.6608 | -DE/DX = 0.0 |
| D323 | D(61,72,73,75) | -178.1201 | -DE/DX = 0.0 |
| D324 | D(61,72,73,76) | -0.3597 | -DE/DX = 0.0 |
| D325 | D(61,72,73,77) | -2.5424 | -DE/DX = 0.0 |
| D326 | D(61,72,73,78) | 178.0921 | -DE/DX = 0.0 |
| D327 | D(61,72,73,79) | 179.9502 | -DE/DX = 0.0 |
| D328 | D(61,72,73,80) | 0.5847 | -DE/DX = 0.0 |
| D329 | D(61,72,73,81) | -178.3594 | -DE/DX = 0.0 |
| D330 | D(61,72,73,82) | 0.2419 | -DE/DX = 0.0 |
| D331 | D(61,72,73,83) | -0.383 | -DE/DX = 0.0 |
| D332 | D(61,72,73,84) | 178.3594 | -DE/DX = 0.0 |
| D333 | D(61,72,73,85) | 179.4453 | -DE/DX = 0.0 |
| D334 | D(61,72,73,86) | -0.3675 | -DE/DX = 0.0 |
| D335 | D(61,72,73,87) | 0.0737 | -DE/DX = 0.0 |
| D336 | D(61,72,73,88) | -179.7391 | -DE/DX = 0.0 |
| D337 | D(61,72,73,89) | -179.9886 | -DE/DX = 0.0 |
| D338 | D(61,72,73,90) | -0.067 | -DE/DX = 0.0 |
| D339 | D(61,72,73,91) | 0.1985 | -DE/DX = 0.0 |
| D340 | D(61,72,73,92) | -179.88 | -DE/DX = 0.0 |
| D341 | D(61,72,73,93) | -179.5087 | -DE/DX = 0.0 |
| D342 | D(61,72,73,94) | 0.278 | -DE/DX = 0.0 |
| D343 | D(61,72,73,95) | 0.4125 | -DE/DX = 0.0 |
| D344 | D(61,72,73,96) | -179.8008 | -DE/DX = 0.0 |
| Index | Index | Index | Index | Index | Value | Value | Value | Value | Value | Value |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| D345  | D(79,81,83,74) | -0.0562 | -DE/DX = 0.0 | ! |
| D346  | D(79,81,83,84) | -178.4429 | -DE/DX = 0.0 | ! |
| D347  | D(82,81,83,74) | 179.733 | -DE/DX = 0.0 | ! |
| D348  | D(82,81,83,84) | -0.0499 | -DE/DX = 0.0 | ! |
| D349  | D(74,83,84,66) | -178.7091 | -DE/DX = 0.0 | ! |
| D350  | D(74,83,84,67) | 178.5109 | -DE/DX = 0.0 | ! |
| D351  | D(81,83,84,66) | -0.1482 | -DE/DX = 0.0 | ! |
| D352  | D(81,83,84,67) | 0.0165 | -DE/DX = 0.0 | ! |
| D353  | D(85,86,87) | -1.72 | -DE/DX = 0.0 | ! |
| D354  | D(85,86,87) | -177.5858 | -DE/DX = 0.0 | ! |
| D355  | D(86,87,88) | -0.6678 | -DE/DX = 0.0 | ! |
| D356  | D(86,87,88) | 177.5858 | -DE/DX = 0.0 | ! |
| D357  | D(87,86,88) | 179.986 | -DE/DX = 0.0 | ! |
| D358  | D(87,86,88) | -0.1989 | -DE/DX = 0.0 | ! |
| D359  | D(91,92,93) | -0.308 | -DE/DX = 0.0 | ! |
| D360  | D(91,92,93) | 179.3528 | -DE/DX = 0.0 | ! |
| D361  | D(93,94,95) | 0.0165 | -DE/DX = 0.0 | ! |
| D362  | D(93,94,95) | 179.2809 | -DE/DX = 0.0 | ! |
| D363  | D(94,95,96) | -0.1213 | -DE/DX = 0.0 | ! |
| D364  | D(94,95,96) | 179.8951 | -DE/DX = 0.0 | ! |
| D365  | D(96,97,98) | -0.2797 | -DE/DX = 0.0 | ! |
| D366  | D(96,97,98) | 179.8951 | -DE/DX = 0.0 | ! |
| D367  | D(97,98,99) | -0.0001 | -DE/DX = 0.0 | ! |
| D368  | D(97,98,99) | 179.8951 | -DE/DX = 0.0 | ! |
| D369  | D(98,99,100) | 179.8951 | -DE/DX = 0.0 | ! |
| D370  | D(98,99,100) | -1.8252 | -DE/DX = 0.0 | ! |
| D371  | D(99,100,101) | 179.986 | -DE/DX = 0.0 | ! |
| D372  | D(99,100,101) | -177.3465 | -DE/DX = 0.0 | ! |
| D373  | D(100,101,102) | 179.986 | -DE/DX = 0.0 | ! |
| D374  | D(100,101,102) | -179.983 | -DE/DX = 0.0 | ! |
| D375  | D(101,102,103) | 1.7993 | -DE/DX = 0.0 | ! |
| D376  | D(101,102,103) | -179.8812 | -DE/DX = 0.0 | ! |
| D377  | D(102,103,104) | -0.0074 | -DE/DX = 0.0 | ! |
| D378  | D(102,103,104) | 179.8395 | -DE/DX = 0.0 | ! |
| Center  | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------|----------------|-------------|------------------------|
| 1       | 30             | Zn          | 3.178962               |
| 2       | 8              | O           | 2.529332               |
| 3       | 1              | H           | 3.165201               |
| 4       | 1              | H           | 1.550903               |
| 5       | 7              | N           | 0.093468               |
| 6       | 7              | N           | 1.945175               |
| 7       | 7              | N           | 3.335758               |
| 8       | 7              | N           | 4.649755               |

Standard orientation (optimized): for (ZnPcH$_2$O)$_2$ dimer
|   |   |   |    |    |    |
|---|---|---|----|----|----|
| 69 | 7  | N  | -6.543596 | -0.015983 | -0.186073 |
| 70 | 7  | N  | -4.661081 | 1.409904  | 0.400395  |
| 71 | 7  | N  | -3.360058 | 3.380457  | 0.976273  |
| 72 | 7  | N  | -1.954595 | 1.419923  | 1.338357  |
| 73 | 6  | C  | -0.678276 | -1.190116 | 1.839040  |
| 74 | 6  | C  | -0.066810 | 2.480171  | 2.188996  |
| 75 | 6  | C  | 1.164013  | 2.842460  | 2.747304  |
| 76 | 1  | H  | 1.916863  | 2.099824  | 2.980929  |
| 77 | 6  | C  | 1.409400  | 4.200401  | 2.987549  |
| 78 | 1  | H  | 2.361459  | -4.503876 | 0.571353  |
| 79 | 6  | C  | 0.442869  | -5.181194 | 2.684455  |
| 80 | 1  | H  | 0.663224  | -6.225565 | 2.882611  |
| 81 | 6  | C  | -0.794114 | -4.824074 | 2.134237  |
| 82 | 1  | H  | -1.548856 | -5.568063 | 1.903973  |
| 83 | 6  | C  | -1.037414 | -3.470760 | 1.890345  |
| 84 | 6  | C  | -2.207995 | -2.771855 | 1.363720  |
| 85 | 6  | C  | -4.451347 | -2.781925 | 0.571353  |
| 86 | 6  | C  | -5.693691 | -3.485662 | 0.244267  |
| 87 | 6  | C  | -6.038205 | -4.839757 | 0.244123  |
| 88 | 1  | H  | -5.310585 | -5.595387 | 0.520019  |
| 89 | 6  | C  | -7.346801 | -5.183939 | -0.120133 |
| 90 | 1  | H  | -7.643808 | -6.228203 | -0.131394 |
| 91 | 6  | C  | -8.289601 | -4.193710 | -0.470228 |
| 92 | 1  | H  | -9.296647 | -4.492184 | -0.745157 |
| 93 | 6  | C  | -9.471900 | -2.834867 | -0.464461 |
| 94 | 1  | H  | -8.669126 | -2.068824 | -0.726115 |
| 95 | 6  | C  | -6.640897 | -2.490856 | -0.107500 |
| 96 | 6  | C  | -5.956858 | -1.201005 | 0.015376  |
| 97 | 6  | C  | -5.963637 | 1.174490  | 0.004460  |
| 98 | 6  | C  | -6.653129 | 2.459343  | -0.139251 |
| 99 | 6  | C  | -7.958362 | 2.792649  | -0.509661 |
| 100| 1  | H  | -8.674973 | 2.020014  | -0.766549 |
| 101| 6  | C  | -8.306924 | 4.149751  | -0.535327 |
| 102| 1  | H  | -9.313359 | 4.440002  | -0.821082 |
| 103| 6  | C  | -7.371017 | 1.486955  | -0.191840 |
| 104| 1  | H  | -7.672579 | 6.191372  | -0.218766 |
| 105| 6  | C  | -6.063322 | 4.815234  | 0.185646  |
| 106| 1  | H  | -5.340952 | 5.577808  | 0.456206  |
| 107| 6  | C  | -5.712795 | 3.462918  | 0.205845  |
| 108| 6  | C  | -4.469627 | 2.768746  | 0.549993  |
| 109| 6  | C  | -2.230704 | 2.777499  | 1.353679  |
| 110| 6  | C  | -1.074386 | 3.489418  | 1.899617  |
| 111| 6  | C  | -0.847611 | 4.839347  | 2.153365  |
| 112| 1  | H  | -1.603918 | 5.577616  | 1.910456  |
| 113| 6  | C  | 0.373753  | 5.205099  | 2.731914  |
| 114| 1  | H  | 0.581043  | 6.250552  | 2.938078  |
| 115| 6  | C  | 1.339841  | 4.230909  | 3.057416  |
| 116| 1  | H  | 2.276978  | 4.540164  | 3.509721  |
| 117| 6  | C  | 1.110064  | 2.872286  | 2.807229  |
| 118| 1  | H  | 1.857608  | 2.134347  | 3.071734  |
| 119| 6  | C  | -0.101585 | 2.501347  | 2.213922  |
| 120| 6  | C  | -0.692980 | 1.207825  | 1.844749  |
Table S5. DFT optimised geometrical parameters (Å,°) for (BePcH₂O)₂ dimer.

View of the optimized (BePcH₂O)₂ dimer

| Item               | Value     | Threshold  | Converged? |
|--------------------|-----------|------------|------------|
| Maximum Force      | 0.000024  | 0.000450   | YES        |
| RMS Force          | 0.000002  | 0.000300   | YES        |
| Maximum Displacement| 0.001354 | 0.001800   | YES        |
| RMS Displacement   | 0.000206  | 0.001200   | YES        |

Predicted change in Energy = -3.440721D-08
Optimization completed. (for (BePcH₂O)₂ dimer)

! Optimized Parameters !
! (Angstroms and Degrees) !

| ! Name   | Definition | Value       | Derivative Info. |
|----------|------------|-------------|------------------|
| ! R1     | R(1,2)     | 1.9126      | -DE/DX = 0.0     |
| ! R2     | R(1,4)     | 1.9492      | -DE/DX = 0.0     |
| ! R3     | R(1,6)     | 1.9731      | -DE/DX = 0.0     |
| ! R4     | R(1,8)     | 1.9515      | -DE/DX = 0.0     |
| ! R5     | R(1,58)    | 1.7242      | -DE/DX = 0.0     |
| ! R6     | R(2,10)    | 1.3839      | -DE/DX = 0.0     |
| ! R7     | R(2,21)    | 1.3955      | -DE/DX = 0.0     |
| ! R8     | R(3,21)    | 1.3244      | -DE/DX = 0.0     |
| ! R9     | R(3,22)    | 1.3275      | -DE/DX = 0.0     |
| ! R10    | R(4,22)    | 1.3872      | -DE/DX = 0.0     |
| ! R11    | R(4,33)    | 1.3896      | -DE/DX = 0.0     |
| ! R12    | R(5,33)    | 1.3287      | -DE/DX = 0.0     |
| ! R13    | R(5,34)    | 1.3282      | -DE/DX = 0.0     |
| ! R14    | R(6,34)    | 1.3913      | -DE/DX = 0.0     |
| ! R15    | R(6,45)    | 1.3891      | -DE/DX = 0.0     |
| ! R16    | R(7,45)    | 1.3277      | -DE/DX = 0.0     |
| ! R17    | R(7,46)    | 1.3251      | -DE/DX = 0.0     |
| ! R18    | R(8,46)    | 1.3933      | -DE/DX = 0.0     |
| ! R19    | R(8,57)    | 1.3823      | -DE/DX = 0.0     |
| ! R20    | R(9,10)    | 1.3387      | -DE/DX = 0.0     |
| ! R21    | R(9,57)    | 1.338       | -DE/DX = 0.0     |
| ! R22    | R(9,119)   | 1.6153      | -DE/DX = 0.0     |
| ! R23    | R(10,11)   | 1.4604      | -DE/DX = 0.0     |
| ! R24    | R(11,12)   | 1.4005      | -DE/DX = 0.0     |
| ! R25    | R(11,20)   | 1.4093      | -DE/DX = 0.0     |
| ! R26    | R(12,13)   | 1.0838      | -DE/DX = 0.0     |
| ! R27    | R(12,14)   | 1.3991      | -DE/DX = 0.0     |
| ! R28    | R(14,15)   | 1.0855      | -DE/DX = 0.0     |
| ! R29    | R(14,16)   | 1.4122      | -DE/DX = 0.0     |
| ! R30    | R(16,17)   | 1.0855      | -DE/DX = 0.0     |

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R91 R(68,106)  1.3933  -DE/DX =  0.0
R92 R(68,117)  1.3823  -DE/DX =  0.0
R93 R(69,70)  1.3387  -DE/DX =  0.0
R94 R(69,117)  1.3380  -DE/DX =  0.0
R95 R(70,71)  1.4604  -DE/DX =  0.0
R96 R(71,72)  1.4005  -DE/DX =  0.0
R97 R(71,80)  1.3993  -DE/DX =  0.0
R98 R(72,73)  1.0838  -DE/DX =  0.0
R99 R(72,74)  1.3991  -DE/DX =  0.0
R100 R(74,75)  1.0855  -DE/DX =  0.0
R101 R(74,76)  1.4122  -DE/DX =  0.0
R102 R(76,77)  1.0855  -DE/DX =  0.0
R103 R(76,78)  1.3988  -DE/DX =  0.0
R104 R(78,79)  1.0843  -DE/DX =  0.0
R105 R(78,80)  1.3979  -DE/DX =  0.0
R106 R(80,81)  1.454  -DE/DX =  0.0
R107 R(82,83)  1.4577  -DE/DX =  0.0
R108 R(83,84)  1.3982  -DE/DX =  0.0
R109 R(83,92)  1.4066  -DE/DX =  0.0
R110 R(84,85)  1.0845  -DE/DX =  0.0
R111 R(84,86)  1.4004  -DE/DX =  0.0
R112 R(86,87)  1.0858  -DE/DX =  0.0
R113 R(86,88)  1.413  -DE/DX =  0.0
R114 R(88,89)  1.0857  -DE/DX =  0.0
R115 R(88,90)  1.4005  -DE/DX =  0.0
R116 R(90,91)  1.0845  -DE/DX =  0.0
R117 R(90,92)  1.3981  -DE/DX =  0.0
R118 R(92,93)  1.4586  -DE/DX =  0.0
R119 R(94,95)  1.4581  -DE/DX =  0.0
R120 R(95,96)  1.3983  -DE/DX =  0.0
R121 R(95,104)  1.4089  -DE/DX =  0.0
R122 R(96,97)  1.0845  -DE/DX =  0.0
R123 R(96,98)  1.4003  -DE/DX =  0.0
R124 R(98,99)  1.0857  -DE/DX =  0.0
R125 R(98,100)  1.4132  -DE/DX =  0.0
R126 R(100,101)  1.0857  -DE/DX =  0.0
R127 R(100,102)  1.4002  -DE/DX =  0.0
R128 R(102,103)  1.0845  -DE/DX =  0.0
R129 R(102,104)  1.3984  -DE/DX =  0.0
R130 R(104,105)  1.4579  -DE/DX =  0.0
R131 R(106,107)  1.4557  -DE/DX =  0.0
R132 R(107,108)  1.3973  -DE/DX =  0.0
R133 R(107,116)  1.4095  -DE/DX =  0.0
R134 R(108,109)  1.0844  -DE/DX =  0.0
R135 R(108,110)  1.3995  -DE/DX =  0.0
R136 R(110,111)  1.0856  -DE/DX =  0.0
R137 R(110,112)  1.4116  -DE/DX =  0.0
R138 R(112,113)  1.0855  -DE/DX =  0.0
R139 R(112,114)  1.3999  -DE/DX =  0.0
R140 R(114,115)  1.0833  -DE/DX =  0.0
R141 R(114,116)  1.4001  -DE/DX =  0.0
R142 R(116,117)  1.4618  -DE/DX =  0.0
R143 R(118,119)  1.0356  -DE/DX =  0.0
R144 R(118,120)  0.9701  -DE/DX =  0.0
A1 A(2,1,4)  89.8052  -DE/DX =  0.0
A2 A(2,1,6)  161.6319  -DE/DX =  0.0
A3 A(2,1,8)  88.5599  -DE/DX =  0.0
A4 A(2,1,58)  101.5172  -DE/DX =  0.0
A5 A(4,1,6)  87.3091  -DE/DX =  0.0
A6 A(4,1,8)  161.0725  -DE/DX =  0.0
| A   | A(4,1,58) | 98.6256 | -DE/DX = 0.0   |
| A8  | A(6,1,8)  | 88.3263 | -DE/DX = 0.0   |
| A9  | A(6,1,58) | 96.8504 | -DE/DX = 0.0   |
| A10 | A(10,2,21)| 122.5069| -DE/DX = 0.0   |
| A11 | A(1,2,10) | 127.3138| -DE/DX = 0.0   |
| A12 | A(1,2,21) | 126.4195| -DE/DX = 0.0   |
| A13 | A(8,1,58) | 100.1779| -DE/DX = 0.0   |
| A14 | A(1,4,22) | 125.9223| -DE/DX = 0.0   |
| A15 | A(1,4,33) | 127.3019| -DE/DX = 0.0   |
| A16 | A(22,4,33)| 106.0209| -DE/DX = 0.0   |
| A17 | A(33,5,34)| 122.0807| -DE/DX = 0.0   |
| A18 | A(10,9,119)| 115.5003| -DE/DX = 0.0   |
| A19 | A(34,6,45)| 115.9239| -DE/DX = 0.0   |
| A20 | A(45,7,46)| 122.6729| -DE/DX = 0.0   |
| A21 | A(1,8,46) | 126.9994| -DE/DX = 0.0   |
| A22 | A(46,8,57)| 126.3693| -DE/DX = 0.0   |
| A23 | A(10,9,57)| 110.6318| -DE/DX = 0.0   |
| A24 | A(11,10,11)| 122.8025| -DE/DX = 0.0   |
| A25 | A(11,10,20)| 120.5054| -DE/DX = 0.0   |
| A26 | A(12,11,13)| 121.5765| -DE/DX = 0.0   |
| A27 | A(12,11,14)| 118.1172| -DE/DX = 0.0   |
| A28 | A(13,12,14)| 120.297 | -DE/DX = 0.0   |
| A29 | A(14,13,15)| 119.5662| -DE/DX = 0.0   |
| A30 | A(14,13,16)| 121.0836| -DE/DX = 0.0   |
| A31 | A(15,14,16)| 119.3497| -DE/DX = 0.0   |
| A32 | A(16,14,17)| 119.3011| -DE/DX = 0.0   |
| A33 | A(16,14,18)| 120.898 | -DE/DX = 0.0   |
| A34 | A(17,15,16)| 119.7986| -DE/DX = 0.0   |
| A35 | A(18,15,16)| 121.6763| -DE/DX = 0.0   |
| A36 | A(19,15,16)| 117.7743| -DE/DX = 0.0   |
| A37 | A(20,15,16)| 120.5476| -DE/DX = 0.0   |
| A38 | A(21,15,16)| 121.5985| -DE/DX = 0.0   |
| A39 | A(22,15,16)| 120.4645| -DE/DX = 0.0   |
| A40 | A(23,15,16)| 131.9127| -DE/DX = 0.0   |
| A41 | A(24,15,16)| 127.3653| -DE/DX = 0.0   |
| A42 | A(25,15,16)| 110.6318| -DE/DX = 0.0   |
| A43 | A(26,15,16)| 122.0029| -DE/DX = 0.0   |
| A44 | A(27,15,16)| 122.4013| -DE/DX = 0.0   |
| A45 | A(28,15,16)| 105.8204| -DE/DX = 0.0   |
| A46 | A(29,15,16)| 121.2703| -DE/DX = 0.0   |
| A47 | A(30,15,16)| 121.5579| -DE/DX = 0.0   |
| A48 | A(31,15,16)| 119.6521| -DE/DX = 0.0   |
| A49 | A(32,15,16)| 121.0924| -DE/DX = 0.0   |
| A50 | A(33,15,16)| 119.2553| -DE/DX = 0.0   |
| A51 | A(34,15,16)| 120.5476| -DE/DX = 0.0   |
| A52 | A(35,15,16)| 119.7986| -DE/DX = 0.0   |
| A53 | A(36,15,16)| 121.6763| -DE/DX = 0.0   |
| A54 | A(37,15,16)| 117.7743| -DE/DX = 0.0   |
| A55 | A(38,15,16)| 120.5476| -DE/DX = 0.0   |
| A56 | A(39,15,16)| 121.0924| -DE/DX = 0.0   |
| A57 | A(40,15,16)| 119.6521| -DE/DX = 0.0   |
| A58 | A(41,15,16)| 121.0924| -DE/DX = 0.0   |
| A59 | A(42,15,16)| 119.2553| -DE/DX = 0.0   |
| A60 | A(43,15,16)| 120.5476| -DE/DX = 0.0   |
| A61 | A(44,15,16)| 119.7986| -DE/DX = 0.0   |
| A62 | A(45,15,16)| 121.6763| -DE/DX = 0.0   |
| A63 | A(46,15,16)| 117.7743| -DE/DX = 0.0   |
| A64 | A(47,15,16)| 120.5476| -DE/DX = 0.0   |
| A65 | A(48,15,16)| 119.6521| -DE/DX = 0.0   |
| A66 | A(49,15,16)| 121.0924| -DE/DX = 0.0   |
|   |   |   |   |   |
|---|---|---|---|---|
| A67 | A(29,28,30) | 119.6376 | -DE/DX = 0.0 | ! |
| A68 | A(28,30,32) | 117.6388 | -DE/DX = 0.0 | ! |
| A69 | A(31,30,32) | 120.8213 | -DE/DX = 0.0 | ! |
| A70 | A(32,30,33) | 121.2556 | -DE/DX = 0.0 | ! |
| A71 | A(23,32,30) | 121.2556 | -DE/DX = 0.0 | ! |
| A72 | A(23,32,33) | 106.1345 | -DE/DX = 0.0 | ! |
| A73 | A(30,32,33) | 120.9654 | -DE/DX = 0.0 | ! |
| A74 | A(33,35) | 126.9721 | -DE/DX = 0.0 | ! |
| A75 | A(33,34,35) | 122.4143 | -DE/DX = 0.0 | ! |
| A76 | A(34,35,36) | 110.8011 | -DE/DX = 0.0 | ! |
| A77 | A(34,35,36) | 132.5992 | -DE/DX = 0.0 | ! |
| A78 | A(35,36,37) | 120.8121 | -DE/DX = 0.0 | ! |
| A79 | A(35,36,38) | 121.2581 | -DE/DX = 0.0 | ! |
| A80 | A(35,36,39) | 117.6395 | -DE/DX = 0.0 | ! |
| A81 | A(36,38,40) | 119.6391 | -DE/DX = 0.0 | ! |
| A82 | A(36,38,40) | 121.0971 | -DE/DX = 0.0 | ! |
| A83 | A(36,38,40) | 119.251 | -DE/DX = 0.0 | ! |
| A84 | A(38,40,42) | 119.2493 | -DE/DX = 0.0 | ! |
| A85 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A86 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A87 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A88 | A(38,40,42) | 119.251 | -DE/DX = 0.0 | ! |
| A89 | A(38,40,42) | 119.2493 | -DE/DX = 0.0 | ! |
| A90 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A91 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A92 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A93 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A94 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A95 | A(38,40,42) | 119.251 | -DE/DX = 0.0 | ! |
| A96 | A(38,40,42) | 119.2493 | -DE/DX = 0.0 | ! |
| A97 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A98 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A99 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A100 | A(38,40,42) | 119.251 | -DE/DX = 0.0 | ! |
| A101 | A(38,40,42) | 119.2493 | -DE/DX = 0.0 | ! |
| A102 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A103 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A104 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A105 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A106 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A107 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A108 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A109 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A110 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A111 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A112 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A113 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A114 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A115 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A116 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A117 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A118 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A119 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A120 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A121 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A122 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A123 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A124 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
| A125 | A(38,40,42) | 119.6391 | -DE/DX = 0.0 | ! |
| A126 | A(38,40,42) | 121.0971 | -DE/DX = 0.0 | ! |
A127 A(59,58,60) 112.9718 -DE/DX = 0.0
A128 A(58,59,69) 173.0325 -DE/DX = 0.0
A129 A(62,61,64) 89.8049 -DE/DX = 0.0
A130 A(62,61,66) 161.6318 -DE/DX = 0.0
A131 A(62,61,68) 88.5595 -DE/DX = 0.0
A132 A(62,61,118) 101.5169 -DE/DX = 0.0
A133 A(64,61,66) 87.3095 -DE/DX = 0.0
A134 A(64,61,68) 161.0720 -DE/DX = 0.0
A135 A(64,61,118) 98.6268 -DE/DX = 0.0
A136 A(66,61,66) 87.3095 -DE/DX = 0.0
A137 A(66,61,68) 161.0720 -DE/DX = 0.0
A138 A(66,61,118) 98.6268 -DE/DX = 0.0
A139 A(61,62,70) 127.3140 -DE/DX = 0.0
A140 A(61,62,81) 126.4199 -DE/DX = 0.0
A141 A(70,62,81) 105.9852 -DE/DX = 0.0
A142 A(81,63,82) 122.5067 -DE/DX = 0.0
A143 A(61,64,82) 125.9231 -DE/DX = 0.0
A144 A(61,64,93) 127.3020 -DE/DX = 0.0
A145 A(82,64,93) 106.0210 -DE/DX = 0.0
A146 A(93,65,94) 122.0806 -DE/DX = 0.0
A147 A(61,66,94) 126.8724 -DE/DX = 0.0
A148 A(61,66,105) 126.8030 -DE/DX = 0.0
A149 A(94,66,105) 106.0030 -DE/DX = 0.0
A150 A(105,67,106) 122.6729 -DE/DX = 0.0
A151 A(61,68,106) 126.9995 -DE/DX = 0.0
A152 A(61,68,117) 126.3697 -DE/DX = 0.0
A153 A(106,68,117) 105.9844 -DE/DX = 0.0
A154 A(59,69,70) 115.4996 -DE/DX = 0.0
A155 A(59,69,117) 115.9246 -DE/DX = 0.0
A156 A(70,69,117) 122.2266 -DE/DX = 0.0
A157 A(62,70,69) 126.2249 -DE/DX = 0.0
A158 A(62,70,71) 111.0810 -DE/DX = 0.0
A159 A(69,70,71) 122.6765 -DE/DX = 0.0
A160 A(70,71,72) 133.5811 -DE/DX = 0.0
A161 A(70,71,80) 105.8203 -DE/DX = 0.0
A162 A(71,71,80) 120.5057 -DE/DX = 0.0
A163 A(71,72,73) 121.5764 -DE/DX = 0.0
A164 A(71,72,74) 118.1170 -DE/DX = 0.0
A165 A(73,72,74) 120.2972 -DE/DX = 0.0
A166 A(72,74,75) 119.5662 -DE/DX = 0.0
A167 A(72,74,76) 121.0837 -DE/DX = 0.0
A168 A(75,74,76) 119.3497 -DE/DX = 0.0
A169 A(74,76,77) 119.3011 -DE/DX = 0.0
A170 A(74,76,78) 120.8981 -DE/DX = 0.0
A171 A(77,76,78) 119.7986 -DE/DX = 0.0
A172 A(76,78,79) 121.6764 -DE/DX = 0.0
A173 A(76,78,80) 117.7743 -DE/DX = 0.0
A174 A(79,78,80) 120.5476 -DE/DX = 0.0
A175 A(71,80,78) 121.5984 -DE/DX = 0.0
A176 A(71,80,81) 106.4645 -DE/DX = 0.0
A177 A(78,80,81) 131.9128 -DE/DX = 0.0
A178 A(62,81,63) 127.3652 -DE/DX = 0.0
A179 A(62,81,80) 110.6317 -DE/DX = 0.0
A180 A(63,81,80) 122.0029 -DE/DX = 0.0
A181 A(63,82,64) 126.6428 -DE/DX = 0.0
A182 A(63,82,83) 122.4013 -DE/DX = 0.0
A183 A(64,82,83) 110.9499 -DE/DX = 0.0
A184 A(82,83,84) 132.6402 -DE/DX = 0.0
A185 A(82,83,92) 106.0888 -DE/DX = 0.0
A186 A(84,83,92) 121.2703 -DE/DX = 0.0
A247 A(107,116,114)  120.694 -DE/DX = 0.0
A248 A(107,116,117)  105.667 -DE/DX = 0.0
A249 A(114,116,117)  133.589 -DE/DX = 0.0
A250 A(68,117,69)   125.771 -DE/DX = 0.0
A251 A(68,117,116)  111.215 -DE/DX = 0.0
A252 A(69,117,116)  122.962 -DE/DX = 0.0
A253 A(61,118,119)  128.311 -DE/DX = 0.0
A254 A(61,118,120)  116.203 -DE/DX = 0.0
A255 A(119,118,120) 112.971 -DE/DX = 0.0
A256 A(9,119,118)   173.033 -DE/DX = 0.0
D1  D(4,1,2,10)   -177.367 -DE/DX = 0.0
D2  D(4,1,2,21)    9.595 -DE/DX = 0.0
D3  D(6,1,2,10)    -96.529 -DE/DX = 0.0
D4  D(6,1,2,21)   90.433 -DE/DX = 0.0
D5  D(8,1,2,10)   -16.226 -DE/DX = 0.0
D6  D(8,1,2,21)  170.736 -DE/DX = 0.0
D7  D(58,1,2,10)   83.869 -DE/DX = 0.0
D8  D(58,1,2,21)  -89.169 -DE/DX = 0.0
D9  D(2,1,4,22)   -12.527 -DE/DX = 0.0
D10 D(2,1,4,33)   178.841 -DE/DX = 0.0
D11 D(6,1,4,22)    14.381 -DE/DX = 0.0
D12 D(6,1,4,33)   -97.514 -DE/DX = 0.0
D13 D(8,1,4,22)   93.854 -DE/DX = 0.0
D14 D(8,1,4,33) -174.381 -DE/DX = 0.0
D15 D(58,1,4,22)  89.093 -DE/DX = 0.0
D16 D(58,1,4,33)  89.093 -DE/DX = 0.0
D17 D(2,1,6,34)  -96.768 -DE/DX = 0.0
D18 D(2,1,6,45)  171.916 -DE/DX = 0.0
D19 D(2,1,6,45)  171.916 -DE/DX = 0.0
D20 D(8,1,6,34) -177.109 -DE/DX = 0.0
D21 D(8,1,6,45)    10.338 -DE/DX = 0.0
D22 D(8,1,6,45)   10.338 -DE/DX = 0.0
D23 D(58,1,6,34)  82.839 -DE/DX = 0.0
D24 D(58,1,6,45)  82.839 -DE/DX = 0.0
D25 D(2,1,8,46) -172.090 -DE/DX = 0.0
D26 D(2,1,8,57)  18.444 -DE/DX = 0.0
D27 D(4,1,8,46)  -86.897 -DE/DX = 0.0
D28 D(4,1,8,57)  103.637 -DE/DX = 0.0
D29 D(6,1,8,46)  -10.195 -DE/DX = 0.0
D30 D(6,1,8,57) -179.661 -DE/DX = 0.0
D31 D(58,1,8,46)  86.465 -DE/DX = 0.0
D32 D(58,1,8,57) -82.999 -DE/DX = 0.0
D33 D(2,1,8,59) -42.173 -DE/DX = 0.0
D34 D(2,1,8,60)  157.239 -DE/DX = 0.0
D35 D(4,1,8,59) -133.743 -DE/DX = 0.0
D36 D(4,1,8,60)  65.669 -DE/DX = 0.0
D37 D(6,1,8,59)  137.953 -DE/DX = 0.0
D38 D(6,1,8,60) -22.634 -DE/DX = 0.0
D39 D(8,1,8,59)  48.430 -DE/DX = 0.0
D40 D(8,1,8,60) -112.158 -DE/DX = 0.0
D41 D(1,2,10,9)  5.989 -DE/DX = 0.0
D42 D(1,2,10,11) -175.559 -DE/DX = 0.0
D43 D(12,2,10,9) -179.834 -DE/DX = 0.0
D44 D(21,2,10,11) -1.383 -DE/DX = 0.0
D45 D(1,2,13) -4.368 -DE/DX = 0.0
D46 D(1,2,21,20) 175.534 -DE/DX = 0.0
D47 D(10,2,21,3) -178.612 -DE/DX = 0.0
D48 D(10,2,21,20) 1.289 -DE/DX = 0.0
D49 D(22,3,21,2) -2.289 -DE/DX = 0.0
D50 D(22,3,21,20) 177.819 -DE/DX = 0.0
| D     | D(1,4,22,3)   | 10.8747 | -DE/DX = 0.0                 |
| D     | D(21,3,22,4) | -1.2219 | -DE/DX = 0.0                 |
| D     | D(1,4,22,23) | 179.551 | -DE/DX = 0.0                 |
| D     | D(22,4,33,5) | 177.4082| -DE/DX = 0.0                 |
| D     | D(22,4,33,32) | -0.885 | -DE/DX = 0.0                 |
| D     | D(33,4,22,3) | -178.5141| -DE/DX = 0.0                 |
| D     | D(33,4,22,23) | 0.6058 | -DE/DX = 0.0                 |
| D     | D(1,4,33,5)  | -12.1517| -DE/DX = 0.0                 |
| D     | D(1,4,33,32) | 169.5551| -DE/DX = 0.0                 |
| D     | D(34,5,33,4) | -1.832 | -DE/DX = 0.0                 |
| D     | D(34,5,33,32) | 176.2813| -DE/DX = 0.0                 |
| D     | D(33,5,34,6) | 3.3874 | -DE/DX = 0.0                 |
| D     | D(33,5,34,35) | -174.8108| -DE/DX = 0.0                 |
| D     | D(1,6,34,5)  | 8.9072 | -DE/DX = 0.0                 |
| D     | D(1,6,34,35) | -172.7199| -DE/DX = 0.0                 |
| D     | D(45,6,34,5) | -177.291| -DE/DX = 0.0                 |
| D     | D(45,6,34,35) | 1.0819 | -DE/DX = 0.0                 |
| D     | D(1,6,45,7)  | -7.4389 | -DE/DX = 0.0                 |
| D     | D(1,6,45,44) | 173.027| -DE/DX = 0.0                 |
| D     | D(34,6,45,7) | 178.7537| -DE/DX = 0.0                 |
| D     | D(34,6,45,44) | -0.7804| -DE/DX = 0.0                 |
| D     | D(46,7,45,6) | 179.3433| -DE/DX = 0.0                 |
| D     | D(46,7,45,44) | 179.6727| -DE/DX = 0.0                 |
| D     | D(46,8,45,7) | 178.3758| -DE/DX = 0.0                 |
| D     | D(46,8,45,44) | 0.4558 | -DE/DX = 0.0                 |
| D     | D(45,7,46,8) | 9.5615 | -DE/DX = 0.0                 |
| D     | D(57,9,10,2) | 9.5615 | -DE/DX = 0.0                 |
| D     | D(57,9,10,11) | -168.7212| -DE/DX = 0.0                 |
| D     | D(119,9,10,2) | -141.2772| -DE/DX = 0.0                 |
| D     | D(119,9,10,11) | 40.4401| -DE/DX = 0.0                 |
| D     | D(10,9,119,118) | 72.3629| -DE/DX = 0.0                 |
| D     | D(10,9,119,118) | -80.3582| -DE/DX = 0.0                 |
| D     | D(10,12,14,15) | 72.3629| -DE/DX = 0.0                 |
| D     | D(10,12,14,16) | -0.6274| -DE/DX = 0.0                 |
| D     | D(13,12,14,15) | -1.4726| -DE/DX = 0.0                 |
| D     | D(13,12,14,16) | 178.2792| -DE/DX = 0.0                 |
| D111  | D(12,14,16,17) | 179.9985 | -DE/DX = 0.0 |
|-------|---------------|----------|--------------|
| D112  | D(12,14,16,18) | -0.5494  | -DE/DX = 0.0 |
| D113  | D(15,14,16,17)| -0.2492  | -DE/DX = 0.0 |
| D114  | D(15,14,16,18)| 179.203  | -DE/DX = 0.0 |
| D115  | D(14,16,18,19)| -178.8592| -DE/DX = 0.0 |
| D116  | D(14,16,18,20)| 0.6615   | -DE/DX = 0.0 |
| D117  | D(17,16,18,19)| 0.5902   | -DE/DX = 0.0 |
| D118  | D(17,16,18,20)| -179.8891| -DE/DX = 0.0 |
| D119  | D(16,18,20,11)| 0.3949   | -DE/DX = 0.0 |
| D120  | D(16,18,20,21)| -177.5515| -DE/DX = 0.0 |
| D121  | D(19,18,20,11)| 179.9213 | -DE/DX = 0.0 |
| D122  | D(19,18,20,21)| 1.9749   | -DE/DX = 0.0 |
| D123  | D(11,20,16,12)| -0.7138  | -DE/DX = 0.0 |
| D124  | D(11,20,16,13)| 179.1938 | -DE/DX = 0.0 |
| D125  | D(18,20,16,12)| 177.4623 | -DE/DX = 0.0 |
| D126  | D(18,20,16,13)| 0.3949   | -DE/DX = 0.0 |
| D127  | D(16,20,18,21)| 179.9213 | -DE/DX = 0.0 |
| D128  | D(16,20,18,22)| -0.5494  | -DE/DX = 0.0 |
| D129  | D(14,20,18,21)| 179.203  | -DE/DX = 0.0 |
| D130  | D(14,20,18,22)| -178.8592| -DE/DX = 0.0 |
| D131  | D(13,20,18,21)| 0.6615   | -DE/DX = 0.0 |
| D132  | D(13,20,18,22)| -0.5494  | -DE/DX = 0.0 |
| D133  | D(16,20,18,21)| 179.9213 | -DE/DX = 0.0 |
| D134  | D(16,20,18,22)| -0.5494  | -DE/DX = 0.0 |
| D135  | D(18,20,18,21)| 179.9213 | -DE/DX = 0.0 |
| D136  | D(18,20,18,22)| -0.5494  | -DE/DX = 0.0 |
| D137  | D(19,20,18,21)| 179.9213 | -DE/DX = 0.0 |
| D138  | D(19,20,18,22)| 0.6615   | -DE/DX = 0.0 |
| D139  | D(20,18,21,22)| -0.5494  | -DE/DX = 0.0 |
| D140  | D(20,18,21,23)| 179.9213 | -DE/DX = 0.0 |
| D141  | D(20,18,21,24)| -0.5494  | -DE/DX = 0.0 |
| D142  | D(20,18,21,25)| 179.9213 | -DE/DX = 0.0 |
| D143  | D(20,18,21,26)| -0.5494  | -DE/DX = 0.0 |
| D144  | D(20,18,21,27)| 179.9213 | -DE/DX = 0.0 |
| D145  | D(20,18,21,28)| -0.5494  | -DE/DX = 0.0 |
| D146  | D(20,18,21,29)| 179.9213 | -DE/DX = 0.0 |
| D147  | D(20,18,21,30)| -0.5494  | -DE/DX = 0.0 |
| D148  | D(20,18,21,31)| 179.9213 | -DE/DX = 0.0 |
| D149  | D(20,18,21,32)| -0.5494  | -DE/DX = 0.0 |
| D150  | D(20,18,21,33)| 179.9213 | -DE/DX = 0.0 |
| D151  | D(20,18,21,34)| -0.5494  | -DE/DX = 0.0 |
| D152  | D(20,18,21,35)| 179.9213 | -DE/DX = 0.0 |
| D153  | D(20,18,21,36)| 0.6615   | -DE/DX = 0.0 |
| D154  | D(20,18,21,37)| -0.5494  | -DE/DX = 0.0 |
| D155  | D(20,18,21,38)| 179.9213 | -DE/DX = 0.0 |
| D156  | D(20,18,21,39)| -0.5494  | -DE/DX = 0.0 |
| D157  | D(20,18,21,40)| 179.9213 | -DE/DX = 0.0 |
| D158  | D(20,18,21,41)| -0.5494  | -DE/DX = 0.0 |
| D159  | D(20,18,21,42)| 179.9213 | -DE/DX = 0.0 |
| D160  | D(20,18,21,43)| -0.5494  | -DE/DX = 0.0 |
| D161  | D(20,18,21,44)| 179.9213 | -DE/DX = 0.0 |
| D162  | D(20,18,21,45)| -0.5494  | -DE/DX = 0.0 |
| D163  | D(20,18,21,46)| 179.9213 | -DE/DX = 0.0 |
| D164  | D(20,18,21,47)| -0.5494  | -DE/DX = 0.0 |
| D165  | D(20,18,21,48)| 179.9213 | -DE/DX = 0.0 |
| D166  | D(20,18,21,49)| -0.5494  | -DE/DX = 0.0 |
| D167  | D(20,18,21,50)| 179.9213 | -DE/DX = 0.0 |
| D168  | D(20,18,21,51)| -0.5494  | -DE/DX = 0.0 |
| D169  | D(20,18,21,52)| 179.9213 | -DE/DX = 0.0 |
| D170  | D(20,18,21,53)| -0.5494  | -DE/DX = 0.0 |
| D171  | D(20,18,21,54)| 179.9213 | -DE/DX = 0.0 |
| D172  | D(20,18,21,55)| -0.5494  | -DE/DX = 0.0 |
| D173  | D(20,18,21,56)| 179.9213 | -DE/DX = 0.0 |
| D171 | D(35,36,38,39) | 179.9238 | -DE/DX = 0.0 |
| D172 | D(35,36,38,40) | -0.2603 | -DE/DX = 0.0 |
| D173 | D(37,36,38,39) | -0.2139 | -DE/DX = 0.0 |
| D174 | D(37,36,38,40) | 179.6020 | -DE/DX = 0.0 |
| D175 | D(36,38,40,41) | -179.7914 | -DE/DX = 0.0 |
| D176 | D(36,38,40,42) | 0.0415 | -DE/DX = 0.0 |
| D177 | D(39,38,40,41) | 0.0252 | -DE/DX = 0.0 |
| D178 | D(39,38,40,42) | 179.8581 | -DE/DX = 0.0 |
| D179 | D(38,40,42,43) | -179.6798 | -DE/DX = 0.0 |
| D180 | D(38,40,42,44) | 0.1992 | -DE/DX = 0.0 |
| D181 | D(41,40,42,43) | 0.1525 | -DE/DX = 0.0 |
| D182 | D(41,40,42,44) | -179.9686 | -DE/DX = 0.0 |
| D183 | D(40,42,44,6) | -0.2192 | -DE/DX = 0.0 |
| D184 | D(40,42,44,7) | -179.3738 | -DE/DX = 0.0 |
| D185 | D(42,44,45,6) | -179.8730 | -DE/DX = 0.0 |
| D186 | D(42,44,45,7) | 179.6608 | -DE/DX = 0.0 |
| D187 | D(35,44,45,6) | 0.1854 | -DE/DX = 0.0 |
| D188 | D(35,44,45,7) | -179.3738 | -DE/DX = 0.0 |
| D189 | D(42,44,45,6) | 179.8764 | -DE/DX = 0.0 |
| D190 | D(42,44,45,7) | 0.3172 | -DE/DX = 0.0 |
| D191 | D(7,46,47,48) | 2.7905 | -DE/DX = 0.0 |
| D192 | D(7,46,47,56) | -178.2135 | -DE/DX = 0.0 |
| D193 | D(8,46,47,48) | -177.7668 | -DE/DX = 0.0 |
| D194 | D(8,46,47,56) | 1.2274 | -DE/DX = 0.0 |
| D195 | D(46,47,48,49) | -0.9520 | -DE/DX = 0.0 |
| D196 | D(46,47,48,50) | 178.7385 | -DE/DX = 0.0 |
| D197 | D(56,47,48,49) | -179.8199 | -DE/DX = 0.0 |
| D198 | D(56,47,48,50) | -0.1293 | -DE/DX = 0.0 |
| D199 | D(46,47,56,54) | -178.6414 | -DE/DX = 0.0 |
| D200 | D(46,47,56,57) | -0.8836 | -DE/DX = 0.0 |
| D201 | D(48,47,56,54) | 0.4812 | -DE/DX = 0.0 |
| D202 | D(48,47,56,57) | 178.2391 | -DE/DX = 0.0 |
| D203 | D(47,48,50,51) | 179.9541 | -DE/DX = 0.0 |
| D204 | D(47,48,50,52) | -0.1121 | -DE/DX = 0.0 |
| D205 | D(49,48,50,51) | -0.3589 | -DE/DX = 0.0 |
| D206 | D(49,48,50,52) | 179.5749 | -DE/DX = 0.0 |
| D207 | D(48,50,52,53) | 179.7758 | -DE/DX = 0.0 |
| D208 | D(48,50,52,54) | 0.0089 | -DE/DX = 0.0 |
| D209 | D(51,50,52,53) | -0.29 | -DE/DX = 0.0 |
| D210 | D(51,50,52,54) | 179.9430 | -DE/DX = 0.0 |
| D211 | D(50,52,54,55) | 179.7506 | -DE/DX = 0.0 |
| D212 | D(50,52,54,56) | 0.3302 | -DE/DX = 0.0 |
| D213 | D(53,52,54,55) | -0.0162 | -DE/DX = 0.0 |
| D214 | D(53,52,54,56) | -179.4365 | -DE/DX = 0.0 |
| D215 | D(52,54,56,47) | -0.5680 | -DE/DX = 0.0 |
| D216 | D(52,54,56,57) | -177.5869 | -DE/DX = 0.0 |
| D217 | D(55,54,56,47) | -179.9821 | -DE/DX = 0.0 |
| D218 | D(55,54,56,57) | 2.9990 | -DE/DX = 0.0 |
| D219 | D(47,56,57,8) | 0.2924 | -DE/DX = 0.0 |
| D220 | D(47,56,57,9) | -177.1972 | -DE/DX = 0.0 |
| D221 | D(54,56,57,8) | 177.6302 | -DE/DX = 0.0 |
| D222 | D(54,56,57,9) | 0.1406 | -DE/DX = 0.0 |
| D223 | D(1,58,59,69) | -6.9545 | -DE/DX = 0.0 |
| D224 | D(60,58,59,69) | 154.1474 | -DE/DX = 0.0 |
| D225 | D(58,59,69,70) | -72.3618 | -DE/DX = 0.0 |
| D226 | D(58,59,69,117) | 80.3591 | -DE/DX = 0.0 |
| D227 | D(64,61,62,70) | 177.3648 | -DE/DX = 0.0 |
| D228 | D(64,61,62,81) | -9.5909 | -DE/DX = 0.0 |
| D229 | D(66,61,62,70) | 96.5262 | -DE/DX = 0.0 |
| D230 | D(66,61,62,81) | -90.4296 | -DE/DX = 0.0 |
| D231 | D(68,61,62,70) | 16.2238 | -DE/DX = 0.0 |
| D232 | D(68,61,62,81) | -170.7319 | -DE/DX = 0.0 |
| D233 | D(118,61,62,70) | -83.8699 | -DE/DX = 0.0 |
| D234 | D(118,61,62,81) | 89.1743 | -DE/DX = 0.0 |
| D235 | D(62,61,64,82) | 12.5243 | -DE/DX = 0.0 |
| D236 | D(62,61,64,93) | -178.8381 | -DE/DX = 0.0 |
| D237 | D(66,61,64,82) | -83.8699 | -DE/DX = 0.0 |
| D238 | D(66,61,64,93) | 89.1743 | -DE/DX = 0.0 |
| D239 | D(68,61,64,82) | 97.5087 | -DE/DX = 0.0 |
| D240 | D(68,61,64,93) | -178.8381 | -DE/DX = 0.0 |
| D241 | D(118,61,64,82) | -93.8536 | -DE/DX = 0.0 |
| D242 | D(118,61,64,93) | 79.5415 | -DE/DX = 0.0 |
| D243 | D(62,61,66,94) | 12.5243 | -DE/DX = 0.0 |
| D244 | D(62,61,66,105) | -178.8381 | -DE/DX = 0.0 |
| D245 | D(64,61,66,94) | 15.5283 | -DE/DX = 0.0 |
| D246 | D(64,61,66,105) | 177.1051 | -DE/DX = 0.0 |
| D247 | D(68,61,66,94) | 177.1051 | -DE/DX = 0.0 |
| D248 | D(68,61,66,105) | -10.3334 | -DE/DX = 0.0 |
| D249 | D(118,61,66,94) | -82.8435 | -DE/DX = 0.0 |
| D250 | D(118,61,66,105) | 97.5087 | -DE/DX = 0.0 |
| D251 | D(62,61,68,106) | -18.4427 | -DE/DX = 0.0 |
| D252 | D(62,61,68,117) | 86.8959 | -DE/DX = 0.0 |
| D253 | D(64,61,68,106) | 178.6136 | -DE/DX = 0.0 |
| D254 | D(64,61,68,117) | -103.634 | -DE/DX = 0.0 |
| D255 | D(66,61,68,106) | 178.6136 | -DE/DX = 0.0 |
| D256 | D(66,61,68,117) | -65.672 | -DE/DX = 0.0 |
| D257 | D(68,61,68,106) | -137.9548 | -DE/DX = 0.0 |
| D258 | D(68,61,68,117) | -65.672 | -DE/DX = 0.0 |
| D259 | D(61,62,70,69) | -137.9548 | -DE/DX = 0.0 |
| D260 | D(61,62,70,71) | -137.9548 | -DE/DX = 0.0 |
| D261 | D(61,62,81,63) | 97.5087 | -DE/DX = 0.0 |
| D262 | D(61,62,81,83) | -178.8381 | -DE/DX = 0.0 |
| D263 | D(93,64,82,63) | 178.6136 | -DE/DX = 0.0 |
| D264 | D(93,64,82,83) | -128.07 | -DE/DX = 0.0 |
| D265 | D(94,65,93,65) | 2.2921 | -DE/DX = 0.0 |
| D266 | D(94,65,93,95) | 2.2921 | -DE/DX = 0.0 |
| D267 | D(93,65,94,66) | -177.8246 | -DE/DX = 0.0 |
| D268 | D(93,65,94,95) | 174.8153 | -DE/DX = 0.0 |
|   |   |   |   |   |
|---|---|---|---|---|
| D291 | D(61,66,94,65) | -8.9034 | -DE/DX = 0.0 |   |
| D292 | D(61,66,94,95) | 172.7174 | -DE/DX = 0.0 |   |
| D293 | D(105,66,94,65) | 177.2883 | -DE/DX = 0.0 |   |
| D294 | D(105,66,94,95) | -1.091 | -DE/DX = 0.0 |   |
| D295 | D(61,66,105,67) | 7.4341 | -DE/DX = 0.0 |   |
| D296 | D(61,66,105,104) | -173.0239 | -DE/DX = 0.0 |   |
| D297 | D(94,66,105,67) | -178.7519 | -DE/DX = 0.0 |   |
| D298 | D(94,66,105,104) | 0.7901 | -DE/DX = 0.0 |   |
| D299 | D(106,67,105,66) | 0.1446 | -DE/DX = 0.0 |   |
| D300 | D(106,67,105,104) | -179.3492 | -DE/DX = 0.0 |   |
| D301 | D(105,67,106,68) | -0.3294 | -DE/DX = 0.0 |   |
| D302 | D(105,67,106,107) | -179.669 | -DE/DX = 0.0 |   |
| D303 | D(61,68,106,67) | -7.1819 | -DE/DX = 0.0 |   |
| D304 | D(61,68,106,107) | 172.2199 | -DE/DX = 0.0 |   |
| D305 | D(117,68,106,67) | -178.3771 | -DE/DX = 0.0 |   |
| D306 | D(117,68,106,107) | 0.7901 | -DE/DX = 0.0 |   |
| D307 | D(61,68,117,69) | 10.8756 | -DE/DX = 0.0 |   |
| D308 | D(61,68,117,116) | -171.7181 | -DE/DX = 0.0 |   |
| D309 | D(106,68,117,69) | -177.8568 | -DE/DX = 0.0 |   |
| D310 | D(106,68,117,116) | -0.4505 | -DE/DX = 0.0 |   |
| D311 | D(59,69,70,62) | 141.276 | -DE/DX = 0.0 |   |
| D312 | D(59,69,70,71) | -40.4357 | -DE/DX = 0.0 |   |
| D313 | D(117,69,70,62) | -9.5627 | -DE/DX = 0.0 |   |
| D314 | D(117,69,70,71) | 168.7256 | -DE/DX = 0.0 |   |
| D315 | D(59,69,117,68) | -143.9115 | -DE/DX = 0.0 |   |
| D316 | D(59,69,117,116) | 38.9706 | -DE/DX = 0.0 |   |
| D317 | D(70,69,117,68) | 6.8128 | -DE/DX = 0.0 |   |
| D318 | D(70,69,117,116) | -170.3052 | -DE/DX = 0.0 |   |
| D319 | D(62,70,71,72) | 175.4176 | -DE/DX = 0.0 |   |
| D320 | D(62,70,71,80) | -0.9546 | -DE/DX = 0.0 |   |
| D321 | D(69,70,71,72) | -3.1026 | -DE/DX = 0.0 |   |
| D322 | D(69,70,71,80) | -179.4748 | -DE/DX = 0.0 |   |
| D323 | D(70,71,72,73) | 1.2747 | -DE/DX = 0.0 |   |
| D324 | D(70,71,72,74) | -177.6163 | -DE/DX = 0.0 |   |
| D325 | D(80,71,72,73) | 177.2229 | -DE/DX = 0.0 |   |
| D326 | D(80,71,72,74) | -1.6682 | -DE/DX = 0.0 |   |
| D327 | D(70,71,80,78) | 178.5434 | -DE/DX = 0.0 |   |
| D328 | D(70,71,80,81) | 0.1373 | -DE/DX = 0.0 |   |
| D329 | D(72,71,80,78) | 1.593 | -DE/DX = 0.0 |   |
| D330 | D(72,71,80,81) | -176.8131 | -DE/DX = 0.0 |   |
| D331 | D(71,72,74,75) | -179.6217 | -DE/DX = 0.0 |   |
| D332 | D(71,72,74,76) | 0.6265 | -DE/DX = 0.0 |   |
| D333 | D(73,72,74,75) | 1.4725 | -DE/DX = 0.0 |   |
| D334 | D(73,72,74,76) | -178.2795 | -DE/DX = 0.0 |   |
| D335 | D(72,74,76,77) | -179.9983 | -DE/DX = 0.0 |   |
| D336 | D(72,74,76,78) | 0.5491 | -DE/DX = 0.0 |   |
| D337 | D(75,74,76,77) | -179.2034 | -DE/DX = 0.0 |   |
| D338 | D(75,74,76,78) | 178.8594 | -DE/DX = 0.0 |   |
| D339 | D(74,76,78,79) | -0.6603 | -DE/DX = 0.0 |   |
| D340 | D(77,76,78,79) | -0.9505 | -DE/DX = 0.0 |   |
| D341 | D(77,76,78,80) | 179.8899 | -DE/DX = 0.0 |   |
| D342 | D(76,78,80,71) | -0.3955 | -DE/DX = 0.0 |   |
| D343 | D(76,78,80,81) | 177.5503 | -DE/DX = 0.0 |   |
| D344 | D(79,78,80,71) | -179.9209 | -DE/DX = 0.0 |   |
| D345 | D(79,78,80,81) | -1.9751 | -DE/DX = 0.0 |   |
| D346 | D(71,80,81,62) | 0.7089 | -DE/DX = 0.0 |   |
| D347 | D(71,80,81,63) | -179.1921 | -DE/DX = 0.0 |   |
| D348 | D(78,80,81,62) | -177.4668 | -DE/DX = 0.0 |   |
| D349 | D(78,80,81,63) | 2.6323 | -DE/DX = 0.0 |   |
| D351 | D(63,82,83,84) | 0.6404 | -DE/DX = 0.0 |
| D352 | D(63,82,83,92) | -179.066 | -DE/DX = 0.0 |
| D353 | D(64,82,83,84) | 179.8083 | -DE/DX = 0.0 |
| D354 | D(64,82,83,92) | 0.1018 | -DE/DX = 0.0 |
| D355 | D(82,83,84,85) | 0.0022 | -DE/DX = 0.0 |
| D356 | D(82,83,84,86) | -179.8744 | -DE/DX = 0.0 |
| D357 | D(92,83,84,85) | 179.6723 | -DE/DX = 0.0 |
| D358 | D(92,83,84,86) | -0.2044 | -DE/DX = 0.0 |
| D359 | D(82,83,92,90) | 179.7472 | -DE/DX = 0.0 |
| D360 | D(82,83,92,93) | 0.4288 | -DE/DX = 0.0 |
| D361 | D(84,83,92,90) | -0.0002 | -DE/DX = 0.0 |
| D362 | D(84,83,92,93) | -179.3186 | -DE/DX = 0.0 |
| D363 | D(83,84,86,87) | -179.9736 | -DE/DX = 0.0 |
| D364 | D(83,84,86,88) | 0.1817 | -DE/DX = 0.0 |
| D365 | D(85,84,86,87) | 0.1507 | -DE/DX = 0.0 |
| D366 | D(85,84,86,88) | -179.694 | -DE/DX = 0.0 |
| D367 | D(84,86,88,89) | 179.8783 | -DE/DX = 0.0 |
| D368 | D(84,86,88,90) | 0.0457 | -DE/DX = 0.0 |
| D369 | D(84,86,88,89) | 0.033 | -DE/DX = 0.0 |
| D370 | D(87,86,88,91) | -179.7996 | -DE/DX = 0.0 |
| D371 | D(86,88,90,91) | 179.6354 | -DE/DX = 0.0 |
| D372 | D(86,88,90,92) | -0.2484 | -DE/DX = 0.0 |
| D373 | D(89,88,90,91) | -0.1965 | -DE/DX = 0.0 |
| D374 | D(89,88,90,92) | 179.9197 | -DE/DX = 0.0 |
| D375 | D(88,90,92,83) | 0.2264 | -DE/DX = 0.0 |
| D376 | D(88,90,92,93) | 179.3368 | -DE/DX = 0.0 |
| D377 | D(91,90,92,83) | -179.6583 | -DE/DX = 0.0 |
| D378 | D(91,90,92,93) | -0.5479 | -DE/DX = 0.0 |
| D379 | D(83,92,93,64) | -0.8398 | -DE/DX = 0.0 |
| D380 | D(83,92,93,65) | 177.5503 | -DE/DX = 0.0 |
| D381 | D(90,92,93,64) | 179.9519 | -DE/DX = 0.0 |
| D382 | D(90,92,93,65) | -1.658 | -DE/DX = 0.0 |
| D383 | D(65,94,95,66) | 1.6755 | -DE/DX = 0.0 |
| D384 | D(65,94,95,104) | -177.4757 | -DE/DX = 0.0 |
| D385 | D(66,94,95,96) | -179.8625 | -DE/DX = 0.0 |
| D386 | D(66,94,95,104) | 0.9863 | -DE/DX = 0.0 |
| D387 | D(94,95,96,97) | 0.5759 | -DE/DX = 0.0 |
| D388 | D(94,95,96,98) | -179.2869 | -DE/DX = 0.0 |
| D389 | D(104,95,96,97) | 179.6221 | -DE/DX = 0.0 |
| D390 | D(104,95,96,98) | -0.2460 | -DE/DX = 0.0 |
| D391 | D(94,95,104,102) | 179.2708 | -DE/DX = 0.0 |
| D392 | D(94,95,104,105) | -0.462 | -DE/DX = 0.0 |
| D393 | D(96,95,104,102) | 0.0017 | -DE/DX = 0.0 |
| D394 | D(96,95,104,105) | -179.7311 | -DE/DX = 0.0 |
| D395 | D(95,96,98,99) | -179.9244 | -DE/DX = 0.0 |
| D396 | D(95,96,98,100) | 0.2597 | -DE/DX = 0.0 |
| D397 | D(97,96,98,99) | 0.2139 | -DE/DX = 0.0 |
| D398 | D(97,96,98,100) | -179.602 | -DE/DX = 0.0 |
| D399 | D(96,98,100,101) | 179.7911 | -DE/DX = 0.0 |
| D400 | D(96,98,100,102) | -0.0414 | -DE/DX = 0.0 |
| D401 | D(99,98,100,101) | -0.0255 | -DE/DX = 0.0 |
| D402 | D(99,98,100,102) | -179.858 | -DE/DX = 0.0 |
| D403 | D(98,100,102,103) | 179.6791 | -DE/DX = 0.0 |
| D404 | D(98,100,102,104) | -0.1986 | -DE/DX = 0.0 |
| D405 | D(101,100,102,103) | -0.1528 | -DE/DX = 0.0 |
| D406 | D(101,100,102,104) | 179.9695 | -DE/DX = 0.0 |
| D407 | D(100,102,104,95) | 0.2185 | -DE/DX = 0.0 |
| D408 | D(100,102,104,105) | 179.8701 | -DE/DX = 0.0 |
| D409 | D(103,102,104,95) | -179.6603 | -DE/DX = 0.0 |
| D410 | D(103,102,104,105) | -0.0087 | -DE/DX = 0.0 |
Standard orientation: (for (BePcH₂O₂) dimer)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------------|--------------|-------------|-------------------------|
|              |              |             | X           | Y           | Z           |
| 1            | 4            | Be          | -3.053111   | -0.013441   | 0.642407    |
| 2            | 7            | N           | -1.862130   | -1.334983   | 1.344627    |
| 3            | 7            | N           | -3.202899   | -3.353532   | 1.075698    |
| 4            | 7            | N           | -4.463244   | -1.354278   | 0.528691    |
| 5            | 7            | N           | -6.382727   | -0.007559   | -0.117137   |
| 6            | 7            | N           | -4.470811   | 1.353356    | 0.518768    |
| 7            | 7            | N           | -6.382727   | -0.007559   | -0.117137   |
| 8            | 7            | N           | -4.470811   | 1.353356    | 0.518768    |
| 9            | 6            | C           | -0.556754   | -1.149267   | 1.765091    |
| 10           | 6            | C           | 0.060090    | -2.418918   | 2.139723    |
| 11           | 6            | C           | 1.299544    | -2.764072   | 2.692920    |
| 12           | 1            | H           | 2.048992    | -2.014291   | 2.918347    |
| 13           | 6            | C           | 1.543710    | -4.112768   | 2.973607    |
| 14           | 1            | H           | 2.498870    | -4.407370   | 3.396949    |
| 15           | 1            | H           | 2.498870    | -4.407370   | 3.396949    |
|   |    |   |     |     |     |     |
|---|----|---|-----|-----|-----|-----|
| 16 | 6  | C | 0.565257 | -5.098999 | 2.720080 |
| 17 | 1  | H | 0.785490 | -6.137014 | 2.948894 |
| 18 | 6  | C | -0.682536 | -4.753494 | 2.190677 |
| 19 | 1  | H | -1.449490 | -5.497902 | 2.008120 |
| 20 | 6  | C | -0.920085 | -3.404958 | 1.909569 |
| 21 | 1  | H | -1.449490 | -5.497902 | 2.008120 |
| 22 | 6  | C | -0.920085 | -3.404958 | 1.909569 |
| 23 | 6  | C | -2.094780 | -2.725159 | 0.657874 |
| 24 | 6  | C | -5.111874 | -3.436830 | 0.286446 |
| 25 | 1  | H | -5.111874 | -3.436830 | 0.286446 |
| 26 | 6  | C | -7.133855 | -5.139612 | -0.163467 |
| 27 | 1  | H | -7.424482 | -6.184983 | -0.203396 |
| 28 | 6  | C | -8.071401 | -4.177711 | -0.529329 |
| 29 | 1  | H | -9.065981 | -4.482323 | -0.844547 |
| 30 | 6  | C | -7.739205 | -2.787831 | -0.488232 |
| 31 | 1  | H | -8.455039 | -2.020481 | -0.761885 |
| 32 | 6  | C | -6.446552 | -2.448059 | -0.077832 |
| 33 | 6  | C | -5.769940 | -1.167411 | 0.094335 |
| 34 | 6  | C | -5.786125 | 1.157217  | 0.110015 |
| 35 | 6  | C | -6.485423 | 2.430770  | -0.013344 |
| 36 | 6  | C | -7.792118 | 2.760837  | -0.386118 |
| 37 | 1  | H | -8.501995 | 1.998634  | -0.664407 |
| 38 | 6  | C | -8.145925 | 4.115707  | -0.383065 |
| 39 | 1  | H | -9.151780 | 4.408621  | -0.668141 |
| 40 | 6  | C | -7.215790 | 5.112441  | -0.010740 |
| 41 | 1  | H | -7.523459 | 6.136677  | -0.015890 |
| 42 | 6  | C | -5.909525 | 4.777921  | 0.366528 |
| 43 | 1  | H | -5.911006 | 5.535949  | 0.658567 |
| 44 | 6  | C | -5.558037 | 3.424420  | 0.357435 |
| 45 | 6  | C | -4.321428 | 2.724566  | 0.683564 |
| 46 | 6  | C | -2.106451 | 2.734885  | 1.399180 |
| 47 | 6  | C | -0.915974 | 3.450292  | 1.835226 |
| 48 | 6  | C | -0.673972 | 4.806164  | 2.070946 |
| 49 | 1  | H | -1.455359 | 5.541630  | 1.914892 |
| 50 | 6  | C | 0.600845  | 5.171905  | 2.517853 |
| 51 | 1  | H | 0.825097  | 6.216473  | 2.710638 |
| 52 | 6  | C | 1.603679  | 4.200921  | 2.724189 |
| 53 | 1  | H | 2.584815  | 4.512526  | 3.067803 |
| 54 | 6  | C | 1.356624  | 2.842432  | 2.489017 |
| 55 | 1  | H | 2.135187  | 2.105932  | 2.646995 |
| 56 | 6  | C | 0.083686  | 2.476856  | 2.035003 |
| 57 | 6  | C | -0.548025 | 1.194128  | 1.730963 |
| 58 | 8  | O | -2.591654 | 0.018045  | -1.018640 |
| 59 | 1  | H | -1.637443 | -0.003967 | -1.420371 |
| 60 | 1  | H | -3.257334 | 0.348944  | -1.641946 |
| 61 | 4  | Be| 3.053134 | 0.013435  | -0.642408 |
| 62 | 7  | N | 1.862114 | 1.334969  | -1.346603 |
| 63 | 7  | N | 3.202883 | 3.355300  | -1.075770 |
| 64 | 7  | N | 4.463240 | 1.354296  | -0.528714 |
| 65 | 7  | N | 6.382776 | 0.007599  | 0.117007 |
| 66 | 7  | N | 4.470854 | -1.353341 | -0.518809 |
| 67 | 7  | N | 3.230655 | -3.363980 | -1.088728 |
| 68 | 7  | N | 1.867741 | -1.362941 | -1.357877 |
| 69 | 7  | N | -0.083913 | -0.022141 | -1.862516 |
| 70 | 6  | C | 0.556748 | 1.149232  | -1.765089 |
| 71 | 6  | C | -0.060153 | 2.418880  | -2.139625 |
| 72 | 6  | C | -1.299660 | 2.764021  | -2.692710 |
| 73 | 1  | H | -2.049109 | 2.014228  | -2.918096 |
| 74 | 6  | C | -1.543868 | 4.112718  | -2.973354 |
| 75 | 1  | H | -2.499063 | 4.407311  | -3.396624 |
|   |   |   |      |      |      |
|---|---|---|------|------|------|
| 76 | 6 | C | -0.565416 | 5.098962 | -2.719873 |
| 77 | 1 | H | -0.785683 | 6.136978 | -2.948649 |
| 78 | 6 | C | 0.682417 | 4.753472 | -2.190552 |
| 79 | 1 | H | 1.449369 | 5.497890 | -2.008029 |
| 80 | 6 | C | 0.920017 | 3.404933 | -1.90504 |
| 81 | 6 | C | 2.094766 | 2.709388 | -1.409137 |
| 82 | 6 | C | 4.295082 | 2.725171 | -0.657950 |
| 83 | 6 | C | 5.118845 | 3.436861 | -0.286484 |
| 84 | 6 | C | 5.841299 | 4.795218 | -0.251344 |
| 85 | 1 | H | 5.117299 | 5.549945 | -0.538479 |
| 86 | 6 | C | 7.133788 | 5.139669 | 0.163468 |
| 87 | 1 | H | 7.424395 | 6.185045 | 0.203415 |
| 88 | 6 | C | 8.071355 | 4.147840 | 0.529310 |
| 89 | 1 | H | 9.065930 | 4.448316 | 0.844532 |
| 90 | 6 | C | 7.739188 | 2.787894 | 0.488187 |
| 91 | 1 | H | 8.455038 | 2.020554 | 0.761824 |
| 92 | 6 | C | 6.446643 | 2.448103 | 0.077774 |
| 93 | 6 | C | 5.769963 | 1.167443 | -0.094432 |
| 94 | 6 | C | 5.786185 | -1.157182 | -0.110141 |
| 95 | 6 | C | 6.485478 | -2.430732 | 0.013272 |
| 96 | 6 | C | 7.792165 | -2.760789 | 0.386082 |
| 97 | 1 | H | 8.502037 | -1.998579 | 0.664364 |
| 98 | 6 | C | 8.145976 | -4.115658 | 0.383062 |
| 99 | 1 | H | 9.151827 | -4.408564 | 0.668157 |
|100 | 6 | C | 7.215847 | -5.112403 | 0.010746 |
|101 | 1 | H | 7.523521 | -6.153627 | 0.015917 |
|102 | 6 | C | 5.909588 | -4.777894 | -0.366549 |
|103 | 1 | H | 5.191078 | -5.535928 | -0.658591 |
|104 | 6 | C | 5.558100 | -3.424392 | -0.357502 |
|105 | 6 | C | 4.321506 | -2.724545 | -0.683701 |
|106 | 6 | C | 2.106514 | -2.734892 | -1.399268 |
|107 | 6 | C | 0.916020 | -3.450318 | -1.855237 |
|108 | 6 | C | 0.674021 | -4.806195 | -2.070931 |
|109 | 1 | H | 1.455425 | -5.541650 | -1.914909 |
|110 | 6 | C | -0.600808 | -5.171953 | -2.517792 |
|111 | 1 | H | -0.825053 | -6.216524 | -2.710567 |
|112 | 6 | C | -1.603660 | -4.200153 | -2.724096 |
|113 | 1 | H | -2.584805 | -4.512600 | -3.067676 |
|114 | 6 | C | -1.356612 | -2.842489 | -2.488942 |
|115 | 1 | H | -2.135189 | -2.105999 | -2.646897 |
|116 | 6 | C | -0.083660 | -2.476895 | -2.034982 |
|117 | 6 | C | 0.548049 | -1.194158 | -1.730978 |
|118 | 8 | O | 2.591676 | -0.018084 | 1.018640 |
|119 | 1 | H | 1.637459 | 0.003927 | 1.420370 |
|120 | 1 | H | 3.257343 | -0.349019 | 1.641941 |
Table S6. TD-DFT results for the low-energy π-π states for MgPc, MgPc(H₂O), ZnPc and ZnPc(H₂O).

(a) MgPc

| λ, nm | E, eV  | f     | Contribution (weight, %)* |
|-------|--------|-------|---------------------------|
| 615   | 2.0154 | 0.4251| 138→139 (94.6), 136→140 (6.4) |
| 612   | 2.0255 | 0.4252| 138→140 (94.4), 136→139 (6.5) |
| 376   | 3.2951 | 0.0151| 137→139 (90.0), 133→140 (7.5) |
| 375   | 3.3052 | 0.0140| 137→140 (88.6), 133→139 (9.1) |

*) HOMO (138) and LUMO (139)

(b) MgPc(H₂O)

| λ, nm | E, eV  | f     | Contribution (weight, %)* |
|-------|--------|-------|---------------------------|
| 612   | 2.0251 | 0.4186| 143→144 (94.0), 141→145 (6.4) |
| 611   | 2.0264 | 0.4184| 143→145 (94.1), 141→144 (6.9) |
| 377   | 3.2890 | 0.0338| 142→145 (89.9), 138→145 (9.1) |
| 375   | 3.3083 | 0.0289| 142→144 (70.5), 141→144 (10.1) |
| 367   | 3.3778 | 0.0006| 137→144 (82.8), 134→144 (15.8) |
| 366   | 3.3806 | 0.0020| 137→145 (81.4), 134→145 (16.9) |

*) HOMO (143), LUMO (144)

(c) ZnPc

| λ, nm | E, eV  | f     | Contribution (weight, %)* |
|-------|--------|-------|---------------------------|
| 594.46| 2.0857 | 0.4084| 147→148 (93.8), 145→149 (6.6) |
| 594.43| 2.0858 | 0.4085| 147→149 (93.8), 145→148 (6.6) |
| 373.77| 3.3171 | 0.0137| 146→148 (90.6), 137→148 (6.7) |
| 373.77| 3.3171 | 0.0137| 146→149 (90.5), 137→149 (6.7) |

*) HOMO (147) and LUMO (148)

(d) ZnPc(H₂O)

| λ, nm | E, eV  | f     | Contribution (weight, %)* |
|-------|--------|-------|---------------------------|
| 603   | 2.0568 | 0.4246| 152→153 (94.2), 148→154 (3.1), 149→154 (3.2) |
| 602   | 2.0584 | 0.4235| 152→154 (94.1), 148→153 (3.1), 149→153 (3.3) |
| 373   | 3.3245 | 0.0057| 148→153 (3.6), 150→153 (5.0), 150→154 (28.6), 151→153 (39.1), 151→154 (13.6) |
| 372   | 3.3278 | 0.0052| 147→154 (2.1), 148→154 (5.3), 149→153 (2.6), 148→154 (4.1), 150→153 (33.4), 150→154 (3.4), 151→153 (13.3) 151→154 (28.7) |
| 369   | 3.3651 | 0.0127| 146→153 (8.1), 147→154 (2.7), 148→154 (18.0), 149→154 (12.9), 150→153 (11.8), 150→154 (2.2), 151→154 (40.0) |
| 368   | 3.6775 | 0.0122| 146→154 (7.3), 147→153 (3.5), 148→153 (19.4), 149→153 (18.4), 150→154 (15.8), 151→153 (31.0) |

*) HOMO (152), LUMO (153)
**Table S7. TD-DFT output for MgPc.**

HOMO: 138, LUMO: 139

Excitation energies and oscillator strengths:

| Excited State | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|---------------|------------|-------------|-----------------|-------------------------|-------|
| 1             |            | 2.0154      | 615.19          | 0.4251                  | 0.000 |
| 136 -> 140    |            | -0.17901    |                 |                         |       |
| 138 -> 139    |            | 0.68768     |                 |                         |       |
| This state for optimization and/or second-order correction. |
| Total Energy, E(TD-HF/TD-KS) = -1867.34625148 |
| Copying the excited state density for this state as the 1-particle RhoCI density. |

| Excited State 2 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 136 -> 139      | 2.0255    | 612.11      | 0.4252          |                         |       |
| 138 -> 140      | 0.18063   |             |                 |                         |       |
| 137 -> 139      | 0.68697   |             |                 |                         |       |

| Excited State 3 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 133 -> 140      | 3.2951    | 376.27      | 0.0151          |                         |       |
| 137 -> 139      | -0.19419  |             |                 |                         |       |
| 136 -> 140      | 0.67092   |             |                 |                         |       |

| Excited State 4 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 133 -> 139      | 3.3052    | 375.12      | 0.0140          |                         |       |
| 137 -> 140      | -0.21355  |             |                 |                         |       |
| 136 -> 140      | 0.66562   |             |                 |                         |       |

| Excited State 5 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 134 -> 139      | 3.3277    | 372.58      | 0.0000          |                         |       |
| 135 -> 140      | 0.50394   |             |                 |                         |       |
| 135 -> 140      | -0.48649  |             |                 |                         |       |

| Excited State 6 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 134 -> 140      | 3.3284    | 372.50      | 0.0000          |                         |       |
| 135 -> 140      | -0.45530  |             |                 |                         |       |
| 134 -> 140      | 0.52681   |             |                 |                         |       |

| Excited State 7 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 129 -> 139      | 3.3482    | 370.30      | 0.0000          |                         |       |
| 129 -> 140      | -0.70277  |             |                 |                         |       |

| Excited State 8 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 129 -> 140      | 3.3614    | 368.84      | 0.0000          |                         |       |
| 129 -> 140      | 0.70272   |             |                 |                         |       |

| Excited State 9 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|-----------------|-----------|-------------|-----------------|-------------------------|-------|
| 131 -> 139      | 3.4000    | 364.66      | 0.0000          |                         |       |
| 132 -> 140      | 0.13229   |             |                 |                         |       |
| 134 -> 140      | 0.12937   |             |                 |                         |       |
| 135 -> 139      | 0.20289   |             |                 |                         |       |
| 135 -> 140      | 0.14778   |             |                 |                         |       |
| 138 -> 141      | 0.62954   |             |                 |                         |       |

| Excited State 10 | Singlet-A | Energy (eV) | Wavelength (nm) | Oscillator Strength (f) | <S^2> |
|------------------|-----------|-------------|-----------------|-------------------------|-------|
| 131 -> 139       | 3.4666    | 357.65      | 0.0000          |                         |       |
| 132 -> 140       | -0.14198  |             |                 |                         |       |
| 134 -> 140       | -0.13227  |             |                 |                         |       |
| 134 -> 140       | 0.48457   |             |                 |                         |       |
| 135 -> 139       | 0.42996   |             |                 |                         |       |
| 138 -> 141       | -0.20161  |             |                 |                         |       |
Table S8. TD-DFT output for MgPcH₂O.

**HOMO: 143, LUMO: 144**

Excitation energies and oscillator strengths:

| Excited State | Singlet-A | Excitation Energy | Oscillator Strength | <S^2> |
|---------------|-----------|-------------------|---------------------|-------|
| 1             | 141 -> 145| 2.0251 eV         | 0.17882             | 0.000 |
|               | 143 -> 144| 0.68566           |                     |       |

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1943.78891632

Copying the excited state density for this state as the 1-particle RhoCI density.

| Excited State | Singlet-A | Excitation Energy | Oscillator Strength | <S^2> |
|---------------|-----------|-------------------|---------------------|-------|
| 2             | 141 -> 144| 2.0264 eV         | -0.18635            | 0.000 |
|               | 143 -> 145| 0.68618           |                     |       |
| 3             | 143 -> 146| 3.1037 eV         | 0.70570             | 0.000 |
| 4             | 138 -> 145| 3.2890 eV         | 0.18785             | 0.000 |
|               | 142 -> 145| 0.67031           |                     |       |
| 5             | 140 -> 145| 3.3072 eV         | 0.69786             | 0.000 |
| 6             | 138 -> 144| 3.3083 eV         | -0.22444            | 0.000 |
|               | 141 -> 144| 0.28490           |                     |       |
|               | 142 -> 144| 0.59361           |                     |       |
| 7             | 139 -> 144| 3.3526 eV         | 0.69707             | 0.000 |
| 8             | 134 -> 144| 3.3778 eV         | -0.28134            | 0.000 |
|               | 137 -> 144| 0.64347           |                     |       |
| 9             | 134 -> 145| 3.3806 eV         | -0.29058            | 0.000 |
|               | 137 -> 145| 0.63802           |                     |       |
| 10            | 135 -> 144| 3.3966 eV         | 0.12140             | 0.000 |
|               | 136 -> 145| 0.12491           |                     |       |
|               | 139 -> 145| 0.10646           |                     |       |
|               | 140 -> 144| 0.13895           |                     |       |
|               | 143 -> 147| 0.65745           |                     |       |
**Table S9. TD-DFT output for ZnPc.**

**HOMO: 147, LUMO: 148**

Excitation energies and oscillator strengths:

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 1             | 2.0857      | 594.46          | 0.1814             | 0               |
| 145 -> 149    |             |                 | 0.68473            |                |

This state for optimization and/or second-order correction.

Total Energy, $E_{TD-HF/TD-DFT} = -3445.90636358$

Copying the excited state density for this state as the 1-particle RhoCl density.

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 2             | 2.0858      | 594.43          | 0.18162            | 0               |
| 145 -> 148    |             |                 | 0.68473            |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 3             | 3.1092      | 398.76          | 0.70409            | 0               |
| 142 -> 148    |             |                 | 0.70400            |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 4             | 3.1093      | 398.75          | 0.70311            | 0               |
| 142 -> 149    |             |                 | 0.70312            |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 5             | 3.2250      | 384.45          | 0.70312            | 0               |
| 141 -> 148    |             |                 | 0.70312            |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 6             | 3.2251      | 384.44          | 0.70312            | 0               |
| 141 -> 149    |             |                 | 0.70312            |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 7             | 3.2847      | 377.45          | 0.49206            | 0               |
| 143 -> 148    |             |                 | 0.49749            |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 8             | 3.2874      | 377.15          | 0.49953            | 0               |
| 143 -> 148    |             |                 | 0.49412            |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 9             | 3.3171      | 373.77          | 0.0137             | 0               |
| 137 -> 148    |             |                 | 0.0137             |                |

| Excited State | Energy (eV) | Wavelength (nm) | Oscillator Strength | Squared Overlap |
|---------------|-------------|-----------------|--------------------|-----------------|
| 10            | 3.3171      | 373.77          | 0.18295            | 0               |
| 137 -> 149    |             |                 | 0.67264            |                |
**Table S10. TD-DFT output for ZnPcH$_2$O.**

**HOMO: 152, LUMO: 153**

Excitation energies and oscillator strengths:

| Excited State | Singlet-A | 2.0568 eV | 602.80 nm | f=0.4246 | <S**2>=0.000 |
|---------------|-----------|-----------|-----------|----------|-------------|
| 148 -> 154    | -0.12564  |           |           |          |             |
| 149 -> 154    | -0.12661  |           |           |          |             |
| 152 -> 153    | 0.68624   |           |           |          |             |

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3522.80700422

Copying the excited state density for this state as the 1-particle RhoCI density.

| Excited State | Singlet-A | 2.0584 eV | 602.32 nm | f=0.4235 | <S**2>=0.000 |
|---------------|-----------|-----------|-----------|----------|-------------|
| 148 -> 153    | 0.12510   |           |           |          |             |
| 149 -> 153    | 0.12804   |           |           |          |             |
| 152 -> 154    | 0.68598   |           |           |          |             |

Excited State 3: Singlet-A 3.1512 eV 393.45 nm f=0.0000 <S**2>=0.000

| Excited State | Singlet-A | 3.1537 eV | 393.14 nm | f=0.0001 | <S**2>=0.000 |
|---------------|-----------|-----------|-----------|----------|-------------|
| 147 -> 153    | 0.65413   |           |           |          |             |
| 148 -> 153    | -0.10696  |           |           |          |             |
| 149 -> 153    | 0.22537   |           |           |          |             |

Excited State 4: Singlet-A 3.3245 eV 372.94 nm f=0.0057 <S**2>=0.000

| Excited State | Singlet-A | 3.3278 eV | 372.57 nm | f=0.0052 | <S**2>=0.000 |
|---------------|-----------|-----------|-----------|----------|-------------|
| 147 -> 154    | 0.10354   |           |           |          |             |
| 148 -> 154    | 0.16243   |           |           |          |             |
| 149 -> 153    | -0.11370  |           |           |          |             |
| 149 -> 154    | -0.14276  |           |           |          |             |
| 150 -> 153    | 0.40871   |           |           |          |             |
| 150 -> 154    | 0.13046   |           |           |          |             |
| 151 -> 153    | 0.25743   |           |           |          |             |
| 151 -> 154    | 0.37913   |           |           |          |             |

Excited State 7: Singlet-A 3.3651 eV 368.44 nm f=0.0127 <S**2>=0.000

| Excited State | Singlet-A | 3.3675 eV | 368.18 nm | f=0.0122 | <S**2>=0.000 |
|---------------|-----------|-----------|-----------|----------|-------------|
| 146 -> 153    | -0.20135  |           |           |          |             |
| 147 -> 154    | -0.11668  |           |           |          |             |
| 148 -> 154    | -0.29978  |           |           |          |             |
| 149 -> 154    | 0.25405   |           |           |          |             |
| 150 -> 153    | -0.24299  |           |           |          |             |
| 150 -> 154    | 0.10571   |           |           |          |             |
| 151 -> 154    | 0.44694   |           |           |          |             |

Excited State 8: Singlet-A 3.3675 eV 368.44 nm f=0.0127 <S**2>=0.000

| Excited State | Singlet-A | 3.3675 eV | 368.18 nm | f=0.0122 | <S**2>=0.000 |
|---------------|-----------|-----------|-----------|----------|-------------|
| 146 -> 153    | -0.19143  |           |           |          |             |
| 147 -> 153    | -0.13311  |           |           |          |             |
| 148 -> 153    | -0.31144  |           |           |          |             |
| 149 -> 153    | 0.30318   |           |           |          |             |
| 150 -> 154    | -0.28114  |           |           |          |             |
| Transition | E (eV) | f | <S^2> | Wavelength (nm) |
|------------|-------|---|-------|----------------|
| 151 -> 153 | 0.39353 |   |       |                 |

**Excited State 9: Singlet-A**  
3.4179 eV 362.75 nm f=0.0001 <S^2>=0.000

| Transition | E (eV) | f | <S^2> | Wavelength (nm) |
|------------|-------|---|-------|----------------|
| 144 -> 154 | 0.11053 |   |       |                 |
| 145 -> 153 | 0.10726 |   |       |                 |
| 148 -> 154 | -0.13065 |   |       |                 |
| 149 -> 154 | 0.11695 |   |       |                 |
| 150 -> 153 | 0.17502 |   |       |                 |
| 152 -> 155 | 0.62874 |   |       |                 |

**Excited State 10: Singlet-A**  
3.4371 eV 360.72 nm f=0.0006 <S^2>=0.000

| Transition | E (eV) | f | <S^2> | Wavelength (nm) |
|------------|-------|---|-------|----------------|
| 142 -> 153 | 0.63997 |   |       |                 |
| 143 -> 153 | 0.28310 |   |       |                 |
Table S11. TD-DFT output for (MgPcH$_2$O)$_2$ dimer.

Excitation energies and oscillator strengths:

| Excited State | Singlet-A | *E* (eV) | *λ* (nm) | f | <S$^2$> |
|---------------|------------|----------|----------|---|---------|
| 1             | 1.6779     | 738.94   | 285 -> 288 | 0.39663 |        |
|               |            |          | 286 -> 287 | 0.58184 |        |

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -3886.74064758

Copying the excited state density for this state as the 1-particle RhoCI density.

| Excited State | Singlet-A | *E* (eV) | *λ* (nm) | f | <S$^2$> |
|---------------|------------|----------|----------|---|---------|
| 2             | 1.6892     | 733.97   | 285 -> 287 | 0.43630 |        |
|               |            |          | 286 -> 288 | 0.55301 |        |
| 3             | 1.8118     | 684.32   | 285 -> 290 | 0.37678 |        |
|               |            |          | 286 -> 289 | 0.59078 |        |
| 4             | 1.8167     | 682.46   | 285 -> 289 | 0.40559 |        |
|               |            |          | 286 -> 290 | 0.57160 |        |
| 5             | 1.9142     | 647.72   | 285 -> 287 | 0.54725 |        |
|               |            |          | 286 -> 288 | -0.42955 |    |
| 6             | 2.0670     | 599.82   | 283 -> 287 | -0.13767 |        |
|               |            |          | 284 -> 288 | -0.12284 |    |
|               |            |          | 285 -> 289 | 0.55644 |        |
|               |            |          | 286 -> 290 | -0.38728 |    |
| 7             | 2.0757     | 597.30   | 283 -> 288 | -0.12961 |        |
|               |            |          | 284 -> 287 | -0.11816 |    |
|               |            |          | 285 -> 290 | 0.57702 |        |
|               |            |          | 286 -> 289 | -0.35935 |    |
| 8             | 2.1006     | 590.25   | 283 -> 290 | 0.13804 |        |
|               |            |          | 284 -> 289 | 0.12611 |        |
|               |            |          | 285 -> 288 | 0.56391 |        |
|               |            |          | 286 -> 287 | -0.37687 |    |
| 9             | 3.1538     | 393.12   | 281 -> 287 | 0.47318 |        |
|               |            |          | 282 -> 288 | 0.41668 |        |
|               |            |          | 283 -> 289 | -0.19241 |   |
|               |            |          | 284 -> 290 | -0.14959 |   |
| 10            | 3.1625     | 392.04   | 281 -> 288 | 0.37960 |        |
|               |            |          | 282 -> 287 | 0.53678 |        |
|               |            |          | 283 -> 290 | -0.11668 |    |
| 11            | 3.1742     | 390.60   | 273 -> 287 | 0.10276 |        |
|               |            |          | 274 -> 287 | 0.12544 |        |
|               |            |          | 275 -> 288 | -0.13615 |    |
|               |            |          | 277 -> 287 | 0.12909 |        |
| 279 -> 289 | -0.12176 |
| 280 -> 288 | -0.18034 |
| 281 -> 290 | -0.13224 |
| 282 -> 289 | -0.10918 |
| 283 -> 288 | -0.13056 |
| 284 -> 287 | 0.56297 |

Excited State 12: Singlet-A 3.1957 eV 387.98 nm f=0.0040 $<S^2>$=0.000
| 273 -> 288 | 0.11311 |
| 278 -> 289 | 0.14299 |
| 279 -> 290 | -0.13310 |
| 280 -> 287 | -0.26394 |
| 283 -> 287 | -0.38826 |
| 284 -> 288 | 0.42863 |

| 269 -> 287 | -0.10813 |
| 271 -> 288 | -0.13560 |
| 274 -> 288 | -0.39269 |
| 275 -> 287 | 0.43490 |
| 280 -> 287 | -0.29544 |

Excited State 13: Singlet-A 3.2016 eV 387.25 nm f=0.0033 $<S^2>$=0.000
| 269 -> 288 | 0.10691 |
| 271 -> 287 | 0.14981 |
| 274 -> 287 | 0.45518 |
| 275 -> 288 | -0.38346 |
| 280 -> 288 | 0.23902 |

Excited State 14: Singlet-A 3.2068 eV 386.63 nm f=0.0000 $<S^2>$=0.000
| 272 -> 287 | -0.10885 |
| 275 -> 287 | -0.17674 |
| 277 -> 288 | 0.22102 |
| 280 -> 287 | -0.13301 |
| 281 -> 289 | -0.32794 |
| 282 -> 290 | -0.32575 |
| 283 -> 287 | 0.33819 |
| 284 -> 288 | 0.15706 |

| 272 -> 287 | -0.10885 |
| 275 -> 287 | -0.17674 |
| 277 -> 288 | 0.22102 |
| 280 -> 287 | -0.13301 |
| 281 -> 289 | -0.32794 |
| 282 -> 290 | -0.32575 |
| 283 -> 287 | 0.33819 |
| 284 -> 288 | 0.15706 |

Excited State 15: Singlet-A 3.2168 eV 385.43 nm f=0.1167 $<S^2>$=0.000
Table S12. TD-DFT output for (ZnPcH2O)2 dimer.

Excitation energies and oscillator strengths:

Excited State 1:  Singlet-A  1.7736 eV  699.05 nm  f=0.0000  <S**2>=0.000
   303 -> 305  -0.43431
   304 -> 306  0.55697
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -7044.77477310
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2:  Singlet-A  1.7745 eV  698.71 nm  f=0.0045  <S**2>=0.000
   303 -> 306  -0.45706
   304 -> 305  0.53851

Excited State 3:  Singlet-A  1.8730 eV  661.96 nm  f=0.0255  <S**2>=0.000
   303 -> 308  -0.41563
   304 -> 307  0.57095

Excited State 4:  Singlet-A  1.8773 eV  660.45 nm  f=0.0000  <S**2>=0.000
   303 -> 307  -0.46566
   304 -> 308  0.53142

Excited State 5:  Singlet-A  1.9781 eV  626.78 nm  f=0.0000  <S**2>=0.000
   302 -> 308  0.10215
   303 -> 305  0.54801
   304 -> 306  0.42394

Excited State 6:  Singlet-A  2.0878 eV  593.86 nm  f=0.0000  <S**2>=0.000
   301 -> 305  0.12076
   302 -> 306  -0.13540
   303 -> 307  0.51314
   304 -> 308  0.44632

Excited State 7:  Singlet-A  2.0977 eV  591.04 nm  f=0.7030  <S**2>=0.000
   301 -> 306  0.11945
   302 -> 305  -0.13036
   303 -> 306  0.17838
   303 -> 308  0.52060
   304 -> 305  0.15288
   304 -> 307  0.36758

Excited State 8:  Singlet-A  2.1081 eV  588.13 nm  f=0.6619  <S**2>=0.000
   301 -> 308  -0.11928
   302 -> 307  0.13164
   303 -> 306  0.48878
   303 -> 308  -0.18692
   304 -> 305  0.40963
   304 -> 307  -0.14158

Excited State 9:  Singlet-A  2.9887 eV  414.84 nm  f=0.0000  <S**2>=0.000
   294 -> 305  0.15820
   297 -> 306  0.46926
   298 -> 305  -0.43905
   299 -> 305  -0.16758

Excited State 10: Singlet-A  2.9888 eV  414.83 nm  f=0.0007  <S**2>=0.000
   294 -> 306  0.15703
   297 -> 305  0.47320
   298 -> 306  -0.43563
   299 -> 306  -0.16651
| Excited State | Singlet-A | 3.0752 eV 403.17 nm f=0.0000 <S**2>=0.000 |
|---------------|-----------|---------------------------------------------|
| 294 -> 307    | 0.15923   |                                             |
| 297 -> 308    | 0.45893   |                                             |
| 298 -> 307    | -0.44764  |                                             |
| 299 -> 307    | -0.16965  |                                             |
| Excited State | Singlet-A | 3.0753 eV 403.16 nm f=0.0004 <S**2>=0.000 |
| 294 -> 308    | 0.15321   |                                             |
| 297 -> 307    | 0.48233   |                                             |
| 298 -> 308    | -0.42644  |                                             |
| 299 -> 308    | -0.16059  |                                             |
| Excited State | Singlet-A | 3.2204 eV 385.00 nm f=0.0000 <S**2>=0.000 |
| 289 -> 305    | 0.40571   |                                             |
| 290 -> 306    | -0.30396  |                                             |
| 291 -> 306    | 0.33495   |                                             |
| 292 -> 305    | -0.17226  |                                             |
| 301 -> 305    | 0.24004   |                                             |
| Excited State | Singlet-A | 3.2209 eV 384.93 nm f=0.0027 <S**2>=0.000 |
| 289 -> 306    | 0.40768   |                                             |
| 290 -> 305    | -0.30966  |                                             |
| 291 -> 305    | 0.34223   |                                             |
| 292 -> 306    | -0.17242  |                                             |
| 301 -> 306    | 0.23167   |                                             |
| Excited State | Singlet-A | 3.2261 eV 384.31 nm f=0.0000 <S**2>=0.000 |
| 298 -> 305    | -0.14139  |                                             |
| 299 -> 305    | 0.41073   |                                             |
| 300 -> 306    | 0.43879   |                                             |
| 301 -> 307    | 0.17839   |                                             |
| 302 -> 308    | -0.15398  |                                             |