Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# The ground-state molecular structures of free-base porphyrin, tetrabenzoporphyrin, tetraphenylporphyrin optimized at the B3LYP level (def2-TZVP).

## Free base porphyrin

The Cartesian coordinates (in angstroms).

| | | | |
|---|---|---|---|
| H | 3.209599995 | 3.172309777 | 0.000000000 |
| N | 0.000000000 | -2.113600613 | 0.000000000 |
| N | 2.031813914 | 0.000000000 | 0.000000000 |
| N | 0.000000000 | 2.113600613 | 0.000000000 |
| N | -2.031813914 | 0.000000000 | 0.000000000 |
| C | 1.126850920 | -2.888627221 | 0.000000000 |
| C | -1.126850920 | -2.888627221 | 0.000000000 |
| C | 1.126850920 | 2.888627221 | 0.000000000 |
| C | -1.126850920 | 2.888627221 | 0.000000000 |
| C | 2.850160984 | -1.083939750 | 0.000000000 |
| C | 2.850160984 | 1.083939750 | 0.000000000 |
| C | -2.850160984 | -1.083939750 | 0.000000000 |
| C | -2.850160984 | 1.083939750 | 0.000000000 |
| C | 0.683827200 | -4.249372023 | 0.000000000 |
| C | -0.683827200 | -4.249372023 | 0.000000000 |
| C | 0.683827200 | 4.249372023 | 0.000000000 |
| C | -0.683827200 | 4.249372023 | 0.000000000 |
| C | 4.248378966 | -0.675836785 | 0.000000000 |
| C | 4.248378966 | 0.675836785 | 0.000000000 |
| C | -4.248378966 | -0.675836785 | 0.000000000 |
| C | -4.248378966 | 0.675836785 | 0.000000000 |
| C | 2.433989580 | -2.416542873 | 0.000000000 |
| C | -2.433989580 | -2.416542873 | 0.000000000 |
| C | -2.433989580 | 2.416542873 | 0.000000000 |
| C | 2.433989580 | 2.416542873 | 0.000000000 |
| H | 1.341416542 | -5.103998738 | 0.000000000 |
| H | -1.341416542 | -5.103998738 | 0.000000000 |
| H | 1.341416542 | 5.103998738 | 0.000000000 |
| H | -1.341416542 | 5.103998738 | 0.000000000 |
| H | 5.096138011 | -1.344322017 | 0.000000000 |
| H | 5.096138011 | 1.344322017 | 0.000000000 |
| H | -5.096138011 | -1.344322017 | 0.000000000 |
| H | -5.096138011 | 1.344322017 | 0.000000000 |
| H | 3.209599995 | -3.172309777 | 0.000000000 |
| H | -3.209599995 | -3.172309777 | 0.000000000 |
| H | -3.209599995 | 3.172309777 | 0.000000000 |
| H | 0.000000000 | -1.102285542 | 0.000000000 |

| | | | |
|---|---|---|---|
| H | 0.000000000 | 1.102285542 | 0.000000000 |

**Tetraphenylporphyrin**

The Cartesian coordinates (in angstroms).

| | | | |
|---|---|---|---|
| N | 0.000000000 | -2.105680682 | 0.021952005 |
| N | 2.039452030 | 0.000000000 | -0.004461212 |
| N | 0.000000000 | 2.105680682 | 0.021952005 |
| N | -2.039452030 | 0.000000000 | -0.004461212 |
| C | 1.129355432 | -2.882536828 | -0.027487004 |
| C | -1.129355432 | -2.882536828 | -0.027487004 |
| C | 1.129355432 | 2.882536828 | -0.027487004 |
| C | -1.129355432 | 2.882536828 | -0.027487004 |
| C | 2.858287624 | -1.086796415 | 0.048401780 |
| C | 2.858287624 | 1.086796415 | 0.048401780 |
| C | -2.858287624 | -1.086796415 | 0.048401780 |
| C | -2.858287624 | 1.086796415 | 0.048401780 |
| C | 0.682467049 | -4.237536572 | -0.127380508 |
| C | -0.682467049 | -4.237536572 | -0.127380508 |
| C | 0.682467049 | 4.237536572 | -0.127380508 |
| C | -0.682467049 | 4.237536572 | -0.127380508 |
| C | 4.250150321 | -0.674623674 | 0.162800348 |
| C | 4.250150321 | 0.674623674 | 0.162800348 |
| C | -4.250150321 | -0.674623674 | 0.162800348 |
| C | -4.250150321 | 0.674623674 | 0.162800348 |
| C | 2.455534292 | -2.434568774 | 0.007870399 |
| C | -2.455534292 | -2.434568774 | 0.007870399 |
| C | -2.455534292 | 2.434568774 | 0.007870399 |
| C | 2.455534292 | 2.434568774 | 0.007870399 |
| H | 1.332626387 | -5.092022433 | -0.200649826 |
| H | -1.332626387 | -5.092022433 | -0.200649826 |
| H | 1.332626387 | 5.092022433 | -0.200649826 |
| H | -1.332626387 | 5.092022433 | -0.200649826 |
| H | 5.098895482 | -1.332382910 | 0.247290919 |
| H | 5.098895482 | 1.332382910 | 0.247290919 |
| H | -5.098895482 | -1.332382910 | 0.247290919 |
| H | -5.098895482 | 1.332382910 | 0.247290919 |
| H | 0.000000000 | -1.095474517 | 0.056508108 |
| H | 0.000000000 | 1.095474517 | 0.056508108 |
| C | -3.517780146 | -3.488958366 | -0.001441992 |
| C | -4.319468881 | -3.684139528 | -1.129278704 |
| C | -3.729974651 | -4.301571916 | 1.115408600 |

| | | | |
|---|---|---|---|
| C | -5.305129307 | -4.664535138 | -1.140745968 |
| C | -4.717404954 | -5.280416386 | 1.106499889 |
| C | -5.507773023 | -5.465677582 | -0.022380786 |
| H | -4.163814823 | -3.063575120 | -2.003179791 |
| H | -3.120542901 | -4.157401921 | 1.999209317 |
| H | -5.913620995 | -4.803474768 | -2.026102195 |
| H | -4.871143414 | -5.895938210 | 1.984535747 |
| H | -6.276514077 | -6.228469685 | -0.030369674 |
| C | -3.517780146 | 3.488958366 | -0.001441992 |
| C | -4.319468881 | 3.684139528 | -1.129278704 |
| C | -3.729974651 | 4.301571916 | 1.115408600 |
| C | -5.305129307 | 4.664535138 | -1.140745968 |
| C | -4.717404954 | 5.280416386 | 1.106499889 |
| C | -5.507773023 | 5.465677582 | -0.022380786 |
| H | -4.163814823 | 3.063575120 | -2.003179791 |
| H | -3.120542901 | 4.157401921 | 1.999209317 |
| H | -5.913620995 | 4.803474768 | -2.026102195 |
| H | -4.871143414 | 5.895938210 | 1.984535747 |
| H | -6.276514077 | 6.228469685 | -0.030369674 |
| C | 3.517780146 | -3.488958366 | -0.001441992 |
| C | 3.729974651 | -4.301571916 | 1.115408600 |
| C | 4.319468881 | -3.684139528 | -1.129278704 |
| C | 4.717404954 | -5.280416386 | 1.106499889 |
| C | 5.305129307 | -4.664535138 | -1.140745968 |
| C | 5.507773023 | -5.465677582 | -0.022380786 |
| H | 3.120542901 | -4.157401921 | 1.999209317 |
| H | 4.163814823 | -3.063575120 | -2.003179791 |
| H | 4.871143414 | -5.895938210 | 1.984535747 |
| H | 5.913620995 | -4.803474768 | -2.026102195 |
| H | 6.276514077 | -6.228469685 | -0.030369674 |
| C | 3.517780146 | 3.488958366 | -0.001441992 |
| C | 3.729974651 | 4.301571916 | 1.115408600 |
| C | 4.319468881 | 3.684139528 | -1.129278704 |
| C | 4.717404954 | 5.280416386 | 1.106499889 |
| C | 5.305129307 | 4.664535138 | -1.140745968 |
| C | 5.507773023 | 5.465677582 | -0.022380786 |
| H | 3.120542901 | 4.157401921 | 1.999209317 |
| H | 4.163814823 | 3.063575120 | -2.003179791 |
| H | 4.871143414 | 5.895938210 | 1.984535747 |
| H | 5.913620995 | 4.803474768 | -2.026102195 |
| H | 6.276514077 | 6.228469685 | -0.030369674 |

**Tetrabenzoporphyrin**

The Cartesian coordinates (in angstroms).

| | | | |
|---|---|---|---|
| H | -1.232086790 | 7.613826839 | 0.000000000 |
| H | -1.232086790 | -7.613826839 | 0.000000000 |
| H | 1.232086790 | 7.613826839 | 0.000000000 |
| H | 1.232086790 | -7.613826839 | 0.000000000 |
| N | -2.145020370 | 0.000000000 | 0.000000000 |
| N | 2.145020370 | 0.000000000 | 0.000000000 |
| N | 0.000000000 | 2.072111312 | 0.000000000 |
| N | 0.000000000 | -2.072111312 | 0.000000000 |
| C | -2.422561120 | 2.438372538 | 0.000000000 |
| C | -2.422561120 | -2.438372538 | 0.000000000 |
| C | 2.422561120 | 2.438372538 | 0.000000000 |
| C | 2.422561120 | -2.438372538 | 0.000000000 |
| C | -2.902486006 | 1.140615555 | 0.000000000 |
| C | -2.902486006 | -1.140615555 | 0.000000000 |
| C | 2.902486006 | 1.140615555 | 0.000000000 |
| C | 2.902486006 | -1.140615555 | 0.000000000 |
| C | -1.096923948 | 2.872391070 | 0.000000000 |
| C | -1.096923948 | -2.872391070 | 0.000000000 |
| C | 1.096923948 | 2.872391070 | 0.000000000 |
| C | 1.096923948 | -2.872391070 | 0.000000000 |
| C | -4.280059357 | 0.706424788 | 0.000000000 |
| C | -4.280059357 | -0.706424788 | 0.000000000 |
| C | 4.280059357 | 0.706424788 | 0.000000000 |
| C | 4.280059357 | -0.706424788 | 0.000000000 |
| C | -0.702021240 | 4.280887586 | 0.000000000 |
| C | -0.702021240 | -4.280887586 | 0.000000000 |
| C | 0.702021240 | 4.280887586 | 0.000000000 |
| C | 0.702021240 | -4.280887586 | 0.000000000 |
| C | -5.484916266 | 1.415557626 | 0.000000000 |
| C | -5.484916266 | -1.415557626 | 0.000000000 |
| C | 5.484916266 | 1.415557626 | 0.000000000 |
| C | 5.484916266 | -1.415557626 | 0.000000000 |
| C | -1.412957239 | 5.478391914 | 0.000000000 |
| C | -1.412957239 | -5.478391914 | 0.000000000 |

| | | | |
|---|---|---|---|
| C | 1.412957239 | 5.478391914 | 0.000000000 |
| C | 1.412957239 | -5.478391914 | 0.000000000 |
| C | -6.669553157 | 0.703167727 | 0.000000000 |
| C | -6.669553157 | -0.703167727 | 0.000000000 |
| C | 6.669553157 | 0.703167727 | 0.000000000 |
| C | 6.669553157 | -0.703167727 | 0.000000000 |
| C | -0.700190457 | 6.670337567 | 0.000000000 |
| C | -0.700190457 | -6.670337567 | 0.000000000 |
| C | 0.700190457 | 6.670337567 | 0.000000000 |
| C | 0.700190457 | -6.670337567 | 0.000000000 |
| H | -5.497366233 | 2.498277563 | 0.000000000 |
| H | -5.497366233 | -2.498277563 | 0.000000000 |
| H | 5.497366233 | 2.498277563 | 0.000000000 |
| H | 5.497366233 | -2.498277563 | 0.000000000 |
| H | -2.496259250 | 5.493226828 | 0.000000000 |
| H | -2.496259250 | -5.493226828 | 0.000000000 |
| H | 2.496259250 | 5.493226828 | 0.000000000 |
| H | 2.496259250 | -5.493226828 | 0.000000000 |
| H | -7.613924994 | 1.233016205 | 0.000000000 |
| H | -7.613924994 | -1.233016205 | 0.000000000 |
| H | 7.613924994 | 1.233016205 | 0.000000000 |
| H | 7.613924994 | -1.233016205 | 0.000000000 |
| H | -1.132864933 | 0.000000000 | 0.000000000 |
| H | 1.132864933 | 0.000000000 | 0.000000000 |
| H | -3.179794239 | 3.211531688 | 0.000000000 |
| H | -3.179794239 | -3.211531688 | 0.000000000 |
| H | 3.179794239 | 3.211531688 | 0.000000000 |
| H | 3.179794239 | -3.211531688 | 0.000000000 |