# Supplementary Information

# Solvent effects in furofuran lignans revealed by vibrational CD spectroscopy

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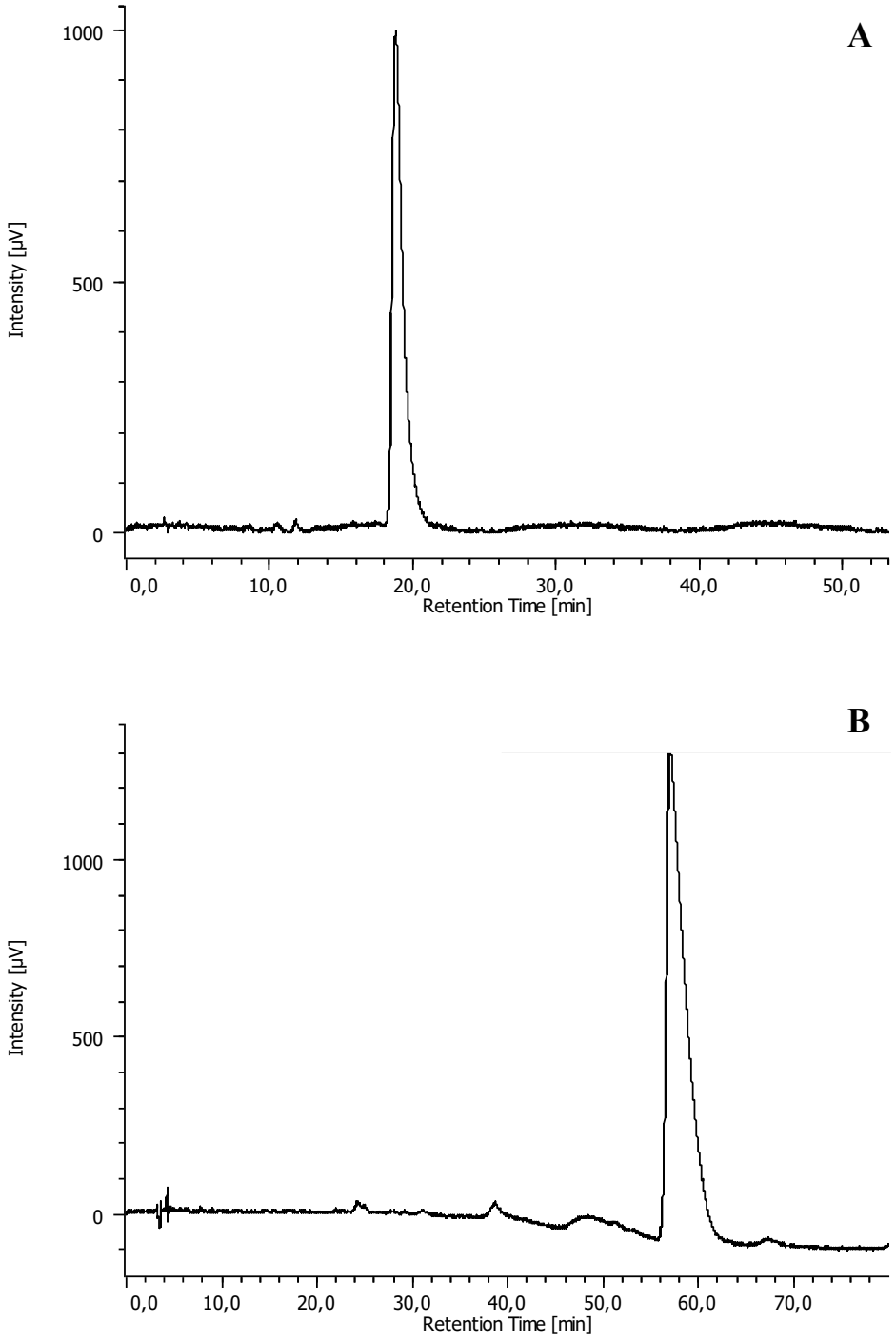


**Figure S1**. Chiral HPLC analysis of (–)-phillygenin (**1**). **A**) Lux Cellulose-1 column (Phenomenex®, 4.6 x 250 mm, 5 μm), Hex/EtOH 75:25, 1.0 mL $min^{-1}$ flow rate, λ = 280 nm, 18.8 min; **B**) CHIRALPAK® IC column (Daicel, 4.6 x 150 mm, 5 μm), Hex/EtOH 80:20, 1 mL $min^{-1}$ flow rate, λ = 280 nm, 56.9 min.

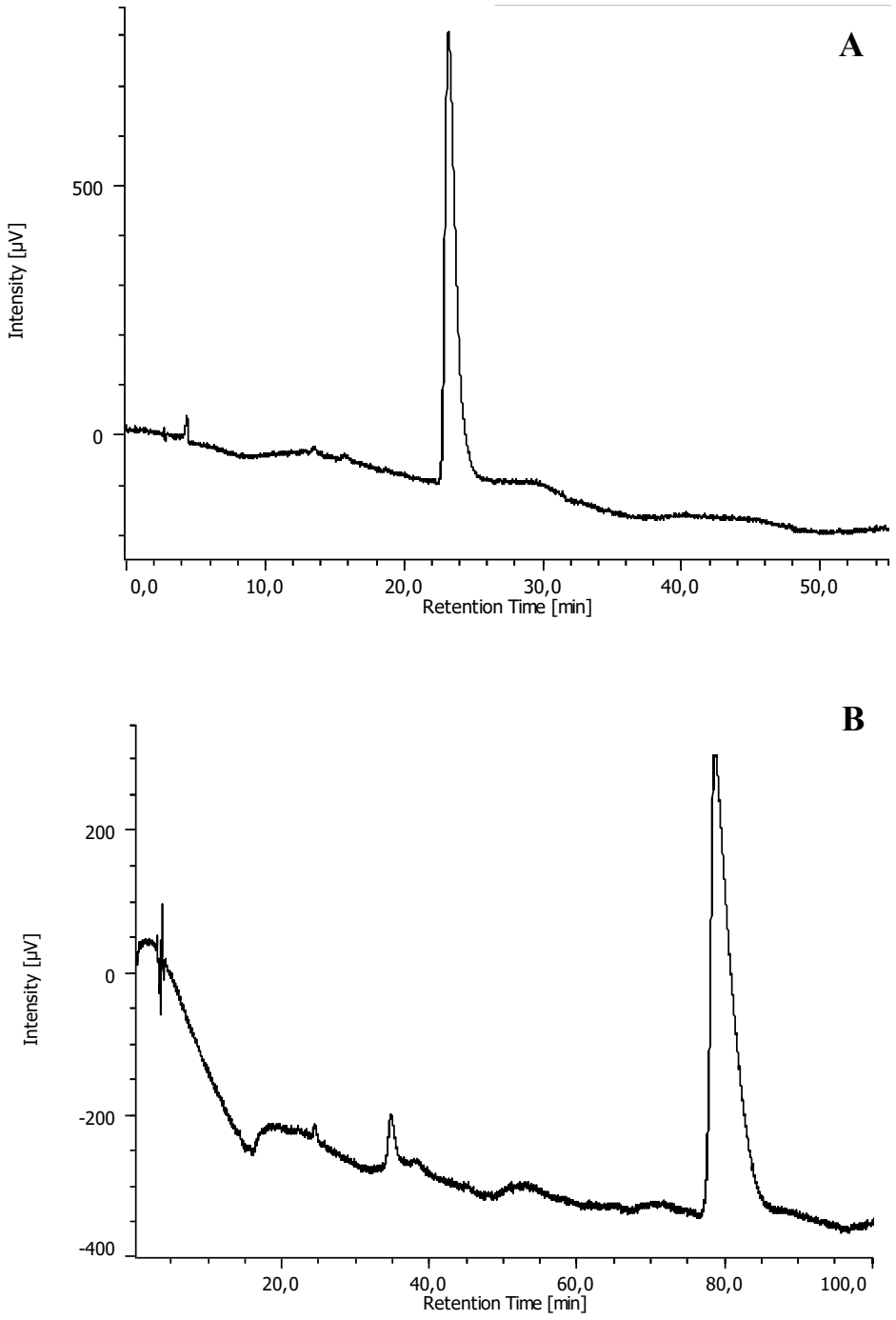


**Figure S2**. Chiral HPLC analysis of (−)-epieudesmin (**2**). **A**) Lux Cellulose-1 column (Phenomenex®, 4.6 x 250 mm, 5 μm), Hex/EtOH 80:20, 1.0 mL $min^{-1}$ flow rate, λ = 280 nm, 23.2 min. **B**) CHIRALPAK® IC column (Daicel, 4.6 x 150 mm, 5 μm), Hex/EtOH 70:30, 1 mL $min^{-1}$ flow rate, λ = 280 nm, 78.6 min.

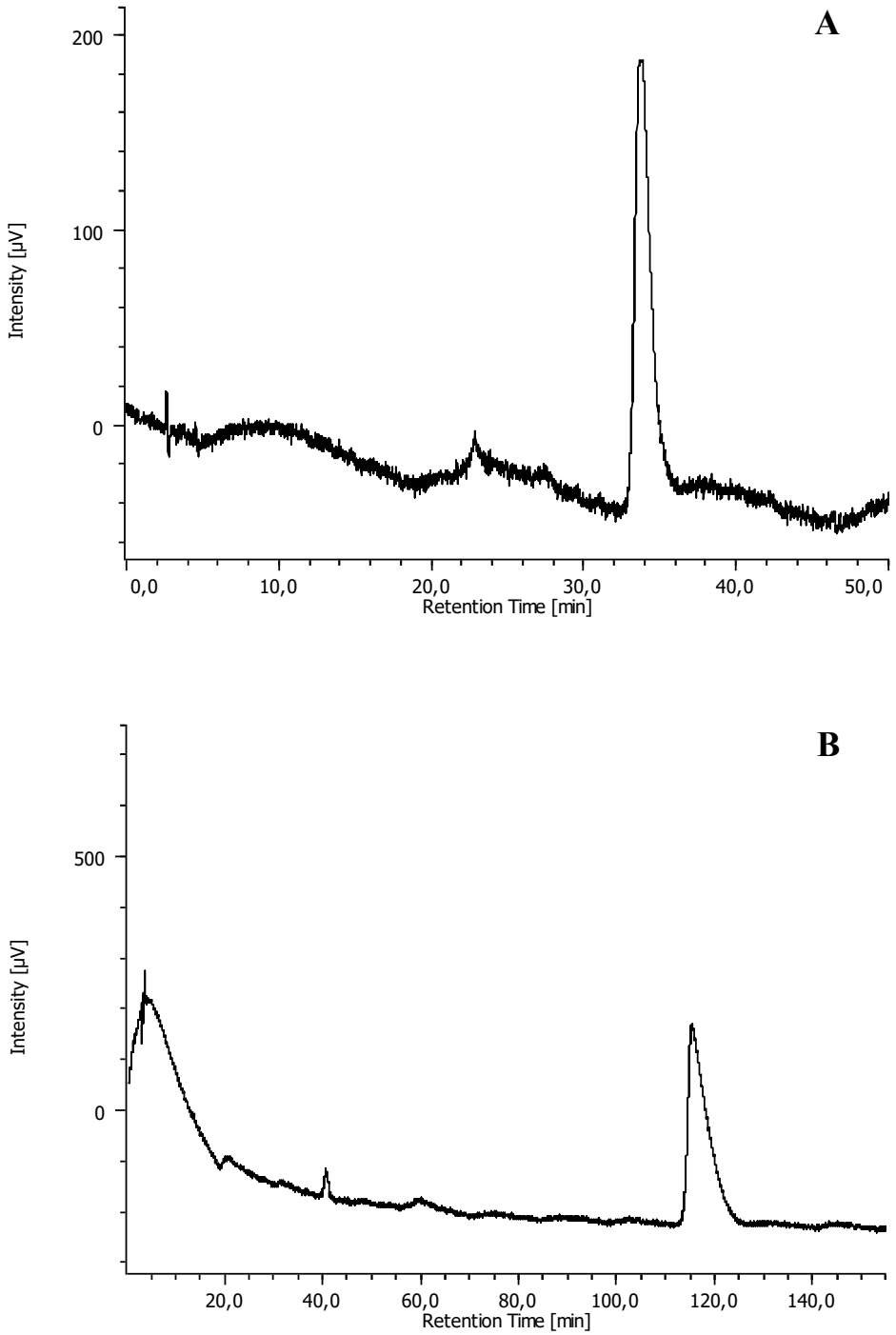


**Figure S3**. Chiral HPLC analysis of (+)-eudesmin (**3**). **A**) Lux Cellulose-1 column (Phenomenex®, 4.6 x 250 mm, 5 μm), Hex/EtOH 80:20, 1.0 mL $min^{-1}$ flow rate, λ = 280 nm, 33.7 min; **B**) CHIRALPAK® IC column (Daicel, 4.6 x 150 mm, 5 μm), Hex/EtOH 70:30, 1 mL $min^{-1}$ flow rate, λ = 280 nm, 115.2 min.

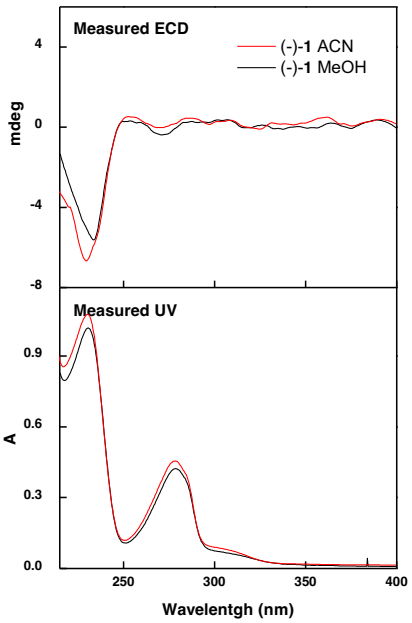


**Figure S4.** Experimental UV and ECD of (-)-**1** in different solvents.

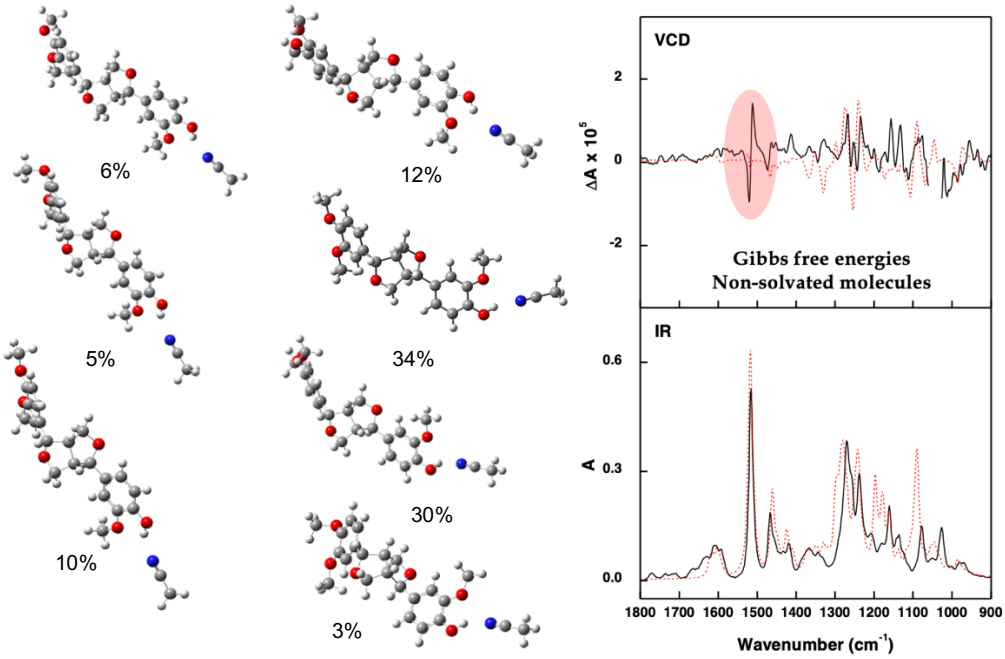


**Figure S5.** (Right) Comparison between experimental IR and VCD spectra of (-)-**1** recorded in MeCN-d3 (black solid trace) with calculated [B3PW91/6-311G(d,p)] data for (7*R*,8*S*,7'*S*,8'*S*)-**1** (red dotted trace) using the micro-solvation approach. Boltzmann weighting (%) based on Gibbs free energies of isolated (non-solvated) molecules. Gap represents intense solvent absorption. The correspondence between experiment and calculations for the 1510 $cm^{-1}$ couplet is highlighted. (Left) Lowest-energy molecular complexes of **1** and MeCN molecules.

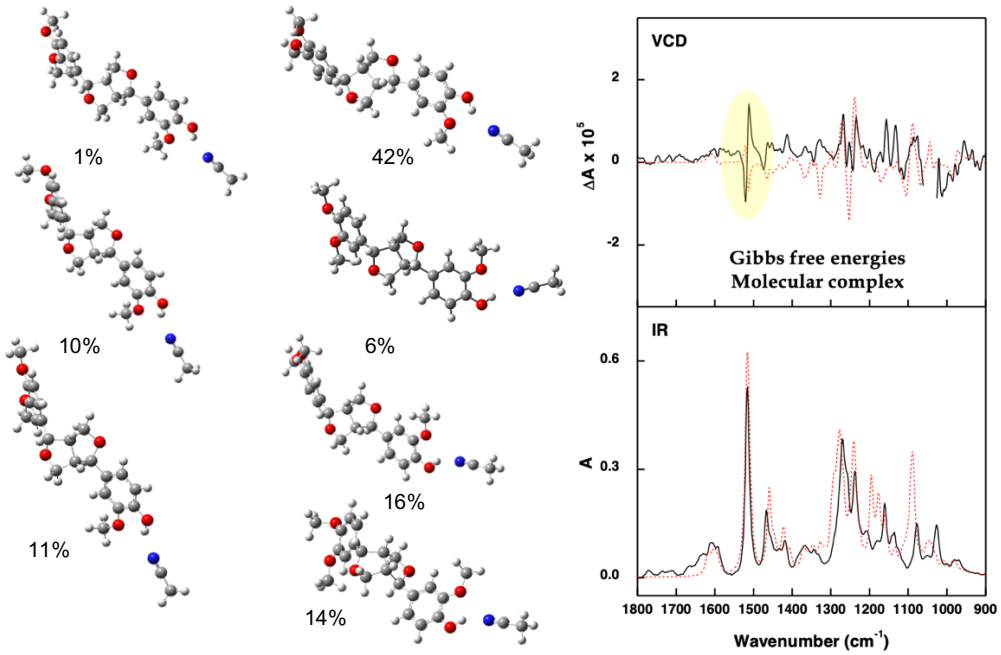


**Figure S6.** (Right) Comparison between experimental IR and VCD spectra of (-)-**1** recorded in MeCN-d3 (black solid trace) with calculated [B3PW91/6-311G(d,p)] data for (7*R*,8*S*,7'*S*,8'*S*)-**1** (red dotted trace) using the micro-solvation approach. Boltzmann weighting (%) based on Gibbs free energies of the molecular complex. Gap represents intense solvent absorption. The correspondence between experiment and calculations for the 1510 $cm^{-1}$ couplet is highlighted. (Left) Lowest-energy molecular complexes of **1** and MeCN molecules.

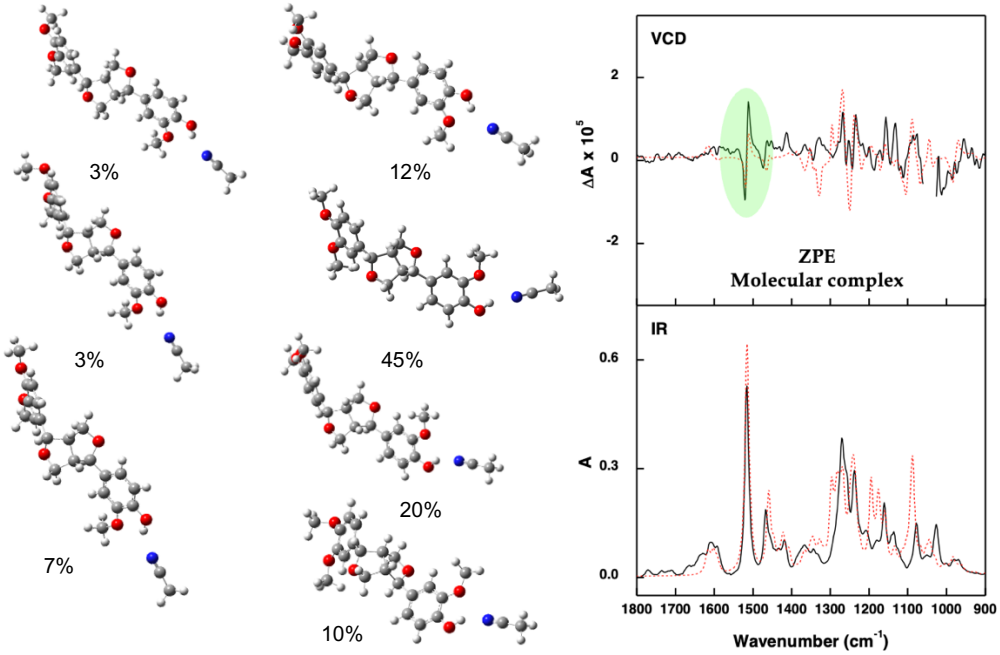


**Figure S7.** (Right) Comparison between experimental IR and VCD spectra of (-)-**1** recorded in MeCN-d3 (black solid trace) with calculated [B3PW91/6-311G(d,p)] data for (7*R*,8*S*,7'*S*,8'*S*)-**1** (red dotted trace) using the micro-solvation approach. Boltzmann weighting (%) based on zero point corrected (ZPE) electronic energies of the molecular complex. The correspondence between experiment and calculations for the 1510 $cm^{-1}$ couplet is highlighted. Gap represents intense solvent absorption. (Left) Lowest-energy molecular complexes of **1** and MeCN molecules.

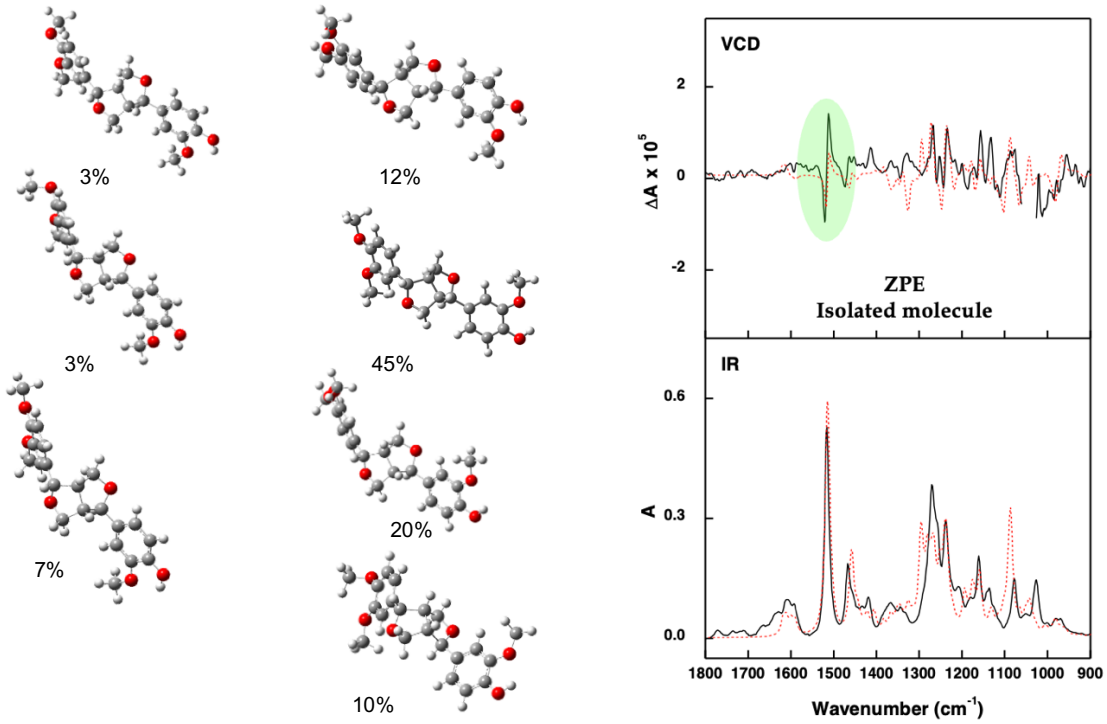


**Figure S8.** (Right) Comparison between experimental IR and VCD spectra of (-)-**1** recorded in MeCN-d3 (black solid trace) with calculated [B3PW91/6-311G(d,p)] data for (7*R*,8*S*,7'*S*,8'*S*)-**1** (red dotted trace) using the micro-solvation approach. Spectra were recalculated after removing explicit solvation. Boltzmann weighting (%) based on zero point corrected electronic energies of the molecular complex. Gap represents intense solvent absorption. The correspondence between experiment and calculations for the 1510 $cm^{-1}$ couplet is highlighted.

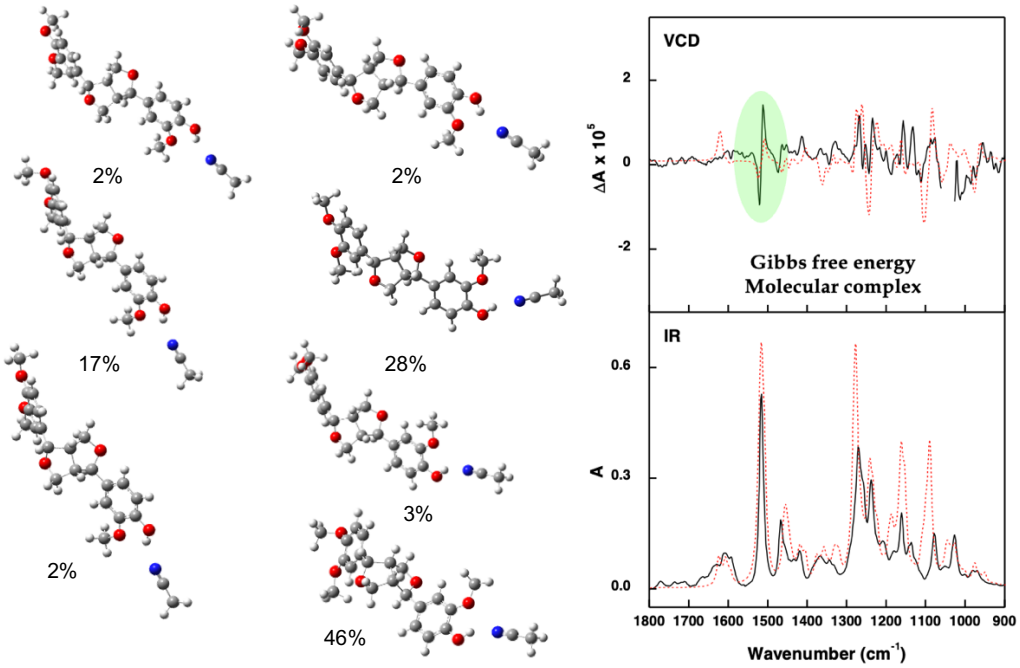


**Figure S9.** (Right) Comparison between experimental IR and VCD spectra of (-)-**1** recorded in MeCN-d3 (black solid trace) with calculated [ωB97XD/6-311G(d,p)] data for (7*R*,8*S*,7'*S*,8'*S*)-**1** (red dotted trace) using the micro-solvation approach. Boltzmann weighting (%) based on Gibbs free energies of the molecular complex. The correspondence between experiment and calculations for the 1510 $cm^{-1}$ couplet is highlighted. Gap represents intense solvent absorption. (Left) Lowest-energy molecular complexes of **1** and MeCN molecules.

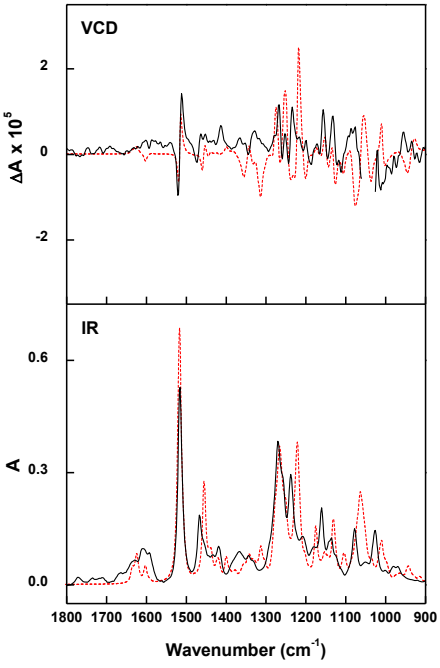


**Figure S10.** Comparison between experimental IR and VCD spectra of (-)-**1** recorded in MeCN-d3 (black solid trace) with calculated [B3PW91/6-311G(d,p)] data for (7*R*,8*S*,7'*S*,8'*S*)-**1** (red dotted trace) using the QM/MM ONIOM geometries. Simple average of snapshots taken over the last 1 ns of the MD simulation. Spectra were recalculated after removing explicit solvation without geometry reoptimization. Gap represents intense solvent absorption.

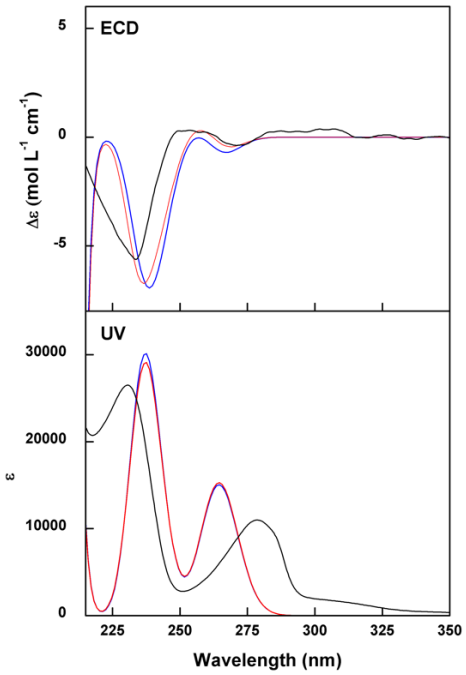


**Figure S11.** Comparison between experimental UV and ECD spectra of (-)-**1** (black solid trace) with calculated [CAM-B3LYP/PCM(MeCN)/TZVP] data for (7*R*,8*S*,7'*S*,8'*S*)-**1** (red and blue traces). Blue trace represents spectra calculated on geometries from the static approach. Red trace represents spectra calculate on geometries from QM/MM method after removal of explicit solvent molecules.

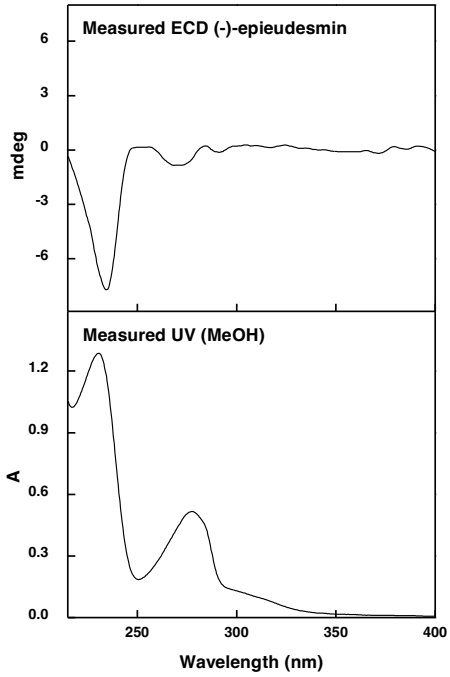


**Figure S12.** Experimental UV and VCD spectra of (-)-**2** in methanol.

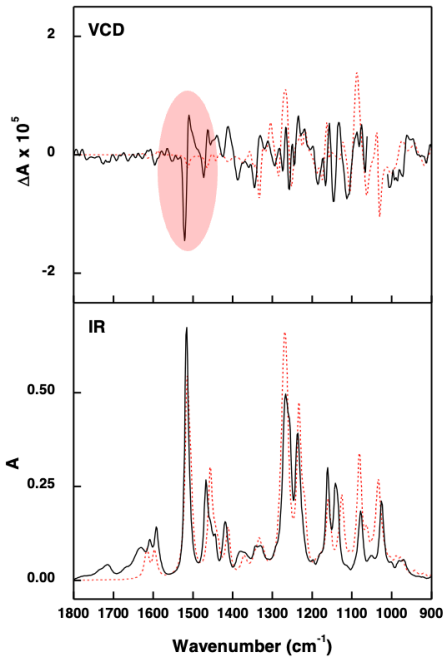


**Figure S13.** Comparison between experimental IR and VCD spectra of (-)-**2** recorded in MeCN-d3 (black solid trace) with calculated [B3PW91/PCM(MeCN)/6-311G(d,p)] data for (7*R*,8*S*,7'*S*,8'*S*)-**2** (red dotted trace). Gap represents intense solvent absorption. The correspondence between experiment and calculations for the 1510 $cm^{-1}$ couplet is highlighted.

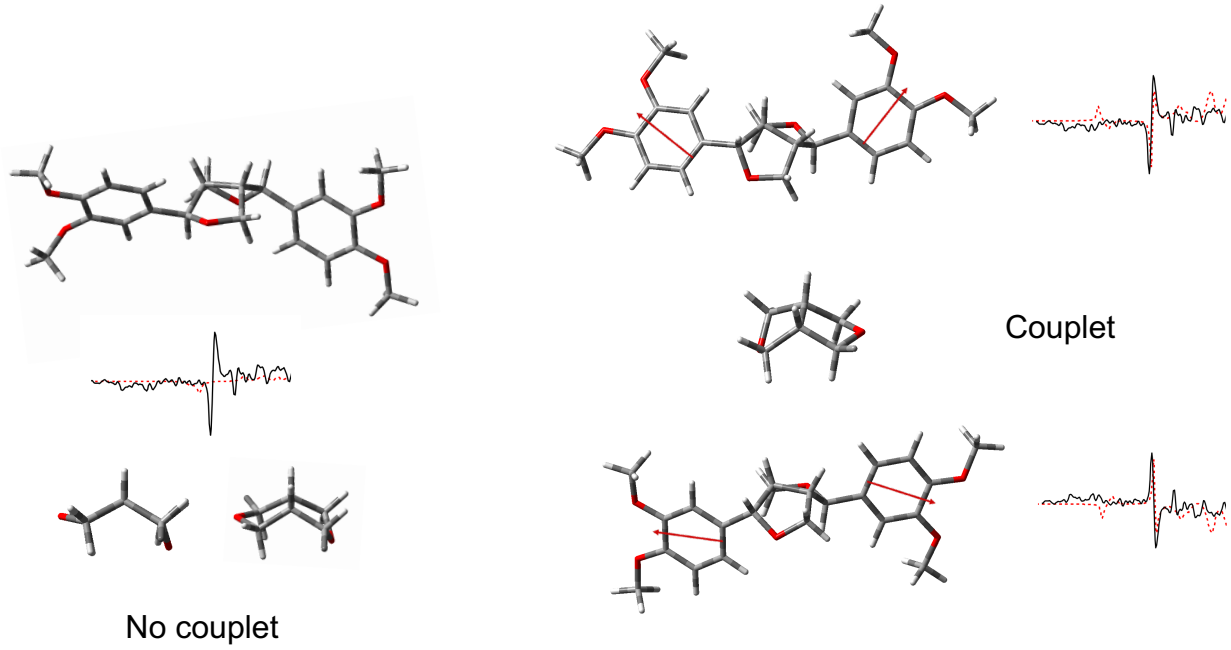


**Figure S14.** Conformational requirements for the couplet signal at 1510 $cm^{-1}$ in (-)-**2**. Aromatic rings omitted for clarity in lateral view of bicyclic core. Red arrows represent dipole moment vectors. Black trace – experimental spectrum; red dotted trace – calculated spectrum.

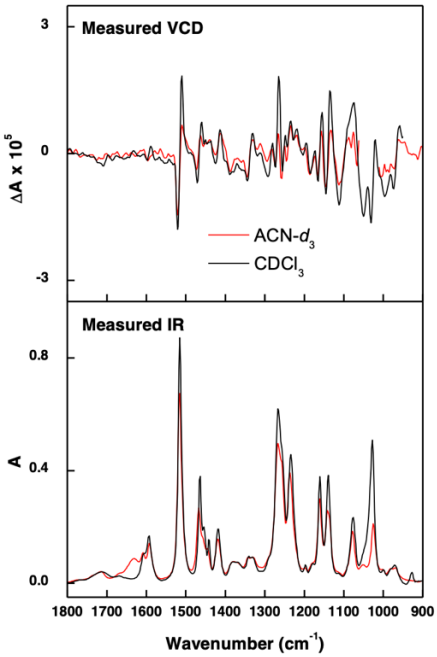


**Figure S15.** Comparison between experimental IR and VCD spectra of (-)-epieudesmin (**2**) in different solvents. Gap represents intense solvent absorption.

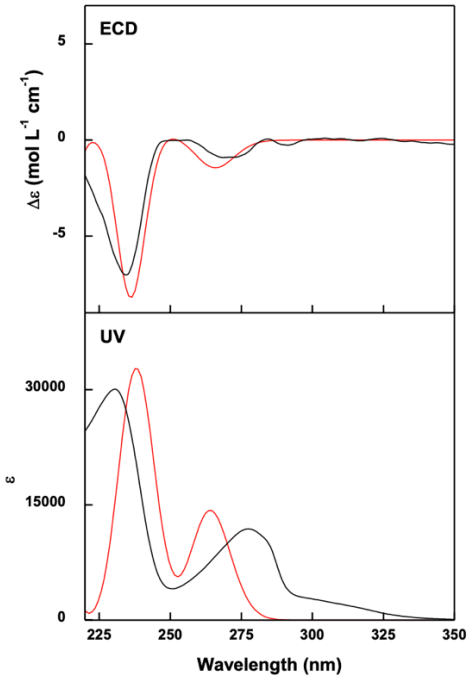


**Figure S16.** Comparison between experimental UV and ECD spectra of (-)-**2** (black trace) with calculated [CAM-B3LYP/PCM(MeCN)/TZVP] data for (7*R*,8*S*,7'*S*,8'*S*)-**2** (red trace).

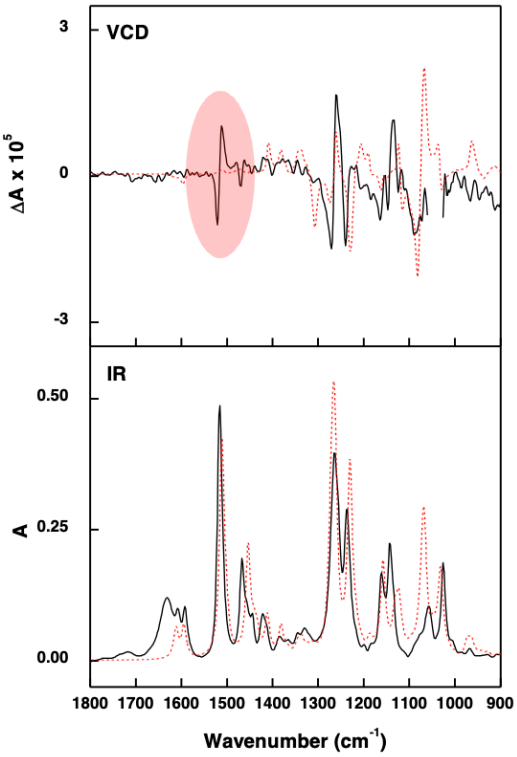


**Figure S17.** Comparison between experimental IR and VCD spectra of (+)-**3** recorded in MeCN-d3 (black solid trace) with calculated [B3PW91/PCM(MeCN)/6-311G(d,p)] data for (7*S*,8*R*,7'*S*,8'*R*)-**3** (red dotted trace). Gap represents intense solvent absorption. The correspondence between experiment and calculations for the 1510 $cm^{-1}$ couplet is highlighted.

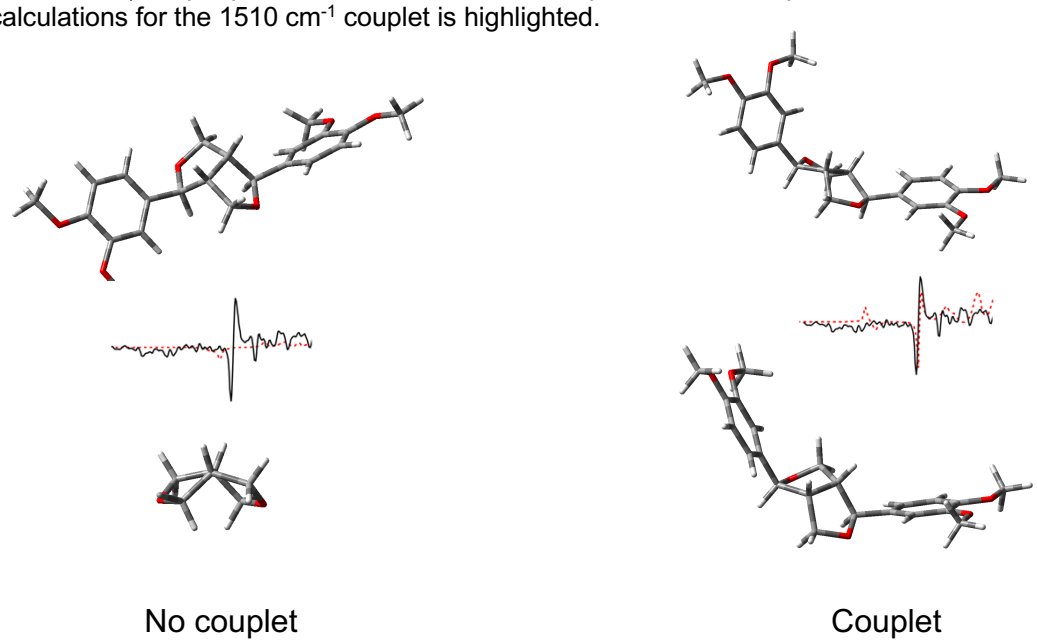


**Figure S18.** Conformational requirements for the couplet signal at 1510 $cm^{-1}$ in (+)-**3**. Black trace – experimental spectrum; red dotted trace – calculated spectrum.

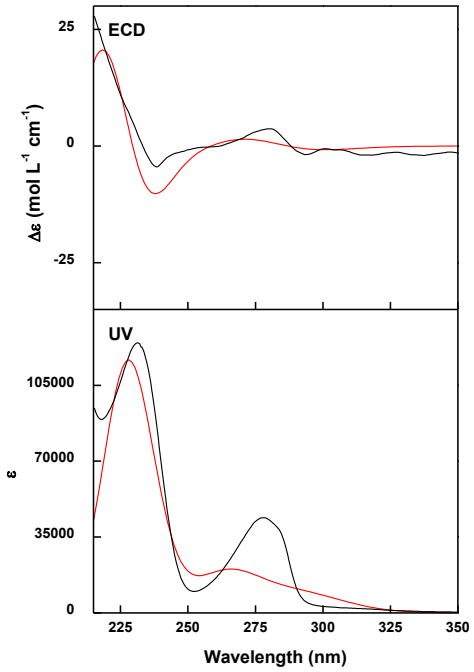


**Figure S19.** Comparison between experimental UV and ECD spectra of (+)-**3** (black trace) with calculated [CAM-B3LYP/PCM(MeCN)/TZVP] data for (7*S*,8*R*,7'*S*,8'*R*)-**3** (red trace).

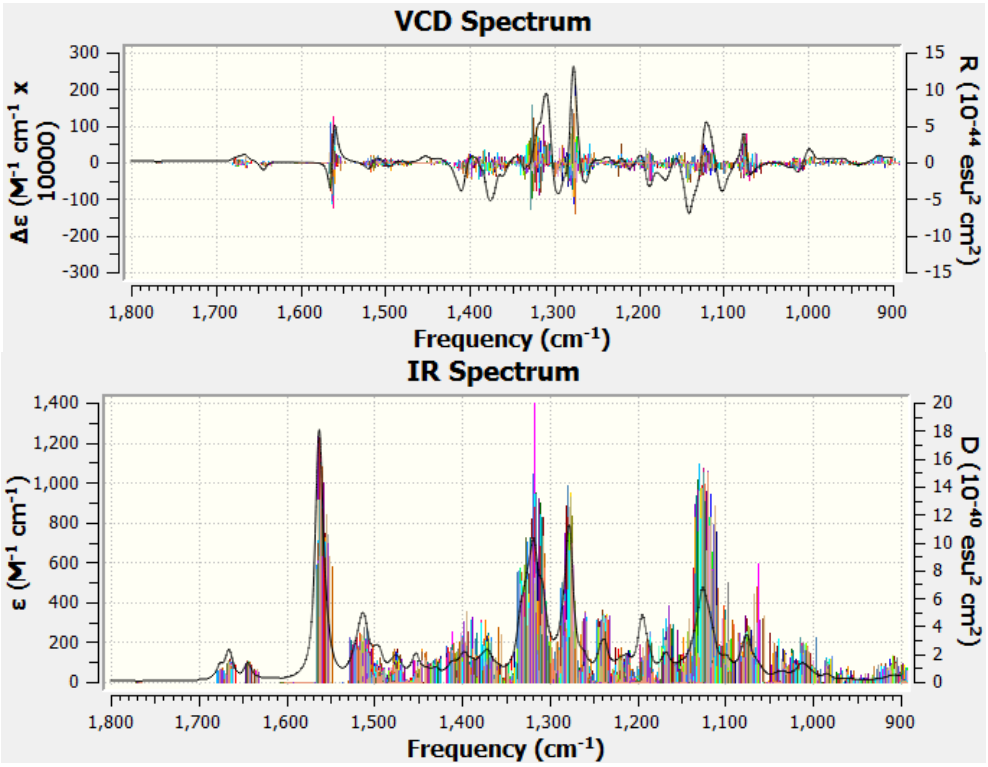


**Figure S20.** IR (bottom) and VCD (top) spectra of individual MD snapshots for (7*R*,8*S*,7'*S*,8'*S*)-**1** at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. Unscaled frequencies.

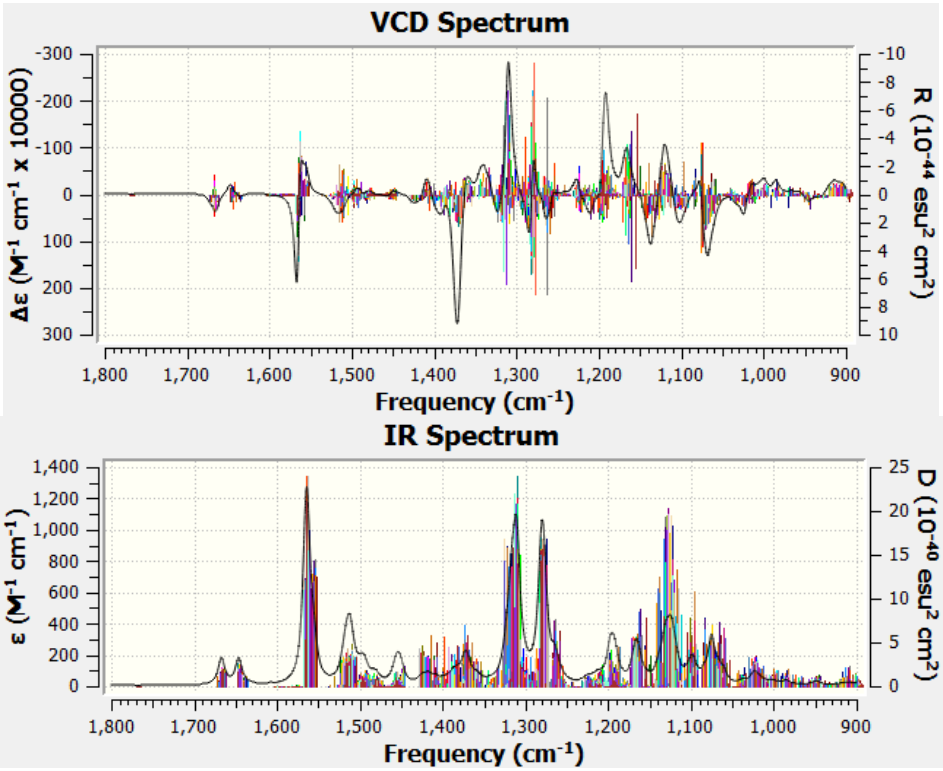


**Figure S21.** IR (bottom) and VCD (top) spectra of individual MD snapshots for (7*R*,8*S*,7'*S*,8'*S*)-**2** (7*S*,8*R*,7'*R*,8'*R* multpl. by -1) at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. Unscaled frequencies.

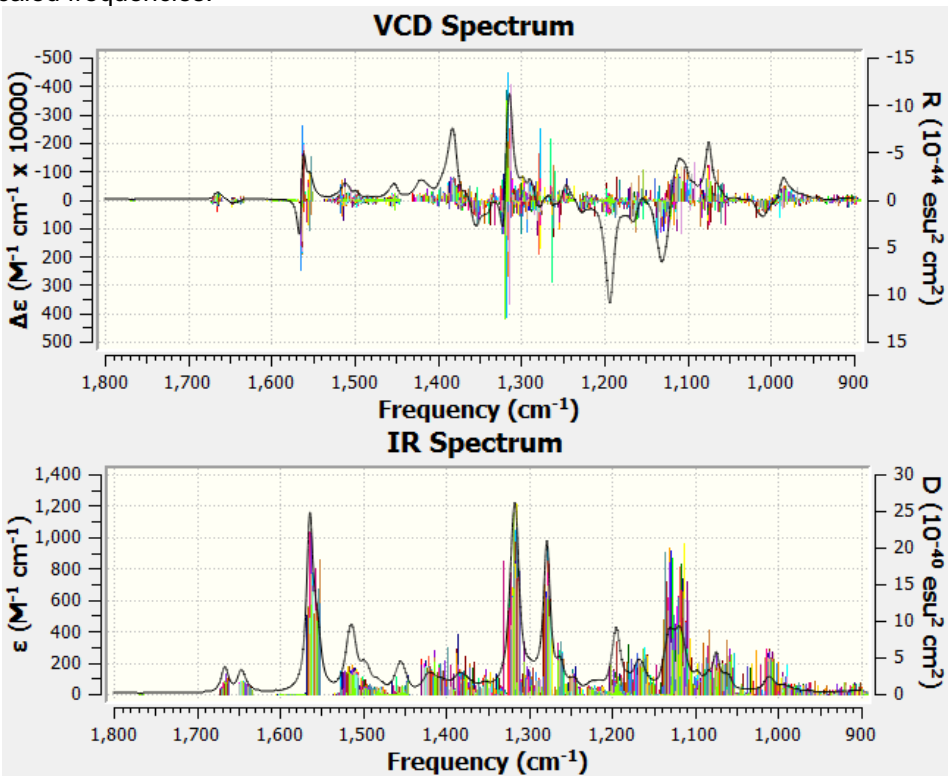


**Figure S22.** IR (bottom) and VCD (top) spectra of individual MD snapshots for (7*S*,8*R*,7'*S*,8'*R*)-**3** (7*R*,8*S*,7'*R*,8'*S* multpl. by -1) at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. Unscaled frequencies.

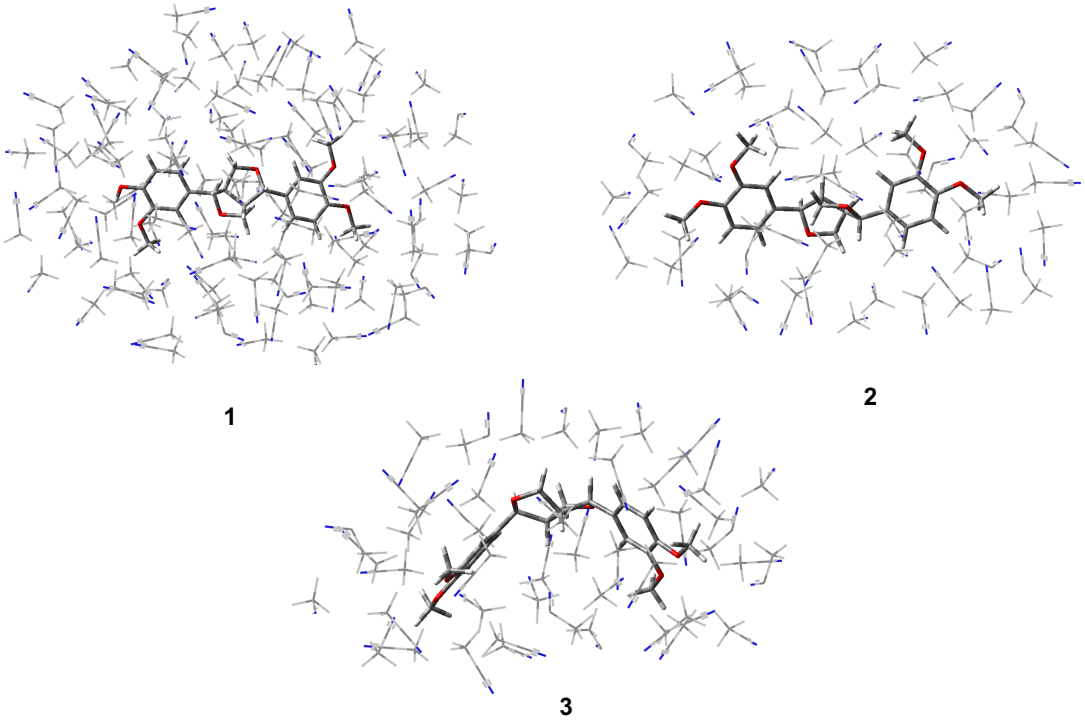


**Figure S23.** Representative snapshots of **1**, **2** and **3** used for IR and VCD calculations at the B3PW91/6-311G(d,p):UFF level using the QM/MM ONIOM approach. See below for cartesian coordinates.

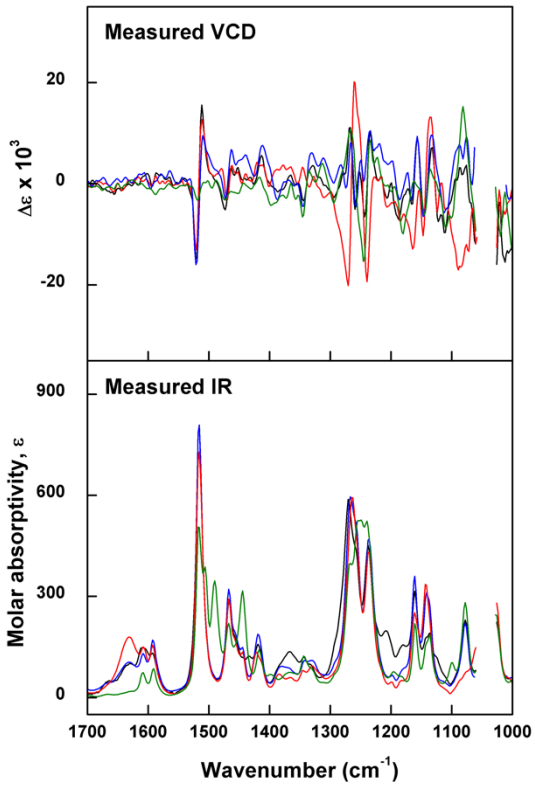


**Figure S24.** Overlaid experimental IR and VCD spectra of (–)-**1** (black trace), (–)-**2** (blue trace), (+)-**3** (red trace) and (–)-fargesin (green trace). Spectra recorded in MeCN-$d_3$.

**Table S1.** Experimental and calculated spectral data for **1** as presented in figure 4 (main text). Experiment: MeCN-d3. Calculations: B3PW91/6-311G(d,p):UFF using the QM/MM ONIOM approach.

| Experiment | | | Calculation | | |
|---|---|---|---|---|---|
| Wn ($cm^{-1}$) | IR, ε ($M^{-1}$ $cm^{-1}$) | VCD, Δε x $10^3$ ($M^{-1}$ $cm^{-1}$) | Wn ($cm^{-1}$) | IR, ε ($M^{-1}$ $cm^{-1}$) | VCD, Δε x $10^3$ ($M^{-1}$ $cm^{-1}$) |
| 900.5 | 13.55184 | -3.04754 | 900.6 | 12.24034 | -0.24366 |
| 902.4 | 12.34803 | -3.68555 | 902.6 | 11.84789 | -0.37142 |
| 904.3 | 11.26624 | -3.40681 | 904.5 | 11.99271 | -0.49095 |
| 906.3 | 10.67915 | -3.23526 | 906.4 | 12.26802 | -0.5938 |
| 908.2 | 10.49288 | -4.09896 | 908.3 | 12.41826 | -0.65889 |
| 910.1 | 10.44446 | -5.212 | 910.3 | 12.32535 | -0.63046 |
| 912.0 | 10.79303 | -6.408 | 912.2 | 12.15026 | -0.52606 |
| 914.0 | 11.65118 | -7.53874 | 913.2 | 12.12098 | -0.46013 |
| 915.9 | 12.80263 | -7.69889 | 915.1 | 12.16449 | -0.29573 |
| 917.8 | 14.22947 | -7.0092 | 917.0 | 12.50844 | -0.09347 |
| 919.8 | 15.43621 | -5.86129 | 919.9 | 14.49106 | 0.32387 |
| 921.7 | 15.60602 | -4.81834 | 921.9 | 16.29522 | 0.66755 |
| 923.6 | 15.0301 | -5.0344 | 923.8 | 17.62607 | 0.93153 |
| 925.5 | 14.57915 | -6.28407 | 925.7 | 18.38524 | 1.051 |
| 927.5 | 14.80565 | -6.63231 | 927.7 | 18.38836 | 1.05192 |
| 929.4 | 15.61802 | -5.31267 | 929.6 | 17.5799 | 1.0017 |
| 931.3 | 16.56991 | -3.31907 | 931.5 | 16.84303 | 0.94212 |
| 933.3 | 17.26232 | -1.76466 | 933.4 | 17.29885 | 0.98116 |
| 935.2 | 17.54726 | -1.23971 | 935.4 | 17.9977 | 1.05738 |
| 937.1 | 17.82732 | -2.12378 | 937.3 | 18.28299 | 1.08275 |
| 939.0 | 18.375 | -3.50162 | 939.2 | 18.86969 | 1.04764 |
| 941.0 | 19.1477 | -4.06469 | 940.2 | 19.46523 | 1.01077 |
| 942.9 | 20.0638 | -4.39107 | 942.1 | 21.73034 | 0.91768 |
| 944.8 | 20.97073 | -4.38962 | 944.1 | 26.02631 | 0.91055 |
| 946.7 | 22.07983 | -3.06849 | 947.0 | 35.32624 | 1.07615 |
| 948.7 | 23.61646 | -1.70097 | 948.9 | 40.57533 | 1.10539 |
| 950.6 | 25.68126 | -0.94378 | 950.8 | 41.80032 | 0.99225 |
| 952.5 | 28.09046 | 0.38924 | 952.8 | 37.97765 | 0.90012 |
| 954.5 | 30.14584 | 1.53433 | 954.7 | 32.19565 | 0.96104 |
| 956.4 | 31.75244 | 1.47215 | 956.6 | 29.3664 | 1.24984 |
| 958.3 | 34.03063 | 0.4107 | 958.5 | 30.64594 | 1.88385 |
| 960.2 | 37.93472 | -1.49657 | 960.5 | 35.59808 | 2.7676 |
| 962.2 | 43.41018 | -3.63371 | 962.4 | 42.76755 | 3.40736 |
| 964.1 | 49.79962 | -5.09466 | 964.3 | 49.78781 | 3.54929 |
| 966.0 | 56.22683 | -5.34358 | 966.3 | 56.32901 | 3.0418 |
| 968.0 | 61.0973 | -5.45303 | 967.2 | 59.80861 | 2.55255 |
| 969.9 | 62.54823 | -6.95754 | 969.2 | 68.09847 | 1.31837 |
| 971.8 | 60.87324 | -8.66782 | 971.1 | 76.99577 | -0.14657 |
| 973.7 | 58.81609 | -8.8992 | 974.0 | 88.45537 | -1.9751 |
| 975.7 | 58.86953 | -7.75306 | 975.9 | 93.56118 | -2.50596 |

| | | | | | |
|---|---|---|---|---|---|
| 977.6 | 61.095 | -6.0311 | 977.8 | 94.30556 | -2.57699 |
| 979.5 | 63.00797 | -5.52369 | 979.8 | 88.92614 | -2.21995 |
| 981.5 | 62.58135 | -7.33314 | 981.7 | 78.12542 | -1.58484 |
| 983.4 | 60.01604 | -9.89535 | 983.6 | 66.33147 | -1.33091 |
| 985.3 | 55.58468 | -10.86818 | 985.6 | 57.32977 | -1.3837 |
| 987.2 | 49.71328 | -10.12051 | 987.5 | 51.64866 | -1.36442 |
| 989.2 | 44.02135 | -9.1907 | 989.4 | 48.19672 | -1.23725 |
| 991.1 | 40.25516 | -8.92088 | 991.4 | 46.25701 | -0.9955 |
| 993.0 | 39.3455 | -8.84657 | 993.3 | 46.85593 | -0.717 |
| 995.0 | 41.18268 | -8.43447 | 994.3 | 48.33355 | -0.60903 |
| 996.9 | 44.64595 | -8.10488 | 996.2 | 52.26778 | -0.42354 |
| 998.8 | 48.07685 | -9.51155 | 998.1 | 55.24556 | -0.25861 |
| 1000.7 | 49.65506 | -11.99883 | 1000.1 | 54.86351 | -0.17168 |
| 1002.7 | 48.99278 | -12.9501 | 1002.9 | 52.12741 | -0.21827 |
| 1004.6 | 47.29025 | -13.26875 | 1004.9 | 49.79987 | -0.24305 |
| 1006.5 | 46.26996 | -13.7334 | 1006.8 | 45.93374 | -0.2487 |
| 1008.5 | 47.1782 | -13.25677 | 1008.7 | 42.2821 | -0.24158 |
| 1010.4 | 49.87569 | -14.06814 | 1010.7 | 39.72863 | -0.23655 |
| 1012.3 | 54.39531 | -15.52477 | 1012.6 | 39.16123 | -0.31702 |
| 1014.2 | 61.85841 | -14.70306 | 1014.5 | 40.66823 | -0.46536 |
| 1016.2 | 74.04682 | -13.96401 | 1016.5 | 45.1946 | -0.67354 |
| 1018.1 | 92.01767 | -10.35948 | 1018.4 | 54.17527 | -0.96704 |
| 1020.0 | 115.1261 | -3.59463 | 1020.3 | 64.81937 | -1.19588 |
| 1021.9 | 142.04543 | -3.74944 | 1021.3 | 70.00955 | -1.24165 |
| 1023.9 | 168.67323 | -9.81213 | 1023.2 | 82.95104 | -1.3224 |
| 1025.8 | 186.11551 | -15.98143 | 1025.1 | 99.31695 | -1.68232 |
| 1027.7 | - | - | 1027.1 | 112.68379 | -2.29905 |
| 1029.7 | - | - | 1029.0 | 123.22097 | -2.89121 |
| 1031.6 | - | - | 1031.9 | 152.05458 | -3.45112 |
| 1033.5 | - | - | 1033.8 | 182.42605 | -1.34277 |
| 1035.4 | - | - | 1035.8 | 216.51818 | 3.47366 |
| 1037.4 | - | - | 1037.7 | 234.08357 | 7.3242 |
| 1039.3 | - | - | 1039.6 | 225.587 | 7.48584 |
| 1041.2 | - | - | 1041.6 | 204.08342 | 4.97293 |
| 1043.2 | - | - | 1043.5 | 175.98413 | 2.51472 |
| 1045.1 | - | - | 1045.4 | 145.46086 | 1.12297 |
| 1047.0 | - | - | 1047.4 | 120.29089 | 0.4159 |
| 1048.9 | - | - | 1048.3 | 110.68316 | 0.06372 |
| 1050.9 | - | - | 1050.2 | 98.03564 | -0.90577 |
| 1052.8 | - | - | 1052.2 | 95.69607 | -1.98454 |
| 1054.7 | - | - | 1054.1 | 100.16868 | -2.86114 |
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| 1058.6 | - | - | 1058.9 | 129.17201 | -5.65634 |
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| 1062.4 | 65.32276 | -11.26608 | 1062.8 | 136.65333 | -7.92508 |
| 1064.4 | 66.42027 | -8.33952 | 1064.7 | 135.83412 | -7.68629 |

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| 1066.3 | 71.84566 | -5.43362 | 1066.7 | 137.39308 | -6.19626 |
| 1068.2 | 83.34409 | -3.79001 | 1068.6 | 146.1558 | -3.67074 |
| 1070.2 | 101.54879 | -3.7047 | 1070.5 | 169.45065 | -0.85944 |
| 1072.1 | 127.31046 | -2.56496 | 1072.4 | 207.50818 | 1.96981 |
| 1074.0 | 157.82491 | 1.17561 | 1074.4 | 250.06377 | 4.89038 |
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| 1077.9 | 191.99294 | 3.23683 | 1077.3 | 314.23526 | 8.51507 |
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| 1081.7 | 152.68864 | 1.85019 | 1081.1 | 393.98717 | 10.99796 |
| 1083.7 | 123.34155 | 1.80482 | 1083.1 | 429.22583 | 10.07832 |
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| 1087.5 | 83.12108 | 3.18628 | 1087.9 | 458.20249 | -0.25159 |
| 1089.4 | 72.05334 | 1.45191 | 1089.8 | 410.61388 | -4.02038 |
| 1091.4 | 63.52098 | 0.70239 | 1091.8 | 353.08491 | -6.28704 |
| 1093.3 | 55.87852 | 1.06201 | 1093.7 | 302.03784 | -7.75785 |
| 1095.2 | 49.16397 | 0.69757 | 1095.6 | 260.71587 | -9.24329 |
| 1097.1 | 43.61511 | -0.61767 | 1097.5 | 220.52456 | -10.9559 |
| 1099.1 | 38.91876 | -2.07817 | 1099.5 | 187.32453 | -13.1016 |
| 1101.0 | 34.34566 | -3.26124 | 1101.4 | 164.08082 | -14.0293 |
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| 1104.9 | 35.8791 | -4.23975 | 1104.3 | 134.33789 | -11.2091 |
| 1106.8 | 41.15527 | -5.48898 | 1106.2 | 120.38688 | -7.97747 |
| 1108.7 | 46.58867 | -7.85062 | 1108.2 | 114.85108 | -5.05161 |
| 1110.6 | 51.50998 | -9.66468 | 1110.1 | 110.77606 | -2.71057 |
| 1112.6 | 55.46168 | -9.65891 | 1112.0 | 103.2172 | -0.73136 |
| 1114.5 | 59.08116 | -7.99463 | 1114.9 | 94.41305 | 0.87584 |
| 1116.4 | 64.23551 | -6.2581 | 1116.9 | 93.86374 | 0.87763 |
| 1118.4 | 71.75359 | -6.14201 | 1118.8 | 96.73845 | 0.0817 |
| 1120.3 | 80.69213 | -6.92632 | 1120.7 | 105.32109 | -0.99227 |
| 1122.2 | 89.74828 | -7.46457 | 1122.6 | 119.96195 | -2.19439 |
| 1124.1 | 97.25472 | -6.59958 | 1124.6 | 136.85467 | -3.49112 |
| 1126.1 | 101.50037 | -3.32779 | 1126.5 | 148.68528 | -4.59911 |
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| 1133.8 | 145.99506 | 7.02234 | 1133.3 | 104.65844 | -3.65661 |
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| 1137.6 | 157.16461 | 2.17432 | 1137.1 | 92.88065 | -2.84745 |
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| 1141.5 | 149.3203 | -2.95158 | 1141.9 | 124.96263 | -4.09877 |
| 1143.4 | 145.76402 | -4.77055 | 1143.9 | 156.44689 | -5.6536 |
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| 1155.0 | 165.34334 | 7.86844 | 1154.5 | 316.09927 | 1.43928 |
| 1156.9 | 203.55386 | 9.15789 | 1156.4 | 261.71362 | 1.94374 |
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| 1160.8 | 263.19702 | 2.74577 | 1160.3 | 160.60651 | 1.09224 |
| 1162.7 | 245.27457 | -1.39763 | 1162.2 | 134.68497 | 0.15499 |
| 1164.6 | 207.02043 | -3.97174 | 1164.2 | 124.41899 | -0.64552 |
| 1166.6 | 171.01967 | -3.99318 | 1166.1 | 126.47893 | -1.19991 |
| 1168.5 | 146.5407 | -2.39045 | 1168.0 | 134.78742 | -1.73375 |
| 1170.4 | 133.76028 | -1.33813 | 1170.9 | 137.98742 | -1.65077 |
| 1172.3 | 128.69438 | -0.9632 | 1172.8 | 134.46876 | -0.66684 |
| 1174.3 | 127.00951 | -1.33745 | 1174.8 | 130.6307 | 0.25475 |
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| 1178.1 | 129.25345 | -2.24713 | 1178.6 | 120.98467 | 0.88568 |
| 1180.1 | 130.51428 | -2.60741 | 1180.6 | 112.74319 | 0.42895 |
| 1182.0 | 128.86411 | -3.59347 | 1181.5 | 109.64583 | 0.09803 |
| 1183.9 | 124.63876 | -5.37378 | 1183.5 | 107.20743 | -0.31764 |
| 1185.8 | 119.31161 | -7.04213 | 1185.4 | 107.89005 | -0.22778 |
| 1187.8 | 113.16808 | -7.07027 | 1187.3 | 113.43093 | 0.1157 |
| 1189.7 | 106.49779 | -6.51751 | 1189.2 | 131.13465 | 0.45266 |
| 1191.6 | 101.24646 | -6.0941 | 1191.2 | 164.22072 | 0.89275 |
| 1193.6 | 100.91085 | -4.9673 | 1193.1 | 199.44398 | 1.35072 |
| 1195.5 | 107.231 | -3.57867 | 1195.0 | 213.48409 | 1.43105 |
| 1197.4 | 117.84177 | -1.58908 | 1197.9 | 203.74321 | 1.09255 |
| 1199.3 | 129.70735 | 0.15979 | 1199.9 | 178.97037 | 0.8394 |
| 1201.3 | 141.37213 | -0.11485 | 1201.8 | 147.25513 | 0.66425 |
| 1203.2 | 151.83047 | -1.51558 | 1203.7 | 120.91521 | 0.51727 |
| 1205.1 | 159.97951 | -2.59769 | 1205.7 | 103.04043 | 0.42973 |
| 1207.1 | 164.70518 | -2.91426 | 1207.6 | 96.8311 | 0.46573 |
| 1209.0 | 165.33835 | -2.38247 | 1208.6 | 97.725 | 0.46612 |
| 1210.9 | 162.40062 | -1.53741 | 1210.5 | 104.36042 | 0.16092 |
| 1212.8 | 157.78612 | -0.46963 | 1212.4 | 114.43676 | -0.51337 |
| 1214.8 | 153.71465 | 0.79723 | 1214.3 | 130.18898 | -1.76194 |
| 1216.7 | 152.07356 | 1.29349 | 1216.3 | 150.49096 | -3.7134 |
| 1218.6 | 154.09071 | 1.00681 | 1218.2 | 165.10433 | -5.25195 |
| 1220.6 | 160.2574 | 0.68295 | 1220.1 | 173.39625 | -5.55097 |
| 1222.5 | 169.65875 | 0.6804 | 1222.1 | 186.49734 | -4.84738 |
| 1224.4 | 179.93018 | 1.37573 | 1224.0 | 217.11241 | -2.40327 |
| 1226.3 | 191.63156 | 2.70548 | 1226.9 | 326.16516 | 5.14201 |
| 1228.3 | 210.31042 | 4.09292 | 1228.8 | 467.89509 | 12.41212 |
| 1230.2 | 240.96365 | 5.94112 | 1230.8 | 655.30515 | 21.17228 |
| 1232.1 | 282.35678 | 8.54668 | 1232.7 | 779.24138 | 26.19502 |
| 1234.1 | 326.25949 | 10.28024 | 1234.6 | 759.92635 | 22.94949 |
| 1236.0 | 361.57416 | 9.14728 | 1235.6 | 708.59028 | 18.56161 |
| 1237.9 | 377.07599 | 4.79171 | 1237.5 | 574.57688 | 7.65546 |
| 1239.8 | 362.23502 | -1.05496 | 1239.4 | 454.62673 | -0.01523 |
| 1241.8 | 321.01178 | -5.46004 | 1241.4 | 365.99172 | -2.93252 |

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| 1243.7 | 275.35358 | -6.54587 | 1243.3 | 301.50144 | -4.01767 |
| 1245.6 | 243.29327 | -4.77053 | 1245.2 | 255.24048 | -5.29845 |
| 1247.5 | 229.32272 | -2.02892 | 1247.2 | 227.91292 | -7.13978 |
| 1249.5 | 232.76929 | 0.45056 | 1249.1 | 213.89754 | -8.37914 |
| 1251.4 | 254.64442 | 2.2705 | 1251.0 | 211.87068 | -8.4778 |
| 1253.3 | 294.26202 | 2.39774 | 1253.9 | 236.51922 | -6.84023 |
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| 1259.1 | 374.66888 | -5.05249 | 1259.7 | 391.69191 | 9.89691 |
| 1261.0 | 383.53415 | -3.62535 | 1261.6 | 471.56553 | 16.11162 |
| 1263.0 | 399.90195 | 1.53748 | 1262.6 | 499.20159 | 17.93132 |
| 1264.9 | 423.34183 | 7.53916 | 1264.5 | 520.8986 | 18.80677 |
| 1266.8 | 454.98853 | 11.11321 | 1266.5 | 539.08859 | 17.52234 |
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| 1270.7 | 489.89981 | 7.88668 | 1270.3 | 672.38588 | 11.3901 |
| 1272.6 | 457.44061 | 4.13162 | 1272.3 | 720.48899 | 10.446 |
| 1274.5 | 405.15948 | 2.14614 | 1274.2 | 695.08696 | 9.61752 |
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| 1280.3 | 274.49445 | 1.84869 | 1281.0 | 522.8431 | 1.09758 |
| 1282.3 | 242.29742 | 0.73104 | 1282.9 | 473.24812 | -0.54634 |
| 1284.2 | 213.00034 | -0.40058 | 1284.8 | 434.3334 | -0.92341 |
| 1286.1 | 187.43333 | -0.91117 | 1286.7 | 393.7034 | -1.36595 |
| 1288.0 | 167.34966 | -1.32111 | 1288.7 | 328.00908 | -1.74525 |
| 1290.0 | 152.59106 | -1.85133 | 1289.6 | 289.83824 | -1.64987 |
| 1291.9 | 140.63788 | -2.38913 | 1291.6 | 220.03158 | -0.92997 |
| 1293.8 | 128.05931 | -2.73127 | 1293.5 | 168.30792 | 0.22583 |
| 1295.8 | 113.10971 | -2.41432 | 1295.4 | 134.23826 | 1.19895 |
| 1297.7 | 97.48571 | -1.82112 | 1297.4 | 111.8942 | 1.59927 |
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| 1301.5 | 73.92268 | -1.31805 | 1301.2 | 87.01621 | 1.19031 |
| 1303.5 | 66.64613 | -1.0973 | 1303.2 | 81.12571 | 0.82609 |
| 1305.4 | 61.37347 | -0.72667 | 1305.1 | 77.52208 | 0.11825 |
| 1307.3 | 57.59697 | -0.35738 | 1307.0 | 77.70059 | -0.76164 |
| 1309.3 | 54.87751 | -0.33318 | 1309.9 | 85.68349 | -2.23117 |
| 1311.2 | 52.76094 | -0.2498 | 1311.8 | 93.54737 | -3.20556 |
| 1313.1 | 51.19708 | 0.2585 | 1313.8 | 100.37343 | -3.7755 |
| 1315.0 | 50.10996 | 0.90061 | 1315.7 | 107.43338 | -3.68048 |
| 1317.0 | 49.56032 | 1.27689 | 1316.7 | 112.45995 | -3.53443 |
| 1318.9 | 49.91428 | 1.26184 | 1318.6 | 127.26084 | -3.77139 |
| 1320.8 | 51.33198 | 1.18702 | 1320.5 | 146.07007 | -5.27495 |
| 1322.7 | 54.27741 | 1.60062 | 1322.5 | 162.45961 | -7.52431 |
| 1324.7 | 59.22147 | 2.50842 | 1324.4 | 165.16332 | -9.16344 |
| 1326.6 | 65.86795 | 3.34396 | 1326.3 | 156.39333 | -10.1416 |
| 1328.5 | 72.92445 | 3.60962 | 1328.3 | 147.00814 | -10.4448 |
| 1330.5 | 78.53312 | 3.46046 | 1330.2 | 138.34732 | -9.65991 |

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| 1332.4 | 81.67515 | 3.18464 | 1332.1 | 127.08317 | -7.55251 |
| 1334.3 | 82.86126 | 2.70868 | 1334.0 | 117.22111 | -4.81154 |
| 1336.2 | 83.64796 | 2.03246 | 1336.9 | 113.35168 | -2.19428 |
| 1338.2 | 86.08099 | 0.89311 | 1338.9 | 117.36599 | -1.511 |
| 1340.1 | 91.45644 | -0.94325 | 1340.8 | 122.40861 | -0.56696 |
| 1342.0 | 97.78961 | -2.66974 | 1342.7 | 124.70037 | 0.60061 |
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| 1345.9 | 97.12516 | -3.11479 | 1345.6 | 138.6294 | 1.36815 |
| 1347.8 | 91.48492 | -2.03393 | 1347.6 | 149.83596 | 1.67293 |
| 1349.7 | 87.85448 | -0.66939 | 1349.5 | 151.43767 | 1.58569 |
| 1351.7 | 87.63065 | 0.07204 | 1351.4 | 142.77821 | 0.98292 |
| 1353.6 | 89.98093 | 0.02206 | 1353.4 | 127.77274 | -0.19661 |
| 1355.5 | 93.6808 | -0.2062 | 1355.3 | 113.5639 | -2.21999 |
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| 1359.4 | 101.57812 | -0.07646 | 1359.1 | 108.27923 | -7.12109 |
| 1361.3 | 105.28819 | 0.45979 | 1361.1 | 107.33574 | -7.81534 |
| 1363.2 | 109.54932 | 1.27065 | 1363.0 | 101.68639 | -7.16118 |
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| 1371.0 | 108.97988 | 0.70719 | 1370.7 | 59.07187 | -2.47357 |
| 1372.9 | 104.77766 | -0.01958 | 1372.7 | 54.16305 | -1.5693 |
| 1374.8 | 100.65696 | -0.63306 | 1374.6 | 55.98836 | -0.94262 |
| 1376.7 | 95.95714 | -0.9813 | 1376.5 | 63.18679 | -0.46297 |
| 1378.7 | 91.09656 | -1.13268 | 1378.4 | 71.90493 | -0.01616 |
| 1380.6 | 86.83716 | -1.19858 | 1380.4 | 76.16082 | 0.36211 |
| 1382.5 | 82.7605 | -1.20366 | 1382.3 | 73.89298 | 0.64478 |
| 1384.5 | 78.24139 | -1.41511 | 1384.2 | 70.33049 | 0.85886 |
| 1386.4 | 73.55123 | -1.65139 | 1386.2 | 69.6085 | 0.99696 |
| 1388.3 | 68.53501 | -1.44803 | 1388.1 | 71.54309 | 1.03423 |
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| 1394.1 | 46.38791 | -0.71157 | 1394.9 | 82.37334 | 0.95875 |
| 1396.0 | 41.14825 | -0.54924 | 1396.8 | 94.70797 | 1.19966 |
| 1397.9 | 37.89286 | -0.34172 | 1397.8 | 104.2546 | 1.31871 |
| 1399.9 | 36.91927 | 0.05968 | 1399.7 | 129.0036 | 1.52786 |
| 1401.8 | 37.12568 | 0.44086 | 1401.6 | 145.09755 | 1.67832 |
| 1403.7 | 39.26091 | 0.72942 | 1403.5 | 137.41814 | 1.58072 |
| 1405.7 | 44.57584 | 1.24872 | 1405.5 | 115.19126 | 1.26421 |
| 1407.6 | 52.80308 | 2.38995 | 1407.4 | 93.04891 | 0.91774 |
| 1409.5 | 64.93549 | 3.91833 | 1409.3 | 78.15699 | 0.6513 |
| 1411.4 | 81.4249 | 5.15724 | 1411.3 | 71.18254 | 0.46225 |
| 1413.4 | 100.451 | 5.60949 | 1413.2 | 70.8549 | 0.31252 |
| 1415.3 | 117.292 | 5.07273 | 1415.1 | 76.66042 | 0.18171 |
| 1417.2 | 128.33768 | 3.83124 | 1417.1 | 88.80611 | 0.04646 |
| 1419.2 | 131.98509 | 2.43749 | 1420.0 | 115.3261 | -0.24592 |

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| 1421.1 | 125.89759 | 1.35553 | 1421.9 | 131.07461 | -0.34682 |
| 1423.0 | 114.15733 | 0.58832 | 1423.8 | 137.29173 | -0.182 |
| 1424.9 | 104.12598 | 0.02108 | 1424.8 | 136.11604 | -0.01266 |
| 1426.9 | 98.20602 | -0.07545 | 1426.7 | 127.82629 | 0.32055 |
| 1428.8 | 96.55506 | 0.57083 | 1428.6 | 116.87391 | 0.39805 |
| 1430.7 | 99.25695 | 1.21175 | 1430.6 | 106.36323 | 0.25416 |
| 1432.7 | 102.41633 | 1.24339 | 1432.5 | 98.39698 | 0.18487 |
| 1434.6 | 102.59612 | 1.05112 | 1434.4 | 96.70391 | 0.10765 |
| 1436.5 | 99.79866 | 0.78689 | 1436.4 | 106.07948 | -0.07827 |
| 1438.4 | 95.66812 | 0.74567 | 1438.3 | 127.47037 | -0.38109 |
| 1440.4 | 94.18577 | 1.05891 | 1440.2 | 155.16579 | -0.78368 |
| 1442.3 | 97.31432 | 1.03791 | 1442.2 | 176.94489 | -1.06148 |
| 1444.2 | 99.66646 | 0.69666 | 1444.1 | 186.21948 | -1.05691 |
| 1446.2 | 99.60055 | 0.79253 | 1446.0 | 185.7433 | -0.78874 |
| 1448.1 | 103.16191 | 1.41546 | 1448.9 | 178.48684 | 0.00829 |
| 1450.0 | 113.45029 | 2.41054 | 1450.8 | 183.17287 | 0.47702 |
| 1451.9 | 126.17843 | 3.22512 | 1451.8 | 191.14042 | 0.63327 |
| 1453.9 | 135.63768 | 3.03255 | 1453.7 | 221.52371 | 0.83219 |
| 1455.8 | 144.26917 | 2.20527 | 1455.7 | 270.55773 | 0.97142 |
| 1457.7 | 153.06413 | 1.67624 | 1457.6 | 320.96252 | 1.13081 |
| 1459.7 | 159.93457 | 1.81686 | 1459.5 | 346.74887 | 0.87121 |
| 1461.6 | 172.71898 | 2.57346 | 1461.5 | 341.32626 | -0.08514 |
| 1463.5 | 199.584 | 3.2911 | 1463.4 | 310.60757 | -1.01804 |
| 1465.4 | 230.87433 | 2.76772 | 1465.3 | 269.63832 | -1.68336 |
| 1467.4 | 238.52652 | 0.66909 | 1467.3 | 228.79354 | -1.78767 |
| 1469.3 | 213.14311 | -1.9346 | 1469.2 | 191.00678 | -1.40234 |
| 1471.2 | 168.19435 | -4.04691 | 1471.1 | 157.41995 | -1.01157 |
| 1473.1 | 126.41836 | -5.14374 | 1473.0 | 130.75099 | -0.66544 |
| 1475.1 | 96.89426 | -4.88492 | 1475.9 | 97.66218 | -0.37603 |
| 1477.0 | 76.16324 | -3.87914 | 1477.9 | 81.26173 | -0.22756 |
| 1478.9 | 62.27174 | -2.86637 | 1478.8 | 75.83511 | -0.15795 |
| 1480.9 | 53.4207 | -1.84201 | 1480.8 | 69.74697 | -0.04322 |
| 1482.8 | 48.24539 | -0.93093 | 1482.7 | 68.44121 | 0.04721 |
| 1484.7 | 45.30732 | -0.28466 | 1484.6 | 70.85779 | 0.1347 |
| 1486.6 | 44.43931 | 0.23212 | 1486.6 | 76.87461 | 0.23171 |
| 1488.6 | 46.37288 | 0.53732 | 1488.5 | 87.17405 | 0.34936 |
| 1490.5 | 51.10649 | 0.72983 | 1490.4 | 103.40283 | 0.508 |
| 1492.4 | 55.78697 | 1.14714 | 1492.4 | 128.60979 | 0.74098 |
| 1494.4 | 61.42448 | 1.66868 | 1494.3 | 166.91608 | 1.09975 |
| 1496.3 | 71.33822 | 1.93879 | 1496.2 | 222.44423 | 1.66163 |
| 1498.2 | 84.92672 | 2.07525 | 1498.1 | 304.00452 | 2.57343 |
| 1500.1 | 102.89185 | 2.59307 | 1500.1 | 417.17828 | 4.01377 |
| 1502.1 | 124.86532 | 3.47916 | 1502.0 | 566.41092 | 6.09632 |
| 1504.0 | 154.43187 | 4.99194 | 1503.9 | 782.61883 | 8.96667 |
| 1505.9 | 206.00772 | 7.29657 | 1505.9 | 1067.32726 | 9.89002 |
| 1507.9 | 275.14774 | 10.31026 | 1507.8 | 1256.10536 | 2.18654 |

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|---|---|---|---|---|---|
| 1509.8 | 358.20636 | 13.82201 | 1509.7 | 1185.54381 | -6.46286 |
| 1511.7 | 469.44293 | 15.5636 | 1511.7 | 910.57651 | -5.95149 |
| 1513.6 | 590.33704 | 12.25756 | 1513.6 | 606.35348 | -3.4425 |
| 1515.6 | 673.75189 | 3.20092 | 1515.5 | 389.94777 | -1.91416 |
| 1517.5 | 654.42053 | -7.60001 | 1517.5 | 261.66923 | -1.09268 |
| 1519.4 | 523.87018 | -14.42276 | 1519.4 | 186.20468 | -0.65773 |
| 1521.4 | 363.45288 | -14.81188 | 1521.3 | 139.40497 | -0.41715 |
| 1523.3 | 253.79094 | -10.62036 | 1523.2 | 108.51041 | -0.27535 |
| 1525.2 | 182.94394 | -5.7256 | 1525.2 | 86.92531 | -0.18773 |
| 1527.1 | 134.07249 | -3.20211 | 1527.1 | 71.20081 | -0.13137 |
| 1529.1 | 98.98112 | -2.42038 | 1529.0 | 59.44556 | -0.09359 |
| 1531.0 | 72.81205 | -1.70364 | 1531.0 | 50.46617 | -0.06811 |
| 1532.9 | 55.35207 | -0.89114 | 1532.9 | 43.48821 | -0.05056 |
| 1534.8 | 44.16912 | 0.07866 | 1534.8 | 37.99113 | -0.03781 |
| 1536.8 | 35.08882 | 0.74783 | 1536.8 | 33.59531 | -0.02856 |
| 1538.7 | 28.49209 | 0.98792 | 1538.7 | 30.0314 | -0.02195 |
| 1540.6 | 25.54791 | 1.10326 | 1540.6 | 27.11164 | -0.01719 |
| 1542.6 | 22.92832 | 0.95887 | 1542.5 | 24.69482 | -0.0138 |
| 1544.5 | 21.05028 | 0.61197 | 1544.5 | 22.66456 | -0.01183 |
| 1546.4 | 19.09705 | 0.34922 | 1546.4 | 20.94277 | -0.01098 |
| 1548.3 | 16.91957 | 0.07295 | 1548.3 | 19.49034 | -0.01054 |
| 1550.3 | 15.11914 | -6.79E-04 | 1550.3 | 18.26945 | -0.0102 |
| 1552.2 | 13.45875 | 0.26959 | 1552.2 | 17.24984 | -0.0103 |
| 1554.1 | 11.50946 | 0.23269 | 1554.1 | 16.41333 | -0.01101 |
| 1556.1 | 8.62021 | -0.16759 | 1556.1 | 15.74592 | -0.01225 |
| 1558.0 | 9.09439 | -0.35139 | 1558.0 | 15.23942 | -0.01398 |
| 1559.9 | 13.08531 | -0.19411 | 1559.9 | 14.89398 | -0.01625 |
| 1561.8 | 13.14293 | 0.38109 | 1561.9 | 14.71988 | -0.01908 |
| 1563.8 | 12.77384 | 1.17694 | 1563.8 | 14.74109 | -0.02244 |
| 1565.7 | 12.90123 | 1.34254 | 1565.7 | 15.00235 | -0.02616 |
| 1567.6 | 13.27707 | 0.96531 | 1567.6 | 15.58376 | -0.02965 |
| 1569.6 | 16.04492 | 0.81259 | 1569.6 | 16.63012 | -0.0313 |
| 1571.5 | 18.21832 | 0.83872 | 1571.5 | 18.40718 | -0.0274 |
| 1573.4 | 19.61162 | 0.98514 | 1573.4 | 21.35804 | -0.01387 |
| 1575.3 | 25.0507 | 1.45493 | 1575.4 | 25.80774 | -0.01442 |
| 1577.3 | 32.18142 | 1.79553 | 1577.3 | 31.06707 | -0.12652 |
| 1579.2 | 38.83056 | 1.68428 | 1579.2 | 37.17037 | -0.35202 |
| 1581.1 | 48.16135 | 1.59743 | 1581.2 | 46.49161 | -0.66736 |
| 1583.1 | 59.07577 | 1.73373 | 1583.1 | 62.36282 | -1.20752 |
| 1585.0 | 69.7963 | 1.99939 | 1584.1 | 73.14019 | -1.53377 |
| 1586.9 | 80.65199 | 2.13823 | 1587.0 | 98.03654 | -2.10295 |
| 1588.8 | 93.25557 | 1.56489 | 1588.9 | 88.37379 | -1.6984 |
| 1590.8 | 105.18612 | 0.40844 | 1590.8 | 66.54008 | -1.03606 |
| 1592.7 | 110.14873 | -0.45333 | 1592.7 | 50.31178 | -0.53625 |
| 1594.6 | 107.80018 | -0.33799 | 1594.7 | 43.03534 | -0.20595 |
| 1596.6 | 104.63988 | 0.61873 | 1596.6 | 42.75321 | 0.04796 |

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|---|---|---|---|---|---|
| 1598.5 | 105.41124 | 1.51954 | 1598.5 | 48.87586 | 0.3013 |
| 1600.4 | 110.20832 | 1.94577 | 1600.5 | 62.66826 | 0.596 |
| 1602.3 | 116.12075 | 2.01532 | 1602.4 | 86.89493 | 0.94975 |
| 1604.3 | 120.21438 | 1.81116 | 1604.3 | 122.53414 | 1.43126 |
| 1606.2 | 122.42463 | 1.59376 | 1606.3 | 154.89274 | 1.9628 |
| 1608.1 | 123.51682 | 1.49322 | 1608.2 | 161.94008 | 2.16955 |
| 1610.0 | 123.74212 | 1.28088 | 1610.1 | 138.78383 | 1.99811 |
| 1612.0 | 121.92665 | 0.73758 | 1611.1 | 123.17055 | 1.89493 |
| 1613.9 | 114.63177 | 0.08143 | 1614.0 | 96.01119 | 1.67363 |
| 1615.8 | 101.62914 | -0.25759 | 1615.9 | 95.981 | 1.5345 |
| 1617.8 | 89.74122 | -0.20841 | 1617.8 | 92.12146 | 1.43751 |
| 1619.7 | 82.14787 | 0.09873 | 1619.8 | 73.886 | 1.21415 |
| 1621.6 | 79.29433 | 0.28321 | 1621.7 | 52.04755 | 0.82549 |
| 1623.5 | 80.4671 | 0.04812 | 1623.6 | 36.10262 | 0.51953 |
| 1625.5 | 82.09895 | -0.31543 | 1625.6 | 26.16972 | 0.35019 |
| 1627.4 | 83.50111 | -0.43678 | 1627.5 | 20.03936 | 0.25222 |
| 1629.3 | 84.6301 | -0.20324 | 1629.4 | 16.06646 | 0.19008 |
| 1631.3 | 83.36643 | -0.01712 | 1631.4 | 13.34169 | 0.14819 |
| 1633.2 | 80.68674 | -0.14383 | 1633.3 | 11.37948 | 0.11864 |
| 1635.1 | 79.58413 | -0.26429 | 1635.2 | 9.90934 | 0.09703 |
| 1637.0 | 77.88659 | -0.53031 | 1637.1 | 8.77205 | 0.08077 |
| 1639.0 | 73.98808 | -0.87378 | 1638.1 | 8.29583 | 0.0741 |
| 1640.9 | 69.26769 | -0.96079 | 1640.0 | 7.48429 | 0.06299 |
| 1642.8 | 63.44296 | -1.26591 | 1642.9 | 6.53038 | 0.05042 |
| 1644.8 | 57.81585 | -1.3828 | 1644.9 | 6.02198 | 0.04398 |
| 1646.7 | 54.17204 | -0.97203 | 1646.8 | 5.58947 | 0.03868 |
| 1648.6 | 49.15911 | -0.89906 | 1648.7 | 5.21723 | 0.03426 |
| 1650.5 | 43.30824 | -0.98072 | 1650.7 | 4.89356 | 0.03055 |
| 1652.5 | 41.96354 | -1.22934 | 1652.6 | 4.60955 | 0.02739 |
| 1654.4 | 42.18645 | -1.97871 | 1654.5 | 4.35834 | 0.02469 |
| 1656.3 | 40.14152 | -2.10274 | 1656.5 | 4.13453 | 0.02236 |
| 1658.3 | 38.87544 | -1.65495 | 1658.4 | 3.93383 | 0.02033 |
| 1660.2 | 38.45308 | -1.73155 | 1660.3 | 3.7528 | 0.01857 |
| 1662.1 | 40.03971 | -1.74496 | 1662.2 | 3.58863 | 0.01701 |
| 1664.0 | 41.60741 | -1.48213 | 1664.2 | 3.43903 | 0.01564 |
| 1666.0 | 40.58072 | -1.4664 | 1665.1 | 3.36908 | 0.01502 |
| 1667.9 | 39.02909 | -1.3744 | 1667.1 | 3.23788 | 0.01387 |
| 1669.8 | 37.56595 | -1.11305 | 1670.0 | 3.06016 | 0.01238 |
| 1671.8 | 33.63433 | -1.02179 | 1671.9 | 2.95269 | 0.01152 |
| 1673.7 | 29.01575 | -1.06524 | 1673.8 | 2.8529 | 0.01073 |
| 1675.6 | 25.62863 | -0.93547 | 1675.8 | 2.75995 | 0.01003 |
| 1677.5 | 21.77616 | -0.64305 | 1677.7 | 2.67314 | 0.00939 |
| 1679.5 | 17.05236 | -0.40594 | 1679.6 | 2.59185 | 0.00881 |
| 1681.4 | 12.60907 | -0.17923 | 1681.6 | 2.51556 | 0.00828 |
| 1683.3 | 11.94922 | -0.00561 | 1683.5 | 2.4438 | 0.00779 |
| 1685.2 | 12.87942 | -0.06437 | 1685.4 | 2.37616 | 0.00735 |

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|---|---|---|---|---|---|
| 1687.2 | 11.0323 | 0.01366 | 1687.3 | 2.31227 | 0.00694 |
| 1689.1 | 10.42669 | 0.40852 | 1689.3 | 2.25183 | 0.00657 |
| 1691.0 | 9.76649 | 0.68369 | 1691.2 | 2.19455 | 0.00622 |
| 1693.0 | 8.23309 | 0.59371 | 1692.2 | 2.16702 | 0.00606 |
| 1694.9 | 9.18372 | 0.27239 | 1694.1 | 2.11403 | 0.00575 |
| 1696.8 | 8.81258 | 0.0758 | 1696.0 | 2.06362 | 0.00546 |
| 1698.7 | 8.99808 | 0.0844 | 1698.9 | 1.99251 | 0.00507 |
| 1700.7 | 13.38677 | -0.01198 | 1700.9 | 1.94789 | 0.00483 |

**Table S2.** Experimental and calculated spectral data for **2** as presented in figure 6 (main text). Experiment: MeCN-d3. Calculations: B3PW91/6-311G(d,p):UFF using the QM/MM ONIOM approach.

| | **Experiment** | | | **Calculation** | |
|---|---|---|---|---|---|
| **Wn ($cm^{-1}$)** | **IR, ε ($M^{-1}$ $cm^{-1}$)** | **VCD, Δε x $10^3$ ($M^{-1}$ $cm^{-1}$)** | **Wn ($cm^{-1}$)** | **IR, ε ($M^{-1}$ $cm^{-1}$)** | **VCD, Δε x $10^3$ ($M^{-1}$ $cm^{-1}$)** |
| 900.5 | 11.62119 | 5.6203 | 900 | 11.70675 | -0.12579 |
| 902.4 | 10.09166 | 6.11789 | 902 | 11.52096 | -0.36895 |
| 904.3 | 8.69421 | 5.95051 | 904 | 11.51117 | -0.48619 |
| 906.3 | 7.57631 | 5.16902 | 907 | 12.15789 | -0.5809 |
| 908.2 | 6.82606 | 4.26069 | 909 | 13.05816 | -0.65031 |
| 910.1 | 6.4301 | 3.29256 | 911 | 14.32602 | -0.74677 |
| 912.0 | 6.27236 | 2.32779 | 913 | 16.67302 | -0.94707 |
| 914.0 | 6.48032 | 2.32135 | 914 | 18.62532 | -1.10082 |
| 915.9 | 7.42818 | 3.13968 | 916 | 24.2889 | -1.41442 |
| 917.8 | 9.08206 | 3.6166 | 918 | 30.50362 | -1.42508 |
| 919.8 | 10.56434 | 3.64703 | 920 | 33.57596 | -1.10643 |
| 921.7 | 11.02627 | 3.6473 | 922 | 32.55461 | -0.72389 |
| 923.6 | 10.7444 | 3.80961 | 923 | 28.73492 | -0.29184 |
| 925.5 | 10.57242 | 3.77523 | 925 | 24.6508 | 0.14633 |
| 927.5 | 10.84683 | 3.53745 | 927 | 21.37784 | 0.47066 |
| 929.4 | 11.44507 | 3.65058 | 929 | 18.62976 | 0.58638 |
| 931.3 | 12.12864 | 3.88163 | 931 | 16.74313 | 0.57368 |
| 933.3 | 12.52641 | 3.89866 | 933 | 16.02093 | 0.60749 |
| 935.2 | 12.51909 | 3.9006 | 935 | 16.14983 | 0.70585 |
| 937.1 | 12.50668 | 4.13723 | 937 | 16.25267 | 0.80636 |
| 939.0 | 12.87151 | 4.72366 | 940 | 15.92819 | 0.743 |
| 941.0 | 13.6412 | 5.44645 | 941 | 15.84875 | 0.66002 |
| 942.9 | 14.77688 | 6.22343 | 943 | 15.97044 | 0.56917 |
| 944.8 | 16.14652 | 6.90151 | 945 | 17.05994 | 0.65545 |
| 946.7 | 17.4627 | 7.08059 | 947 | 19.15954 | 0.84166 |
| 948.7 | 18.62065 | 6.97356 | 949 | 21.94923 | 1.10122 |
| 950.6 | 20.03919 | 6.91348 | 951 | 26.35097 | 1.52375 |
| 952.5 | 22.30618 | 6.87965 | 953 | 33.19997 | 2.20508 |
| 954.5 | 25.43528 | 6.91177 | 954 | 39.40776 | 2.87155 |
| 956.4 | 28.91543 | 7.11823 | 956 | 39.81566 | 2.9601 |

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|---|---|---|---|---|---|
| 958.3 | 32.51427 | 7.37162 | 958 | 35.39757 | 2.51539 |
| 960.2 | 36.73885 | 7.64961 | 960 | 30.57199 | 1.95766 |
| 962.2 | 42.48958 | 7.75939 | 962 | 27.85255 | 1.66161 |
| 964.1 | 50.06886 | 6.91755 | 964 | 28.40104 | 1.87172 |
| 966.0 | 58.0617 | 5.02798 | 966 | 32.19072 | 2.46149 |
| 968.0 | 63.96656 | 2.67125 | 967 | 34.64622 | 2.7994 |
| 969.9 | 66.34174 | 0.46148 | 969 | 39.00886 | 3.29424 |
| 971.8 | 65.50679 | -0.63293 | 972 | 42.8769 | 3.22648 |
| 973.7 | 62.87276 | -0.51588 | 974 | 43.88731 | 2.87701 |
| 975.7 | 60.81668 | -0.23399 | 976 | 43.52488 | 2.4601 |
| 977.6 | 61.14859 | 0.02723 | 978 | 43.47886 | 2.20961 |
| 979.5 | 62.73492 | 0.6634 | 980 | 46.32509 | 2.18869 |
| 981.5 | 62.7862 | 0.7039 | 982 | 51.95364 | 2.31393 |
| 983.4 | 60.34858 | -0.55256 | 984 | 58.70711 | 2.20853 |
| 985.3 | 56.19666 | -1.57545 | 986 | 66.52838 | 1.61485 |
| 987.2 | 50.70525 | -1.42655 | 987 | 76.67499 | 0.50307 |
| 989.2 | 44.81411 | -0.95969 | 989 | 89.16478 | -1.11216 |
| 991.1 | 40.80893 | -1.16171 | 991 | 99.55942 | -3.02772 |
| 993.0 | 40.44332 | -1.48108 | 993 | 99.62215 | -4.21245 |
| 995.0 | 43.82874 | -0.42079 | 994 | 94.46645 | -4.25028 |
| 996.9 | 49.70513 | 0.55904 | 996 | 77.80768 | -3.53628 |
| 998.8 | 55.57384 | -0.59908 | 998 | 62.03726 | -2.72291 |
| 1000.7 | 58.75119 | -2.21037 | 1000 | 53.72746 | -2.34959 |
| 1002.7 | 58.76796 | -2.83652 | 1003 | 51.16472 | -2.0068 |
| 1004.6 | 57.76263 | -2.97428 | 1005 | 50.76163 | -1.52428 |
| 1006.5 | 58.08174 | -3.02822 | 1007 | 48.0207 | -1.02899 |
| 1008.5 | 60.50964 | -2.28699 | 1009 | 43.52621 | -0.72342 |
| 1010.4 | 64.90914 | -0.31475 | 1011 | 39.18125 | -0.64814 |
| 1012.3 | - | - | 1013 | 36.30903 | -0.69515 |
| 1014.2 | - | - | 1015 | 35.07167 | -0.80728 |
| 1016.2 | - | - | 1017 | 35.73096 | -1.00714 |
| 1018.1 | - | - | 1019 | 39.17405 | -1.31214 |
| 1020.0 | - | - | 1020 | 46.24783 | -1.77992 |
| 1021.9 | - | - | 1021 | 51.44637 | -2.09294 |
| 1023.9 | - | - | 1023 | 65.57374 | -2.86962 |
| 1025.8 | - | - | 1025 | 86.21191 | -3.90409 |
| 1027.7 | - | - | 1027 | 112.1152 | -5.32113 |
| 1029.7 | - | - | 1029 | 132.8006 | -6.99396 |
| 1031.6 | - | - | 1031 | 145.6224 | -8.70711 |
| 1033.5 | - | - | 1033 | 161.5162 | -10.9057 |
| 1035.4 | - | - | 1036 | 188.3246 | -13.1256 |
| 1037.4 | - | - | 1038 | 212.2547 | -12.0067 |
| 1039.3 | - | - | 1040 | 259.1597 | -9.33123 |
| 1041.2 | - | - | 1042 | 319.1892 | -4.60808 |
| 1043.2 | - | - | 1044 | 326.8329 | 0.83488 |
| 1045.1 | - | - | 1046 | 264.3004 | 2.80332 |

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|---|---|---|---|---|---|
| 1047.0 | - | - | 1048 | 200.0343 | 1.97017 |
| 1048.9 | - | - | 1049 | 180.4028 | 1.50237 |
| 1050.9 | - | - | 1051 | 158.5427 | 0.93398 |
| 1052.8 | - | - | 1052 | 139.0674 | 0.46362 |
| 1054.7 | - | - | 1054 | 118.4286 | -0.06918 |
| 1056.7 | - | - | 1056 | 107.6699 | -0.69869 |
| 1058.6 | - | - | 1058 | 112.8903 | -1.47399 |
| 1060.5 | - | - | 1060 | 135.2067 | -2.41083 |
| 1062.4 | 60.68814 | 7.10195 | 1062 | 169.2068 | -3.37273 |
| 1064.4 | 62.20008 | 2.24909 | 1064 | 196.6851 | -4.27686 |
| 1066.3 | 69.03925 | -0.16743 | 1066 | 201.1669 | -5.27026 |
| 1068.2 | 82.98269 | 0.38604 | 1069 | 174.5597 | -6.08206 |
| 1070.2 | 105.7306 | 2.53375 | 1071 | 151.9359 | -5.71772 |
| 1072.1 | 137.9143 | 5.6694 | 1073 | 135.3246 | -4.53771 |
| 1074.0 | 175.7731 | 8.50331 | 1075 | 126.3891 | -2.51382 |
| 1075.9 | 208.1145 | 9.37752 | 1076 | 125.6497 | -1.29065 |
| 1077.9 | 220.9022 | 8.17303 | 1078 | 134.5869 | 1.26459 |
| 1079.8 | 208.3697 | 5.88838 | 1080 | 158.7097 | 3.80356 |
| 1081.7 | 178.019 | 4.91858 | 1082 | 198.9361 | 6.44339 |
| 1083.7 | 143.5974 | 5.93417 | 1083 | 253.7023 | 8.93051 |
| 1085.6 | 114.7062 | 7.30571 | 1085 | 315.492 | 10.43547 |
| 1087.5 | 93.88254 | 7.83404 | 1087 | 379.936 | 10.25351 |
| 1089.4 | 79.6173 | 7.33753 | 1089 | 434.5747 | 8.1191 |
| 1091.4 | 69.22295 | 6.80247 | 1091 | 458.9013 | 4.88129 |
| 1093.3 | 60.53227 | 6.39034 | 1093 | 447.9567 | 1.23984 |
| 1095.2 | 52.84116 | 5.4686 | 1095 | 431.9988 | -2.0236 |
| 1097.1 | 46.57856 | 4.26913 | 1097 | 407.115 | -4.71227 |
| 1099.1 | 41.69626 | 2.49634 | 1099 | 352.3557 | -7.05156 |
| 1101.0 | 36.97696 | 0.83866 | 1102 | 268.6514 | -10.2585 |
| 1102.9 | 34.05647 | -1.028 | 1103 | 249.5243 | -10.6781 |
| 1104.9 | 35.23496 | -3.58925 | 1105 | 214.5378 | -9.75771 |
| 1106.8 | 38.22912 | -4.82057 | 1107 | 175.7237 | -7.79563 |
| 1108.7 | 41.38712 | -4.84098 | 1109 | 140.4509 | -5.82967 |
| 1110.6 | 44.41097 | -5.31513 | 1111 | 114.2695 | -3.91298 |
| 1112.6 | 46.87202 | -5.75687 | 1113 | 99.49768 | -2.21852 |
| 1114.5 | 48.3399 | -5.33416 | 1115 | 94.77023 | -0.77505 |
| 1116.4 | 49.19832 | -3.67484 | 1116 | 96.65575 | 0.42367 |
| 1118.4 | 50.38546 | -1.76909 | 1118 | 104.827 | 1.24971 |
| 1120.3 | 52.94468 | -0.16006 | 1120 | 118.9458 | 1.85764 |
| 1122.2 | 57.90205 | 1.35118 | 1122 | 136.3482 | 2.64347 |
| 1124.1 | 66.01644 | 2.3623 | 1124 | 166.1764 | 3.99395 |
| 1126.1 | 78.07287 | 3.69919 | 1126 | 215.3078 | 5.73757 |
| 1128.0 | 96.33724 | 6.10953 | 1127 | 243.5731 | 6.73614 |
| 1129.9 | 125.6577 | 8.55284 | 1129 | 289.9379 | 8.80528 |
| 1131.9 | 171.0503 | 9.5567 | 1132 | 290.0775 | 9.87691 |
| 1133.8 | 227.4945 | 9.61172 | 1134 | 251.1411 | 8.56626 |

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|---|---|---|---|---|---|
| 1135.7 | 271.5935 | 8.70618 | 1136 | 201.5811 | 6.63808 |
| 1137.6 | 289.6286 | 5.43694 | 1138 | 153.0519 | 4.91365 |
| 1139.6 | 301.017 | 0.86851 | 1140 | 119.4905 | 3.87507 |
| 1141.5 | 310.3965 | -2.82206 | 1142 | 102.7966 | 3.59315 |
| 1143.4 | 291.1404 | -5.09776 | 1144 | 98.13599 | 3.96452 |
| 1145.4 | 242.3956 | -6.36987 | 1146 | 101.7449 | 4.75502 |
| 1147.3 | 194.9635 | -6.44505 | 1148 | 112.7385 | 6.01449 |
| 1149.2 | 167.7372 | -4.46945 | 1149 | 133.9097 | 8.2178 |
| 1151.1 | 161.3 | -0.73197 | 1151 | 170.6577 | 11.91397 |
| 1153.1 | 172.2075 | 3.75708 | 1153 | 223.4395 | 17.02083 |
| 1155.0 | 201.364 | 7.80692 | 1154 | 252.875 | 19.53627 |
| 1156.9 | 252.1718 | 9.3651 | 1156 | 305.6661 | 21.69992 |
| 1158.9 | 316.7398 | 7.63533 | 1158 | 338.4296 | 17.83046 |
| 1160.8 | 359.8712 | 4.24037 | 1160 | 342.3617 | 9.79357 |
| 1162.7 | 342.4518 | 0.6962 | 1162 | 310.9288 | 2.87374 |
| 1164.6 | 276.0914 | -2.202 | 1165 | 218.8968 | -0.45989 |
| 1166.6 | 203.9089 | -3.34558 | 1167 | 166.0795 | -0.87356 |
| 1168.5 | 150.5144 | -2.05115 | 1169 | 132.9751 | -1.36947 |
| 1170.4 | 118.494 | 0.55476 | 1171 | 116.6902 | -2.39675 |
| 1172.3 | 101.6054 | 2.19676 | 1173 | 110.7809 | -3.70088 |
| 1174.3 | 93.31759 | 2.01542 | 1175 | 107.7589 | -4.19874 |
| 1176.2 | 89.57216 | 0.99085 | 1177 | 102.6404 | -3.65492 |
| 1178.1 | 87.68741 | -0.08233 | 1179 | 96.08184 | -2.81982 |
| 1180.1 | 85.52103 | -0.92528 | 1180 | 89.71201 | -1.89356 |
| 1182.0 | 81.67785 | -1.76824 | 1181 | 86.63391 | -1.51528 |
| 1183.9 | 75.76968 | -2.81292 | 1183 | 80.98999 | -0.8811 |
| 1185.8 | 68.38387 | -3.15743 | 1185 | 77.16948 | 0.13859 |
| 1187.8 | 60.37841 | -2.74031 | 1187 | 75.60981 | 1.83656 |
| 1189.7 | 53.54335 | -1.94042 | 1189 | 72.84537 | 3.08892 |
| 1191.6 | 50.90298 | -0.30736 | 1191 | 66.57376 | 3.04942 |
| 1193.6 | 54.34429 | 1.80459 | 1193 | 57.32758 | 2.37948 |
| 1195.5 | 61.47346 | 3.56002 | 1195 | 48.64459 | 1.63762 |
| 1197.4 | 66.1655 | 4.49403 | 1198 | 41.31671 | 0.88149 |
| 1199.3 | 65.53114 | 4.47641 | 1200 | 39.68907 | 0.64476 |
| 1201.3 | 62.40321 | 4.15592 | 1202 | 39.7714 | 0.54628 |
| 1203.2 | 60.3201 | 3.92373 | 1204 | 41.16199 | 0.52788 |
| 1205.1 | 60.42762 | 3.78373 | 1206 | 43.60548 | 0.47886 |
| 1207.1 | 62.49995 | 3.95499 | 1208 | 47.09853 | 0.35936 |
| 1209.0 | 66.33244 | 4.25532 | 1209 | 49.37725 | 0.309 |
| 1210.9 | 72.11368 | 4.40311 | 1211 | 55.49397 | 0.26011 |
| 1212.8 | 80.2387 | 4.78391 | 1213 | 64.47254 | 0.27125 |
| 1214.8 | 91.21695 | 5.74418 | 1214 | 77.44365 | 0.32059 |
| 1216.7 | 105.7134 | 6.97546 | 1216 | 95.6332 | 0.34481 |
| 1218.6 | 124.4443 | 7.91171 | 1218 | 118.8942 | -0.16788 |
| 1220.6 | 147.6807 | 7.83597 | 1220 | 148.3983 | -1.69931 |
| 1222.5 | 174.2086 | 7.26627 | 1222 | 184.9477 | -3.56397 |

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| 1224.4 | 202.2831 | 7.12515 | 1224 | 226.408 | -4.76974 |
| 1226.3 | 234.7408 | 6.90749 | 1226 | 263.5547 | -5.22848 |
| 1228.3 | 278.6539 | 6.51101 | 1228 | 281.9191 | -4.18504 |
| 1230.2 | 335.1654 | 7.12594 | 1231 | 305.9305 | -1.34985 |
| 1232.1 | 394.742 | 9.00934 | 1233 | 370.4638 | -0.2988 |
| 1234.1 | 443.4623 | 10.47923 | 1235 | 506.5096 | 0.41617 |
| 1236.0 | 470.7165 | 10.25318 | 1236 | 603.9256 | 0.79952 |
| 1237.9 | 466.5805 | 8.74917 | 1238 | 827.983 | 2.37495 |
| 1239.8 | 421.7695 | 6.58299 | 1240 | 1009.765 | 5.888 |
| 1241.8 | 351.3644 | 3.68535 | 1242 | 1060.074 | 6.57147 |
| 1243.7 | 289.7978 | 0.89947 | 1244 | 913.7875 | -1.34978 |
| 1245.6 | 257.1693 | 0.46387 | 1245 | 671.4388 | -7.66133 |
| 1247.5 | 255.5091 | 2.64678 | 1247 | 475.3567 | -7.59386 |
| 1249.5 | 282.5614 | 4.71905 | 1249 | 351.4796 | -5.57199 |
| 1251.4 | 336.9359 | 4.2544 | 1251 | 279.3508 | -3.27489 |
| 1253.3 | 411.1757 | 1.33106 | 1253 | 241.2809 | -1.48472 |
| 1255.3 | 480.2833 | -2.18293 | 1255 | 226.6299 | -0.34112 |
| 1257.2 | 516.3412 | -4.5134 | 1257 | 229.4789 | 0.93438 |
| 1259.1 | 527.2471 | -4.29409 | 1259 | 249.2956 | 2.7399 |
| 1261.0 | 540.2502 | -0.8701 | 1261 | 287.3791 | 4.93335 |
| 1263.0 | 562.3852 | 4.27051 | 1263 | 349.1376 | 7.41842 |
| 1264.9 | 584.8609 | 7.92528 | 1265 | 450.1072 | 11.14888 |
| 1266.8 | 596.1002 | 8.05742 | 1267 | 617.8888 | 17.24547 |
| 1268.8 | 581.1121 | 5.39447 | 1269 | 854.3327 | 24.6256 |
| 1270.7 | 527.7568 | 1.93245 | 1271 | 1057.594 | 28.26641 |
| 1272.6 | 445.0998 | -0.43546 | 1273 | 1092.316 | 22.08198 |
| 1274.5 | 359.1031 | -0.84702 | 1275 | 1017.913 | 10.8624 |
| 1276.5 | 287.6481 | 0.26189 | 1277 | 916.0222 | 3.74601 |
| 1278.4 | 233.4632 | 1.94412 | 1278 | 777.1372 | 0.33235 |
| 1280.3 | 192.9188 | 3.22625 | 1280 | 628.5101 | -1.93003 |
| 1282.3 | 162.8633 | 3.75402 | 1282 | 501.8613 | -3.47112 |
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| 1288.0 | 119.1235 | 2.18739 | 1288 | 218.6061 | -1.2741 |
| 1290.0 | 113.4039 | 1.43608 | 1289 | 188.8971 | -0.51112 |
| 1291.9 | 107.4672 | 0.64509 | 1291 | 145.1326 | 1.22191 |
| 1293.8 | 99.67972 | 0.11394 | 1294 | 108.0393 | 3.59524 |
| 1295.8 | 90.7177 | 0.2416 | 1296 | 93.15375 | 4.62385 |
| 1297.7 | 82.42881 | 0.76266 | 1298 | 82.84493 | 5.59571 |
| 1299.6 | 75.97302 | 1.2921 | 1300 | 75.52413 | 6.23907 |
| 1301.5 | 71.3685 | 1.92827 | 1302 | 69.89961 | 6.17564 |
| 1303.5 | 68.35699 | 2.6857 | 1304 | 65.69575 | 5.55935 |
| 1305.4 | 66.95383 | 3.4029 | 1306 | 62.28339 | 4.50663 |
| 1307.3 | 66.80045 | 4.07651 | 1308 | 59.94824 | 3.3304 |
| 1309.3 | 67.14239 | 4.73782 | 1310 | 60.35717 | 2.54142 |
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| 1313.1 | 68.31546 | 4.95851 | 1313 | 72.89282 | 2.57352 |
| 1315.0 | 69.44958 | 4.42233 | 1315 | 83.35684 | 3.13372 |
| 1317.0 | 71.82728 | 3.80904 | 1316 | 89.10761 | 3.45953 |
| 1318.9 | 75.98794 | 3.49917 | 1318 | 99.61022 | 3.86415 |
| 1320.8 | 82.1937 | 3.50726 | 1320 | 108.0894 | 3.21604 |
| 1322.7 | 90.32864 | 3.8305 | 1322 | 117.7425 | 0.48786 |
| 1324.7 | 98.97288 | 4.46388 | 1324 | 134.351 | -4.69339 |
| 1326.6 | 105.8854 | 5.19281 | 1327 | 181.0395 | -16.6677 |
| 1328.5 | 109.7319 | 5.84239 | 1329 | 216.4105 | -24.5979 |
| 1330.5 | 110.7666 | 6.13043 | 1331 | 231.7387 | -27.6878 |
| 1332.4 | 110.2188 | 6.03347 | 1333 | 217.4433 | -25.0563 |
| 1334.3 | 108.9569 | 5.44644 | 1335 | 183.9563 | -18.9024 |
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| 1338.2 | 106.8071 | 1.34486 | 1339 | 141.6025 | -7.52306 |
| 1340.1 | 108.1243 | -1.29685 | 1341 | 138.3563 | -4.43237 |
| 1342.0 | 110.3827 | -3.33451 | 1342 | 131.6252 | -2.92699 |
| 1344.0 | 108.4021 | -4.43451 | 1343 | 127.3764 | -2.55717 |
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| 1351.7 | 72.28233 | -0.63199 | 1351 | 84.28472 | -4.28137 |
| 1353.6 | 70.15385 | 0.09024 | 1353 | 75.60692 | -3.9437 |
| 1355.5 | 70.1997 | 0.1257 | 1355 | 70.22984 | -3.36948 |
| 1357.5 | 71.60996 | -0.2339 | 1357 | 69.02845 | -2.65052 |
| 1359.4 | 73.95852 | -0.45715 | 1360 | 64.52087 | -0.83536 |
| 1361.3 | 77.00232 | -0.2479 | 1362 | 64.29979 | 0.64124 |
| 1363.2 | 80.52361 | 0.09155 | 1364 | 70.11136 | 2.15429 |
| 1365.2 | 84.08567 | 0.32036 | 1366 | 76.28044 | 3.1706 |
| 1367.1 | 86.93243 | 0.58214 | 1368 | 79.08525 | 3.01631 |
| 1369.0 | 88.59997 | 0.73216 | 1370 | 81.38711 | 1.90773 |
| 1371.0 | 89.4145 | 0.62737 | 1371 | 83.23332 | 1.22863 |
| 1372.9 | 89.98762 | 0.41696 | 1373 | 88.59404 | -0.03435 |
| 1374.8 | 90.72552 | 0.35576 | 1374 | 92.48015 | -0.9433 |
| 1376.7 | 91.66209 | 0.35658 | 1376 | 93.19953 | -1.48776 |
| 1378.7 | 92.43523 | -0.14328 | 1378 | 89.48233 | -1.70896 |
| 1380.6 | 92.4874 | -1.02367 | 1380 | 85.56983 | -1.81319 |
| 1382.5 | 91.31682 | -1.82863 | 1382 | 82.22547 | -1.81369 |
| 1384.5 | 88.50096 | -2.59727 | 1384 | 73.91376 | -1.60239 |
| 1386.4 | 83.51588 | -3.09992 | 1386 | 62.75063 | -1.29054 |
| 1388.3 | 76.30778 | -3.06557 | 1388 | 51.79182 | -0.92436 |
| 1390.2 | 67.6662 | -2.44952 | 1390 | 43.85525 | -0.60142 |
| 1392.2 | 58.83847 | -1.38587 | 1393 | 40.0137 | -0.31144 |
| 1394.1 | 51.17368 | -0.21326 | 1395 | 41.78026 | -0.1897 |
| 1396.0 | 45.72079 | 1.09011 | 1397 | 47.06534 | -0.08172 |
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| 1399.9 | 42.52921 | 3.38505 | 1400 | 65.11218 | 0.124 |

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| 1401.8 | 44.75137 | 4.01842 | 1402 | 88.7351 | 0.33513 |
| 1403.7 | 49.85971 | 4.61436 | 1404 | 124.2009 | 0.56964 |
| 1405.7 | 58.48489 | 5.48969 | 1406 | 165.6119 | 0.64824 |
| 1407.6 | 71.53163 | 6.52037 | 1407 | 201.9208 | 0.44543 |
| 1409.5 | 90.07463 | 7.25042 | 1409 | 220.7651 | 0.06134 |
| 1411.4 | 114.3202 | 7.57981 | 1411 | 216.1468 | -0.26703 |
| 1413.4 | 142.2493 | 7.46328 | 1413 | 189.7716 | -0.39524 |
| 1415.3 | 168.121 | 6.67174 | 1415 | 151.6081 | -0.39735 |
| 1417.2 | 184.6635 | 5.22528 | 1417 | 114.9896 | -0.31994 |
| 1419.2 | 187.5123 | 3.6464 | 1419 | 87.56029 | -0.22017 |
| 1421.1 | 176.2539 | 2.43464 | 1421 | 70.13453 | -0.14389 |
| 1423.0 | 153.5672 | 1.70008 | 1424 | 57.58174 | -0.06375 |
| 1424.9 | 126.2361 | 1.47348 | 1425 | 56.0121 | -0.04106 |
| 1426.9 | 101.6469 | 1.62797 | 1427 | 56.20609 | 0.01398 |
| 1428.8 | 82.52153 | 2.06632 | 1429 | 60.68343 | 0.12831 |
| 1430.7 | 69.47466 | 2.81425 | 1431 | 69.50992 | 0.3523 |
| 1432.7 | 62.86841 | 3.60297 | 1433 | 82.85664 | 0.61503 |
| 1434.6 | 62.88514 | 4.32073 | 1435 | 97.36125 | 0.77611 |
| 1436.5 | 70.07638 | 5.07592 | 1437 | 107.5574 | 0.69285 |
| 1438.4 | 85.30875 | 5.62827 | 1439 | 111.857 | 0.35975 |
| 1440.4 | 108.9095 | 5.67212 | 1440 | 112.044 | 0.1393 |
| 1442.3 | 134.8117 | 5.34269 | 1442 | 115.7275 | 0.29796 |
| 1444.2 | 148.8334 | 4.99651 | 1444 | 130.1731 | 0.73174 |
| 1446.2 | 146.7756 | 4.80734 | 1446 | 155.3125 | 1.0901 |
| 1448.1 | 142.369 | 4.7249 | 1448 | 183.845 | 1.2245 |
| 1450.0 | 147.1871 | 4.63017 | 1450 | 205.2829 | 1.25496 |
| 1451.9 | 159.5024 | 4.49185 | 1451 | 211.0582 | 1.04052 |
| 1453.9 | 173.839 | 4.11996 | 1453 | 213.8043 | 0.25145 |
| 1455.8 | 187.392 | 3.68548 | 1456 | 207.8358 | -0.15846 |
| 1457.7 | 196.6152 | 4.07354 | 1458 | 217.6806 | -0.42956 |
| 1459.7 | 203.4756 | 5.34283 | 1460 | 250.4494 | -1.01894 |
| 1461.6 | 220.0692 | 6.57802 | 1462 | 303.9876 | -1.71639 |
| 1463.5 | 256.6798 | 6.73698 | 1464 | 377.385 | -2.59172 |
| 1465.4 | 302.6382 | 5.18324 | 1466 | 443.7692 | -3.45084 |
| 1467.4 | 321.3721 | 2.48677 | 1468 | 463.6907 | -3.89615 |
| 1469.3 | 290.4012 | -0.36226 | 1470 | 440.5039 | -3.93869 |
| 1471.2 | 228.9044 | -2.44071 | 1471 | 388.2745 | -3.96334 |
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| 1475.1 | 126.458 | -2.13117 | 1475 | 246.9311 | -3.28886 |
| 1477.0 | 96.89811 | -0.59814 | 1477 | 185.8067 | -2.56931 |
| 1478.9 | 77.7044 | 0.74156 | 1478 | 160.5061 | -2.23051 |
| 1480.9 | 65.95901 | 1.41852 | 1480 | 121.5578 | -1.62312 |
| 1482.8 | 59.37566 | 1.83452 | 1482 | 96.53251 | -1.14169 |
| 1484.7 | 56.39388 | 2.27567 | 1484 | 81.85497 | -0.80213 |
| 1486.6 | 55.9842 | 2.5693 | 1486 | 73.46611 | -0.55024 |
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| 1490.5 | 61.04392 | 2.8129 | 1491 | 68.83565 | -0.11768 |
| 1492.4 | 66.26816 | 3.12888 | 1493 | 72.29534 | -0.00584 |
| 1494.4 | 73.86624 | 3.61195 | 1495 | 78.98942 | 0.10918 |
| 1496.3 | 84.91288 | 4.24644 | 1497 | 89.82319 | 0.26085 |
| 1498.2 | 100.5153 | 4.97369 | 1499 | 106.5268 | 0.48363 |
| 1500.1 | 122.65 | 5.55957 | 1501 | 132.3885 | 0.83785 |
| 1502.1 | 153.2184 | 6.01972 | 1503 | 173.6272 | 1.44076 |
| 1504.0 | 195.3992 | 6.52625 | 1504 | 203.1786 | 1.89559 |
| 1505.9 | 255.2089 | 7.38035 | 1505 | 287.5689 | 3.23789 |
| 1507.9 | 333.2568 | 8.66696 | 1507 | 403.8292 | 5.006 |
| 1509.8 | 431.5012 | 9.52273 | 1509 | 524.1231 | 6.26001 |
| 1511.7 | 557.5932 | 8.17239 | 1511 | 648.1204 | 6.41791 |
| 1513.6 | 700.7724 | 3.21671 | 1513 | 845.8602 | 7.03374 |
| 1515.6 | 808.6866 | -4.10657 | 1515 | 1125.515 | 6.0537 |
| 1517.5 | 785.9183 | -10.9543 | 1517 | 1274.702 | -4.45394 |
| 1519.4 | 619.2576 | -15.3227 | 1519 | 1125.919 | -17.268 |
| 1521.4 | 422.0506 | -15.9874 | 1522 | 659.9108 | -14.4803 |
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| 1525.2 | 186.0234 | -7.32614 | 1526 | 285.4436 | -5.2592 |
| 1527.1 | 130.1513 | -2.18442 | 1528 | 202.6372 | -3.31572 |
| 1529.1 | 96.48034 | 0.43155 | 1530 | 151.013 | -2.21149 |
| 1531.0 | 75.14649 | 0.96379 | 1531 | 132.1651 | -1.83852 |
| 1532.9 | 60.88164 | 0.82435 | 1533 | 103.522 | -1.31112 |
| 1534.8 | 51.15504 | 0.6363 | 1535 | 83.30974 | -0.97301 |
| 1536.8 | 44.18606 | 0.50916 | 1536 | 68.62214 | -0.74636 |
| 1538.7 | 38.49489 | 0.48987 | 1538 | 57.67563 | -0.58772 |
| 1540.6 | 34.30013 | 0.73209 | 1540 | 49.34568 | -0.47374 |
| 1542.6 | 31.24986 | 1.13356 | 1542 | 42.85647 | -0.38926 |
| 1544.5 | 28.74331 | 1.20535 | 1544 | 37.71402 | -0.3251 |
| 1546.4 | 26.69535 | 0.76193 | 1546 | 33.58931 | -0.27567 |
| 1548.3 | 25.02534 | 0.29449 | 1548 | 30.24228 | -0.23697 |
| 1550.3 | 23.64488 | 0.05279 | 1550 | 27.48438 | -0.20619 |
| 1552.2 | 22.5389 | -0.05647 | 1552 | 25.17301 | -0.18124 |
| 1554.1 | 21.62887 | 0.04829 | 1555 | 22.39706 | -0.15196 |
| 1556.1 | 20.92542 | 0.39333 | 1557 | 20.93555 | -0.13676 |
| 1558.0 | 20.26248 | 0.95126 | 1558 | 20.30393 | -0.13022 |
| 1559.9 | 19.74472 | 1.57123 | 1560 | 19.21679 | -0.1189 |
| 1561.8 | 19.56116 | 2.1057 | 1562 | 18.34292 | -0.10961 |
| 1563.8 | 19.76069 | 2.51276 | 1564 | 17.66509 | -0.10209 |
| 1565.7 | 20.45429 | 2.49459 | 1566 | 17.1753 | -0.0962 |
| 1567.6 | 21.79485 | 1.87068 | 1568 | 16.87475 | -0.09193 |
| 1569.6 | 23.94562 | 1.21603 | 1569 | 16.7751 | -0.08945 |
| 1571.5 | 26.98581 | 1.09392 | 1571 | 16.9014 | -0.08917 |
| 1573.4 | 31.13539 | 1.26965 | 1573 | 17.29773 | -0.09199 |
| 1575.3 | 36.91954 | 1.50907 | 1575 | 18.03749 | -0.09964 |
| 1577.3 | 44.45521 | 1.83343 | 1577 | 19.24299 | -0.11563 |

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| 1579.2 | 53.91771 | 1.94322 | 1579 | 21.12332 | -0.14718 |
| 1581.1 | 65.7816 | 1.71382 | 1581 | 24.04791 | -0.20906 |
| 1583.1 | 79.88625 | 1.28549 | 1583 | 28.65773 | -0.32566 |
| 1585.0 | 96.31706 | 0.77837 | 1585 | 35.80607 | -0.49037 |
| 1586.9 | 116.7069 | 0.51488 | 1587 | 45.95027 | -0.52777 |
| 1588.8 | 142.2637 | 0.43188 | 1589 | 59.56537 | -0.29482 |
| 1590.8 | 165.478 | 0.17845 | 1591 | 78.76156 | 0.04848 |
| 1592.7 | 170.6512 | -0.28955 | 1593 | 109.5496 | 0.48197 |
| 1594.6 | 153.7791 | -0.84753 | 1595 | 152.3464 | 1.05534 |
| 1596.6 | 129.9032 | -1.00037 | 1597 | 179.9418 | 1.80183 |
| 1598.5 | 113.1436 | -0.49496 | 1599 | 162.396 | 2.0281 |
| 1600.4 | 106.0733 | 0.16747 | 1601 | 118.4899 | 1.40955 |
| 1602.3 | 106.6514 | 0.84667 | 1602 | 82.81656 | 0.67358 |
| 1604.3 | 113.6342 | 1.67227 | 1604 | 63.79719 | 0.13993 |
| 1606.2 | 123.9874 | 2.17042 | 1606 | 56.87913 | -0.28735 |
| 1608.1 | 130.2488 | 2.06116 | 1608 | 59.30581 | -0.7528 |
| 1610.0 | 126.1415 | 1.8284 | 1610 | 72.03341 | -1.40802 |
| 1612.0 | 114.2791 | 1.78508 | 1611 | 83.40572 | -1.84547 |
| 1613.9 | 102.3581 | 1.90493 | 1613 | 117.9537 | -2.84823 |
| 1615.8 | 94.40605 | 1.8454 | 1615 | 161.7704 | -3.56824 |
| 1617.8 | 91.2926 | 1.41818 | 1618 | 177.2856 | -3.15013 |
| 1619.7 | 91.81873 | 1.16364 | 1620 | 133.6119 | -2.43164 |
| 1621.6 | 94.05269 | 1.04432 | 1622 | 89.18815 | -1.95026 |
| 1623.5 | 97.05444 | 0.65901 | 1624 | 59.39966 | -1.41773 |
| 1625.5 | 100.2239 | 0.2888 | 1626 | 41.25615 | -0.9353 |
| 1627.4 | 102.8854 | 0.18792 | 1628 | 30.33166 | -0.62695 |
| 1629.3 | 104.6018 | 0.31 | 1630 | 23.46566 | -0.44278 |
| 1631.3 | 105.1491 | 0.51087 | 1632 | 18.90264 | -0.32838 |
| 1633.2 | 104.4088 | 0.71509 | 1633 | 15.71379 | -0.25331 |
| 1635.1 | 102.3998 | 1.02045 | 1635 | 13.38992 | -0.20159 |
| 1637.0 | 99.1811 | 1.25653 | 1637 | 11.63688 | -0.16447 |
| 1639.0 | 95.01822 | 1.15565 | 1638 | 10.91566 | -0.14973 |
| 1640.9 | 90.22495 | 0.76923 | 1640 | 9.70549 | -0.12578 |
| 1642.8 | 84.97904 | 0.40516 | 1642 | 8.73298 | -0.1073 |
| 1644.8 | 79.52543 | 0.29869 | 1644 | 7.93661 | -0.09275 |
| 1646.7 | 74.03476 | 0.49341 | 1646 | 7.27384 | -0.08108 |
| 1648.6 | 68.55466 | 0.79263 | 1648 | 6.71445 | -0.07157 |
| 1650.5 | 63.32047 | 0.97282 | 1651 | 6.02277 | -0.0603 |
| 1652.5 | 58.60166 | 0.91721 | 1653 | 5.63768 | -0.05428 |
| 1654.4 | 54.42329 | 0.64925 | 1655 | 5.30037 | -0.04917 |
| 1656.3 | 50.89642 | 0.4165 | 1657 | 5.00251 | -0.04479 |
| 1658.3 | 48.19213 | 0.18598 | 1659 | 4.73758 | -0.04101 |
| 1660.2 | 46.28573 | -0.13283 | 1661 | 4.50037 | -0.03772 |
| 1662.1 | 45.09044 | -0.38905 | 1663 | 4.28673 | -0.03484 |
| 1664.0 | 44.38173 | -0.43461 | 1665 | 4.09328 | -0.0323 |
| 1666.0 | 43.79431 | -0.22257 | 1665 | 4.00324 | -0.03115 |

| | | | | | |
|---|---|---|---|---|---|
| 1667.9 | 42.96638 | 0.13477 | 1667 | 3.83502 | -0.02902 |
| 1669.8 | 41.61509 | 0.57927 | 1669 | 3.68092 | -0.02713 |
| 1671.8 | 39.63741 | 1.0316 | 1671 | 3.53921 | -0.02542 |
| 1673.7 | 37.0954 | 1.24085 | 1673 | 3.40841 | -0.02389 |
| 1675.6 | 34.26928 | 1.10141 | 1675 | 3.28728 | -0.0225 |
| 1677.5 | 31.55337 | 0.82284 | 1677 | 3.17474 | -0.02124 |
| 1679.5 | 29.12985 | 0.6482 | 1679 | 3.06989 | -0.02009 |
| 1681.4 | 27.08578 | 0.54061 | 1681 | 2.97194 | -0.01904 |
| 1683.3 | 25.33617 | 0.56882 | 1684 | 2.83649 | -0.01762 |
| 1685.2 | 23.89885 | 0.65178 | 1686 | 2.75299 | -0.01677 |
| 1687.2 | 22.83108 | 0.414 | 1688 | 2.67437 | -0.01598 |
| 1689.1 | 22.06577 | -0.0473 | 1690 | 2.60018 | -0.01525 |
| 1691.0 | 21.59301 | -0.43652 | 1692 | 2.53004 | -0.01457 |
| 1693.0 | 21.47857 | -0.52846 | 1693 | 2.49639 | -0.01425 |
| 1694.9 | 21.74267 | -0.25327 | 1695 | 2.43173 | -0.01364 |
| 1696.8 | 22.44959 | 0.14486 | 1697 | 2.37035 | -0.01308 |
| 1698.7 | 23.90129 | 0.48207 | 1698 | 2.312 | -0.01255 |
| 1700.7 | 26.3038 | 0.63544 | 1700 | 2.25646 | -0.01205 |

**Table S3.** Experimental and calculated spectral data for **3** as presented in figure 7 (main text). Experiment: MeCN-d3. Calculations: B3PW91/6-311G(d,p):UFF using the QM/MM ONIOM approach.

| | **Experiment** | | | **Calculation** | |
|---|---|---|---|---|---|
| **Wn ($cm^{-1}$)** | **IR, ε ($M^{-1}$ $cm^{-1}$)** | **VCD, Δε x $10^3$ ($M^{-1}$ $cm^{-1}$)** | **Wn ($cm^{-1}$)** | **IR, ε ($M^{-1}$ $cm^{-1}$)** | **VCD, Δε x $10^3$ ($M^{-1}$ $cm^{-1}$)** |
| 900.5 | 21.4046 | -10.949 | 900.7 | 13.98344 | -0.16379 |
| 902.4 | 21.30333 | -11.874 | 902.7 | 13.77057 | -0.04623 |
| 904.3 | 21.27034 | -11.7114 | 904.6 | 13.88329 | 0.04147 |
| 906.3 | 21.90425 | -11.2488 | 906.5 | 13.60742 | 0.1527 |
| 908.2 | 22.40151 | -11.5534 | 908.5 | 13.07081 | 0.32443 |
| 910.1 | 21.17996 | -12.3184 | 910.4 | 13.08683 | 0.50879 |
| 912.0 | 18.24099 | -12.9268 | 912.4 | 13.29832 | 0.62059 |
| 914.0 | 15.16865 | -12.4921 | 913.3 | 13.32927 | 0.65437 |
| 915.9 | 12.89743 | -10.8033 | 915.3 | 13.44958 | 0.76163 |
| 917.8 | 12.12498 | -8.97925 | 917.2 | 13.08293 | 0.8505 |
| 919.8 | 13.16468 | -7.57834 | 919.1 | 12.40327 | 0.88004 |
| 921.7 | 15.09295 | -7.27641 | 921.1 | 12.35323 | 0.89167 |
| 923.6 | 17.2021 | -8.0698 | 924.0 | 13.16548 | 0.8355 |
| 925.5 | 19.12275 | -8.3611 | 925.9 | 14.48265 | 0.82912 |
| 927.5 | 20.40839 | -7.68238 | 927.8 | 16.61403 | 0.92365 |
| 929.4 | 20.82981 | -6.48381 | 929.8 | 19.0004 | 1.11741 |
| 931.3 | 20.60174 | -5.53654 | 931.7 | 20.65646 | 1.35677 |
| 933.3 | 20.01812 | -5.76301 | 933.6 | 22.18117 | 1.64137 |
| 935.2 | 19.32605 | -6.3572 | 935.6 | 23.89174 | 2.07912 |
| 937.1 | 18.92618 | -6.92193 | 937.5 | 25.216 | 2.61159 |

| | | | | | |
|---|---|---|---|---|---|
| 939.0 | 18.61455 | -7.41086 | 939.4 | 25.82814 | 2.87785 |
| 941.0 | 18.00272 | -7.46375 | 940.4 | 25.86943 | 2.8864 |
| 942.9 | 17.21531 | -8.20973 | 942.3 | 25.95532 | 2.90387 |
| 944.8 | 16.59937 | -9.38913 | 944.3 | 26.68074 | 3.10613 |
| 946.7 | 16.41922 | -9.54833 | 946.2 | 27.08396 | 3.40215 |
| 948.7 | 16.45657 | -8.81682 | 948.2 | 27.89417 | 3.94987 |
| 950.6 | 16.44137 | -7.11895 | 950.1 | 30.5912 | 4.86574 |
| 952.5 | 16.42653 | -5.05388 | 952.0 | 35.02063 | 5.78193 |
| 954.5 | 16.62476 | -4.02401 | 954.9 | 42.55676 | 5.60641 |
| 956.4 | 17.76363 | -3.57952 | 956.9 | 48.43179 | 4.52998 |
| 958.3 | 20.76606 | -3.84607 | 958.8 | 54.79508 | 3.10423 |
| 960.2 | 25.62967 | -5.32052 | 960.7 | 60.55269 | 1.49862 |
| 962.2 | 31.19492 | -7.1958 | 962.7 | 64.30662 | 0.11105 |
| 964.1 | 36.17407 | -8.96721 | 964.6 | 65.03707 | -0.67767 |
| 966.0 | 39.9709 | -9.85836 | 966.5 | 65.84729 | -1.06698 |
| 968.0 | 41.60538 | -9.4672 | 967.5 | 66.74295 | -1.21041 |
| 969.9 | 39.87727 | -8.47131 | 969.4 | 68.92665 | -1.59314 |
| 971.8 | 35.39407 | -7.4911 | 971.4 | 73.02316 | -2.17895 |
| 973.7 | 30.2724 | -6.6545 | 973.3 | 78.70099 | -2.79886 |
| 975.7 | 26.22741 | -5.26788 | 975.2 | 86.04283 | -3.51656 |
| 977.6 | 24.05039 | -3.25649 | 977.2 | 92.75559 | -4.18916 |
| 979.5 | 24.03998 | -2.27559 | 979.1 | 93.67415 | -4.35766 |
| 981.5 | 25.85448 | -3.03656 | 981.0 | 87.14065 | -3.88699 |
| 983.4 | 27.98475 | -4.64032 | 983.9 | 79.64789 | -3.23382 |
| 985.3 | 28.94335 | -5.80996 | 985.9 | 77.47234 | -3.36642 |
| 987.2 | 28.81009 | -5.61817 | 987.8 | 70.22268 | -3.2602 |
| 989.2 | 28.20274 | -4.48756 | 989.8 | 59.55321 | -2.49036 |
| 991.1 | 27.54944 | -3.53245 | 991.7 | 52.12121 | -1.71452 |
| 993.0 | 27.65798 | -2.92467 | 993.6 | 46.87998 | -1.19119 |
| 995.0 | 29.55403 | -1.95161 | 994.6 | 43.4902 | -0.95249 |
| 996.9 | 33.9748 | -1.01967 | 996.5 | 36.47294 | -0.46752 |
| 998.8 | 41.19601 | -0.95162 | 998.5 | 32.51917 | -0.0711 |
| 1000.7 | 50.77962 | -1.14846 | 1000.4 | 31.56122 | 0.14166 |
| 1002.7 | 60.41703 | -2.22225 | 1002.3 | 31.82527 | 0.23944 |
| 1004.6 | 67.25904 | -3.90078 | 1004.3 | 32.11432 | 0.31741 |
| 1006.5 | 70.54085 | -4.18319 | 1006.2 | 31.70832 | 0.34206 |
| 1008.5 | 71.46396 | -4.61234 | 1008.1 | 31.74051 | 0.31029 |
| 1010.4 | 72.7713 | -6.57162 | 1010.1 | 33.28064 | 0.2295 |
| 1012.3 | 77.62564 | -7.0886 | 1012.0 | 35.69626 | 0.3141 |
| 1014.2 | 88.70628 | -6.35151 | 1014.9 | 41.98641 | 0.87353 |
| 1016.2 | 108.276 | -7.95474 | 1016.8 | 49.25193 | 1.23658 |
| 1018.1 | 138.3324 | -8.00345 | 1018.8 | 60.78847 | 1.43296 |
| 1020.0 | 182.0941 | -3.50046 | 1020.7 | 79.23071 | 1.71026 |
| 1021.9 | 241.0374 | -1.44167 | 1021.7 | 90.78271 | 1.9574 |
| 1023.9 | 303.7568 | -5.13272 | 1023.6 | 114.4574 | 2.61561 |
| 1025.8 | 336.2549 | -14.8765 | 1025.6 | 129.311 | 3.43419 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 1027.7 | -- | | - | 1027.5 | 132.3867 | 4.24422 |
| 1029.7 | -- | | - | 1029.4 | 134.1651 | 4.85412 |
| 1031.6 | -- | | - | 1031.4 | 141.475 | 5.5813 |
| 1033.5 | -- | | - | 1033.3 | 154.81 | 6.80244 |
| 1035.4 | -- | | - | 1035.2 | 179.5631 | 8.84246 |
| 1037.4 | -- | | - | 1037.2 | 225.7282 | 11.77736 |
| 1039.3 | -- | | - | 1039.1 | 275.4786 | 14.01344 |
| 1041.2 | -- | | - | 1041.0 | 274.9529 | 13.38574 |
| 1043.2 | -- | | - | 1043.9 | 205.7424 | 9.445 |
| 1045.1 | -- | | - | 1045.9 | 182.1779 | 7.34841 |
| 1047.0 | -- | | - | 1047.8 | 172.9658 | 6.00829 |
| 1048.9 | -- | | - | 1048.8 | 165.4815 | 5.49067 |
| 1050.9 | -- | | - | 1050.7 | 142.6161 | 4.5478 |
| 1052.8 | -- | | - | 1052.6 | 116.8409 | 4.03324 |
| 1054.7 | -- | | - | 1054.6 | 100.7292 | 4.14173 |
| 1056.7 | -- | | - | 1056.5 | 100.089 | 4.94373 |
| 1058.6 | -- | | -12.4766 | 1058.4 | 114.3783 | 6.38802 |
| 1060.5 | | 177.6809 | -13.9474 | 1060.4 | 136.2857 | 8.11664 |
| 1062.4 | | 163.7025 | -10.6879 | 1062.3 | 148.1843 | 10.35305 |
| 1064.4 | | 146.1307 | -7.00328 | 1064.3 | 142.5978 | 13.13441 |
| 1066.3 | | 127.2993 | -5.66337 | 1066.2 | 132.7311 | 14.79756 |
| 1068.2 | | 111.6552 | -8.10155 | 1068.1 | 128.2694 | 14.16789 |
| 1070.2 | | 101.8786 | -12.7774 | 1070.1 | 135.3175 | 13.39928 |
| 1072.1 | | 96.92404 | -15.7654 | 1073.0 | 182.4032 | 14.67821 |
| 1074.0 | | 94.47342 | -15.4062 | 1074.9 | 237.5768 | 15.33191 |
| 1075.9 | | 92.17092 | -14.1341 | 1075.9 | 269.066 | 15.23804 |
| 1077.9 | | 87.79427 | -14.8306 | 1077.8 | 333.885 | 14.2589 |
| 1079.8 | | 81.00926 | -16.7947 | 1079.7 | 385.8694 | 12.98556 |
| 1081.7 | | 73.55084 | -18.2519 | 1081.7 | 409.5591 | 10.59316 |
| 1083.7 | | 67.70932 | -19.226 | 1083.6 | 410.5401 | 5.02115 |
| 1085.6 | | 64.04575 | -19.4054 | 1085.5 | 412.8586 | -3.32398 |
| 1087.5 | | 60.40271 | -19.2476 | 1087.5 | 425.5592 | -12.4818 |
| 1089.4 | | 54.37208 | -20.0649 | 1089.4 | 446.2225 | -19.9444 |
| 1091.4 | | 46.02973 | -19.1758 | 1091.3 | 444.8753 | -23.3105 |
| 1093.3 | | 38.01473 | -16.0956 | 1093.3 | 431.8803 | -24.1402 |
| 1095.2 | | 31.91673 | -14.4777 | 1095.2 | 421.4499 | -24.4293 |
| 1097.1 | | 26.91477 | -13.6741 | 1097.1 | 404.3405 | -24.1307 |
| 1099.1 | | 22.20246 | -12.3652 | 1099.1 | 374.7792 | -22.6623 |
| 1101.0 | | 16.72768 | -10.8752 | 1101.0 | 309.4773 | -18.1437 |
| 1102.9 | | 14.04738 | -8.53566 | 1103.0 | 226.0178 | -11.939 |
| 1104.9 | | 17.54713 | -6.61245 | 1104.9 | 163.6691 | -7.39444 |
| 1106.8 | | 22.46694 | -5.92172 | 1106.8 | 127.8367 | -4.83655 |
| 1108.7 | | 26.17676 | -5.69002 | 1108.8 | 108.8004 | -3.25044 |
| 1110.6 | | 29.20322 | -6.15333 | 1110.7 | 99.11238 | -2.0643 |
| 1112.6 | | 32.29582 | -5.18148 | 1112.6 | 97.22367 | -1.11623 |
| 1114.5 | | 35.32683 | -1.97544 | 1114.6 | 101.1205 | -0.23804 |

| | | | | | |
|---|---|---|---|---|---|
| 1116.4 | 37.97011 | 0.12883 | 1116.5 | 106.7378 | 0.36026 |
| 1118.4 | 41.03835 | 0.09738 | 1118.4 | 113.7412 | 0.53482 |
| 1120.3 | 45.48516 | -1.61896 | 1120.4 | 129.1018 | 0.66562 |
| 1122.2 | 51.83884 | -4.95065 | 1122.3 | 153.8826 | 0.6035 |
| 1124.1 | 61.24263 | -6.69662 | 1124.2 | 180.3873 | -0.00544 |
| 1126.1 | 74.61487 | -4.44822 | 1126.2 | 202.5704 | -1.1895 |
| 1128.0 | 93.83921 | 0.58718 | 1127.1 | 211.9193 | -1.78609 |
| 1129.9 | 123.9203 | 7.17868 | 1129.1 | 225.3899 | -2.67719 |
| 1131.9 | 169.4001 | 13.04693 | 1132.0 | 213.6822 | -3.73764 |
| 1133.8 | 224.5442 | 15.448 | 1133.9 | 184.1943 | -3.43664 |
| 1135.7 | 271.9232 | 15.50507 | 1135.8 | 149.7253 | -3.14273 |
| 1137.6 | 308.9173 | 14.67492 | 1137.8 | 123.5875 | -3.31196 |
| 1139.6 | 353.4418 | 11.65622 | 1139.7 | 110.6962 | -3.78419 |
| 1141.5 | 398.3778 | 5.56908 | 1141.7 | 108.5263 | -4.46643 |
| 1143.4 | 403.6868 | -2.43822 | 1143.6 | 116.2283 | -5.53774 |
| 1145.4 | 354.9986 | -9.42288 | 1145.5 | 133.5673 | -7.3539 |
| 1147.3 | 286.1465 | -12.0996 | 1147.5 | 157.8951 | -9.9274 |
| 1149.2 | 235.3179 | -9.45668 | 1149.4 | 193.8105 | -13.5056 |
| 1151.1 | 215.1285 | -4.39323 | 1151.3 | 247.12 | -18.7677 |
| 1153.1 | 218.5382 | -1.45871 | 1153.3 | 313.6463 | -24.9251 |
| 1155.0 | 234.2681 | -1.69581 | 1154.2 | 347.183 | -27.2317 |
| 1156.9 | 256.5576 | -4.07021 | 1156.2 | 392.4375 | -28.2389 |
| 1158.9 | 283.2331 | -8.47037 | 1158.1 | 384.1153 | -24.6035 |
| 1160.8 | 301.9322 | -12.628 | 1160.0 | 329.2125 | -19.2937 |
| 1162.7 | 291.4093 | -14.6549 | 1162.9 | 224.1326 | -11.8153 |
| 1164.6 | 246.6485 | -15.1731 | 1164.9 | 166.9412 | -8.20454 |
| 1166.6 | 187.125 | -13.804 | 1166.8 | 127.7464 | -5.64211 |
| 1168.5 | 135.3919 | -11.4718 | 1168.7 | 104.4113 | -4.07215 |
| 1170.4 | 100.4175 | -10.2119 | 1170.7 | 92.38391 | -3.07109 |
| 1172.3 | 80.00856 | -9.26515 | 1172.6 | 87.48208 | -2.45388 |
| 1174.3 | 68.97675 | -8.41791 | 1174.5 | 86.82161 | -2.18299 |
| 1176.2 | 63.29134 | -7.81327 | 1176.5 | 85.90321 | -2.26521 |
| 1178.1 | 60.67643 | -7.06049 | 1178.4 | 84.16704 | -3.00132 |
| 1180.1 | 60.04206 | -7.07486 | 1180.4 | 83.50062 | -4.36862 |
| 1182.0 | 60.51485 | -7.88393 | 1181.3 | 83.79583 | -5.00398 |
| 1183.9 | 59.7989 | -8.75661 | 1183.3 | 85.27835 | -5.56502 |
| 1185.8 | 55.56858 | -8.60525 | 1185.2 | 85.24621 | -5.36473 |
| 1187.8 | 47.93154 | -6.96193 | 1187.1 | 80.70712 | -4.83182 |
| 1189.7 | 39.55789 | -5.48173 | 1189.1 | 71.98052 | -4.13491 |
| 1191.6 | 34.66012 | -4.74533 | 1192.0 | 57.79889 | -2.35619 |
| 1193.6 | 36.58431 | -4.11542 | 1193.9 | 52.72213 | -1.10585 |
| 1195.5 | 44.65887 | -4.27061 | 1195.8 | 52.3283 | -0.11685 |
| 1197.4 | 52.75526 | -4.49464 | 1197.8 | 56.26866 | 0.67439 |
| 1199.3 | 55.52492 | -4.40585 | 1199.7 | 65.58514 | 1.63937 |
| 1201.3 | 53.16189 | -4.77417 | 1201.6 | 81.03568 | 2.96688 |
| 1203.2 | 49.53444 | -5.08273 | 1203.6 | 98.43517 | 3.96928 |

| | | | | | |
|---|---|---|---|---|---|
| 1205.1 | 48.07777 | -5.25569 | 1205.5 | 108.9094 | 3.8368 |
| 1207.1 | 49.98864 | -5.46648 | 1207.4 | 110.5992 | 2.98676 |
| 1209.0 | 55.47494 | -4.91934 | 1208.4 | 110.6311 | 2.52895 |
| 1210.9 | 64.55854 | -3.25145 | 1210.3 | 112.0394 | 1.33976 |
| 1212.8 | 77.01303 | -0.8347 | 1212.3 | 115.1905 | -0.08918 |
| 1214.8 | 91.40708 | 1.37885 | 1214.2 | 123.0682 | -1.37717 |
| 1216.7 | 105.2958 | 1.8812 | 1216.1 | 139.3226 | -1.86547 |
| 1218.6 | 118.0589 | 1.08729 | 1218.1 | 164.2632 | -1.06123 |
| 1220.6 | 132.7113 | 0.62276 | 1220.0 | 198.5809 | 0.68378 |
| 1222.5 | 153.3574 | 0.71417 | 1222.9 | 239.7062 | 2.06492 |
| 1224.4 | 183.115 | 1.02168 | 1224.9 | 248.8147 | 1.57062 |
| 1226.3 | 225.0183 | 1.53134 | 1226.8 | 261.0478 | 0.93292 |
| 1228.3 | 280.2184 | 1.49065 | 1228.7 | 296.8237 | 0.10513 |
| 1230.2 | 345.305 | 0.63836 | 1230.7 | 382.7433 | -1.24507 |
| 1232.1 | 413.6291 | -1.65029 | 1232.6 | 549.2519 | -2.74475 |
| 1234.1 | 476.1586 | -6.91242 | 1234.5 | 779.6911 | -4.28349 |
| 1236.0 | 517.5845 | -14.0745 | 1235.5 | 875.7932 | -5.0758 |
| 1237.9 | 517.9751 | -20.2449 | 1237.4 | 911.7998 | -6.02987 |
| 1239.8 | 471.179 | -22.7987 | 1239.4 | 758.7649 | -4.74554 |
| 1241.8 | 399.6381 | -20.234 | 1241.3 | 556.5128 | -1.44869 |
| 1243.7 | 337.1074 | -13.8596 | 1243.2 | 395.5475 | 1.3 |
| 1245.6 | 303.408 | -6.16287 | 1245.2 | 301.58 | 3.47823 |
| 1247.5 | 302.6751 | 1.23726 | 1247.1 | 253.6467 | 5.91259 |
| 1249.5 | 333.1981 | 7.47341 | 1249.0 | 229.2717 | 7.52118 |
| 1251.4 | 390.7643 | 12.20244 | 1251.9 | 215.3221 | 8.34258 |
| 1253.3 | 463.8909 | 14.76384 | 1253.9 | 216.708 | 7.68973 |
| 1255.3 | 531.8488 | 16.28726 | 1255.8 | 223.0746 | 6.5059 |
| 1257.2 | 581.6762 | 19.57416 | 1257.8 | 231.4046 | 6.21113 |
| 1259.1 | 624.0587 | 23.49281 | 1259.7 | 245.2245 | 7.16504 |
| 1261.0 | 671.9054 | 23.70726 | 1261.6 | 276.5355 | 8.35782 |
| 1263.0 | 711.2594 | 16.98296 | 1262.6 | 301.2068 | 8.88549 |
| 1264.9 | 712.0449 | 3.37239 | 1264.5 | 367.0158 | 9.97983 |
| 1266.8 | 665.675 | -11.6932 | 1266.5 | 465.9986 | 11.78434 |
| 1268.8 | 591.5047 | -21.3031 | 1268.4 | 628.6982 | 15.4007 |
| 1270.7 | 510.3357 | -23.7181 | 1270.3 | 852.7734 | 19.40951 |
| 1272.6 | 431.8475 | -22.2374 | 1272.3 | 1058.218 | 20.23849 |
| 1274.5 | 359.6385 | -19.9589 | 1274.2 | 1131.229 | 16.66096 |
| 1276.5 | 296.2982 | -17.8877 | 1276.1 | 1071.201 | 7.92804 |
| 1278.4 | 243.6125 | -15.9805 | 1278.1 | 931.1308 | -1.63585 |
| 1280.3 | 201.7799 | -14.13 | 1280.0 | 733.3881 | -4.96147 |
| 1282.3 | 169.6145 | -12.3504 | 1282.9 | 461.6893 | -3.31279 |
| 1284.2 | 145.3397 | -10.8653 | 1284.8 | 332.5084 | -2.33414 |
| 1286.1 | 127.4693 | -9.86766 | 1286.8 | 241.929 | -1.80113 |
| 1288.0 | 114.447 | -9.08352 | 1288.7 | 183.417 | -2.13339 |
| 1290.0 | 104.5248 | -8.01547 | 1289.7 | 163.4501 | -2.65383 |
| 1291.9 | 96.42857 | -6.52063 | 1291.6 | 136.4502 | -4.35092 |

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| 1293.8 | 89.44945 | -4.85309 | 1293.5 | 118.9814 | -6.39271 |
| 1295.8 | 83.69811 | -3.20576 | 1295.5 | 107.2268 | -7.98536 |
| 1297.7 | 79.39124 | -2.08822 | 1297.4 | 100.673 | -9.23424 |
| 1299.6 | 75.85727 | -1.85879 | 1299.4 | 95.55207 | -9.92382 |
| 1301.5 | 72.45938 | -2.13022 | 1301.3 | 87.34883 | -9.41098 |
| 1303.5 | 69.52008 | -2.38858 | 1303.2 | 79.35153 | -8.22227 |
| 1305.4 | 67.5521 | -2.63109 | 1305.2 | 76.31898 | -7.21553 |
| 1307.3 | 66.81635 | -2.92239 | 1307.1 | 79.78116 | -6.99139 |
| 1309.3 | 67.64351 | -3.14519 | 1309.0 | 86.21096 | -6.98824 |
| 1311.2 | 70.12571 | -3.22893 | 1311.9 | 89.14722 | -6.02156 |
| 1313.1 | 74.1276 | -2.9277 | 1313.9 | 88.15613 | -5.12597 |
| 1315.0 | 79.06089 | -2.07262 | 1315.8 | 85.67398 | -3.36661 |
| 1317.0 | 83.9203 | -1.28446 | 1316.8 | 84.58288 | -2.3597 |
| 1318.9 | 88.04186 | -0.95709 | 1318.7 | 83.09026 | -0.49422 |
| 1320.8 | 91.7602 | -0.73864 | 1320.6 | 82.34156 | 0.86234 |
| 1322.7 | 96.11312 | -0.2281 | 1322.6 | 83.64725 | 1.76492 |
| 1324.7 | 101.6137 | 0.75263 | 1324.5 | 87.59131 | 2.43058 |
| 1326.6 | 107.5417 | 1.6532 | 1326.4 | 92.9614 | 2.51131 |
| 1328.5 | 111.8505 | 1.62749 | 1328.4 | 101.6822 | 3.42408 |
| 1330.5 | 112.4819 | 0.76283 | 1330.3 | 114.4842 | 6.62459 |
| 1332.4 | 108.9456 | -0.22435 | 1332.2 | 130.6002 | 11.77928 |
| 1334.3 | 102.5212 | -0.74795 | 1334.2 | 148.296 | 18.64865 |
| 1336.2 | 95.74313 | -0.58353 | 1336.1 | 160.7948 | 24.00008 |
| 1338.2 | 91.26946 | 0.05841 | 1338.1 | 160.4682 | 24.6389 |
| 1340.1 | 90.41153 | 1.02747 | 1341.0 | 147.948 | 20.5152 |
| 1342.0 | 92.67566 | 2.32311 | 1342.9 | 131.615 | 16.95015 |
| 1344.0 | 95.73837 | 3.49903 | 1343.9 | 121.6984 | 15.27061 |
| 1345.9 | 95.18054 | 3.82292 | 1345.8 | 106.046 | 12.18166 |
| 1347.8 | 88.00226 | 3.04069 | 1347.7 | 99.08402 | 9.5523 |
| 1349.7 | 76.70549 | 1.66209 | 1349.7 | 98.06372 | 7.65872 |
| 1351.7 | 66.65698 | 0.46073 | 1351.6 | 101.8029 | 6.4412 |
| 1353.6 | 60.78604 | -0.146 | 1353.5 | 107.8539 | 5.56458 |
| 1355.5 | 58.91338 | -0.00301 | 1355.5 | 114.6839 | 4.87302 |
| 1357.5 | 59.72122 | 0.90121 | 1357.4 | 123.2219 | 4.60773 |
| 1359.4 | 62.05077 | 1.96211 | 1359.3 | 126.8116 | 4.47431 |
| 1361.3 | 65.55259 | 2.74486 | 1361.3 | 123.6403 | 4.36843 |
| 1363.2 | 69.4345 | 3.50113 | 1363.2 | 119.1244 | 4.51569 |
| 1365.2 | 71.75865 | 3.92557 | 1365.1 | 115.8304 | 4.85673 |
| 1367.1 | 71.62636 | 3.76934 | 1367.1 | 112.6583 | 5.1372 |
| 1369.0 | 69.78798 | 3.5582 | 1369.0 | 114.9711 | 5.61548 |
| 1371.0 | 67.45062 | 3.37652 | 1370.9 | 117.1125 | 5.89363 |
| 1372.9 | 66.09521 | 3.27745 | 1372.9 | 112.5262 | 5.61311 |
| 1374.8 | 66.79454 | 3.73222 | 1374.8 | 107.1708 | 5.21308 |
| 1376.7 | 69.30803 | 4.32955 | 1376.8 | 100.9509 | 4.80888 |
| 1378.7 | 73.27001 | 4.32597 | 1378.7 | 93.45832 | 4.35507 |
| 1380.6 | 78.05334 | 3.87765 | 1380.6 | 84.18966 | 3.78933 |

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| 1382.5 | 82.13943 | 3.32494 | 1382.6 | 69.73699 | 3.0027 |
| 1384.5 | 83.65439 | 3.13106 | 1384.5 | 55.03232 | 2.24231 |
| 1386.4 | 81.36216 | 3.34812 | 1386.4 | 45.97792 | 1.76079 |
| 1388.3 | 74.85721 | 3.3137 | 1388.4 | 42.0508 | 1.52058 |
| 1390.2 | 65.1306 | 3.12383 | 1390.3 | 41.83591 | 1.44857 |
| 1392.2 | 54.70671 | 2.88307 | 1392.2 | 44.97847 | 1.52153 |
| 1394.1 | 45.97912 | 2.26222 | 1394.2 | 52.29049 | 1.76874 |
| 1396.0 | 39.91488 | 1.4481 | 1396.1 | 65.9072 | 2.27862 |
| 1397.9 | 36.90953 | 0.40951 | 1397.1 | 75.97495 | 2.66965 |
| 1399.9 | 37.13034 | -0.57714 | 1400.0 | 118.9806 | 4.28343 |
| 1401.8 | 39.96634 | -0.614 | 1401.9 | 152.0286 | 5.35996 |
| 1403.7 | 46.3511 | 0.36952 | 1403.8 | 182.8323 | 6.07419 |
| 1405.7 | 57.2664 | 1.82514 | 1405.8 | 202.1239 | 5.97418 |
| 1407.6 | 72.43973 | 3.16749 | 1407.7 | 202.0799 | 5.21169 |
| 1409.5 | 91.34675 | 4.01316 | 1409.6 | 186.8124 | 4.2034 |
| 1411.4 | 110.958 | 4.3428 | 1411.6 | 162.2849 | 3.20609 |
| 1413.4 | 126.4204 | 4.24512 | 1413.5 | 132.3465 | 2.49882 |
| 1415.3 | 135.5079 | 4.19362 | 1415.5 | 102.9457 | 1.98312 |
| 1417.2 | 142.9992 | 4.4417 | 1417.4 | 80.65657 | 1.49921 |
| 1419.2 | 153.6875 | 4.82328 | 1419.3 | 67.21954 | 1.15653 |
| 1421.1 | 160.9919 | 4.98858 | 1421.3 | 60.68061 | 0.94699 |
| 1423.0 | 157.0716 | 4.14065 | 1423.2 | 59.25441 | 0.77475 |
| 1424.9 | 140.6012 | 2.49524 | 1424.2 | 60.20902 | 0.67508 |
| 1426.9 | 116.8077 | 1.13145 | 1426.1 | 65.23418 | 0.40507 |
| 1428.8 | 92.81602 | 0.53517 | 1428.0 | 73.82591 | 0.07005 |
| 1430.7 | 74.20433 | 0.61717 | 1430.9 | 89.67777 | -0.23277 |
| 1432.7 | 63.14306 | 0.77933 | 1432.9 | 98.30027 | -0.22874 |
| 1434.6 | 60.79662 | 0.9164 | 1434.8 | 103.2341 | 0.03138 |
| 1436.5 | 69.15581 | 1.56409 | 1436.7 | 105.9925 | 0.36979 |
| 1438.4 | 86.94423 | 2.27888 | 1438.7 | 112.5495 | 0.55311 |
| 1440.4 | 114.2884 | 2.22355 | 1440.6 | 126.9687 | 0.66059 |
| 1442.3 | 145.5613 | 1.40402 | 1442.5 | 147.9413 | 0.94932 |
| 1444.2 | 162.1369 | 0.38635 | 1444.5 | 172.7577 | 1.30327 |
| 1446.2 | 158.5519 | 0.00443 | 1446.4 | 197.4775 | 1.43196 |
| 1448.1 | 151.1722 | 0.63713 | 1448.3 | 214.9105 | 1.504 |
| 1450.0 | 154.078 | 1.89443 | 1450.3 | 220.277 | 1.88291 |
| 1451.9 | 165.7593 | 2.7455 | 1451.3 | 220.0666 | 2.11888 |
| 1453.9 | 180.3616 | 2.59031 | 1453.2 | 219.106 | 2.46542 |
| 1455.8 | 197.24 | 2.30285 | 1455.1 | 228.8387 | 2.5873 |
| 1457.7 | 210.8519 | 2.61123 | 1457.1 | 263.6327 | 2.86641 |
| 1459.7 | 219.2969 | 3.32445 | 1460.0 | 350.0701 | 3.78864 |
| 1461.6 | 237.4452 | 4.22135 | 1461.9 | 400.3878 | 4.36868 |
| 1463.5 | 279.3899 | 4.03862 | 1463.8 | 426.7446 | 4.37312 |
| 1465.4 | 332.3396 | 1.55216 | 1465.8 | 414.6705 | 3.75281 |
| 1467.4 | 351.5049 | -1.75443 | 1467.7 | 367.4858 | 3.29765 |
| 1469.3 | 315.4586 | -3.67014 | 1469.6 | 310.0921 | 2.65328 |

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|---|---|---|---|---|---|
| 1471.2 | 244.2841 | -3.53534 | 1471.6 | 247.0928 | 1.8725 |
| 1473.1 | 176.8472 | -1.62468 | 1473.5 | 191.5969 | 1.34933 |
| 1475.1 | 130.8508 | 1.10297 | 1475.4 | 150.3957 | 1.10821 |
| 1477.0 | 100.671 | 3.00422 | 1477.4 | 119.082 | 1.01886 |
| 1478.9 | 81.3495 | 3.57035 | 1478.3 | 106.6331 | 0.95525 |
| 1480.9 | 69.1374 | 3.38798 | 1480.3 | 88.88861 | 0.81048 |
| 1482.8 | 61.86881 | 2.81104 | 1482.2 | 79.16854 | 0.70447 |
| 1484.7 | 58.41859 | 2.35854 | 1484.1 | 74.97872 | 0.64921 |
| 1486.6 | 58.37175 | 2.33946 | 1486.1 | 74.79808 | 0.64115 |
| 1488.6 | 61.49135 | 2.15725 | 1489.0 | 81.75531 | 0.71117 |
| 1490.5 | 66.7189 | 1.7891 | 1490.9 | 92.3649 | 0.84405 |
| 1492.4 | 72.26699 | 1.78953 | 1492.9 | 109.4207 | 1.08239 |
| 1494.4 | 80.29093 | 2.03849 | 1494.8 | 135.9412 | 1.46824 |
| 1496.3 | 93.82755 | 2.39758 | 1496.7 | 174.4646 | 1.93274 |
| 1498.2 | 112.8901 | 2.66779 | 1498.7 | 231.4917 | 2.43645 |
| 1500.1 | 140.0232 | 3.36881 | 1500.6 | 323.9416 | 3.18955 |
| 1502.1 | 176.4473 | 5.06442 | 1502.5 | 455.8392 | 4.00121 |
| 1504.0 | 226.5653 | 7.22899 | 1503.5 | 523.4149 | 4.24365 |
| 1505.9 | 304.2644 | 9.40054 | 1505.4 | 617.1168 | 4.59018 |
| 1507.9 | 402.306 | 11.8023 | 1507.4 | 686.4562 | 6.1226 |
| 1509.8 | 515.5791 | 14.02683 | 1509.3 | 824.7066 | 8.68313 |
| 1511.7 | 654.4885 | 14.92722 | 1511.2 | 1039.448 | 7.41675 |
| 1513.6 | 792.2811 | 12.45139 | 1513.2 | 1128.248 | -3.34495 |
| 1515.6 | 874.9989 | 4.48313 | 1515.1 | 947.5732 | -9.32929 |
| 1517.5 | 842.3974 | -6.13254 | 1517.0 | 664.3789 | -6.72134 |
| 1519.4 | 686.9791 | -13.6635 | 1519.9 | 350.9381 | -2.96136 |
| 1521.4 | 482.9257 | -15.4594 | 1521.9 | 238.8709 | -1.71744 |
| 1523.3 | 324.498 | -12.1763 | 1523.8 | 172.3645 | -1.04097 |
| 1525.2 | 215.9284 | -6.84479 | 1525.7 | 130.2701 | -0.66222 |
| 1527.1 | 146.5564 | -3.23827 | 1527.7 | 101.7916 | -0.43454 |
| 1529.1 | 105.0814 | -1.69097 | 1529.6 | 81.64584 | -0.28838 |
| 1531.0 | 78.61566 | -0.76183 | 1530.6 | 73.76402 | -0.23558 |
| 1532.9 | 61.18597 | -0.13889 | 1532.5 | 61.21463 | -0.1587 |
| 1534.8 | 49.29952 | 0.18971 | 1534.5 | 51.83848 | -0.10845 |
| 1536.8 | 40.54067 | -0.05907 | 1536.4 | 44.66181 | -0.07487 |
| 1538.7 | 34.00276 | -0.49954 | 1538.3 | 39.02524 | -0.05115 |
| 1540.6 | 29.82136 | -0.41772 | 1540.3 | 34.52281 | -0.03388 |
| 1542.6 | 26.03291 | 0.19564 | 1542.2 | 30.8946 | -0.02151 |
| 1544.5 | 22.98959 | 0.83601 | 1544.1 | 27.93663 | -0.01258 |
| 1546.4 | 20.32883 | 0.84115 | 1546.1 | 25.49384 | -0.00631 |
| 1548.3 | 17.95039 | 0.24609 | 1548.0 | 23.45952 | -0.00212 |
| 1550.3 | 16.07139 | -0.15291 | 1550.9 | 21.02891 | 0.00136 |
| 1552.2 | 14.78054 | -0.10803 | 1552.8 | 19.75411 | 0.00223 |
| 1554.1 | 13.68979 | -0.10603 | 1554.8 | 18.71388 | 0.00212 |
| 1556.1 | 12.55312 | -0.26697 | 1556.7 | 17.88341 | 0.0011 |
| 1558.0 | 13.52827 | -0.42582 | 1557.7 | 17.54178 | 2.53E-04 |

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| 1559.9 | 15.58735 | -0.55504 | 1559.6 | 17.00083 | -0.00216 |
| 1561.8 | 15.0973 | -0.30121 | 1561.5 | 16.65035 | -0.00561 |
| 1563.8 | 15.23345 | 0.39894 | 1563.5 | 16.50114 | -0.01031 |
| 1565.7 | 16.29206 | 0.76761 | 1565.4 | 16.57861 | -0.01658 |
| 1567.6 | 17.9543 | 0.6356 | 1567.4 | 16.92965 | -0.02494 |
| 1569.6 | 21.13098 | 0.41663 | 1569.3 | 17.63594 | -0.03622 |
| 1571.5 | 23.97243 | 0.08943 | 1571.2 | 18.84047 | -0.05178 |
| 1573.4 | 27.34581 | 0.12576 | 1573.2 | 20.80078 | -0.07397 |
| 1575.3 | 34.19338 | 0.59517 | 1575.1 | 23.98225 | -0.10682 |
| 1577.3 | 42.07886 | 0.60746 | 1577.0 | 29.08091 | -0.15635 |
| 1579.2 | 50.23068 | 0.1994 | 1579.9 | 40.64414 | -0.29482 |
| 1581.1 | 61.61077 | 0.04211 | 1581.9 | 50.27813 | -0.43898 |
| 1583.1 | 76.13841 | 0.3484 | 1583.8 | 61.43795 | -0.49799 |
| 1585.0 | 94.66906 | 1.12628 | 1584.8 | 67.58115 | -0.50629 |
| 1586.9 | 119.1116 | 1.75759 | 1586.7 | 83.21244 | -0.66147 |
| 1588.8 | 149.1715 | 1.5712 | 1588.6 | 108.0441 | -1.17869 |
| 1590.8 | 176.5823 | 0.75046 | 1590.6 | 140.0179 | -1.78642 |
| 1592.7 | 186.1559 | -0.18758 | 1592.5 | 159.0185 | -2.03277 |
| 1594.6 | 172.2589 | -0.61272 | 1594.4 | 145.9695 | -1.90846 |
| 1596.6 | 148.9248 | -0.30556 | 1596.4 | 109.8834 | -1.41022 |
| 1598.5 | 133.7054 | 0.20585 | 1598.3 | 78.50014 | -0.79203 |
| 1600.4 | 132.444 | 0.68066 | 1600.2 | 61.62142 | -0.33341 |
| 1602.3 | 143.0528 | 1.09012 | 1602.2 | 56.32007 | 0.00719 |
| 1604.3 | 160.2875 | 1.07557 | 1604.1 | 60.60352 | 0.33685 |
| 1606.2 | 175.4067 | 0.7895 | 1606.1 | 76.13028 | 0.77374 |
| 1608.1 | 179.8179 | 0.59632 | 1609.0 | 127.5727 | 1.95517 |
| 1610.0 | 172.7855 | 0.55406 | 1610.9 | 166.1426 | 2.70883 |
| 1612.0 | 161.6128 | 0.81137 | 1611.9 | 174.0572 | 2.65263 |
| 1613.9 | 154.4462 | 1.28462 | 1613.8 | 156.4994 | 1.7055 |
| 1615.8 | 155.0639 | 1.53845 | 1615.7 | 115.7104 | 1.0071 |
| 1617.8 | 161.0007 | 1.38587 | 1617.7 | 79.80405 | 0.84959 |
| 1619.7 | 168.7506 | 1.03131 | 1619.6 | 54.77176 | 0.71345 |
| 1621.6 | 179.3062 | 0.68424 | 1621.5 | 38.51397 | 0.50603 |
| 1623.5 | 191.0943 | 0.38545 | 1623.5 | 28.41134 | 0.34088 |
| 1625.5 | 201.2636 | 0.11733 | 1625.4 | 22.02844 | 0.23845 |
| 1627.4 | 209.3197 | 0.10818 | 1627.3 | 17.78917 | 0.17553 |
| 1629.3 | 214.5767 | 0.53785 | 1629.3 | 14.82721 | 0.13494 |
| 1631.3 | 215.8061 | 0.90706 | 1631.2 | 12.66693 | 0.10738 |
| 1633.2 | 213.5029 | 0.73897 | 1633.1 | 11.03487 | 0.08784 |
| 1635.1 | 208.5984 | 0.18661 | 1635.1 | 9.76559 | 0.07349 |
| 1637.0 | 200.8265 | -0.4698 | 1637.0 | 8.75434 | 0.06265 |
| 1639.0 | 190.0776 | -1.05492 | 1638.9 | 7.93209 | 0.05427 |
| 1640.9 | 177.3493 | -1.39746 | 1640.9 | 7.25181 | 0.04766 |
| 1642.8 | 163.2997 | -1.63735 | 1642.8 | 6.68049 | 0.04235 |
| 1644.8 | 148.6159 | -1.4473 | 1644.8 | 6.19441 | 0.03803 |
| 1646.7 | 134.3057 | -0.65618 | 1646.7 | 5.77608 | 0.03446 |

| | | | | | |
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| 1648.6 | 120.3769 | -0.01197 | 1648.6 | 5.41244 | 0.03148 |
| 1650.5 | 107.3517 | 0.13032 | 1650.6 | 5.09347 | 0.02896 |
| 1652.5 | 95.81896 | -0.45498 | 1652.5 | 4.81146 | 0.02682 |
| 1654.4 | 86.05495 | -1.48555 | 1654.4 | 4.56032 | 0.02497 |
| 1656.3 | 76.66046 | -1.95548 | 1656.4 | 4.33522 | 0.02337 |
| 1658.3 | 68.73805 | -1.75062 | 1658.3 | 4.13227 | 0.02197 |
| 1660.2 | 62.20318 | -1.52241 | 1660.2 | 3.94831 | 0.02075 |
| 1662.1 | 57.08322 | -1.16994 | 1662.2 | 3.78077 | 0.01966 |
| 1664.0 | 52.45974 | -0.54769 | 1664.1 | 3.62748 | 0.01869 |
| 1666.0 | 47.70345 | -0.12289 | 1665.1 | 3.55562 | 0.01825 |
| 1667.9 | 43.85031 | -0.01998 | 1668.0 | 3.35684 | 0.01704 |
| 1669.8 | 40.59298 | 0.06515 | 1669.9 | 3.23672 | 0.01634 |
| 1671.8 | 36.56248 | 0.0499 | 1671.8 | 3.12521 | 0.0157 |
| 1673.7 | 32.86968 | -0.10878 | 1673.8 | 3.02141 | 0.01511 |
| 1675.6 | 29.91612 | 0.06367 | 1675.7 | 2.92451 | 0.01457 |
| 1677.5 | 26.75581 | 0.33946 | 1677.6 | 2.83381 | 0.01408 |
| 1679.5 | 23.406 | 0.42477 | 1679.6 | 2.74873 | 0.01363 |
| 1681.4 | 20.5865 | 0.52175 | 1681.5 | 2.66873 | 0.0132 |
| 1683.3 | 20.10231 | 0.41048 | 1683.5 | 2.59336 | 0.01281 |
| 1685.2 | 19.86704 | -0.14154 | 1685.4 | 2.52221 | 0.01245 |
| 1687.2 | 17.6697 | -0.68693 | 1687.3 | 2.45492 | 0.0121 |
| 1689.1 | 16.74878 | -0.73947 | 1689.3 | 2.39117 | 0.01178 |
| 1691.0 | 16.1158 | -0.45723 | 1691.2 | 2.33068 | 0.01148 |
| 1693.0 | 15.57571 | -0.33724 | 1692.2 | 2.30158 | 0.01134 |
| 1694.9 | 16.64246 | -0.50167 | 1694.1 | 2.24552 | 0.01106 |
| 1696.8 | 16.26027 | -0.67063 | 1696.0 | 2.19213 | 0.0108 |
| 1698.7 | 16.43162 | -0.77772 | 1698.9 | 2.11666 | 0.01044 |
| 1700.7 | 18.96738 | -0.79279 | 1700.9 | 2.06917 | 0.01021 |

**Cartesian Coordinates**

QM/MM B3PW91/6-311G(d,p):UFF

(7*R*,8*S*,7'*S*,8'*S*)-**1**

| Symbol | X | Y | Z |
|---|---|---|---|
| H | -7.70344 | -1.05146 | 0.038447 |
| O | -7.45776 | -0.12189 | 0.120938 |
| C | -6.10704 | -0.09298 | 0.213676 |
| C | -5.43001 | 1.105366 | 0.355969 |
| C | -5.37685 | -1.29008 | 0.161115 |
| H | -6.00366 | 2.022646 | 0.3897 |
| C | -4.04134 | 1.115408 | 0.448932 |
| O | -6.16338 | -2.39881 | 0.009405 |
| C | -3.99546 | -1.28174 | 0.260361 |
| H | -3.5271 | 2.065466 | 0.547831 |
| C | -3.31586 | -0.06996 | 0.412853 |
| C | -5.52384 | -3.64851 | -0.15123 |
| H | -3.42053 | -2.19649 | 0.213371 |
| C | -1.81388 | -0.04992 | 0.503434 |

| | | | |
|---|---|---|---|
| H | -6.31936 | -4.38727 | -0.23507 |
| H | -4.89987 | -3.88593 | 0.715675 |
| H | -4.90871 | -3.66484 | -1.05818 |
| H | -1.4078 | 0.515952 | -0.3502 |
| O | -1.30064 | -1.36734 | 0.446296 |
| C | -1.21459 | 0.553455 | 1.797601 |
| C | 0.056907 | -1.25101 | 0.825841 |
| H | -1.92872 | 0.468772 | 2.61421 |
| C | -0.67853 | 1.980188 | 1.665137 |
| C | 0.068825 | -0.28977 | 2.024057 |
| H | 0.42982 | -2.25086 | 1.044236 |
| H | 0.645081 | -0.82577 | 0.002528 |
| H | -1.20206 | 2.589379 | 0.927047 |
| H | -0.71853 | 2.497473 | 2.634124 |
| O | 0.664995 | 1.839683 | 1.243148 |
| H | 0.032252 | -0.83463 | 2.968197 |
| C | 1.187845 | 0.768008 | 2.024577 |
| H | 1.298989 | 1.135468 | 3.058786 |
| C | 2.54711 | 0.3732 | 1.506954 |
| C | 3.091279 | -0.88326 | 1.724996 |
| C | 3.317017 | 1.335485 | 0.843632 |
| H | 2.530814 | -1.64624 | 2.254105 |
| C | 4.376949 | -1.18586 | 1.268626 |
| H | 2.877709 | 2.306256 | 0.665824 |
| C | 4.599372 | 1.053941 | 0.401807 |
| H | 4.787536 | -2.17094 | 1.448761 |
| C | 5.137 | -0.23735 | 0.600673 |
| O | 5.40394 | 1.94199 | -0.22926 |
| O | 6.384972 | -0.44011 | 0.114844 |
| C | 4.975504 | 3.287433 | -0.25567 |
| C | 6.838824 | -1.77185 | 0.011878 |
| H | 4.830028 | 3.67769 | 0.757562 |
| H | 4.044036 | 3.406909 | -0.81912 |
| H | 5.768091 | 3.846121 | -0.74879 |
| H | 6.124556 | -2.39276 | -0.54042 |
| H | 7.029461 | -2.22426 | 0.991869 |
| H | 7.773044 | -1.7233 | -0.54243 |
| C | 2.42465 | -2.88419 | 9.367966 |
| C | 2.640742 | -1.85507 | 8.35181 |
| H | 3.63837 | -1.39188 | 8.496472 |
| H | 2.592263 | -2.31931 | 7.346515 |
| H | 1.854934 | -1.07681 | 8.436825 |
| N | 2.253693 | -3.69992 | 10.17059 |
| C | 10.2479 | 7.352153 | -2.33264 |
| C | 10.52273 | 7.318736 | -0.8963 |
| H | 10.51542 | 8.352004 | -0.49313 |
| H | 9.743309 | 6.71921 | -0.38569 |
| H | 11.51618 | 6.859024 | -0.71837 |
| N | 10.03245 | 7.377955 | -3.46915 |
| C | 9.140305 | -7.61207 | 1.035281 |

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| C | 10.37341 | -7.05721 | 0.476548 |
| H | 10.2965 | -5.95212 | 0.437221 |
| H | 11.23233 | -7.3439 | 1.117241 |
| H | 10.52638 | -7.45311 | -0.54813 |
| N | 8.164585 | -8.05031 | 1.476369 |
| C | -1.89133 | -6.80359 | 3.806356 |
| C | -1.17566 | -6.16348 | 4.909063 |
| H | -0.15097 | -5.8996 | 4.579653 |
| H | -1.71202 | -5.24262 | 5.211535 |
| H | -1.11988 | -6.85995 | 5.770426 |
| N | -2.45615 | -7.30987 | 2.932973 |
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| H | -1.89046 | -4.47905 | -6.52316 |
| H | -1.66401 | -5.80331 | -7.73623 |
| H | -0.38474 | -4.53913 | -7.52747 |
| N | -2.64004 | -3.254 | -9.34396 |
| C | 3.196846 | -7.32418 | -3.51958 |
| C | 2.312461 | -6.18578 | -3.1302 |
| H | 2.151315 | -6.2028 | -2.03414 |
| H | 2.76396 | -5.21104 | -3.41485 |
| H | 1.334019 | -6.29975 | -3.63758 |
| N | 4.318558 | -7.1153 | -4.10267 |
| C | -0.37588 | 9.417882 | -2.66326 |
| C | -0.06998 | 9.034962 | -1.28558 |
| H | -1.00049 | 9.03995 | -0.68298 |
| H | 0.371001 | 8.017795 | -1.27287 |
| H | 0.652011 | 9.757514 | -0.8544 |
| N | -0.61919 | 9.719819 | -3.75342 |
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| C | -4.31623 | -0.33487 | -8.07377 |
| H | -4.38417 | -1.38184 | -7.71447 |
| H | -5.17552 | -0.11686 | -8.7407 |
| H | -3.36762 | -0.197 | -8.63203 |
| N | -4.36789 | 1.294639 | -6.02454 |
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| C | -0.87593 | 2.351217 | -5.50185 |
| H | -0.47469 | 1.385929 | -5.13355 |
| H | -0.13976 | 3.155629 | -5.302 |
| H | -1.82537 | 2.579689 | -4.97756 |
| N | -1.31312 | 2.186239 | -8.07905 |
| C | -13.5562 | -2.82408 | -2.84426 |
| C | -13.3055 | -4.14653 | -2.27102 |
| H | -12.9423 | -4.0356 | -1.22913 |
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| N | -13.7533 | -1.77782 | -3.29763 |
| C | 12.76011 | 5.000309 | -2.95628 |
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| H | 11.99594 | 3.100799 | -2.3329 |

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| H | 13.66013 | 3.493904 | -1.73226 |
| H | 12.21798 | 4.312319 | -1.01139 |
| N | 13.24582 | 4.765563 | -4.11842 |
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| H | 10.26278 | -5.92615 | 3.348695 |
| H | 9.291579 | -4.67327 | 4.225505 |
| H | 9.78496 | -4.39767 | 2.508719 |
| N | 11.91244 | -4.54083 | 5.031457 |
| C | -14.012 | 1.621186 | 0.210759 |
| C | -13.2619 | 1.942606 | 1.424571 |
| H | -13.4611 | 1.173469 | 2.198717 |
| H | -12.1776 | 1.961102 | 1.194645 |
| H | -13.5771 | 2.937423 | 1.800127 |
| N | -14.6046 | 1.365874 | -0.74973 |
| C | 1.879488 | -1.14703 | -3.20633 |
| C | 2.565833 | -1.70295 | -2.04167 |
| H | 2.820068 | -0.88311 | -1.34108 |
| H | 1.908941 | -2.43661 | -1.53291 |
| H | 3.494052 | -2.21047 | -2.36842 |
| N | 1.33603 | -0.70753 | -4.128 |
| C | -5.62807 | -6.85735 | -1.75288 |
| C | -6.39517 | -6.30873 | -2.86829 |
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| H | -6.5355 | -5.21986 | -2.71922 |
| N | -5.02308 | -7.29223 | -0.86858 |
| C | 3.220312 | 3.898762 | -4.46431 |
| C | 4.211956 | 3.051473 | -3.80556 |
| H | 4.867387 | 3.676558 | -3.16889 |
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| N | 2.434692 | 4.567107 | -4.98745 |
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| C | -1.14275 | -7.30819 | -0.84518 |
| H | -1.75971 | -7.96352 | -1.49168 |
| H | -0.32269 | -6.8641 | -1.44515 |
| H | -0.71659 | -7.90637 | -0.01433 |
| N | -2.63506 | -5.397 | 0.139499 |
| C | -8.79866 | -1.53482 | 6.589825 |
| C | -8.52785 | -2.96698 | 6.716155 |
| H | -8.76104 | -3.47432 | 5.757948 |
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| H | -9.15929 | -3.3931 | 7.522336 |

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| N | -9.0127 | -0.40209 | 6.490502 |
| C | 1.746003 | 9.245582 | 1.912972 |
| C | 1.236457 | 7.877041 | 1.981219 |
| H | 0.23092 | 7.834088 | 1.518657 |
| H | 1.920952 | 7.199213 | 1.433137 |
| H | 1.1678 | 7.56054 | 3.041011 |
| N | 2.149358 | 10.32859 | 1.857201 |
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| C | -3.69158 | -9.97546 | -2.89067 |
| H | -3.63064 | -8.89085 | -3.11004 |
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| H | -3.46756 | -10.5515 | -3.81167 |
| N | -6.10759 | -10.5532 | -2.05784 |
| C | 12.11581 | 0.223952 | -4.79858 |
| C | 11.13156 | -0.58913 | -5.51232 |
| H | 11.64017 | -1.45371 | -5.98558 |
| H | 10.36509 | -0.95672 | -4.80069 |
| H | 10.64247 | 0.025512 | -6.2954 |
| N | 12.89528 | 0.867667 | -4.23562 |
| C | -11.7176 | 2.878618 | 4.613154 |
| C | -11.9089 | 4.239027 | 4.111089 |
| H | -11.2855 | 4.94215 | 4.700403 |
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| H | -12.9771 | 4.521706 | 4.207523 |
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| C | 2.265661 | -6.7228 | 6.133795 |
| C | 2.335797 | -5.41724 | 6.788348 |
| H | 1.323936 | -5.12015 | 7.129256 |
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| H | 2.716421 | -4.66318 | 6.071687 |
| N | 2.210143 | -7.75637 | 5.616857 |
| C | -5.8917 | 7.054926 | 5.29107 |
| C | -5.39446 | 7.894108 | 4.201313 |
| H | -4.87488 | 8.77748 | 4.623936 |
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| H | -6.24557 | 8.231402 | 3.57539 |
| N | -6.28617 | 6.391248 | 6.152744 |
| C | -4.09077 | 4.41541 | -7.67091 |
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| H | -4.63877 | 5.382816 | -5.87724 |
| H | -2.96138 | 4.703423 | -5.91456 |
| H | -3.34839 | 6.208918 | -6.84169 |
| N | -4.36956 | 3.773108 | -8.59218 |
| C | -6.64979 | 8.008913 | 0.558795 |
| C | -5.4475 | 7.177594 | 0.573297 |
| H | -4.59843 | 7.759643 | 0.984616 |
| H | -5.62393 | 6.283544 | 1.203546 |
| H | -5.20759 | 6.86003 | -0.46061 |
| N | -7.60057 | 8.668032 | 0.546239 |
| C | 2.945584 | -0.36028 | 5.224232 |

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| C | 4.305512 | -0.80033 | 4.930222 |
| H | 4.276159 | -1.82024 | 4.497284 |
| H | 4.770675 | -0.10272 | 4.205195 |
| H | 4.898838 | -0.80994 | 5.866213 |
| N | 1.869013 | -0.01214 | 5.460347 |
| C | 7.652868 | -5.81171 | -1.54652 |
| C | 7.623442 | -6.89474 | -2.52791 |
| H | 6.727055 | -7.52467 | -2.35656 |
| H | 7.585159 | -6.46572 | -3.5498 |
| H | 8.53637 | -7.51534 | -2.42073 |
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| C | 9.941223 | 6.046362 | 2.496062 |
| C | 10.34458 | 4.675804 | 2.183483 |
| H | 10.98244 | 4.281151 | 3.000545 |
| H | 9.441946 | 4.040974 | 2.081033 |
| H | 10.91373 | 4.665466 | 1.231545 |
| N | 9.621829 | 7.130981 | 2.742073 |
| C | 6.167896 | -4.76375 | -7.16024 |
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| H | 7.849675 | -6.06171 | -7.54085 |
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| C | 1.209226 | -6.47153 | 1.924223 |
| C | 1.025474 | -5.17247 | 1.279789 |
| H | 0.009969 | -4.78997 | 1.504104 |
| H | 1.780667 | -4.45713 | 1.661345 |
| H | 1.145662 | -5.28473 | 0.183616 |
| N | 1.352438 | -7.50097 | 2.432257 |
| C | 3.496906 | 7.650225 | -5.60579 |
| C | 2.553477 | 8.322939 | -4.71323 |
| H | 3.094757 | 9.064959 | -4.0917 |
| H | 1.780518 | 8.841102 | -5.31655 |
| H | 2.066967 | 7.574085 | -4.05601 |
| N | 4.242992 | 7.118225 | -6.3123 |
| C | 15.23156 | -2.35179 | 1.731046 |
| C | 13.88655 | -2.07015 | 2.311158 |
| H | 13.69528 | -0.97702 | 2.310514 |
| H | 13.10437 | -2.58484 | 1.716183 |
| H | 13.85289 | -2.44269 | 3.355248 |
| N | 15.50551 | -2.00665 | 0.527937 |
| C | 5.584248 | 2.817858 | -8.47438 |
| C | 5.26823 | 3.954166 | -7.60924 |
| H | 5.661769 | 3.762083 | -6.59126 |
| H | 5.7359 | 4.872804 | -8.01855 |
| H | 4.168419 | 4.089269 | -7.56053 |
| N | 5.834216 | 1.91776 | -9.15728 |
| C | 3.151304 | 3.458738 | 3.552061 |
| C | 2.353774 | 4.481275 | 2.878764 |
| H | 2.642912 | 4.5335 | 1.81013 |

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| H | 1.277232 | 4.227922 | 2.962429 |
| H | 2.542399 | 5.462768 | 3.355753 |
| N | 3.78519 | 2.65079 | 4.083814 |
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| N | -3.82855 | 1.87546 | 4.070968 |
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| H | -3.42921 | 8.489133 | -1.43385 |
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| N | -3.8973 | 6.890472 | -3.36608 |
| C | -3.53945 | 11.28604 | 0.514365 |
| C | -4.83911 | 11.09976 | 1.159342 |
| H | -5.07873 | 11.99252 | 1.772425 |
| H | -5.61963 | 10.96355 | 0.383186 |
| H | -4.80606 | 10.20426 | 1.8125 |
| N | -2.51156 | 11.43477 | 0.004265 |
| C | -4.90588 | -9.71853 | 1.490296 |
| C | -3.54594 | -9.9929 | 1.026324 |
| H | -3.18576 | -9.14169 | 0.414623 |
| H | -2.87632 | -10.1287 | 1.900165 |
| H | -3.54401 | -10.9165 | 0.412029 |
| N | -5.98175 | -9.50212 | 1.856956 |
| C | 4.505581 | 6.233693 | 5.800128 |
| C | 3.85564 | 7.527277 | 5.588586 |
| H | 4.594763 | 8.252407 | 5.190742 |
| H | 3.02589 | 7.412224 | 4.862366 |
| H | 3.452815 | 7.900241 | 6.552353 |
| N | 5.020047 | 5.210946 | 5.967845 |
| C | -4.33806 | -3.86428 | 7.09719 |
| C | -4.64831 | -4.8897 | 6.060243 |
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| H | -4.16976 | -4.59761 | 5.104501 |
| N | -4.80045 | -3.98322 | 8.285961 |
| C | -0.48617 | 1.692318 | 6.951889 |
| C | -0.70071 | 2.020802 | 5.543176 |
| H | -0.98727 | 1.103715 | 4.989423 |
| H | -1.50904 | 2.774063 | 5.459157 |
| H | 0.233686 | 2.435606 | 5.112728 |
| N | -0.31505 | 1.433227 | 8.066483 |
| C | -0.50005 | 6.259277 | -5.04341 |
| C | -0.7312 | 5.753606 | -3.69112 |
| H | 0.176305 | 5.229536 | -3.32912 |
| H | -0.96195 | 6.599238 | -3.01426 |
| H | -1.58741 | 5.049485 | -3.70352 |

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| N | -0.31726 | 6.65809 | -6.11406 |
| C | -7.11929 | -5.78676 | 3.24175 |
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| H | -5.14245 | -5.15651 | 2.855103 |
| H | -5.32437 | -6.88714 | 3.351701 |
| H | -5.81529 | -6.36553 | 1.688181 |
| N | -8.18731 | -5.56706 | 3.628921 |
| C | 10.4233 | -1.91168 | -1.40262 |
| C | 10.60623 | -3.16024 | -0.6651 |
| H | 9.819431 | -3.25001 | 0.110996 |
| H | 10.53414 | -4.01667 | -1.36508 |
| H | 11.6025 | -3.16036 | -0.17994 |
| N | 10.27535 | -0.92352 | -1.98521 |
| C | -2.26533 | -6.54898 | -4.17231 |
| C | -1.31938 | -7.46814 | -4.80319 |
| H | -0.7425 | -7.99954 | -4.01921 |
| H | -1.87438 | -8.20565 | -5.41806 |
| H | -0.62308 | -6.89622 | -5.44925 |
| N | -3.01215 | -5.82226 | -3.67031 |
| C | -8.38117 | 3.629229 | 0.630018 |
| C | -9.01876 | 2.51887 | 1.33596 |
| H | -9.45542 | 1.813404 | 0.600381 |
| H | -8.26354 | 1.992313 | 1.952724 |
| H | -9.822 | 2.908011 | 1.992367 |
| N | -7.87632 | 4.507843 | 0.071884 |
| C | -2.69714 | -2.71736 | 3.272602 |
| C | -3.24668 | -1.60641 | 4.045598 |
| H | -3.9073 | -2.00181 | 4.841098 |
| H | -2.42053 | -1.03028 | 4.508198 |
| H | -3.82942 | -0.94508 | 3.374185 |
| N | -2.26195 | -3.59685 | 2.660935 |
| C | -3.9936 | -0.35018 | 7.358913 |
| C | -5.37346 | -0.16777 | 6.914322 |
| H | -5.39586 | 0.563207 | 6.082043 |
| H | -5.77877 | -1.13817 | 6.565068 |
| H | -5.9891 | 0.20942 | 7.756279 |
| N | -2.90116 | -0.49651 | 7.708572 |
| C | 7.177468 | -3.26798 | -3.75782 |
| C | 5.771159 | -3.66436 | -3.72455 |
| H | 5.157228 | -2.8808 | -4.21228 |
| H | 5.642792 | -4.62455 | -4.26192 |
| H | 5.44904 | -3.78849 | -2.67212 |
| N | 8.289503 | -2.95153 | -3.78337 |
| C | 7.516516 | 6.017053 | -5.54352 |
| C | 6.98776 | 5.429776 | -4.31338 |
| H | 7.612542 | 5.748878 | -3.45566 |
| H | 5.943283 | 5.768991 | -4.15998 |
| H | 7.009346 | 4.324423 | -4.39168 |
| N | 7.935376 | 6.481806 | -6.51676 |
| C | 0.620716 | 5.099815 | 6.908745 |

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| C | -0.26819 | 5.105752 | 8.069098 |
| H | 0.258634 | 4.665572 | 8.940401 |
| H | -0.56645 | 6.148649 | 8.301467 |
| H | -1.17216 | 4.505251 | 7.842132 |
| N | 1.322397 | 5.094616 | 5.989523 |
| C | -7.44532 | 6.605137 | -4.17829 |
| C | -7.51882 | 6.746348 | -2.72425 |
| H | -8.56907 | 6.621366 | -2.38983 |
| H | -6.88523 | 5.972491 | -2.24697 |
| H | -7.15655 | 7.75303 | -2.4326 |
| N | -7.38693 | 6.493988 | -5.32849 |
| C | -10.6628 | -1.6805 | 3.467349 |
| C | -10.119 | -0.45637 | 2.88082 |
| H | -9.60959 | 0.137417 | 3.666085 |
| H | -9.39135 | -0.7183 | 2.087169 |
| H | -10.9424 | 0.142473 | 2.443768 |
| N | -11.0923 | -2.64958 | 3.931173 |
| C | 3.381346 | 7.752761 | -1.23694 |
| C | 3.180963 | 6.319733 | -1.44728 |
| H | 3.255122 | 5.79342 | -0.4742 |
| H | 2.178234 | 6.145012 | -1.88713 |
| H | 3.95799 | 5.935521 | -2.13902 |
| N | 3.540494 | 8.88649 | -1.06993 |
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| C | 0.906794 | 2.227652 | -2.0839 |
| H | 1.087942 | 1.308199 | -1.49101 |
| H | 1.173045 | 2.041225 | -3.14346 |
| H | 1.529711 | 3.054451 | -1.68568 |
| N | -1.6243 | 2.880857 | -1.92849 |
| C | 1.084294 | -9.83998 | -1.66433 |
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| H | 3.075791 | -9.47852 | -1.06863 |
| H | 1.871806 | -8.22796 | -0.55556 |
| H | 1.91536 | -9.83407 | 0.276797 |
| N | 0.323565 | -10.2552 | -2.43107 |
| C | 4.514006 | 2.051375 | 7.371545 |
| C | 3.121302 | 2.369946 | 7.685707 |
| H | 2.669713 | 1.530447 | 8.252785 |
| H | 3.080477 | 3.295184 | 8.296275 |
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| N | 5.615438 | 1.799464 | 7.122043 |
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| H | 7.825774 | 1.115423 | 2.48859 |
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| H | 7.185081 | 2.691791 | 1.878857 |
| N | 7.924789 | 3.138045 | 4.925525 |
| C | 2.749293 | -4.20596 | -6.3527 |
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| H | 2.175546 | -5.46074 | -7.94784 |

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| H | 3.385512 | -6.16717 | -6.79913 |
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| N | 2.965776 | -3.14997 | -5.93326 |
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| C | -9.77369 | -4.38115 | -1.23285 |
| H | -8.91918 | -4.84784 | -1.76193 |
| H | -10.5683 | -5.13862 | -1.08509 |
| H | -10.1718 | -3.54046 | -1.83508 |
| N | -8.97524 | -3.48508 | 1.093141 |
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| N | 11.19782 | -6.15806 | -3.19636 |
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| C | 6.282718 | 5.609862 | 2.625468 |
| H | 6.96229 | 5.883993 | 3.45779 |
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| N | 4.691229 | 7.621815 | 2.101441 |
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| H | -6.46996 | -3.89357 | -4.92004 |
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| C | -0.42678 | -2.50165 | 6.247333 |
| H | -1.45559 | -2.90463 | 6.157744 |
| H | 0.042094 | -2.89414 | 7.17084 |
| H | -0.46755 | -1.39487 | 6.295795 |
| N | 0.994264 | -3.23655 | 4.173414 |
| C | -2.4144 | 10.31689 | 3.940355 |
| C | -1.90881 | 9.320211 | 2.997822 |
| H | -2.75926 | 8.807178 | 2.50555 |
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| H | -1.29646 | 8.575993 | 3.543893 |
| N | -2.81468 | 11.10544 | 4.686461 |
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| C | 7.460109 | -1.78212 | 4.02359 |
| H | 6.941245 | -1.19715 | 3.238026 |
| H | 8.34657 | -2.28497 | 3.589307 |
| H | 6.769918 | -2.54693 | 4.430406 |
| N | 8.214374 | -0.17848 | 5.952077 |
| C | 6.910083 | 7.596513 | -0.59145 |
| C | 7.311079 | 8.901089 | -0.0679 |
| H | 7.975942 | 9.404114 | -0.79963 |
| H | 6.40872 | 9.52369 | 0.101477 |
| H | 7.851717 | 8.763236 | 0.890733 |

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| N | 6.591361 | 6.564498 | -1.00467 |
| C | 4.249158 | -5.34681 | -0.16729 |
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| H | 3.871573 | -7.19595 | 0.765084 |
| H | 4.569784 | -7.29755 | -0.90212 |
| H | 5.617665 | -6.81223 | 0.489781 |
| N | 3.968905 | -4.23892 | -0.34404 |
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| H | 10.57107 | -3.1302 | 7.419586 |
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| C | -7.05626 | -3.44839 | -8.80826 |

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| C | 8.808692 | 3.870416 | -1.16174 |
| H | 8.398437 | 4.51057 | -0.35514 |
| H | 9.621405 | 4.409774 | -1.68802 |
| H | 8.005044 | 3.624453 | -1.88355 |
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| H | -8.48605 | -1.39629 | -2.37847 |
| N | -5.56738 | -0.54092 | -3.2559 |
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| C | -1.27649 | -5.18738 | 8.836947 |
| H | -1.52554 | -4.97182 | 7.778751 |
| H | -2.19571 | -5.09643 | 9.450746 |
| H | -0.52718 | -4.44835 | 9.192401 |
| N | 0.424764 | -6.80407 | 9.407966 |
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| C | 7.444299 | 0.81073 | -3.12698 |
| H | 8.335503 | 0.518946 | -3.7179 |
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| H | 7.687523 | 0.743725 | -2.04733 |
| N | 5.193129 | 0.010956 | -2.85713 |
| C | 5.759147 | -4.11633 | 8.476158 |
| C | 5.863541 | -3.42305 | 7.193241 |
| H | 6.519046 | -4.00217 | 6.511482 |
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| N | 5.676294 | -4.66592 | 9.490951 |
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| H | -11.1729 | -1.10326 | -1.83492 |
| H | -11.2942 | 0.421923 | -0.86393 |
| N | -12.9441 | -1.78017 | 0.702657 |
| C | -2.42758 | -1.12607 | -4.45338 |
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| H | -1.26191 | -0.06314 | -3.0531 |
| H | -2.86202 | 0.684176 | -3.45851 |
| N | -2.50733 | -1.80593 | -5.38584 |
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| N | -3.1795 | -2.51065 | 10.82925 |
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| N | -4.7574 | -8.9142 | -6.01824 |
| C | 5.048481 | -9.70123 | 1.920734 |
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| H | 5.503085 | -7.92094 | 2.956825 |
| H | 3.861938 | -8.60968 | 3.282121 |
| H | 5.330361 | -9.39903 | 3.989382 |
| N | 5.144106 | -10.3676 | 0.979599 |
| C | -12.3348 | -6.37353 | 0.881476 |
| C | -11.9427 | -5.40594 | 1.905933 |
| H | -12.0111 | -4.3805 | 1.489822 |
| H | -12.6193 | -5.49618 | 2.78019 |
| H | -10.899 | -5.60551 | 2.223875 |
| N | -12.6435 | -7.13817 | 0.069675 |
| C | 13.88465 | -3.65301 | -2.14867 |
| C | 13.94677 | -2.41341 | -2.9227 |
| H | 14.81614 | -1.81081 | -2.58891 |
| H | 14.05296 | -2.65364 | -4.00042 |
| H | 13.01551 | -1.83391 | -2.766 |
| N | 13.83491 | -4.63328 | -1.53582 |
| C | 1.183698 | -1.48537 | -8.44346 |
| C | 0.141437 | -1.27905 | -7.397 |
| H | 0.143216 | -2.13286 | -6.68893 |
| H | 0.362696 | -0.34881 | -6.83855 |
| H | -0.85844 | -1.18779 | -7.87008 |

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| C | -2.4292 | 5.541839 | 5.040367 |
| C | -1.809 | 5.558143 | 3.685107 |
| H | -1.85498 | 4.540521 | 3.24992 |
| H | -2.36599 | 6.255964 | 3.027654 |
| H | -0.7485 | 5.877458 | 3.75617 |
| N | -2.50289 | 6.616328 | 5.733737 |
| C | -0.3703 | -3.72288 | -3.44658 |
| C | -0.86534 | -3.36665 | -2.11943 |
| H | -0.3606 | -3.99102 | -1.35584 |
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| H | -1.96188 | -3.52778 | -2.07397 |
| N | 0.021742 | -3.99962 | -4.49863 |
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| C | -6.71743 | -2.31122 | 3.601135 |
| H | -6.07128 | -2.70739 | 2.792918 |
| H | -6.34032 | -2.6694 | 4.57953 |
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| C | -9.1475 | -8.07398 | 1.294218 |
| C | -8.55998 | -7.60635 | 0.039529 |
| H | -7.85023 | -8.36857 | -0.34185 |
| H | -9.36311 | -7.44484 | -0.70805 |
| H | -8.02069 | -6.65335 | 0.216207 |
| N | -9.61199 | -8.44414 | 2.28726 |
| C | -9.58505 | 6.491427 | 2.345867 |
| C | -8.62754 | 5.904967 | 3.282874 |
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| H | -8.69202 | 6.432757 | 4.25598 |
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| H | -6.72518 | 3.841597 | -6.36707 |
| N | -9.8312 | 3.638199 | -6.94272 |
| C | 13.25582 | 1.392068 | 0.467459 |
| C | 13.26188 | 0.490333 | -0.68421 |
| H | 12.43591 | 0.765158 | -1.3699 |
| H | 14.22979 | 0.577536 | -1.21875 |
| H | 13.12167 | -0.55465 | -0.34085 |
| N | 13.25007 | 2.106907 | 1.377281 |
| C | -8.19055 | -0.51324 | -7.07607 |

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| C | -9.20462 | -0.38991 | -8.12171 |
| H | -8.72643 | -0.51156 | -9.11522 |
| H | -9.97541 | -1.17547 | -7.98333 |
| H | -9.68061 | 0.609985 | -8.05855 |
| N | -7.38871 | -0.61104 | -6.24855 |
| C | 0.933746 | 9.781038 | 5.573184 |
| C | 0.275314 | 8.614753 | 6.160265 |
| H | 0.821268 | 8.3012 | 7.073455 |
| H | -0.7699 | 8.874971 | 6.424866 |
| H | 0.275076 | 7.783176 | 5.42719 |
| N | 1.45466 | 10.70418 | 5.109387 |
| C | -4.15597 | 4.511046 | 8.141256 |
| C | -4.48207 | 3.431427 | 7.210492 |
| H | -3.60713 | 2.75832 | 7.102001 |
| H | -5.34722 | 2.857331 | 7.599954 |
| H | -4.74144 | 3.863039 | 6.223088 |
| N | -3.89801 | 5.366333 | 8.876688 |
| C | -0.7012 | 5.465462 | 0.090721 |
| C | -2.06247 | 5.995291 | 0.050216 |
| H | -2.07637 | 7.016757 | 0.481455 |
| H | -2.41574 | 6.030861 | -0.99965 |
| H | -2.72937 | 5.336629 | 0.640914 |
| N | 0.375908 | 5.04552 | 0.123366 |
| C | 10.75547 | -0.06786 | 3.270201 |
| C | 10.43329 | -0.84923 | 2.04181 |
| H | 10.56484 | -1.92861 | 2.251556 |
| H | 9.383166 | -0.66533 | 1.734374 |
| H | 11.11573 | -0.55655 | 1.219267 |
| N | 10.67848 | 1.210867 | 3.264928 |
| C | -11.7227 | 1.126295 | -3.96327 |
| C | -10.7336 | 0.395129 | -4.75414 |
| H | -11.252 | -0.231 | -5.50863 |
| H | -10.0658 | 1.115527 | -5.2674 |
| H | -10.1295 | -0.25099 | -4.08622 |
| N | -12.5044 | 1.705492 | -3.33714 |

QM/MM B3PW91/6-311G(d,p):UFF
(7S,8*R*,7'*R*,8'*R*)-**2**

| Symbol | X | Y | Z |
|---|---|---|---|
| H | -6.43145 | -2.60632 | -0.84329 |
| C | -5.74835 | -1.79467 | -0.63129 |
| C | -6.18825 | -0.68755 | 0.078275 |
| C | -4.42864 | -1.88194 | -1.07694 |
| O | -7.43912 | -0.51753 | 0.567467 |
| C | -5.28197 | 0.364005 | 0.341718 |
| H | -4.09375 | -2.7611 | -1.6107 |
| C | -3.53805 | -0.84972 | -0.83716 |
| C | -8.40386 | -1.4909 | 0.23809 |
| O | -5.78441 | 1.399291 | 1.05635 |
| C | -3.98001 | 0.276687 | -0.12734 |

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| C | -2.14038 | -0.89379 | -1.39629 |
| H | -8.11803 | -2.48655 | 0.596106 |
| H | -9.32115 | -1.18264 | 0.735602 |
| H | -8.57458 | -1.5321 | -0.84301 |
| C | -4.90855 | 2.443597 | 1.414717 |
| H | -3.2945 | 1.094074 | 0.059061 |
| H | -2.13591 | -0.39694 | -2.38171 |
| O | -1.71383 | -2.2377 | -1.5746 |
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| H | -5.49233 | 3.124479 | 2.031731 |
| H | -4.05737 | 2.07409 | 1.99785 |
| H | -4.54012 | 2.982851 | 0.534776 |
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| H | -0.96474 | 0.812187 | -0.6762 |
| C | -1.05195 | -0.66694 | 0.923222 |
| C | 0.243877 | -0.99297 | -1.05565 |
| H | -0.19877 | -1.9695 | -2.95686 |
| H | 0.119156 | -3.12628 | -1.64568 |
| H | -1.54804 | -1.63959 | 1.033208 |
| H | -1.54596 | 0.049807 | 1.577598 |
| O | 0.304967 | -0.74443 | 1.309342 |
| H | 0.872282 | -0.3567 | -1.67847 |
| C | 1.007673 | -1.37908 | 0.246542 |
| H | 0.958941 | -2.47029 | 0.378469 |
| C | 2.44625 | -0.94104 | 0.284766 |
| C | 3.487895 | -1.82843 | 0.090664 |
| C | 2.739903 | 0.40801 | 0.518885 |
| H | 3.281947 | -2.88233 | -0.05876 |
| C | 4.813144 | -1.38162 | 0.105282 |
| H | 1.920381 | 1.083222 | 0.715634 |
| C | 4.044544 | 0.8653 | 0.546896 |
| H | 5.613347 | -2.09313 | -0.05016 |
| C | 5.106174 | -0.04444 | 0.32774 |
| O | 4.408856 | 2.148767 | 0.778544 |
| O | 6.348393 | 0.493615 | 0.354568 |
| C | 3.383868 | 3.096425 | 0.982017 |
| C | 7.439212 | -0.35378 | 0.075814 |
| H | 2.719242 | 2.814442 | 1.805537 |
| H | 2.783545 | 3.242758 | 0.077076 |
| H | 3.888269 | 4.026361 | 1.23567 |
| H | 8.317208 | 0.289234 | 0.052701 |
| H | 7.571126 | -1.11392 | 0.854016 |
| H | 7.327732 | -0.84819 | -0.89587 |
| C | 7.095348 | 2.870381 | 4.51471 |
| C | 6.863747 | 2.746328 | 3.046708 |
| H | 7.832701 | 2.772135 | 2.506332 |
| H | 6.344002 | 1.792702 | 2.825016 |
| H | 6.230927 | 3.590724 | 2.70479 |
| N | 7.795161 | 1.996923 | 5.138308 |
| C | 11.24799 | 1.912789 | -1.17731 |

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| C | 10.16383 | 2.673495 | -0.55754 |
| H | 10.04924 | 2.365968 | 0.501348 |
| H | 10.39786 | 3.756483 | -0.60482 |
| H | 9.218764 | 2.476309 | -1.101 |
| N | 12.10546 | 1.311026 | -1.66874 |
| C | -8.20894 | -3.08117 | -3.37418 |
| C | -8.99603 | -3.95793 | -2.50756 |
| H | -9.94708 | -3.45485 | -2.24013 |
| H | -9.21623 | -4.90543 | -3.04021 |
| H | -8.42307 | -4.17768 | -1.58434 |
| N | -7.58639 | -2.38842 | -4.06039 |
| C | 3.920599 | 1.432887 | 5.717558 |
| C | 3.510523 | 2.008927 | 4.437836 |
| H | 3.92517 | 3.033155 | 4.340837 |
| H | 3.891157 | 1.376584 | 3.610771 |
| H | 2.404293 | 2.053436 | 4.38795 |
| N | 4.246554 | 0.975907 | 6.729324 |
| C | 9.688818 | -4.16799 | 3.491651 |
| C | 10.31839 | -5.10157 | 2.510066 |
| H | 9.605671 | -5.91781 | 2.272567 |
| H | 10.58972 | -4.57165 | 1.572032 |
| H | 11.23454 | -5.53891 | 2.957108 |
| N | 9.526397 | -2.92908 | 3.208019 |
| C | 5.485818 | -4.77654 | 2.836391 |
| C | 6.315883 | -5.82907 | 3.419898 |
| H | 6.95939 | -6.27119 | 2.632054 |
| H | 6.952503 | -5.39819 | 4.219216 |
| H | 5.664038 | -6.61699 | 3.849708 |
| N | 4.828887 | -3.94544 | 2.372502 |
| C | -1.31035 | 3.751779 | 0.008458 |
| C | -0.79304 | 3.149533 | 1.269221 |
| H | -0.437 | 3.94663 | 1.952436 |
| H | -1.59574 | 2.567315 | 1.765462 |
| H | 0.050946 | 2.474554 | 1.030842 |
| N | -2.28643 | 4.580206 | 0.038358 |
| C | -11.8539 | -2.62438 | -0.04064 |
| C | -11.3096 | -3.70625 | 0.77973 |
| H | -11.2729 | -3.38277 | 1.839862 |
| H | -11.958 | -4.60152 | 0.688888 |
| H | -10.286 | -3.95612 | 0.433686 |
| N | -12.2845 | -1.76796 | -0.68853 |
| C | -8.49967 | -3.89562 | 3.196873 |
| C | -8.58717 | -2.5076 | 3.650152 |
| H | -7.71386 | -1.93963 | 3.271979 |
| H | -9.51788 | -2.05064 | 3.258993 |
| H | -8.59652 | -2.47743 | 4.758816 |
| N | -8.4304 | -4.99297 | 2.836306 |
| C | -6.68032 | 0.726088 | -3.15714 |
| C | -7.18339 | 1.91117 | -2.40564 |
| H | -6.39467 | 2.689354 | -2.35241 |

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| H | -8.0805 | 2.325375 | -2.91103 |
| H | -7.45809 | 1.603517 | -1.37753 |
| N | -6.32664 | 0.839398 | -4.38327 |
| C | -5.32325 | -5.21985 | -5.35344 |
| C | -5.92712 | -5.67876 | -4.06676 |
| H | -5.7848 | -4.89354 | -3.29644 |
| H | -7.0125 | -5.85246 | -4.21371 |
| H | -5.4552 | -6.62131 | -3.71697 |
| N | -4.3767 | -5.88262 | -5.90772 |
| C | -1.56136 | 6.601379 | -3.50058 |
| C | -0.83151 | 5.345153 | -3.66795 |
| H | 0.258934 | 5.545558 | -3.64941 |
| H | -1.09416 | 4.654479 | -2.84195 |
| H | -1.10404 | 4.882092 | -4.63818 |
| N | -2.13831 | 7.595412 | -3.3667 |
| C | -7.26227 | 0.969593 | 4.131103 |
| C | -8.36886 | 1.466386 | 3.314463 |
| H | -7.9892 | 2.216211 | 2.591897 |
| H | -8.83011 | 0.621743 | 2.76401 |
| H | -9.12865 | 1.939528 | 3.969274 |
| N | -6.38778 | 0.575862 | 4.778329 |
| C | -11.2809 | 2.608392 | 0.546694 |
| C | -10.3555 | 1.706511 | -0.20181 |
| H | -10.1232 | 2.159583 | -1.18658 |
| H | -9.40943 | 1.551973 | 0.358215 |
| H | -10.8478 | 0.725981 | -0.36089 |
| N | -10.9443 | 3.098894 | 1.681854 |
| C | -5.63773 | 6.939914 | -1.56319 |
| C | -5.1077 | 5.606461 | -1.84395 |
| H | -5.28586 | 4.945046 | -0.97239 |
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| C | 2.746061 | -1.53791 | 3.605546 |
| H | 2.316191 | -2.366 | 3.007654 |
| H | 2.017806 | -0.70452 | 3.659804 |
| H | 3.675903 | -1.18054 | 3.121197 |
| N | 3.28633 | -2.3947 | 6.020409 |
| C | 0.168358 | 0.176592 | -5.14844 |
| C | -1.07603 | 0.923723 | -5.32821 |
| H | -1.4103 | 0.838587 | -6.3823 |
| H | -1.85624 | 0.507653 | -4.66108 |
| H | -0.90745 | 1.991286 | -5.07834 |
| N | 1.154172 | -0.41221 | -5.00698 |
| C | 1.75526 | -5.28082 | 2.579438 |
| C | 1.869901 | -5.6722 | 3.983297 |
| H | 2.86769 | -6.12323 | 4.160992 |
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| H | 1.079023 | -6.41119 | 4.226097 |

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| N | 1.665286 | -4.96826 | 1.46963 |
| C | -11.1242 | -1.05574 | -3.88675 |
| C | -10.22 | 0.046777 | -3.56143 |
| H | -10.8068 | 0.977046 | -3.41817 |
| H | -9.66878 | -0.19018 | -2.62922 |
| H | -9.49754 | 0.18945 | -4.39086 |
| N | -11.8388 | -1.92872 | -4.14402 |
| C | 10.78068 | -3.01105 | -1.17112 |
| C | 10.74695 | -1.87385 | -0.25252 |
| H | 10.02231 | -2.07584 | 0.560953 |
| H | 11.75578 | -1.72015 | 0.181243 |
| H | 10.43767 | -0.96277 | -0.8021 |
| N | 10.80895 | -3.91141 | -1.8972 |
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| C | -12.0821 | -0.26063 | 2.78314 |
| H | -12.6616 | -1.20292 | 2.702131 |
| H | -12.7381 | 0.599567 | 2.538245 |
| H | -11.2308 | -0.28893 | 2.073959 |
| N | -11.1711 | -0.00206 | 5.225772 |
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| C | -8.91116 | 5.227363 | -1.65117 |
| H | -8.95812 | 6.326248 | -1.50718 |
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| N | -7.79055 | 4.118236 | 0.439688 |
| C | 3.256199 | -3.24655 | -4.59478 |
| C | 2.905582 | -3.08686 | -3.18467 |
| H | 2.361373 | -2.13296 | -3.04548 |
| H | 2.260696 | -3.92914 | -2.8641 |
| H | 3.829572 | -3.0715 | -2.57383 |
| N | 3.534862 | -3.37205 | -5.71071 |
| C | 1.286929 | 5.168937 | 4.222279 |
| C | 2.037491 | 5.734393 | 3.101992 |
| H | 1.684598 | 5.280441 | 2.154668 |
| H | 1.879518 | 6.831656 | 3.065321 |
| H | 3.117669 | 5.520166 | 3.235393 |
| N | 0.694075 | 4.722458 | 5.109788 |
| C | -2.84652 | -6.60993 | -2.27584 |
| C | -2.37307 | -5.39268 | -2.93328 |
| H | -1.51462 | -4.97759 | -2.36946 |
| H | -2.05333 | -5.63077 | -3.96813 |
| H | -3.191 | -4.64562 | -2.96024 |
| N | -3.22073 | -7.57325 | -1.75556 |
| C | -3.96711 | 3.925112 | 4.707091 |
| C | -2.80994 | 4.490362 | 4.014891 |
| H | -1.93092 | 3.832748 | 4.165859 |
| H | -3.02912 | 4.569918 | 2.931056 |
| H | -2.59105 | 5.497172 | 4.424373 |
| N | -4.8829 | 3.478171 | 5.254967 |
| C | 1.611615 | 7.316089 | -1.63296 |

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| C | 0.951034 | 6.576754 | -0.55806 |
| H | 1.399913 | 5.566613 | -0.47046 |
| H | 1.082501 | 7.123248 | 0.397424 |
| H | -0.12959 | 6.481645 | -0.78508 |
| N | 2.134759 | 7.900255 | -2.4838 |
| C | -5.45622 | -6.54634 | 0.683259 |
| C | -6.01699 | -5.55914 | -0.23811 |
| H | -6.67172 | -4.86144 | 0.322841 |
| H | -5.19402 | -4.99144 | -0.71747 |
| H | -6.61158 | -6.07742 | -1.01782 |
| N | -5.01289 | -7.32745 | 1.412727 |
| C | -5.05199 | -3.341 | 2.508484 |
| C | -4.49971 | -2.02054 | 2.931337 |
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| H | -4.08245 | -2.07381 | 3.959392 |
| H | -3.69915 | -1.71698 | 2.228299 |
| N | -4.99941 | -4.35391 | 3.291674 |
| C | -3.66093 | 3.162116 | -4.01405 |
| C | -3.35515 | 2.405149 | -2.8014 |
| H | -3.79051 | 2.919206 | -1.92189 |
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| C | 1.112422 | -6.72251 | -2.74906 |
| C | 0.719406 | -6.81163 | -1.34312 |
| H | 1.545505 | -7.25803 | -0.75331 |
| H | 0.496891 | -5.79532 | -0.96003 |
| H | -0.18295 | -7.44894 | -1.24948 |
| N | 1.423062 | -6.6503 | -3.86134 |
| C | 4.900203 | 1.549655 | -2.98521 |
| C | 4.437932 | 0.139488 | -3.14395 |
| H | 5.208709 | -0.57603 | -2.78609 |
| H | 3.508285 | -0.0046 | -2.5577 |
| H | 4.227172 | -0.05976 | -4.2145 |
| N | 6.047917 | 1.811218 | -2.48023 |
| C | 7.810796 | 5.149449 | 0.504446 |
| C | 6.929442 | 4.290824 | -0.28526 |
| H | 5.87716 | 4.59238 | -0.12 |
| H | 7.178067 | 4.394464 | -1.35985 |
| H | 7.062435 | 3.234895 | 0.024645 |
| N | 8.508083 | 5.828436 | 1.130071 |
| C | -1.38857 | -3.99983 | 4.411314 |
| C | -0.7193 | -2.79792 | 3.915828 |
| H | -0.00025 | -2.43507 | 4.677651 |
| H | -0.17875 | -3.03608 | 2.977821 |
| H | -1.47306 | -2.01146 | 3.714294 |
| N | -1.91789 | -4.95169 | 4.801879 |
| C | -1.75699 | -5.93537 | 1.252403 |
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| H | -2.75607 | -4.57728 | -0.0188 |

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| H | -2.36307 | -3.95271 | 1.629356 |
| H | -1.04856 | -4.14238 | 0.403775 |
| N | -1.56602 | -7.01543 | 1.620761 |
| C | 6.718104 | -2.03522 | 4.91844 |
| C | 6.578099 | -1.05663 | 3.84125 |
| H | 7.558953 | -0.58086 | 3.641827 |
| H | 6.221914 | -1.56435 | 2.923073 |
| H | 5.845993 | -0.2816 | 4.142883 |
| N | 6.828445 | -2.80971 | 5.770935 |
| C | 7.85181 | -4.90424 | -0.05133 |
| C | 8.015046 | -6.20918 | -0.68935 |
| H | 7.711842 | -7.00656 | 0.019739 |
| H | 7.378589 | -6.25919 | -1.59651 |
| H | 9.077842 | -6.35052 | -0.9737 |
| N | 7.722463 | -3.87242 | 0.454682 |
| C | 9.748523 | 4.804068 | -3.83447 |
| C | 9.100284 | 3.484144 | -4.09695 |
| H | 8.645791 | 3.4928 | -5.10881 |
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| H | 8.309183 | 3.27219 | -3.34798 |
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| C | -5.35003 | 6.459684 | 2.156106 |
| H | -5.77185 | 7.293167 | 1.55864 |
| H | -4.57634 | 6.854845 | 2.845473 |
| H | -4.89218 | 5.712245 | 1.476585 |
| N | -7.25967 | 5.325949 | 3.546058 |
| C | 8.028013 | -0.09875 | -4.49735 |
| C | 8.978154 | -0.2129 | -3.39149 |
| H | 8.895029 | -1.2188 | -2.93354 |
| H | 10.00972 | -0.06376 | -3.77064 |
| H | 8.750176 | 0.558343 | -2.62931 |
| N | 7.275715 | -0.00826 | -5.37183 |
| C | 4.441201 | -6.69598 | 0.051179 |
| C | 4.294624 | -5.62217 | -0.93056 |
| H | 4.526917 | -6.01143 | -1.94272 |
| H | 3.252983 | -5.24567 | -0.9118 |
| H | 4.987692 | -4.79322 | -0.68218 |
| N | 4.555998 | -7.54575 | 0.828033 |
| C | 5.249149 | 7.61242 | -0.34803 |
| C | 4.461266 | 7.150169 | 0.794423 |
| H | 3.76143 | 6.358626 | 0.461287 |
| H | 5.138624 | 6.739057 | 1.570922 |
| H | 3.883539 | 7.998305 | 1.215486 |
| N | 5.872679 | 7.976102 | -1.25239 |
| C | 11.66731 | 0.519647 | 2.368058 |
| C | 10.31698 | 0.539244 | 2.929363 |
| H | 10.01683 | 1.587573 | 3.130326 |
| H | 9.610588 | 0.084364 | 2.206673 |
| H | 10.29981 | -0.03814 | 3.876318 |

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| N | 12.73543 | 0.505115 | 1.923288 |
| C | 4.619284 | 5.042221 | -2.93999 |
| C | 5.618722 | 5.255418 | -3.98582 |
| H | 6.482075 | 5.809434 | -3.56404 |
| H | 5.962512 | 4.274845 | -4.37407 |
| H | 5.169371 | 5.843496 | -4.81199 |
| N | 3.830343 | 4.87159 | -2.1115 |
| C | 8.007555 | -3.98811 | -3.75632 |
| C | 6.704669 | -3.44018 | -3.2751 |
| H | 6.299134 | -2.68991 | -3.98692 |
| H | 5.97941 | -4.272 | -3.17246 |
| H | 6.849678 | -2.95983 | -2.28637 |
| N | 8.519071 | -3.59015 | -4.86196 |
| C | -2.771 | -2.38992 | -4.98758 |
| C | -4.08453 | -1.84099 | -4.65254 |
| H | -4.6373 | -1.60725 | -5.5852 |
| H | -4.65622 | -2.58441 | -4.06203 |
| H | -3.95927 | -0.91535 | -4.05617 |
| N | -1.73227 | -2.82468 | -5.25375 |
| C | -1.8378 | 0.837803 | 4.368886 |
| C | -0.3945 | 1.045774 | 4.47851 |
| H | 0.061061 | 0.195202 | 5.025061 |
| H | 0.049715 | 1.115933 | 3.464739 |
| H | -0.19855 | 1.985525 | 5.032879 |
| N | -2.97952 | 0.672985 | 4.281756 |
| C | 1.748812 | 2.892055 | -3.76267 |
| C | 1.211217 | 2.545435 | -2.44789 |
| H | 1.935038 | 1.899867 | -1.91277 |
| H | 1.040907 | 3.47062 | -1.8622 |
| H | 0.251805 | 2.004677 | -2.57198 |
| N | 2.174039 | 3.166384 | -4.80324 |
| C | -2.13544 | 7.776206 | 1.047858 |
| C | -1.35664 | 7.465535 | 2.246464 |
| H | -1.9796 | 7.639048 | 3.14735 |
| H | -1.03685 | 6.404328 | 2.214956 |
| H | -0.46132 | 8.119042 | 2.286028 |
| N | -2.75079 | 8.020873 | 0.099015 |

QM/MM B3PW91/6-311G(d,p):UFF
(7*R*,8*S*,7'*R*,8'*S*)-**3**

| Symbol | X | Y | Z |
|---|---|---|---|
| H | -5.4214 | -1.65863 | -0.99508 |
| C | -4.78307 | -0.82048 | -0.75233 |
| C | -5.08149 | -0.02649 | 0.343967 |
| C | -3.67712 | -0.53834 | -1.55651 |
| O | -6.11888 | -0.22178 | 1.191358 |
| C | -4.25569 | 1.083376 | 0.63263 |
| H | -3.4781 | -1.16391 | -2.41991 |
| C | -2.85003 | 0.532684 | -1.26447 |
| C | -6.99497 | -1.29383 | 0.929857 |

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| O | -4.62072 | 1.817795 | 1.709308 |
| C | -3.15397 | 1.345076 | -0.1666 |
| C | -1.62079 | 0.801937 | -2.09326 |
| H | -7.73289 | -1.2746 | 1.730398 |
| H | -7.50439 | -1.17235 | -0.0323 |
| H | -6.47614 | -2.25958 | 0.941886 |
| C | -3.75285 | 2.853764 | 2.111548 |
| H | -2.5226 | 2.20001 | 0.028312 |
| H | -1.82889 | 0.495747 | -3.1298 |
| O | -1.31782 | 2.195798 | -2.07515 |
| C | -0.3318 | 0.084678 | -1.61271 |
| H | -2.74972 | 2.470189 | 2.327178 |
| H | -3.68049 | 3.6403 | 1.35371 |
| H | -4.18383 | 3.270323 | 3.019673 |
| C | 0.074835 | 2.338061 | -2.26257 |
| H | -0.5046 | -0.44756 | -0.67737 |
| C | 0.351177 | -0.82567 | -2.63381 |
| C | 0.711159 | 1.208308 | -1.45466 |
| H | 0.35506 | 3.339373 | -1.93493 |
| H | 0.33613 | 2.242712 | -3.32747 |
| H | 0.132722 | -0.48186 | -3.65702 |
| H | 0.072897 | -1.87749 | -2.56142 |
| O | 1.734945 | -0.73124 | -2.36461 |
| H | 0.831829 | 1.510575 | -0.41566 |
| C | 2.027589 | 0.618874 | -2.02201 |
| H | 2.298735 | 1.167009 | -2.93829 |
| C | 3.198725 | 0.672392 | -1.0752 |
| C | 3.873898 | 1.864826 | -0.87437 |
| C | 3.598885 | -0.46418 | -0.36704 |
| H | 3.598178 | 2.752651 | -1.43507 |
| C | 4.918784 | 1.93766 | 0.046901 |
| H | 3.084505 | -1.39437 | -0.56101 |
| C | 4.644885 | -0.40857 | 0.542487 |
| H | 5.434957 | 2.876796 | 0.191717 |
| C | 5.309175 | 0.818047 | 0.766691 |
| O | 5.107507 | -1.46483 | 1.252284 |
| O | 6.309788 | 0.793467 | 1.679727 |
| C | 4.541475 | -2.7324 | 0.996413 |
| C | 7.019541 | 1.990699 | 1.900671 |
| H | 3.472194 | -2.7571 | 1.231322 |
| H | 4.685613 | -3.03534 | -0.04694 |
| H | 5.064483 | -3.42768 | 1.650774 |
| H | 6.36554 | 2.794621 | 2.256635 |
| H | 7.754291 | 1.764365 | 2.670214 |
| H | 7.538012 | 2.325517 | 0.995026 |
| C | -7.18726 | 5.498124 | -0.67483 |
| C | -6.24383 | 4.768464 | 0.223453 |
| H | -6.63507 | 4.793612 | 1.259821 |
| H | -5.25434 | 5.26849 | 0.197219 |
| H | -6.12675 | 3.710362 | -0.09256 |

| | | | |
|---|---|---|---|
| N | -7.73751 | 4.906621 | -1.66951 |
| C | -1.20704 | -4.86651 | -1.09696 |
| C | -1.47697 | -3.51313 | -0.61513 |
| H | -0.52826 | -3.04103 | -0.29201 |
| H | -2.17922 | -3.55751 | 0.241177 |
| H | -1.9289 | -2.91627 | -1.43208 |
| N | -0.99484 | -5.93821 | -1.47792 |
| C | -7.53626 | 1.872364 | -3.48105 |
| C | -7.10313 | 1.48696 | -2.13908 |
| H | -7.17179 | 0.386785 | -2.03309 |
| H | -7.75461 | 1.973837 | -1.38662 |
| H | -6.05368 | 1.803994 | -1.9805 |
| N | -7.87915 | 2.176138 | -4.54351 |
| C | 7.124945 | -1.5919 | -3.48906 |
| C | 6.216669 | -1.48236 | -2.34884 |
| H | 5.273809 | -2.0194 | -2.57073 |
| H | 5.995233 | -0.41449 | -2.15464 |
| H | 6.689113 | -1.93023 | -1.45243 |
| N | 7.843743 | -1.67843 | -4.39152 |
| C | 1.123946 | -0.54193 | 1.92895 |
| C | 1.321789 | 0.834037 | 2.378174 |
| H | 1.463303 | 0.847001 | 3.477923 |
| H | 0.430228 | 1.436707 | 2.110675 |
| H | 2.218253 | 1.259961 | 1.883846 |
| N | 0.964741 | -1.63056 | 1.572546 |
| C | 2.657432 | -5.75804 | 2.015028 |
| C | 1.641254 | -5.53265 | 0.988509 |
| H | 1.454823 | -4.44474 | 0.88562 |
| H | 0.702094 | -6.04383 | 1.280912 |
| H | 1.993135 | -5.94167 | 0.020662 |
| N | 3.461001 | -5.93736 | 2.827721 |
| C | -1.56372 | -1.84946 | -6.31107 |
| C | -1.58103 | -2.67876 | -5.07168 |
| H | -0.54489 | -2.96069 | -4.79258 |
| H | -2.1702 | -3.59979 | -5.25679 |
| H | -2.04744 | -2.10817 | -4.24218 |
| N | -0.94811 | -0.72629 | -6.33244 |
| C | 2.014063 | 5.267512 | -0.54973 |
| C | 2.155571 | 4.579772 | 0.732661 |
| H | 1.846021 | 5.260297 | 1.551552 |
| H | 3.213891 | 4.28579 | 0.878187 |
| H | 1.515083 | 3.674656 | 0.741013 |
| N | 1.899421 | 5.811645 | -1.56449 |
| C | -10.6058 | -1.26995 | 3.17759 |
| C | -11.0107 | -0.82218 | 1.81392 |
| H | -11.249 | 0.260858 | 1.838512 |
| H | -11.9068 | -1.38572 | 1.479691 |
| H | -10.1796 | -0.99448 | 1.100965 |
| N | -10.2964 | -2.4946 | 3.391952 |
| C | 11.92669 | -0.99702 | 1.758084 |

| | | | |
|---|---|---|---|
| C | 11.54612 | -2.40299 | 1.622616 |
| H | 12.42404 | -3.04644 | 1.836001 |
| H | 11.19321 | -2.59167 | 0.588651 |
| H | 10.73328 | -2.63824 | 2.339201 |
| N | 12.22681 | 0.115494 | 1.86407 |
| C | 6.251666 | 6.213783 | -2.87263 |
| C | 5.344163 | 5.338945 | -2.07612 |
| H | 4.576293 | 4.88673 | -2.73803 |
| H | 4.842426 | 5.947486 | -1.29738 |
| H | 5.929626 | 4.535549 | -1.58619 |
| N | 6.938663 | 5.727537 | -3.83865 |
| C | 8.913678 | -4.00118 | -1.30395 |
| C | 8.283532 | -4.356 | 0.000378 |
| H | 8.290652 | -5.45745 | 0.135883 |
| H | 7.235322 | -3.99453 | 0.011723 |
| H | 8.84149 | -3.87902 | 0.832266 |
| N | 10.12985 | -4.32285 | -1.54653 |
| C | -3.56443 | -7.27993 | 0.527873 |
| C | -2.88522 | -6.5797 | 1.617489 |
| H | -3.27835 | -5.54553 | 1.694334 |
| H | -1.79615 | -6.54707 | 1.413582 |
| H | -3.06395 | -7.11564 | 2.571786 |
| N | -4.10222 | -7.83244 | -0.33493 |
| C | -8.09817 | 3.307943 | 4.940058 |
| C | -7.11627 | 4.164227 | 4.275261 |
| H | -6.61783 | 3.593531 | 3.466843 |
| H | -6.35665 | 4.499347 | 5.010946 |
| H | -7.62895 | 5.046688 | 3.840807 |
| N | -8.87444 | 2.628632 | 5.464355 |
| C | -4.96348 | 1.290168 | 5.17596 |
| C | -5.94254 | 0.450946 | 4.48654 |
| H | -6.44683 | 1.041812 | 3.696825 |
| H | -6.69792 | 0.092219 | 5.214552 |
| H | -5.42789 | -0.41508 | 4.024388 |
| N | -4.18991 | 1.955531 | 5.721456 |
| C | 4.16461 | -0.07137 | 5.702053 |
| C | 4.792294 | -0.29098 | 4.399929 |
| H | 5.701984 | 0.337999 | 4.320588 |
| H | 4.079491 | -0.01677 | 3.595783 |
| H | 5.071548 | -1.35919 | 4.296797 |
| N | 3.666899 | 0.103216 | 6.731902 |
| C | -0.89027 | -4.7558 | 3.929226 |
| C | -2.03999 | -4.4896 | 4.840071 |
| H | -2.99475 | -4.66105 | 4.301244 |
| H | -2.00019 | -3.4403 | 5.200825 |
| H | -1.98571 | -5.17662 | 5.709054 |
| N | -0.73983 | -4.0686 | 2.858949 |
| C | -3.31547 | -1.94528 | 2.557799 |
| C | -2.33772 | -0.87829 | 2.764819 |
| H | -1.52753 | -1.2433 | 3.427089 |

| | | | |
|---|---|---|---|
| H | -2.83487 | -0.00743 | 3.237586 |
| H | -1.90923 | -0.57588 | 1.78755 |
| N | -4.08888 | -2.78965 | 2.393458 |
| C | -5.88037 | -6.17359 | 3.520689 |
| C | -6.59188 | -5.76097 | 2.311228 |
| H | -6.37789 | -6.47666 | 1.491474 |
| H | -6.25713 | -4.74708 | 2.01284 |
| H | -7.68251 | -5.74502 | 2.512484 |
| N | -5.31836 | -6.49935 | 4.478263 |
| C | -5.9205 | -3.02155 | 5.447695 |
| C | -7.1611 | -3.00683 | 4.672946 |
| H | -6.92786 | -2.81109 | 3.607205 |
| H | -7.82823 | -2.20865 | 5.057266 |
| H | -7.66931 | -3.98817 | 4.766678 |
| N | -4.93908 | -3.0309 | 6.060377 |
| C | -8.59996 | -4.87107 | -0.59783 |
| C | -9.31575 | -3.92212 | 0.254271 |
| H | -9.43164 | -2.95999 | -0.28291 |
| H | -8.74213 | -3.75651 | 1.188527 |
| H | -10.3175 | -4.32815 | 0.503094 |
| N | -8.03444 | -5.62221 | -1.27226 |
| C | -9.35721 | 3.129025 | 1.411229 |
| C | -8.56407 | 1.908833 | 1.549592 |
| H | -8.77142 | 1.439419 | 2.532724 |
| H | -7.48691 | 2.159535 | 1.47845 |
| H | -8.83187 | 1.200739 | 0.740645 |
| N | -9.98376 | 4.095518 | 1.301862 |
| C | -4.94064 | -1.0458 | -5.62254 |
| C | -4.6046 | 0.238264 | -5.00911 |
| H | -5.00808 | 1.064671 | -5.62922 |
| H | -3.50314 | 0.334052 | -4.93628 |
| H | -5.04715 | 0.288812 | -3.99472 |
| N | -5.20582 | -2.06265 | -6.10693 |
| C | -1.1283 | 6.269104 | 0.567656 |
| C | -1.54306 | 5.173085 | -0.30681 |
| H | -1.17098 | 5.359091 | -1.33487 |
| H | -2.64962 | 5.109551 | -0.32323 |
| H | -1.12016 | 4.221138 | 0.072433 |
| N | -0.79856 | 7.135593 | 1.259973 |
| C | 6.340823 | -4.80519 | 4.226732 |
| C | 6.987671 | -5.59896 | 3.181959 |
| H | 6.958011 | -6.67232 | 3.460086 |
| H | 8.042345 | -5.27377 | 3.069932 |
| H | 6.452538 | -5.45303 | 2.222354 |
| N | 5.829711 | -4.17649 | 5.052716 |
| C | -4.91749 | 4.295449 | -3.92123 |
| C | -4.00151 | 3.693233 | -2.95426 |
| H | -4.44237 | 3.744414 | -1.93941 |
| H | -3.04141 | 4.246339 | -2.96075 |
| H | -3.82388 | 2.634039 | -3.22855 |

| | | | |
|---|---|---|---|
| N | -5.64175 | 4.773035 | -4.68673 |
| C | -8.31072 | -1.66838 | -4.24001 |
| C | -7.50633 | -2.36398 | -3.23655 |
| H | -6.488 | -1.92735 | -3.21461 |
| H | -7.44244 | -3.44084 | -3.49367 |
| H | -7.97803 | -2.24938 | -2.24073 |
| N | -8.94682 | -1.11754 | -5.03417 |
| C | 1.303861 | -2.09298 | 5.110612 |
| C | 2.34833 | -3.01682 | 4.668341 |
| H | 2.760297 | -2.67454 | 3.697519 |
| H | 1.920111 | -4.03257 | 4.551406 |
| H | 3.159223 | -3.04477 | 5.424113 |
| N | 0.478937 | -1.36138 | 5.461512 |
| C | -1.18142 | 4.0211 | -5.21438 |
| C | -1.73098 | 2.796718 | -5.79637 |
| H | -1.43554 | 1.928097 | -5.17456 |
| H | -1.3352 | 2.664817 | -6.82406 |
| H | -2.83727 | 2.867004 | -5.83173 |
| N | -0.74606 | 4.988198 | -4.75152 |
| C | 6.243865 | 2.129407 | -3.52913 |
| C | 7.520386 | 2.202645 | -2.81902 |
| H | 8.104773 | 1.280334 | -3.01148 |
| H | 7.332635 | 2.301427 | -1.73092 |
| H | 8.093103 | 3.082378 | -3.17599 |
| N | 5.233318 | 2.070965 | -4.08935 |
| C | -3.98232 | 7.976988 | -0.79802 |
| C | -4.06285 | 7.394823 | -2.13733 |
| H | -4.26153 | 8.196013 | -2.87819 |
| H | -4.88605 | 6.653504 | -2.16696 |
| H | -3.10436 | 6.894007 | -2.38342 |
| N | -3.91863 | 8.437742 | 0.261398 |
| C | 1.592825 | 1.453407 | -7.33903 |
| C | 1.83734 | 1.764024 | -5.93131 |
| H | 2.918901 | 1.661994 | -5.71205 |
| H | 1.263502 | 1.059723 | -5.29684 |
| H | 1.515498 | 2.803441 | -5.71806 |
| N | 1.398307 | 1.206401 | -8.45256 |
| C | 2.404826 | -1.78166 | -5.42095 |
| C | 3.791353 | -1.27437 | -5.20874 |
| H | 3.81372 | -0.63663 | -4.30181 |
| H | 4.111632 | -0.67185 | -6.08414 |
| H | 4.488538 | -2.12656 | -5.07164 |
| N | 2.135862 | -2.53956 | -6.4182 |
| C | 9.903782 | 3.741859 | 3.297747 |
| C | 8.764274 | 4.652192 | 3.411308 |
| H | 9.105772 | 5.626224 | 3.81739 |
| H | 8.004326 | 4.212703 | 4.089763 |
| H | 8.316593 | 4.807009 | 2.409567 |
| N | 10.8044 | 3.021079 | 3.206992 |
| C | 6.563873 | 7.031764 | 0.997235 |

| | | | |
|---|---|---|---|
| C | 5.669219 | 6.090559 | 1.669841 |
| H | 4.621246 | 6.439296 | 1.567695 |
| H | 5.936913 | 6.028707 | 2.7444 |
| H | 5.771866 | 5.089237 | 1.20669 |
| N | 7.271508 | 7.775909 | 0.463996 |
| C | 1.744258 | -4.65141 | -3.17977 |
| C | 2.535465 | -3.89186 | -2.21336 |
| H | 3.275323 | -4.56018 | -1.73042 |
| H | 1.864973 | -3.46313 | -1.44161 |
| H | 3.069733 | -3.07552 | -2.73764 |
| N | 1.119665 | -5.25237 | -3.94623 |
| C | 8.2919 | -1.33968 | 3.448872 |
| C | 9.102149 | -0.3768 | 4.193192 |
| H | 9.666257 | 0.258583 | 3.480723 |
| H | 9.81487 | -0.92032 | 4.846609 |
| H | 8.440647 | 0.261475 | 4.814317 |
| N | 7.652237 | -2.1017 | 2.859068 |
| C | 3.55953 | 4.576542 | 4.151843 |
| C | 3.900148 | 3.164902 | 3.980204 |
| H | 3.150991 | 2.539615 | 4.50679 |
| H | 4.90671 | 2.972594 | 4.404731 |
| H | 3.898661 | 2.910592 | 2.90117 |
| N | 3.287529 | 5.692999 | 4.287701 |
| C | 4.303018 | -7.30285 | -1.25179 |
| C | 5.273677 | -6.75555 | -0.3041 |
| H | 6.297246 | -6.87631 | -0.71344 |
| H | 5.195278 | -7.29706 | 0.660737 |
| H | 5.065449 | -5.67841 | -0.14112 |
| N | 3.534405 | -7.73388 | -2.00175 |
| C | -4.59887 | 6.633 | 3.231447 |
| C | -3.34348 | 6.074345 | 3.732221 |
| H | -2.80569 | 5.575064 | 2.901923 |
| H | -3.55908 | 5.334756 | 4.53056 |
| H | -2.71192 | 6.888881 | 4.142029 |
| N | -5.59196 | 7.076175 | 2.836193 |
| C | -4.73317 | -4.40287 | -1.69398 |
| C | -4.37444 | -4.37132 | -3.11107 |
| H | -5.15944 | -4.88442 | -3.70321 |
| H | -3.40333 | -4.88626 | -3.25846 |
| H | -4.28862 | -3.31841 | -3.4468 |
| N | -5.0156 | -4.4259 | -0.57242 |
| C | 9.923773 | 3.627864 | -0.4033 |
| C | 9.019643 | 4.769277 | -0.54019 |
| H | 9.398083 | 5.615006 | 0.069499 |
| H | 8.007972 | 4.484604 | -0.18795 |
| H | 8.967278 | 5.075142 | -1.60485 |
| N | 10.64007 | 2.7258 | -0.29476 |
| C | 9.838044 | -0.5078 | -1.21143 |
| C | 8.881913 | -0.3334 | -0.11929 |
| H | 9.347094 | 0.260934 | 0.693 |

| | | | |
|---|---|---|---|
| H | 8.58407 | -1.3253 | 0.273895 |
| H | 7.985689 | 0.195858 | -0.49756 |
| N | 10.59434 | -0.64604 | -2.07605 |
| C | -11.2167 | -1.21631 | -1.96778 |
| C | -10.4576 | 0.014234 | -1.74818 |
| H | -10.2919 | 0.526726 | -2.71775 |
| H | -9.48013 | -0.23716 | -1.2917 |
| H | -11.0216 | 0.682942 | -1.06613 |
| N | -11.8156 | -2.19112 | -2.14065 |
| C | 5.498246 | -5.11197 | -3.91592 |
| C | 4.653657 | -5.46516 | -5.05629 |
| H | 5.292313 | -5.68017 | -5.93733 |
| H | 3.974484 | -4.62071 | -5.28994 |
| H | 4.052346 | -6.36317 | -4.80609 |
| N | 6.166054 | -4.83456 | -3.01307 |
| C | -0.91666 | 3.357914 | 4.652247 |
| C | -0.18328 | 4.037106 | 3.545089 |
| H | -0.18331 | 5.132208 | 3.721026 |
| H | -0.67785 | 3.825133 | 2.575181 |
| H | 0.863721 | 3.673929 | 3.510128 |
| N | -1.03355 | 2.081989 | 4.666988 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*R*,8'*R*)-**1**
**Conf 1** – E = −1265.456416 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 6.161564 | -1.51575 | -0.453 |
| O | 7.226948 | 0.889683 | -0.3761 |
| C | 5.268427 | -0.48773 | -0.37913 |
| C | 5.874438 | 0.783215 | -0.34191 |
| C | 5.0789 | 1.914517 | -0.28068 |
| C | 3.688889 | 1.791915 | -0.25495 |
| C | 3.085494 | 0.540166 | -0.27774 |
| C | 3.888853 | -0.60638 | -0.34285 |
| C | -4.50357 | 2.87439 | -1.22535 |
| O | -5.14801 | 1.619333 | -1.08881 |
| C | -5.20018 | -0.57481 | -0.26446 |
| C | -3.27344 | 0.810109 | 0.231436 |
| C | -2.69196 | -0.23524 | 0.958 |
| C | -3.37583 | -1.43697 | 1.073414 |
| C | -4.6194 | -1.60704 | 0.461362 |
| C | -4.51378 | 0.656539 | -0.37525 |
| O | -0.92838 | 1.28747 | 1.593388 |
| C | 0.44179 | 1.268373 | 1.972762 |
| C | 1.052241 | 0.074986 | 1.23431 |
| C | 1.591553 | 0.403583 | -0.18195 |
| O | 1.13573 | -0.66555 | -1.00193 |

| | | | |
|---|---|---|---|
| C | -1.34185 | -0.07367 | 1.608208 |
| C | -0.16601 | -0.84075 | 0.957954 |
| C | -0.19209 | -0.93581 | -0.57505 |
| O | -6.40239 | -0.64024 | -0.88942 |
| H | 5.557106 | 2.887683 | -0.26438 |
| H | 3.077131 | 2.687974 | -0.22336 |
| H | 3.412996 | -1.5779 | -0.38665 |
| H | -5.17511 | 3.489801 | -1.82226 |
| H | -4.34415 | 3.351328 | -0.25199 |
| H | -3.54348 | 2.777953 | -1.74433 |
| H | -2.73959 | 1.748094 | 0.1609 |
| H | -2.95163 | -2.25743 | 1.644101 |
| H | -5.13372 | -2.55449 | 0.562892 |
| H | 0.528792 | 1.139294 | 3.060999 |
| H | 0.880342 | 2.230636 | 1.700525 |
| H | 1.122701 | 1.341593 | -0.52046 |
| H | -1.41859 | -0.4057 | 2.656541 |
| H | -0.4721 | -1.9206 | -0.95094 |
| H | -0.88175 | -0.19141 | -0.99612 |
| C | -7.12863 | -1.85318 | -0.79716 |
| H | -0.05002 | -1.8287 | 1.406322 |
| H | 1.826125 | -0.41746 | 1.825379 |
| C | 5.656642 | -2.84171 | -0.50113 |
| H | 7.579911 | -0.00845 | -0.42975 |
| H | -6.57526 | -2.68782 | -1.24234 |
| H | -7.37652 | -2.09472 | 0.242648 |
| H | -8.04853 | -1.69312 | -1.35764 |
| H | 6.526833 | -3.49372 | -0.55503 |
| H | 5.080292 | -3.07612 | 0.39983 |
| H | 5.031512 | -2.99334 | -1.38694 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*R*,8'*R*)-**1**
**Conf 2** – E = −1265.456296 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -6.09694 | 1.644611 | -0.50935 |
| O | -7.33139 | -0.66601 | -0.25779 |
| C | -5.27887 | 0.560192 | -0.38674 |
| C | -5.97432 | -0.65779 | -0.25673 |
| C | -5.26154 | -1.83858 | -0.13887 |
| C | -3.86604 | -1.81703 | -0.14784 |
| C | -3.17402 | -0.61716 | -0.26142 |
| C | -3.89386 | 0.579148 | -0.38444 |
| C | 5.252983 | 2.983714 | 0.843846 |
| O | 5.608071 | 1.813888 | 0.127946 |
| C | 5.142408 | -0.37113 | -0.58817 |

| | | | |
|---|---|---|---|
| C | 3.512162 | 0.772597 | 0.790265 |
| C | 2.666622 | -0.34633 | 0.743123 |
| C | 3.07453 | -1.46733 | 0.040344 |
| C | 4.307535 | -1.47857 | -0.61977 |
| C | 4.734694 | 0.776782 | 0.134364 |
| O | 0.773949 | -1.58583 | 1.574222 |
| C | -0.56677 | -1.37471 | 1.99512 |
| C | -1.06931 | -0.19306 | 1.164909 |
| C | -1.67223 | -0.58912 | -0.20634 |
| O | -1.15615 | 0.3721 | -1.11869 |
| C | 1.34052 | -0.28696 | 1.454362 |
| C | 0.22931 | 0.561871 | 0.785639 |
| C | 0.204474 | 0.554279 | -0.75129 |
| O | 6.351139 | -0.28501 | -1.19649 |
| H | -5.80812 | -2.77112 | -0.05163 |
| H | -3.31964 | -2.75189 | -0.07212 |
| H | -3.35163 | 1.509231 | -0.49944 |
| H | 4.335044 | 3.433376 | 0.448605 |
| H | 5.126557 | 2.777322 | 1.912593 |
| H | 6.08034 | 3.678613 | 0.707882 |
| H | 3.204307 | 1.644981 | 1.355347 |
| H | 2.43805 | -2.34266 | 0.011463 |
| H | 4.608104 | -2.36818 | -1.15919 |
| H | -0.59278 | -1.13727 | 3.06839 |
| H | -1.12197 | -2.3006 | 1.830701 |
| H | -1.28639 | -1.58531 | -0.47606 |
| H | 1.505076 | 0.119647 | 2.466113 |
| H | 0.551365 | 1.48552 | -1.20105 |
| H | 0.814217 | -0.27138 | -1.14246 |
| C | 6.80163 | -1.41274 | -1.92694 |
| H | 0.238611 | 1.583415 | 1.168949 |
| H | -1.77413 | 0.428576 | 1.71972 |
| C | -5.49905 | 2.923696 | -0.65642 |
| H | -7.61974 | 0.250717 | -0.36053 |
| H | 6.913867 | -2.29048 | -1.28062 |
| H | 6.122339 | -1.65363 | -2.75237 |
| H | 7.774632 | -1.13689 | -2.33083 |
| H | -6.32101 | 3.633309 | -0.73448 |
| H | -4.88339 | 3.17307 | 0.214035 |
| H | -4.88846 | 2.971031 | -1.56384 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*R*,8'*R*)-**1**
**Conf 3** – E = −1265.455454 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 6.149285 | 1.57148 | 0.038077 |

| | | | |
|---|---|---|---|
| O | 7.218754 | -0.74263 | -0.6298 |
| C | 5.259929 | 0.56603 | -0.20545 |
| C | 5.866179 | -0.65226 | -0.55917 |
| C | 5.070592 | -1.7515 | -0.84223 |
| C | 3.682724 | -1.65293 | -0.76627 |
| C | 3.075897 | -0.45148 | -0.41434 |
| C | 3.87694 | 0.66418 | -0.14123 |
| C | -3.86949 | 3.203746 | -0.8508 |
| O | -4.76568 | 2.105981 | -0.82904 |
| C | -5.27354 | -0.1095 | -0.25508 |
| C | -3.09163 | 0.772506 | 0.324981 |
| C | -2.73712 | -0.45034 | 0.907221 |
| C | -3.65972 | -1.48634 | 0.911214 |
| C | -4.91756 | -1.31872 | 0.328184 |
| C | -4.34238 | 0.955012 | -0.25066 |
| O | -0.72322 | 0.589662 | 1.740932 |
| C | 0.624332 | 0.258058 | 2.050147 |
| C | 1.006876 | -0.85239 | 1.069242 |
| C | 1.58101 | -0.34845 | -0.28006 |
| O | 0.9389 | -1.14099 | -1.26886 |
| C | -1.37273 | -0.65607 | 1.512404 |
| C | -0.35741 | -1.47199 | 0.675844 |
| C | -0.41157 | -1.26457 | -0.84551 |
| O | -6.46927 | 0.153646 | -0.83864 |
| H | 5.551947 | -2.68169 | -1.12418 |
| H | 3.065679 | -2.51277 | -0.99867 |
| H | 3.410086 | 1.609227 | 0.112603 |
| H | -3.60215 | 3.523854 | 0.16235 |
| H | -2.95732 | 2.965665 | -1.40914 |
| H | -4.39985 | 4.010303 | -1.35498 |
| H | -2.3729 | 1.580554 | 0.34456 |
| H | -3.41338 | -2.43827 | 1.371579 |
| H | -5.62087 | -2.14191 | 0.341953 |
| H | 0.69542 | -0.09704 | 3.088162 |
| H | 1.224775 | 1.164937 | 1.951913 |
| H | 1.277483 | 0.703662 | -0.40974 |
| H | -1.49623 | -1.1702 | 2.479292 |
| H | -0.8576 | -2.09976 | -1.38684 |
| H | -0.96862 | -0.35063 | -1.09283 |
| C | -7.43242 | -0.88524 | -0.86586 |
| H | -0.41546 | -2.53273 | 0.924412 |
| H | 1.687131 | -1.57818 | 1.517528 |
| C | 5.641789 | 2.848157 | 0.393624 |
| H | 7.573257 | 0.127594 | -0.40406 |
| H | -7.06852 | -1.75535 | -1.42395 |
| H | -7.71753 | -1.19521 | 0.145839 |

| | | | |
|---|---|---|---|
| H | -8.30271 | -0.47162 | -1.37329 |
| H | 6.510578 | 3.486507 | 0.545095 |
| H | 5.020821 | 3.262929 | -0.40722 |
| H | 5.061649 | 2.797344 | 1.321002 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*R*,8'*R*)-**1**
**Conf 4** – E = −1265.455317 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -6.22791 | 0.421253 | 1.021194 |
| O | -6.31351 | 2.292883 | -0.82791 |
| C | -5.16581 | 0.4405 | 0.165187 |
| C | -5.24812 | 1.451501 | -0.81081 |
| C | -4.23805 | 1.569508 | -1.74939 |
| C | -3.14834 | 0.697535 | -1.72391 |
| C | -3.04943 | -0.29146 | -0.75366 |
| C | -4.07824 | -0.41879 | 0.191755 |
| C | 4.236556 | 2.839889 | 2.096389 |
| O | 4.935142 | 2.085373 | 1.121714 |
| C | 5.088984 | 0.237419 | -0.31581 |
| C | 3.112126 | 0.476636 | 1.062226 |
| C | 2.575821 | -0.70218 | 0.521714 |
| C | 3.305347 | -1.4 | -0.42562 |
| C | 4.556972 | -0.93186 | -0.83926 |
| C | 4.348295 | 0.955912 | 0.654479 |
| O | 0.962885 | -2.48962 | 0.562831 |
| C | -0.41691 | -2.72237 | 0.808286 |
| C | -1.15367 | -1.38187 | 0.593733 |
| C | -1.88964 | -1.27736 | -0.75185 |
| O | -0.87555 | -0.93269 | -1.68232 |
| C | 1.219465 | -1.16101 | 0.984721 |
| C | 0.003973 | -0.36163 | 0.465118 |
| C | 0.026925 | -0.03309 | -1.0367 |
| O | 6.290003 | 0.769438 | -0.65242 |
| H | -4.31568 | 2.345807 | -2.50295 |
| H | -2.37175 | 0.780575 | -2.47479 |
| H | -4.03125 | -1.20002 | 0.942092 |
| H | 3.276106 | 3.201154 | 1.711677 |
| H | 4.067542 | 2.258147 | 3.009566 |
| H | 4.874395 | 3.691894 | 2.326787 |
| H | 2.548848 | 1.01771 | 1.814006 |
| H | 2.906651 | -2.31671 | -0.84137 |
| H | 5.112224 | -1.49679 | -1.57768 |
| H | -0.55797 | -3.07129 | 1.840996 |
| H | -0.74545 | -3.50997 | 0.127089 |
| H | -2.26968 | -2.25665 | -1.06519 |

| | | | |
|---|---|---|---|
| H | 1.195031 | -1.11936 | 2.08777 |
| H | -0.2867 | 1.004408 | -1.20375 |
| H | 1.007799 | -0.17851 | -1.49226 |
| C | 7.064527 | 0.083721 | -1.62099 |
| H | -0.15575 | 0.536515 | 1.063157 |
| H | -1.81155 | -1.16255 | 1.434561 |
| C | -6.26443 | -0.57472 | 2.031039 |
| H | -6.89601 | 2.027085 | -0.10408 |
| H | 7.326463 | -0.9256 | -1.2842 |
| H | 6.541457 | 0.022015 | -2.58187 |
| H | 7.974521 | 0.669172 | -1.7438 |
| H | -7.18981 | -0.41259 | 2.581146 |
| H | -6.27195 | -1.57893 | 1.59447 |
| H | -5.41403 | -0.47631 | 2.713986 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*R*,8'*R*)-**1**
**Conf 5** – E = −1265.454822 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 6.086737 | 1.698011 | -0.15127 |
| O | 7.212171 | -0.63321 | -0.6425 |
| C | 5.223175 | 0.65171 | -0.29434 |
| C | 5.858919 | -0.57456 | -0.55614 |
| C | 5.091368 | -1.71535 | -0.73352 |
| C | 3.702723 | -1.64862 | -0.64398 |
| C | 3.066487 | -0.43875 | -0.38364 |
| C | 3.83886 | 0.716789 | -0.21522 |
| C | -4.23463 | 3.140871 | -0.33859 |
| O | -5.00608 | 1.957982 | -0.47817 |
| C | -5.28614 | -0.35122 | -0.1628 |
| C | -3.19962 | 0.669267 | 0.519479 |
| C | -2.73465 | -0.56543 | 0.975706 |
| C | -3.55447 | -1.68632 | 0.874375 |
| C | -4.81558 | -1.57295 | 0.296783 |
| C | -4.47072 | 0.790698 | -0.04059 |
| O | -0.75361 | 0.573467 | 1.760643 |
| C | 0.606917 | 0.299214 | 2.071145 |
| C | 1.018692 | -0.83601 | 1.131387 |
| C | 1.570793 | -0.36744 | -0.23991 |
| O | 0.941979 | -1.21185 | -1.19484 |
| C | -1.36185 | -0.69974 | 1.583619 |
| C | -0.32732 | -1.51292 | 0.770786 |
| C | -0.4007 | -1.3551 | -0.75582 |
| O | -6.55836 | -0.26885 | -0.66291 |
| H | 5.595264 | -2.65227 | -0.94497 |
| H | 3.108258 | -2.54212 | -0.79456 |

| | | | |
|---|---|---|---|
| H | 3.348344 | 1.665999 | -0.03149 |
| H | -3.3043 | 3.08277 | -0.91355 |
| H | -4.85217 | 3.946625 | -0.73237 |
| H | -4.00263 | 3.34249 | 0.712403 |
| H | -2.5568 | 1.532543 | 0.625556 |
| H | -3.21465 | -2.65019 | 1.240213 |
| H | -5.46928 | -2.43402 | 0.206928 |
| H | 0.69772 | -0.01087 | 3.12177 |
| H | 1.175664 | 1.220779 | 1.93052 |
| H | 1.239623 | 0.670954 | -0.4058 |
| H | -1.46605 | -1.17898 | 2.570827 |
| H | -0.83114 | -2.21672 | -1.26734 |
| H | -0.9825 | -0.46194 | -1.02343 |
| C | -6.64377 | -0.01852 | -2.0661 |
| H | -0.34773 | -2.56619 | 1.054204 |
| H | 1.722783 | -1.52242 | 1.603983 |
| C | 5.548332 | 2.988427 | 0.091582 |
| H | 7.544326 | 0.263154 | -0.50058 |
| H | -6.1465 | -0.81445 | -2.63203 |
| H | -7.70597 | -0.01237 | -2.31149 |
| H | -6.20452 | 0.947911 | -2.32464 |
| H | 6.400639 | 3.662011 | 0.162938 |
| H | 4.900651 | 3.307011 | -0.73175 |
| H | 4.987296 | 3.011586 | 1.031691 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*R*,8'*R*)-**1**
**Conf 6** – E = −1265.454517 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -6.37213 | 0.45068 | 0.249216 |
| O | -6.55807 | -1.93457 | -0.85161 |
| C | -5.18618 | -0.19763 | 0.06286 |
| C | -5.32502 | -1.46916 | -0.52506 |
| C | -4.19506 | -2.23235 | -0.76064 |
| C | -2.93223 | -1.74462 | -0.4201 |
| C | -2.78435 | -0.48553 | 0.14678 |
| C | -3.92976 | 0.286274 | 0.393641 |
| C | 3.654313 | -1.90524 | 2.276536 |
| O | 4.532622 | -1.54029 | 1.222104 |
| C | 5.022316 | -0.25094 | -0.67849 |
| C | 2.946142 | 0.154182 | 0.498179 |
| C | 2.605498 | 1.143545 | -0.42883 |
| C | 3.474865 | 1.4289 | -1.47603 |
| C | 4.675987 | 0.73238 | -1.59242 |
| C | 4.141201 | -0.55014 | 0.381691 |
| O | 0.930074 | 2.033435 | 1.047288 |

| | | | |
|---|---|---|---|
| C | -0.44382 | 2.380117 | 1.037585 |
| C | -1.08859 | 1.450055 | 0.010135 |
| C | -1.41562 | 0.035094 | 0.560542 |
| O | -0.36458 | -0.8156 | 0.118088 |
| C | 1.292499 | 1.869193 | -0.31944 |
| C | 0.057312 | 1.200719 | -1.00597 |
| C | 0.080109 | -0.31641 | -1.13817 |
| O | 6.185186 | -0.95161 | -0.85602 |
| H | -4.31361 | -3.2126 | -1.20966 |
| H | -2.05223 | -2.35247 | -0.5921 |
| H | -3.835 | 1.264714 | 0.851299 |
| H | 2.688881 | -2.24661 | 1.88916 |
| H | 4.144217 | -2.72423 | 2.800869 |
| H | 3.495194 | -1.07324 | 2.970758 |
| H | 2.256661 | -0.05568 | 1.304476 |
| H | 3.226872 | 2.201452 | -2.19717 |
| H | 5.368736 | 0.940791 | -2.40081 |
| H | -0.56985 | 3.431026 | 0.734116 |
| H | -0.83032 | 2.261343 | 2.051771 |
| H | -1.36061 | 0.032294 | 1.655182 |
| H | 1.412067 | 2.865957 | -0.77235 |
| H | -0.60002 | -0.63222 | -1.94146 |
| H | 1.069155 | -0.73408 | -1.33011 |
| C | 7.203589 | -0.69542 | 0.111619 |
| H | -0.12459 | 1.673133 | -1.97286 |
| H | -1.96636 | 1.904812 | -0.45021 |
| C | -6.34936 | 1.744042 | 0.832175 |
| H | -7.19418 | -1.25192 | -0.60032 |
| H | 6.876799 | -0.9756 | 1.115737 |
| H | 8.059185 | -1.30669 | -0.17625 |
| H | 7.493127 | 0.361455 | 0.097622 |
| H | -7.38674 | 2.070384 | 0.883099 |
| H | -5.9276 | 1.714345 | 1.842262 |
| H | -5.77753 | 2.444824 | 0.214805 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*R*,8'*R*)-**1**
**Conf 7** – E = −1265.454143 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 6.22983 | -1.3486 | -0.52298 |
| O | 7.21325 | 1.076925 | -0.25336 |
| C | 5.301859 | -0.3593 | -0.38191 |
| C | 5.864916 | 0.924363 | -0.24233 |
| C | 5.031936 | 2.021473 | -0.10556 |
| C | 3.646566 | 1.851925 | -0.10462 |
| C | 3.085309 | 0.586747 | -0.22791 |

| | | | |
|---|---|---|---|
| C | 3.92679 | -0.52522 | -0.3705 |
| C | -4.53448 | 2.736437 | -1.09271 |
| O | -5.15666 | 1.461946 | -1.04009 |
| C | -5.15402 | -0.79226 | -0.38697 |
| C | -3.27848 | 0.602154 | 0.245325 |
| C | -2.67112 | -0.48551 | 0.875792 |
| C | -3.30993 | -1.72244 | 0.874126 |
| C | -4.54377 | -1.86553 | 0.246072 |
| C | -4.5115 | 0.461248 | -0.3902 |
| O | -0.96124 | 1.027128 | 1.663802 |
| C | 0.406208 | 1.014115 | 2.055061 |
| C | 1.058704 | -0.08519 | 1.213758 |
| C | 1.596133 | 0.394171 | -0.15951 |
| O | 1.181237 | -0.60593 | -1.082 |
| C | -1.33034 | -0.34105 | 1.54868 |
| C | -0.12791 | -1.00791 | 0.839354 |
| C | -0.13969 | -0.95823 | -0.69638 |
| O | -6.34053 | -0.98654 | -1.04262 |
| H | 5.477331 | 3.005704 | -0.01144 |
| H | 3.004782 | 2.722447 | -0.01346 |
| H | 3.484288 | -1.50581 | -0.4935 |
| H | -5.20968 | 3.373185 | -1.6622 |
| H | -4.39739 | 3.15735 | -0.09099 |
| H | -3.56719 | 2.686319 | -1.60364 |
| H | -2.77086 | 1.55697 | 0.262566 |
| H | -2.85546 | -2.57551 | 1.368249 |
| H | -5.05623 | -2.82159 | 0.230852 |
| H | 0.487554 | 0.785929 | 3.127328 |
| H | 0.81647 | 2.010681 | 1.879354 |
| H | 1.098384 | 1.344636 | -0.41082 |
| H | -1.40266 | -0.77204 | 2.560615 |
| H | -0.3842 | -1.91179 | -1.1658 |
| H | -0.85072 | -0.20038 | -1.05274 |
| C | -7.47774 | -0.37355 | -0.43464 |
| H | 0.015228 | -2.02972 | 1.194015 |
| H | 1.84383 | -0.60774 | 1.762507 |
| C | 5.771091 | -2.68289 | -0.67994 |
| H | 7.596514 | 0.197763 | -0.37322 |
| H | -8.33666 | -0.64582 | -1.04843 |
| H | -7.62475 | -0.75418 | 0.582472 |
| H | -7.37743 | 0.714198 | -0.41066 |
| H | 6.6636 | -3.29906 | -0.77488 |
| H | 5.195722 | -3.00672 | 0.193523 |
| H | 5.159119 | -2.78562 | -1.58178 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 1** – E = −1304.716345 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -0.72535 | -0.79995 | -1.23242 |
| C | 0.644599 | -0.8115 | -0.8536 |
| C | -1.38176 | 0.019842 | -0.27312 |
| C | -0.72713 | -0.34964 | 1.083119 |
| C | 0.655571 | -0.91934 | 0.677924 |
| C | 1.651106 | 0.010771 | 1.412905 |
| O | 0.940332 | 1.232029 | 1.577229 |
| C | -0.37464 | 0.850276 | 1.965047 |
| C | -2.87081 | -0.18535 | -0.34105 |
| C | 2.976396 | 0.24656 | 0.736951 |
| C | 3.285617 | 1.443654 | 0.112687 |
| C | 3.925711 | -0.78705 | 0.736251 |
| C | 4.523349 | 1.614729 | -0.51708 |
| C | 5.154007 | -0.63239 | 0.110085 |
| C | 5.461203 | 0.592608 | -0.53166 |
| C | -3.73125 | 0.90008 | -0.1293 |
| C | -3.41558 | -1.43996 | -0.57272 |
| C | -4.8007 | -1.61736 | -0.59152 |
| C | -5.6584 | -0.54652 | -0.37158 |
| C | -5.11079 | 0.736346 | -0.13562 |
| O | -6.01008 | 1.732588 | 0.060382 |
| O | -7.01314 | -0.61973 | -0.36927 |
| O | 6.123712 | -1.57901 | 0.059879 |
| O | 6.683846 | 0.660313 | -1.11575 |
| C | 5.867366 | -2.82636 | 0.686722 |
| C | 7.035816 | 1.869323 | -1.77057 |
| C | -5.51125 | 3.040765 | 0.294341 |
| C | -7.60602 | -1.8867 | -0.61026 |
| H | 1.131783 | 0.118465 | -1.17773 |
| H | 1.125203 | -1.65132 | -1.35695 |
| H | -1.15268 | 1.076282 | -0.48878 |
| H | -1.34379 | -1.07785 | 1.611909 |
| H | 0.783984 | -1.95519 | 0.994622 |
| H | 1.839027 | -0.42376 | 2.408355 |
| H | -1.0295 | 1.712875 | 1.825963 |
| H | -0.38626 | 0.56861 | 3.027289 |
| H | 2.567791 | 2.254247 | 0.118006 |
| H | 3.692675 | -1.71964 | 1.237147 |
| H | 4.744427 | 2.560231 | -0.99649 |
| H | -3.30841 | 1.884299 | 0.034088 |
| H | -2.76309 | -2.28613 | -0.75331 |
| H | -5.20478 | -2.60399 | -0.78127 |

| | | | |
|---|---|---|---|
| H | 5.002644 | -3.32833 | 0.239552 |
| H | 6.758601 | -3.43008 | 0.523012 |
| H | 5.703889 | -2.70729 | 1.763234 |
| H | 7.050461 | 2.713095 | -1.07224 |
| H | 8.03789 | 1.71264 | -2.1668 |
| H | 6.350662 | 2.091378 | -2.59582 |
| H | -6.38739 | 3.673432 | 0.427543 |
| H | -4.89633 | 3.078777 | 1.199975 |
| H | -4.92808 | 3.405373 | -0.55812 |
| H | -8.68197 | -1.72467 | -0.56838 |
| H | -7.3362 | -2.27324 | -1.59894 |
| H | -7.31954 | -2.61496 | 0.156113 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 2** – E = −1304.715081 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -0.73343 | -0.81392 | -0.96814 |
| C | 0.608569 | -1.09824 | -0.59174 |
| C | -1.20177 | 0.140148 | -0.02082 |
| C | -0.64932 | -0.35194 | 1.338325 |
| C | 0.615396 | -1.15484 | 0.944558 |
| C | 1.758569 | -0.38939 | 1.659122 |
| O | 1.251486 | 0.929451 | 1.839456 |
| C | -0.10551 | 0.762456 | 2.232577 |
| C | -2.69687 | 0.265097 | -0.10245 |
| C | 3.094339 | -0.35601 | 0.962466 |
| C | 3.935745 | -1.45806 | 1.018125 |
| C | 3.501462 | 0.772935 | 0.240642 |
| C | 5.162462 | -1.4489 | 0.350067 |
| C | 4.722587 | 0.79863 | -0.42053 |
| C | 5.568734 | -0.33395 | -0.37231 |
| C | -3.5026 | -0.87578 | -0.18871 |
| C | -3.31548 | 1.508786 | -0.068 |
| C | -4.70598 | 1.623557 | -0.09446 |
| C | -5.50468 | 0.485147 | -0.16811 |
| C | -4.88328 | -0.78148 | -0.22471 |
| O | -5.63295 | -1.92823 | -0.25611 |
| O | -6.85984 | 0.487821 | -0.1835 |
| O | 5.192541 | 1.853302 | -1.13283 |
| O | 6.740169 | -0.22699 | -1.04875 |
| C | 4.380028 | 3.014757 | -1.21173 |
| C | 7.621353 | -1.33918 | -1.02192 |
| C | -6.28173 | -2.18954 | -1.50311 |
| C | -7.52443 | 1.742754 | -0.1286 |
| H | 1.27487 | -0.30474 | -0.95555 |

| | | | |
|---|---|---|---|
| H | 0.896573 | -2.03816 | -1.06442 |
| H | -0.74732 | 1.119265 | -0.24164 |
| H | -1.39433 | -0.96261 | 1.850764 |
| H | 0.572449 | -2.18731 | 1.293577 |
| H | 1.895699 | -0.85174 | 2.649323 |
| H | -0.61351 | 1.720842 | 2.106307 |
| H | -0.15821 | 0.473833 | 3.291722 |
| H | 3.649263 | -2.33856 | 1.584797 |
| H | 2.8486 | 1.634862 | 0.218771 |
| H | 5.80157 | -2.32109 | 0.406933 |
| H | -3.05583 | -1.86301 | -0.23413 |
| H | -2.71435 | 2.411554 | -0.01999 |
| H | -5.15672 | 2.607347 | -0.05741 |
| H | 4.936502 | 3.725637 | -1.82058 |
| H | 3.419723 | 2.799721 | -1.69249 |
| H | 4.202536 | 3.447171 | -0.22125 |
| H | 7.948042 | -1.5668 | -0.00145 |
| H | 7.157443 | -2.2284 | -1.46241 |
| H | 8.484307 | -1.04999 | -1.61975 |
| H | -6.81985 | -3.12922 | -1.37791 |
| H | -6.98879 | -1.39569 | -1.75576 |
| H | -5.54452 | -2.29886 | -2.30598 |
| H | -7.26779 | 2.367817 | -0.99013 |
| H | -8.58912 | 1.516742 | -0.15082 |
| H | -7.28676 | 2.27814 | 0.796396 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 3** – E = −1304.71496 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 0.788135 | 0.547755 | -1.04244 |
| C | -0.58395 | 0.673182 | -0.69044 |
| C | 1.322668 | -0.43008 | -0.15659 |
| C | 0.683377 | -0.11073 | 1.216999 |
| C | -0.63357 | 0.615673 | 0.844288 |
| C | -1.72606 | -0.29592 | 1.457917 |
| O | -1.11825 | -1.58064 | 1.53475 |
| C | 0.208122 | -1.34146 | 1.989667 |
| C | 2.824896 | -0.39827 | -0.18884 |
| C | -3.03834 | -0.36955 | 0.722443 |
| C | -3.39867 | -1.47246 | -0.03402 |
| C | -3.92198 | 0.717663 | 0.804424 |
| C | -4.62232 | -1.49754 | -0.7114 |
| C | -5.13512 | 0.708937 | 0.130823 |
| C | -5.49496 | -0.42098 | -0.64414 |
| C | 3.51242 | 0.820309 | -0.17819 |

| | | | |
|---|---|---|---|
| C | 3.565597 | -1.57386 | -0.19998 |
| C | 4.960635 | -1.54797 | -0.1751 |
| C | 5.641027 | -0.33317 | -0.15107 |
| C | 4.895983 | 0.865999 | -0.16333 |
| O | 5.526519 | 2.081324 | -0.10202 |
| O | 6.989111 | -0.19914 | -0.10896 |
| O | -6.0416 | 1.717574 | 0.154115 |
| O | -6.69896 | -0.35118 | -1.26523 |
| C | -5.7273 | 2.874487 | 0.914082 |
| C | -7.09931 | -1.46211 | -2.0527 |
| C | 6.18447 | 2.478368 | -1.30766 |
| C | 7.776075 | -1.38241 | -0.09006 |
| H | -1.16095 | -0.15343 | -1.127 |
| H | -0.9518 | 1.612382 | -1.10561 |
| H | 0.979933 | -1.4282 | -0.47338 |
| H | 1.354425 | 0.512285 | 1.810462 |
| H | -0.68414 | 1.618958 | 1.269116 |
| H | -1.91955 | 0.063037 | 2.481847 |
| H | 0.797439 | -2.24081 | 1.798897 |
| H | 0.2062 | -1.14555 | 3.071089 |
| H | -2.73261 | -2.32396 | -0.09394 |
| H | -3.65027 | 1.57541 | 1.408791 |
| H | -4.88483 | -2.3724 | -1.2931 |
| H | 2.969218 | 1.758912 | -0.18601 |
| H | 3.057865 | -2.53305 | -0.22857 |
| H | 5.508007 | -2.48226 | -0.17574 |
| H | -6.57254 | 3.549767 | 0.790986 |
| H | -5.607 | 2.635282 | 1.976122 |
| H | -4.81821 | 3.360935 | 0.54442 |
| H | -8.07634 | -1.20334 | -2.45784 |
| H | -6.40067 | -1.64021 | -2.87728 |
| H | -7.18732 | -2.37083 | -1.44746 |
| H | 6.629161 | 3.453365 | -1.10792 |
| H | 6.969334 | 1.769458 | -1.58235 |
| H | 5.464252 | 2.570278 | -2.12799 |
| H | 8.812056 | -1.05026 | -0.05091 |
| H | 7.556621 | -1.9909 | 0.793252 |
| H | 7.619885 | -1.97929 | -0.99448 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 4** – E = −1304.714933 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -0.70198 | -0.53967 | -1.26974 |
| C | 0.675954 | -0.63201 | -0.93169 |
| C | -1.32847 | 0.084813 | -0.15411 |

| | | | |
|---|---|---|---|
| C | -0.6531 | -0.54915 | 1.087836 |
| C | 0.718484 | -1.02963 | 0.551133 |
| C | 1.732524 | -0.25887 | 1.431198 |
| O | 1.028216 | 0.903314 | 1.852111 |
| C | -0.27851 | 0.449466 | 2.184834 |
| C | -2.81996 | -0.09093 | -0.23057 |
| C | 3.041714 | 0.11213 | 0.785133 |
| C | 3.346988 | 1.415157 | 0.428675 |
| C | 3.981927 | -0.89986 | 0.536764 |
| C | 4.572137 | 1.715123 | -0.17699 |
| C | 5.197422 | -0.61671 | -0.06906 |
| C | 5.500839 | 0.717535 | -0.43567 |
| C | -3.67625 | 0.964473 | 0.090071 |
| C | -3.38333 | -1.31163 | -0.59187 |
| C | -4.76501 | -1.48355 | -0.6176 |
| C | -5.61694 | -0.43364 | -0.27305 |
| C | -5.05517 | 0.809445 | 0.07851 |
| O | -5.84699 | 1.860669 | 0.46014 |
| O | -6.97011 | -0.51314 | -0.24027 |
| O | 6.158064 | -1.53316 | -0.34546 |
| O | 6.710746 | 0.90692 | -1.01926 |
| C | 5.905545 | -2.88536 | 0.004295 |
| C | 7.057843 | 2.228694 | -1.40218 |
| C | -6.58729 | 2.474725 | -0.59795 |
| C | -7.57449 | -1.75359 | -0.58052 |
| H | 1.166582 | 0.339104 | -1.08543 |
| H | 1.135918 | -1.36457 | -1.59614 |
| H | -1.09041 | 1.160575 | -0.16506 |
| H | -1.26451 | -1.36673 | 1.472548 |
| H | 0.848885 | -2.107 | 0.660827 |
| H | 1.94373 | -0.88134 | 2.316123 |
| H | -0.93455 | 1.320841 | 2.236971 |
| H | -0.26704 | -0.0407 | 3.16847 |
| H | 2.636277 | 2.207588 | 0.626701 |
| H | 3.753063 | -1.91831 | 0.828632 |
| H | 4.79066 | 2.741705 | -0.44385 |
| H | -3.28136 | 1.938849 | 0.36134 |
| H | -2.73856 | -2.13964 | -0.86438 |
| H | -5.17301 | -2.44619 | -0.8998 |
| H | 5.029384 | -3.27804 | -0.52284 |
| H | 6.789679 | -3.44193 | -0.30249 |
| H | 5.762704 | -2.99955 | 1.084278 |
| H | 8.049867 | 2.159572 | -1.84583 |
| H | 6.356757 | 2.6278 | -2.1432 |
| H | 7.094097 | 2.899505 | -0.53701 |
| H | -7.14602 | 3.294065 | -0.14548 |

| | | | |
|---|---|---|---|
| H | -5.91026 | 2.875722 | -1.36008 |
| H | -7.28329 | 1.76829 | -1.05646 |
| H | -8.6476 | -1.59781 | -0.48386 |
| H | -7.34104 | -2.04222 | -1.61049 |
| H | -7.26075 | -2.54897 | 0.103262 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 5** – E = −1304.714869 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 0.848024 | 0.627137 | -0.96487 |
| C | -0.49254 | 0.900325 | -0.57745 |
| C | 1.299897 | -0.39868 | -0.08862 |
| C | 0.718754 | -0.02521 | 1.299337 |
| C | -0.49748 | 0.87117 | 0.957551 |
| C | -1.68288 | 0.12578 | 1.613485 |
| O | -1.26607 | -1.23426 | 1.656942 |
| C | 0.097119 | -1.19672 | 2.064079 |
| C | 2.799747 | -0.50672 | -0.13747 |
| C | -3.02057 | 0.258481 | 0.931178 |
| C | -3.70347 | 1.466104 | 0.975747 |
| C | -3.59171 | -0.81972 | 0.245027 |
| C | -4.93545 | 1.609071 | 0.333805 |
| C | -4.8207 | -0.69267 | -0.39074 |
| C | -5.50566 | 0.543766 | -0.35207 |
| C | 3.579466 | 0.65313 | -0.20531 |
| C | 3.422238 | -1.74733 | -0.06338 |
| C | 4.814475 | -1.82695 | -0.05462 |
| C | 5.594554 | -0.68356 | -0.11812 |
| C | 4.969147 | 0.579686 | -0.19421 |
| O | 5.797716 | 1.651744 | -0.23956 |
| O | 6.958859 | -0.79165 | -0.05217 |
| O | -5.44469 | -1.6877 | -1.06991 |
| O | -6.69603 | 0.580993 | -1.00257 |
| C | -4.79761 | -2.94902 | -1.14156 |
| C | -7.42092 | 1.8009 | -0.98405 |
| C | 5.214177 | 2.94628 | -0.29813 |
| C | 7.645036 | -0.52531 | -1.27783 |
| H | -1.16414 | 0.130146 | -0.98109 |
| H | -0.77361 | 1.865403 | -1.00057 |
| H | 0.861243 | -1.35914 | -0.40243 |
| H | 1.470264 | 0.495207 | 1.894832 |
| H | -0.39543 | 1.877532 | 1.365551 |
| H | -1.77922 | 0.496654 | 2.646611 |
| H | 0.544185 | -2.16576 | 1.833421 |
| H | 0.160484 | -1.02952 | 3.148302 |

| | | | |
|---|---|---|---|
| H | -3.2869 | 2.312852 | 1.512363 |
| H | -3.05931 | -1.76086 | 0.225966 |
| H | -5.44808 | 2.561734 | 0.379817 |
| H | 3.078722 | 1.610281 | -0.27433 |
| H | 2.829231 | -2.65525 | -0.02266 |
| H | 5.319108 | -2.78557 | 0.003714 |
| H | -4.65542 | -3.38337 | -0.14621 |
| H | -5.4591 | -3.58967 | -1.72273 |
| H | -3.82925 | -2.87397 | -1.6478 |
| H | -7.68853 | 2.092232 | 0.037474 |
| H | -6.85477 | 2.610605 | -1.45709 |
| H | -8.32953 | 1.616176 | -1.55505 |
| H | 6.04714 | 3.647071 | -0.31429 |
| H | 4.615184 | 3.073512 | -1.20561 |
| H | 4.592468 | 3.14165 | 0.581561 |
| H | 7.469051 | 0.498831 | -1.61555 |
| H | 8.706532 | -0.66271 | -1.07128 |
| H | 7.33339 | -1.23093 | -2.05571 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 6** – E = −1304.714791 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -0.65018 | -1.17629 | -1.11852 |
| C | 0.689942 | -1.36878 | -0.68522 |
| C | -1.24089 | -0.30399 | -0.16297 |
| C | -0.70858 | -0.79734 | 1.205805 |
| C | 0.623901 | -1.50093 | 0.844377 |
| C | 1.677743 | -0.69723 | 1.646136 |
| O | 1.08392 | 0.581348 | 1.838611 |
| C | -0.27822 | 0.319937 | 2.157145 |
| C | -2.73841 | -0.30724 | -0.30584 |
| C | 3.043659 | -0.56737 | 1.02205 |
| C | 3.907488 | -1.65954 | 1.022703 |
| C | 3.455014 | 0.634518 | 0.440985 |
| C | 5.159186 | -1.55424 | 0.421911 |
| C | 4.714773 | 0.74934 | -0.14527 |
| C | 5.575159 | -0.36602 | -0.16096 |
| C | -3.45897 | 0.875555 | -0.09298 |
| C | -3.43065 | -1.47088 | -0.60787 |
| C | -4.82445 | -1.46227 | -0.69639 |
| C | -5.54456 | -0.2948 | -0.47477 |
| C | -4.84618 | 0.895988 | -0.16536 |
| O | -5.61603 | 1.995464 | 0.030645 |
| O | -6.89537 | -0.18719 | -0.53684 |
| O | 5.198846 | 1.884373 | -0.70746 |

| | | | |
|---|---|---|---|
| O | 6.838685 | -0.2762 | -0.68474 |
| C | 4.367101 | 3.036653 | -0.7127 |
| C | 6.893873 | -0.21859 | -2.11193 |
| C | -4.96334 | 3.214774 | 0.350225 |
| C | -7.63722 | -1.35401 | -0.85776 |
| H | 1.30439 | -0.50515 | -0.97408 |
| H | 1.079651 | -2.25649 | -1.18493 |
| H | -0.86339 | 0.718117 | -0.3291 |
| H | -1.42958 | -1.47337 | 1.667655 |
| H | 0.629796 | -2.54957 | 1.144004 |
| H | 1.791412 | -1.1842 | 2.627577 |
| H | -0.83611 | 1.250305 | 2.034129 |
| H | -0.364 | -0.00457 | 3.203497 |
| H | 3.609792 | -2.5944 | 1.486905 |
| H | 2.780596 | 1.479672 | 0.470277 |
| H | 5.845629 | -2.39435 | 0.411309 |
| H | -2.91988 | 1.790475 | 0.122688 |
| H | -2.88661 | -2.39023 | -0.78995 |
| H | -5.34402 | -2.38029 | -0.94131 |
| H | 4.124185 | 3.356364 | 0.305758 |
| H | 4.943536 | 3.81653 | -1.20748 |
| H | 3.442408 | 2.858731 | -1.27111 |
| H | 6.375677 | 0.66489 | -2.49282 |
| H | 7.949905 | -0.16268 | -2.3767 |
| H | 6.457739 | -1.12209 | -2.5521 |
| H | -4.29558 | 3.535386 | -0.45667 |
| H | -5.75504 | 3.951704 | 0.475692 |
| H | -4.39482 | 3.131393 | 1.282757 |
| H | -8.68303 | -1.05081 | -0.85883 |
| H | -7.37051 | -1.73777 | -1.84837 |
| H | -7.48936 | -2.14095 | -0.11031 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 7** – E = −1304.714628 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 0.87328 | 0.335044 | -1.06094 |
| C | -0.49805 | 0.528313 | -0.73598 |
| C | 1.371704 | -0.57237 | -0.08552 |
| C | 0.732918 | -0.11105 | 1.247737 |
| C | -0.56076 | 0.612836 | 0.796961 |
| C | -1.68222 | -0.20964 | 1.48074 |
| O | -1.11029 | -1.49723 | 1.68135 |
| C | 0.218796 | -1.25288 | 2.125311 |
| C | 2.875644 | -0.58793 | -0.10287 |
| C | -2.99063 | -0.31624 | 0.742235 |

| | | | |
|---|---|---|---|
| C | -3.37016 | -1.4708 | 0.077657 |
| C | -3.84933 | 0.793498 | 0.724007 |
| C | -4.58888 | -1.52574 | -0.60706 |
| C | -5.05769 | 0.754431 | 0.042987 |
| C | -5.43694 | -0.42813 | -0.63847 |
| C | 3.584665 | 0.609393 | -0.25052 |
| C | 3.571349 | -1.77879 | 0.070418 |
| C | 4.965653 | -1.77257 | 0.096854 |
| C | 5.67571 | -0.59176 | -0.04796 |
| C | 4.976123 | 0.621681 | -0.2236 |
| O | 5.739547 | 1.73552 | -0.3448 |
| O | 7.043312 | -0.61108 | 0.033222 |
| O | -5.94246 | 1.779925 | -0.02564 |
| O | -6.63403 | -0.38298 | -1.2749 |
| C | -5.61174 | 2.98784 | 0.64233 |
| C | -7.05694 | -1.54784 | -1.96683 |
| C | 5.080349 | 2.982858 | -0.51566 |
| C | 7.723632 | -0.39864 | -1.20623 |
| H | -1.09224 | -0.32023 | -1.1014 |
| H | -0.83689 | 1.434554 | -1.23952 |
| H | 1.00198 | -1.58473 | -0.31321 |
| H | 1.417369 | 0.545174 | 1.787528 |
| H | -0.58737 | 1.651701 | 1.128047 |
| H | -1.87347 | 0.247432 | 2.465189 |
| H | 0.7846 | -2.18118 | 2.023543 |
| H | 0.214287 | -0.95839 | 3.184192 |
| H | -2.72356 | -2.33912 | 0.096783 |
| H | -3.5631 | 1.692764 | 1.257205 |
| H | -4.86692 | -2.44041 | -1.11571 |
| H | 3.029231 | 1.527205 | -0.39497 |
| H | 3.033648 | -2.71587 | 0.172829 |
| H | 5.526298 | -2.69162 | 0.231046 |
| H | -4.68964 | 3.425486 | 0.244842 |
| H | -6.44193 | 3.667363 | 0.456252 |
| H | -5.50641 | 2.832484 | 1.721441 |
| H | -6.35969 | -1.81179 | -2.76928 |
| H | -7.16828 | -2.39913 | -1.28659 |
| H | -8.02618 | -1.30255 | -2.39822 |
| H | 4.486677 | 2.997645 | -1.4354 |
| H | 4.436488 | 3.212334 | 0.3395 |
| H | 5.869949 | 3.729278 | -0.5834 |
| H | 8.78947 | -0.45733 | -0.98522 |
| H | 7.460405 | -1.17831 | -1.92935 |
| H | 7.49116 | 0.584817 | -1.62181 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 8** – E = −1304.714607 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 0.807445 | 0.549467 | -1.07769 |
| C | -0.52522 | 0.853825 | -0.68792 |
| C | 1.31839 | -0.30565 | -0.0589 |
| C | 0.788794 | 0.296855 | 1.265935 |
| C | -0.4791 | 1.0739 | 0.831927 |
| C | -1.60529 | 0.398476 | 1.651922 |
| O | -1.11688 | -0.91092 | 1.919003 |
| C | 0.254371 | -0.73792 | 2.258005 |
| C | 2.81397 | -0.40813 | -0.16516 |
| C | -2.96706 | 0.34034 | 1.009644 |
| C | -3.74106 | 1.493341 | 0.9123 |
| C | -3.48223 | -0.84977 | 0.492144 |
| C | -4.99677 | 1.467526 | 0.309455 |
| C | -4.73399 | -0.89461 | -0.1046 |
| C | -5.5113 | 0.276107 | -0.20103 |
| C | 3.580396 | 0.746256 | -0.38588 |
| C | 3.459173 | -1.62449 | -0.0122 |
| C | 4.85509 | -1.70053 | -0.06259 |
| C | 5.617338 | -0.56149 | -0.27951 |
| C | 4.963922 | 0.684869 | -0.44978 |
| O | 5.777942 | 1.747034 | -0.67032 |
| O | 6.970829 | -0.53068 | -0.35279 |
| O | -5.22201 | -2.09948 | -0.54008 |
| O | -6.73144 | 0.143029 | -0.7784 |
| C | -5.2732 | -2.24968 | -1.96063 |
| C | -7.54698 | 1.30123 | -0.88844 |
| C | 5.172951 | 3.019438 | -0.8445 |
| C | 7.668781 | -1.75714 | -0.19942 |
| H | -1.18946 | 0.015123 | -0.93789 |
| H | -0.84693 | 1.732347 | -1.24869 |
| H | 0.88064 | -1.30909 | -0.18088 |
| H | 1.544847 | 0.941704 | 1.716508 |
| H | -0.41292 | 2.136598 | 1.068833 |
| H | -1.69279 | 0.942926 | 2.605835 |
| H | 0.743625 | -1.71184 | 2.190309 |
| H | 0.342889 | -0.37045 | 3.289937 |
| H | -3.37222 | 2.432068 | 1.314683 |
| H | -2.913 | -1.76877 | 0.563431 |
| H | -5.57631 | 2.380694 | 0.25602 |
| H | 3.069113 | 1.690211 | -0.52523 |
| H | 2.884305 | -2.53169 | 0.144008 |
| H | 5.338122 | -2.66162 | 0.061168 |

| | | | |
|---|---|---|---|
| H | -5.66655 | -3.24862 | -2.14977 |
| H | -5.93356 | -1.5064 | -2.41398 |
| H | -4.27034 | -2.16792 | -2.39404 |
| H | -7.78563 | 1.714851 | 0.096819 |
| H | -7.0672 | 2.070508 | -1.50239 |
| H | -8.46505 | 0.973653 | -1.37334 |
| H | 5.992182 | 3.718854 | -1.00356 |
| H | 4.51136 | 3.031538 | -1.71728 |
| H | 4.607972 | 3.318785 | 0.044813 |
| H | 8.725502 | -1.51214 | -0.29379 |
| H | 7.486329 | -2.20086 | 0.785254 |
| H | 7.392031 | -2.47466 | -0.97932 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 9** – E = −1304.714314 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 0.669306 | 0.814807 | -1.21566 |
| C | -0.69845 | 0.827634 | -0.82783 |
| C | 1.320462 | -0.04855 | -0.29012 |
| C | 0.683495 | 0.286276 | 1.082303 |
| C | -0.69939 | 0.875797 | 0.707243 |
| C | -1.69362 | -0.07808 | 1.413752 |
| O | -0.98395 | -1.30498 | 1.535459 |
| C | 0.332805 | -0.93779 | 1.930558 |
| C | 2.811109 | 0.134307 | -0.36906 |
| C | -3.02147 | -0.29068 | 0.735074 |
| C | -3.33831 | -1.471 | 0.08338 |
| C | -3.96576 | 0.747191 | 0.761936 |
| C | -4.57862 | -1.62093 | -0.54676 |
| C | -5.19661 | 0.613461 | 0.135917 |
| C | -5.51152 | -0.59429 | -0.53424 |
| C | 3.665285 | -0.96816 | -0.2962 |
| C | 3.376774 | 1.401266 | -0.48178 |
| C | 4.758598 | 1.567674 | -0.5292 |
| C | 5.608607 | 0.463571 | -0.45917 |
| C | 5.044474 | -0.82122 | -0.33403 |
| O | 5.835104 | -1.94045 | -0.32109 |
| O | 6.961697 | 0.522682 | -0.52157 |
| O | -6.16187 | 1.565692 | 0.111762 |
| O | -6.73602 | -0.64224 | -1.11638 |
| C | -5.89658 | 2.796931 | 0.766062 |
| C | -7.0952 | -1.83329 | -1.79962 |
| C | 6.575821 | -2.14175 | 0.88509 |
| C | 7.567793 | 1.799714 | -0.66879 |
| H | -1.19873 | -0.08289 | -1.18544 |

| | | | |
|---|---|---|---|
| H | -1.17161 | 1.692372 | -1.2947 |
| H | 1.072357 | -1.09289 | -0.539 |
| H | 1.309768 | 0.995097 | 1.626128 |
| H | -0.82211 | 1.89908 | 1.064414 |
| H | -1.87778 | 0.323175 | 2.423773 |
| H | 0.986228 | -1.79667 | 1.764013 |
| H | 0.348234 | -0.68678 | 3.000425 |
| H | -2.62457 | -2.28503 | 0.067133 |
| H | -3.72661 | 1.666356 | 1.284299 |
| H | -4.80553 | -2.55361 | -1.04804 |
| H | 3.26852 | -1.97622 | -0.22332 |
| H | 2.733392 | 2.271093 | -0.55184 |
| H | 5.1679 | 2.56499 | -0.63182 |
| H | -5.73029 | 2.652381 | 1.839008 |
| H | -5.03052 | 3.304202 | 0.327538 |
| H | -6.78496 | 3.40912 | 0.619172 |
| H | -7.11109 | -2.69403 | -1.12234 |
| H | -8.09792 | -1.66275 | -2.18843 |
| H | -6.41373 | -2.03764 | -2.63246 |
| H | 5.899577 | -2.2502 | 1.740114 |
| H | 7.136368 | -3.06681 | 0.749814 |
| H | 7.2704 | -1.31785 | 1.065525 |
| H | 8.640396 | 1.6172 | -0.70591 |
| H | 7.250335 | 2.285406 | -1.5972 |
| H | 7.339635 | 2.450268 | 0.181771 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 10** – E = −1304.714086 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -0.77701 | -1.16109 | -1.11509 |
| C | 0.576595 | -1.30196 | -0.70436 |
| C | -1.36256 | -0.24366 | -0.19864 |
| C | -0.78196 | -0.63682 | 1.18333 |
| C | 0.54734 | -1.35037 | 0.830738 |
| C | 1.612882 | -0.49612 | 1.560545 |
| O | 1.017096 | 0.791177 | 1.678975 |
| C | -0.33621 | 0.54674 | 2.044037 |
| C | -2.86303 | -0.28947 | -0.29823 |
| C | 2.9671 | -0.39892 | 0.90846 |
| C | 3.867271 | -1.45565 | 1.009795 |
| C | 3.353266 | 0.734177 | 0.189219 |
| C | 5.11308 | -1.40124 | 0.388103 |
| C | 4.592329 | 0.807655 | -0.43013 |
| C | 5.489186 | -0.27526 | -0.34349 |
| C | -3.60438 | 0.892541 | -0.16959 |

| | | | |
|---|---|---|---|
| C | -3.53629 | -1.48913 | -0.4775 |
| C | -4.93153 | -1.51681 | -0.52765 |
| C | -5.67185 | -0.34907 | -0.38964 |
| C | -4.99322 | 0.878419 | -0.20548 |
| O | -5.78298 | 1.974849 | -0.08649 |
| O | -7.02595 | -0.27524 | -0.42364 |
| O | 4.903425 | 1.919056 | -1.16982 |
| O | 6.668754 | -0.13383 | -0.99774 |
| C | 5.882086 | 2.778484 | -0.58067 |
| C | 7.596527 | -1.20843 | -0.93918 |
| C | -5.15051 | 3.232551 | 0.095247 |
| C | -7.74937 | -1.48141 | -0.61449 |
| H | 1.165444 | -0.44327 | -1.05476 |
| H | 0.97415 | -2.20763 | -1.16421 |
| H | -1.01615 | 0.774291 | -0.44014 |
| H | -1.48026 | -1.28648 | 1.712971 |
| H | 0.56905 | -2.38119 | 1.186461 |
| H | 1.742957 | -0.91933 | 2.569397 |
| H | -0.90263 | 1.46351 | 1.867981 |
| H | -0.39816 | 0.295844 | 3.112169 |
| H | 3.603543 | -2.34224 | 1.578653 |
| H | 2.684555 | 1.582416 | 0.104631 |
| H | 5.786309 | -2.24439 | 0.479352 |
| H | -3.07966 | 1.832978 | -0.04864 |
| H | -2.97708 | -2.41026 | -0.59263 |
| H | -5.43645 | -2.46301 | -0.67725 |
| H | 5.529202 | 3.161848 | 0.383029 |
| H | 6.834639 | 2.260263 | -0.44568 |
| H | 6.016116 | 3.610657 | -1.27194 |
| H | 7.175343 | -2.12142 | -1.37265 |
| H | 8.455265 | -0.89249 | -1.52909 |
| H | 7.915854 | -1.40484 | 0.089577 |
| H | -4.51102 | 3.486203 | -0.75705 |
| H | -5.95551 | 3.961912 | 0.170282 |
| H | -4.55675 | 3.252869 | 1.015467 |
| H | -8.80165 | -1.20147 | -0.60781 |
| H | -7.505 | -1.94716 | -1.57529 |
| H | -7.55938 | -2.19459 | 0.194831 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 11** – E = −1304.713919 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -0.66672 | -1.15014 | -1.16798 |
| C | 0.694327 | -1.27097 | -0.77365 |
| C | -1.28226 | -0.33553 | -0.17947 |

| | | | |
|---|---|---|---|
| C | -0.67604 | -0.81013 | 1.165925 |
| C | 0.675323 | -1.44525 | 0.751917 |
| C | 1.714545 | -0.61646 | 1.545348 |
| O | 1.076894 | 0.638007 | 1.761798 |
| C | -0.26537 | 0.320762 | 2.1116 |
| C | -2.78083 | -0.44458 | -0.2707 |
| C | 3.065098 | -0.43041 | 0.903425 |
| C | 3.988299 | -1.46629 | 0.921409 |
| C | 3.40589 | 0.772591 | 0.272717 |
| C | 5.232849 | -1.31874 | 0.304988 |
| C | 4.643447 | 0.934967 | -0.3372 |
| C | 5.574693 | -0.12963 | -0.32667 |
| C | -3.57168 | 0.671584 | 0.018306 |
| C | -3.39233 | -1.65267 | -0.59114 |
| C | -4.782 | -1.73594 | -0.62767 |
| C | -5.57509 | -0.63728 | -0.32966 |
| C | -4.96333 | 0.587258 | 0.005467 |
| O | -5.79918 | 1.613367 | 0.299703 |
| O | -6.93884 | -0.77226 | -0.3135 |
| O | 5.053023 | 2.066263 | -0.96403 |
| O | 6.757602 | 0.113049 | -0.94535 |
| C | 4.1552 | 3.165018 | -1.00204 |
| C | 7.721044 | -0.92907 | -0.96001 |
| C | -5.22599 | 2.863701 | 0.656784 |
| C | -7.61967 | -0.13991 | -1.39998 |
| H | 1.247168 | -0.36433 | -1.05454 |
| H | 1.123233 | -2.12013 | -1.30702 |
| H | -0.98537 | 0.713281 | -0.34169 |
| H | -1.34539 | -1.52323 | 1.649269 |
| H | 0.735014 | -2.50014 | 1.022616 |
| H | 1.858407 | -1.11082 | 2.519178 |
| H | -0.8635 | 1.228179 | 2.007807 |
| H | -0.31198 | -0.01209 | 3.157852 |
| H | 3.752256 | -2.40232 | 1.418071 |
| H | 2.687939 | 1.58164 | 0.279733 |
| H | 5.936585 | -2.14125 | 0.330607 |
| H | -3.08963 | 1.612749 | 0.255637 |
| H | -2.78468 | -2.51801 | -0.82734 |
| H | -5.27874 | -2.667 | -0.88037 |
| H | 3.912357 | 3.518882 | 0.005634 |
| H | 4.673502 | 3.953613 | -1.54537 |
| H | 3.230765 | 2.908214 | -1.53022 |
| H | 8.027287 | -1.20572 | 0.054642 |
| H | 7.34374 | -1.8156 | -1.48117 |
| H | 8.579976 | -0.53296 | -1.4995 |
| H | -4.60463 | 2.773705 | 1.553702 |

| | | | |
|---|---|---|---|
| H | -4.62997 | 3.278446 | -0.16263 |
| H | -6.06443 | 3.526455 | 0.863896 |
| H | -8.68081 | -0.346 | -1.25907 |
| H | -7.45486 | 0.940339 | -1.39547 |
| H | -7.29332 | -0.5604 | -2.3575 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*R*,8*S*,7'*S*,8'*S*)-**2**
**Conf 12** – E = −1304.713897 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -0.80079 | -0.87153 | -1.22058 |
| C | 0.570656 | -0.89317 | -0.84846 |
| C | -1.44219 | -0.02831 | -0.27128 |
| C | -0.78565 | -0.38455 | 1.087502 |
| C | 0.587633 | -0.97833 | 0.684596 |
| C | 1.597622 | -0.05029 | 1.401067 |
| O | 0.904338 | 1.182937 | 1.548303 |
| C | -0.41386 | 0.824985 | 1.948302 |
| C | -2.93402 | -0.21504 | -0.32885 |
| C | 2.923283 | 0.158302 | 0.717373 |
| C | 3.2534 | 1.350324 | 0.084711 |
| C | 3.863358 | -0.8779 | 0.714781 |
| C | 4.484573 | 1.505646 | -0.55457 |
| C | 5.087017 | -0.74283 | 0.079834 |
| C | 5.409505 | 0.464952 | -0.57436 |
| C | -3.77909 | 0.886419 | -0.13971 |
| C | -3.49631 | -1.46747 | -0.52845 |
| C | -4.88368 | -1.62673 | -0.53763 |
| C | -5.72626 | -0.53956 | -0.34009 |
| C | -5.16073 | 0.741149 | -0.13711 |
| O | -6.04564 | 1.754056 | 0.037893 |
| O | -7.08185 | -0.59481 | -0.33082 |
| O | 5.946668 | -1.80957 | 0.052344 |
| O | 6.617787 | 0.509064 | -1.18866 |
| C | 7.11037 | -1.66767 | 0.870778 |
| C | 6.976509 | 1.704303 | -1.86816 |
| C | -5.52838 | 3.060974 | 0.236201 |
| C | -7.69241 | -1.85929 | -0.53847 |
| H | 1.066531 | 0.026351 | -1.18924 |
| H | 1.039424 | -1.74574 | -1.34142 |
| H | -1.20044 | 1.021449 | -0.50486 |
| H | -1.40866 | -1.09629 | 1.631004 |
| H | 0.704666 | -2.01087 | 1.01602 |
| H | 1.783952 | -0.47148 | 2.402374 |
| H | -1.05801 | 1.693693 | 1.797794 |
| H | -0.42392 | 0.560928 | 3.014995 |

| | | | |
|---|---|---|---|
| H | 2.546629 | 2.171038 | 0.090503 |
| H | 3.654144 | -1.82268 | 1.207812 |
| H | 4.709472 | 2.445531 | -1.04324 |
| H | -3.34253 | 1.868428 | -0.00124 |
| H | -2.85606 | -2.3265 | -0.69146 |
| H | -5.3015 | -2.61215 | -0.70228 |
| H | 7.680717 | -2.58937 | 0.755172 |
| H | 7.719357 | -0.81938 | 0.549504 |
| H | 6.829398 | -1.54522 | 1.922513 |
| H | 6.273536 | 1.927328 | -2.67733 |
| H | 7.025793 | 2.555026 | -1.18062 |
| H | 7.964203 | 1.522612 | -2.28851 |
| H | -4.94336 | 3.395325 | -0.62734 |
| H | -6.39547 | 3.708667 | 0.355684 |
| H | -4.90984 | 3.114333 | 1.138586 |
| H | -8.76592 | -1.68216 | -0.49519 |
| H | -7.43288 | -2.27285 | -1.51894 |
| H | -7.41147 | -2.57274 | 0.24371 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 1** – E = −1304.715986 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.140643 | -0.28311 | 1.585955 |
| C | 1.534787 | -0.65483 | 0.267126 |
| C | 0.716771 | 0.280483 | -0.6458 |
| C | 0.298262 | -0.28908 | -2.00871 |
| O | -1.12892 | -0.35092 | -2.01442 |
| C | -1.56168 | -0.48131 | -0.6636 |
| C | -0.60372 | 0.43287 | 0.127821 |
| C | -0.26089 | -0.00701 | 1.558528 |
| C | -3.02282 | -0.13784 | -0.55181 |
| C | -3.56361 | 0.9378 | -1.24168 |
| C | -3.85105 | -0.88869 | 0.292442 |
| C | -5.1918 | -0.56451 | 0.459316 |
| C | -4.91132 | 1.269908 | -1.09027 |
| C | -5.73419 | 0.536635 | -0.24351 |
| C | 3.028553 | -0.55397 | 0.125638 |
| C | 3.706792 | 0.55918 | 0.644388 |
| C | 3.749381 | -1.52801 | -0.54599 |
| C | 5.131416 | -1.39733 | -0.71937 |
| C | 5.806529 | -0.29709 | -0.21017 |
| C | 5.077573 | 0.697022 | 0.489847 |
| O | -6.05823 | -1.23851 | 1.255691 |
| O | -7.05044 | 0.783537 | -0.02801 |
| O | 7.141057 | -0.08244 | -0.31643 |

| | | | |
|---|---|---|---|
| O | 5.811253 | 1.732384 | 0.96782 |
| C | -5.5635 | -2.35398 | 1.980891 |
| C | -7.63886 | 1.876422 | -0.71663 |
| C | 5.129728 | 2.754878 | 1.678723 |
| C | 7.915022 | -1.05881 | -0.99677 |
| H | 1.231746 | -1.69602 | 0.071803 |
| H | 1.239745 | 1.233563 | -0.7452 |
| H | 0.716906 | -1.29359 | -2.16289 |
| H | 0.602065 | 0.340186 | -2.84688 |
| H | -1.41385 | -1.52132 | -0.32934 |
| H | -0.97735 | 1.45793 | 0.093454 |
| H | -0.8237 | -0.90727 | 1.842084 |
| H | -0.45711 | 0.766866 | 2.302476 |
| H | -2.94073 | 1.517463 | -1.91306 |
| H | -3.43574 | -1.74086 | 0.817264 |
| H | -5.31416 | 2.109811 | -1.64262 |
| H | 3.141529 | 1.304934 | 1.188518 |
| H | 3.246383 | -2.40467 | -0.94144 |
| H | 5.674113 | -2.17017 | -1.24893 |
| H | -4.76594 | -2.0603 | 2.671831 |
| H | -6.40917 | -2.73743 | 2.54956 |
| H | -5.19465 | -3.13649 | 1.309106 |
| H | -7.58995 | 1.738724 | -1.80217 |
| H | -8.68145 | 1.898994 | -0.40336 |
| H | -7.15931 | 2.823641 | -0.44741 |
| H | 4.382477 | 3.249995 | 1.049409 |
| H | 4.645111 | 2.361244 | 2.578558 |
| H | 5.893108 | 3.475934 | 1.966722 |
| H | 7.599716 | -1.16336 | -2.0405 |
| H | 8.942255 | -0.6991 | -0.96539 |
| H | 7.856648 | -2.03268 | -0.49896 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 2** – E = −1304.715781 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.718241 | -0.9053 | 0.40625 |
| C | 0.400379 | -1.46057 | 0.366754 |
| C | -0.36393 | -0.67262 | -0.72117 |
| C | -1.79203 | -0.29943 | -0.36379 |
| O | -1.71824 | 0.905297 | 0.40625 |
| C | -0.40038 | 1.460573 | 0.366754 |
| C | 0.36393 | 0.672619 | -0.72117 |
| C | 1.792033 | 0.299431 | -0.36379 |
| C | -0.45286 | 2.94965 | 0.1294 |
| C | -1.41452 | 3.517543 | -0.69244 |

| | | | |
|---|---|---|---|
| C | 0.513504 | 3.777929 | 0.71626 |
| C | 0.532757 | 5.145596 | 0.472839 |
| C | -1.41235 | 4.89234 | -0.93976 |
| C | -0.44775 | 5.715955 | -0.37281 |
| C | 0.452859 | -2.94965 | 0.1294 |
| C | -0.5135 | -3.77793 | 0.71626 |
| C | 1.414521 | -3.51754 | -0.69244 |
| C | 1.412353 | -4.89234 | -0.93976 |
| C | 0.447748 | -5.71596 | -0.37281 |
| C | -0.53276 | -5.1456 | 0.472839 |
| O | 1.431508 | 6.013749 | 1.000612 |
| O | -0.36393 | 7.058207 | -0.55305 |
| O | 0.36393 | -7.05821 | -0.55305 |
| O | -1.43151 | -6.01375 | 1.000612 |
| C | 2.436004 | 5.490064 | 1.855906 |
| C | -1.33809 | 7.674311 | -1.38126 |
| C | -2.436 | -5.49006 | 1.855906 |
| C | 1.338092 | -7.67431 | -1.38126 |
| H | -0.08131 | -1.2798 | 1.338745 |
| H | -0.29666 | -1.18609 | -1.68271 |
| H | -2.29991 | -1.06378 | 0.232852 |
| H | -2.38701 | -0.11939 | -1.26694 |
| H | 0.081306 | 1.279804 | 1.338745 |
| H | 0.296663 | 1.186094 | -1.68271 |
| H | 2.299914 | 1.063784 | 0.232852 |
| H | 2.387005 | 0.11939 | -1.26694 |
| H | -2.18282 | 2.893923 | -1.13446 |
| H | 1.25072 | 3.341237 | 1.379861 |
| H | -2.1763 | 5.315654 | -1.58017 |
| H | -1.25072 | -3.34124 | 1.379861 |
| H | 2.182817 | -2.89392 | -1.13446 |
| H | 2.176303 | -5.31565 | -1.58017 |
| H | 3.045734 | 6.341331 | 2.154557 |
| H | 2.000801 | 5.026342 | 2.747701 |
| H | 3.063977 | 4.759747 | 1.33442 |
| H | -2.34791 | 7.539955 | -0.97869 |
| H | -1.0926 | 8.735125 | -1.39131 |
| H | -1.299 | 7.283854 | -2.40389 |
| H | -2.0008 | -5.02634 | 2.747701 |
| H | -3.06398 | -4.75975 | 1.33442 |
| H | -3.04573 | -6.34133 | 2.154557 |
| H | 1.0926 | -8.73513 | -1.39131 |
| H | 1.299002 | -7.28385 | -2.40389 |
| H | 2.347911 | -7.53996 | -0.97869 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 3** – E = −1304.715561 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | -1.8103 | -1.10393 | -0.58762 |
| C | -0.47265 | -1.53046 | -0.83607 |
| C | 0.37892 | -0.66834 | 0.117188 |
| C | 1.7897 | -0.3085 | -0.36771 |
| O | 1.8103 | 1.103928 | -0.58762 |
| C | 0.472649 | 1.530461 | -0.83607 |
| C | -0.37892 | 0.668342 | 0.117188 |
| C | -1.7897 | 0.308497 | -0.36771 |
| C | 0.35936 | 3.017413 | -0.64212 |
| C | -0.35936 | 3.799283 | -1.53182 |
| C | 0.955899 | 3.627027 | 0.47194 |
| C | 0.830892 | 4.989847 | 0.693626 |
| C | -0.50343 | 5.173864 | -1.31554 |
| C | 0.082255 | 5.780871 | -0.21378 |
| C | -0.35936 | -3.01741 | -0.64212 |
| C | -0.9559 | -3.62703 | 0.47194 |
| C | 0.35936 | -3.79928 | -1.53182 |
| C | 0.503425 | -5.17386 | -1.31554 |
| C | -0.08226 | -5.78087 | -0.21378 |
| C | -0.83089 | -4.98985 | 0.693626 |
| O | 1.382983 | 5.659598 | 1.735671 |
| O | 0.009227 | 7.102228 | 0.07979 |
| O | -0.00923 | -7.10223 | 0.07979 |
| O | -1.38298 | -5.6596 | 1.735671 |
| C | 2.145956 | 4.913634 | 2.672035 |
| C | -0.72182 | 7.93651 | -0.80616 |
| C | -2.14596 | -4.91363 | 2.672035 |
| C | 0.721818 | -7.93651 | -0.80616 |
| H | -0.19476 | -1.29157 | -1.87509 |
| H | 0.390429 | -1.1296 | 1.106615 |
| H | 2.036003 | -0.83551 | -1.29971 |
| H | 2.562964 | -0.53704 | 0.367943 |
| H | 0.194757 | 1.291566 | -1.87509 |
| H | -0.39043 | 1.129602 | 1.106615 |
| H | -2.036 | 0.835512 | -1.29971 |
| H | -2.56296 | 0.537041 | 0.367943 |
| H | -0.81491 | 3.35058 | -2.40882 |
| H | 1.536093 | 3.015761 | 1.151369 |
| H | -1.07036 | 5.764707 | -2.02394 |
| H | -1.53609 | -3.01576 | 1.151369 |
| H | 0.814912 | -3.35058 | -2.40882 |
| H | 1.070359 | -5.76471 | -2.02394 |

| | | | |
|---|---|---|---|
| H | 2.491408 | 5.632182 | 3.413622 |
| H | 1.537104 | 4.148188 | 3.164974 |
| H | 3.01098 | 4.439945 | 2.195719 |
| H | -1.77421 | 7.637723 | -0.86004 |
| H | -0.65355 | 8.941557 | -0.39291 |
| H | -0.28848 | 7.928032 | -1.81203 |
| H | -1.5371 | -4.14819 | 3.164974 |
| H | -3.01098 | -4.43995 | 2.195719 |
| H | -2.49141 | -5.63218 | 3.413622 |
| H | 0.653546 | -8.94156 | -0.39291 |
| H | 0.288475 | -7.92803 | -1.81203 |
| H | 1.77421 | -7.63772 | -0.86004 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 4** – E = −1304.714363 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.122025 | -1.95748 | -0.69002 |
| C | 1.51742 | -0.59067 | -0.54035 |
| C | 0.591351 | 0.00197 | 0.544949 |
| C | 0.095991 | 1.412339 | 0.273836 |
| O | -1.07214 | 1.287595 | -0.54728 |
| C | -1.464 | -0.08102 | -0.67594 |
| C | -0.66773 | -0.85376 | 0.399004 |
| C | -0.12993 | -2.20482 | -0.0405 |
| C | -2.96071 | -0.22432 | -0.55148 |
| C | -3.64003 | -1.18651 | -1.29041 |
| C | -3.66781 | 0.577582 | 0.350056 |
| C | -5.03918 | 0.415893 | 0.524984 |
| C | -5.01438 | -1.35168 | -1.12048 |
| C | -5.72123 | -0.5675 | -0.22299 |
| C | 2.988649 | -0.49427 | -0.22164 |
| C | 3.746699 | 0.558565 | -0.75114 |
| C | 3.604255 | -1.40784 | 0.621195 |
| C | 4.955866 | -1.27339 | 0.945138 |
| C | 5.70872 | -0.22308 | 0.434286 |
| C | 5.090582 | 0.709198 | -0.43154 |
| O | -5.79641 | 1.140332 | 1.385483 |
| O | -7.06148 | -0.78766 | -0.03936 |
| O | 7.023799 | -0.00913 | 0.690502 |
| O | 5.892481 | 1.697979 | -0.89972 |
| C | -5.15388 | 2.145068 | 2.158292 |
| C | -7.91653 | 0.21447 | -0.59481 |
| C | 5.321152 | 2.656473 | -1.77706 |
| C | 7.686542 | -0.92602 | 1.547672 |
| H | 1.33129 | -0.06616 | -1.48905 |

| | | | |
|---|---|---|---|
| H | 1.051556 | -0.09323 | 1.530771 |
| H | 0.83042 | 2.030528 | -0.25229 |
| H | -0.17331 | 1.920237 | 1.206762 |
| H | -1.16439 | -0.44203 | -1.67038 |
| H | -1.24257 | -0.9181 | 1.325555 |
| H | -0.794 | -2.72177 | -0.74082 |
| H | 0.034362 | -2.86071 | 0.822094 |
| H | -3.10844 | -1.80192 | -2.00908 |
| H | -3.12776 | 1.336697 | 0.901186 |
| H | -5.56113 | -2.09827 | -1.68684 |
| H | 3.27513 | 1.259293 | -1.43021 |
| H | 3.037472 | -2.24093 | 1.020514 |
| H | 5.417778 | -2.00113 | 1.600647 |
| H | -5.93415 | 2.592246 | 2.771901 |
| H | -4.38365 | 1.715911 | 2.807211 |
| H | -4.70807 | 2.914725 | 1.519998 |
| H | -7.77801 | 0.282325 | -1.67935 |
| H | -8.93814 | -0.10026 | -0.38101 |
| H | -7.73254 | 1.189361 | -0.13667 |
| H | 6.123606 | 3.350345 | -2.02252 |
| H | 4.953792 | 2.188638 | -2.69678 |
| H | 4.504275 | 3.203673 | -1.29442 |
| H | 7.676373 | -1.94005 | 1.133671 |
| H | 8.715423 | -0.57663 | 1.61888 |
| H | 7.237567 | -0.93595 | 2.546746 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 5** – E = −1304.714249 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.558813 | 0.029146 | 2.33933 |
| C | 1.722157 | -0.82792 | 1.21189 |
| C | 0.474277 | -0.56221 | 0.335707 |
| C | -0.13806 | -1.81148 | -0.28621 |
| O | -1.03993 | -2.31543 | 0.69888 |
| C | -1.68255 | -1.18787 | 1.290758 |
| C | -0.59266 | -0.09658 | 1.356892 |
| C | 0.184461 | -0.05139 | 2.684905 |
| C | -2.93958 | -0.78056 | 0.538017 |
| C | -3.48423 | -1.59291 | -0.44859 |
| C | -3.61964 | 0.396371 | 0.87044 |
| C | -4.80056 | 0.755287 | 0.240374 |
| C | -4.66752 | -1.24397 | -1.10063 |
| C | -5.3423 | -0.07331 | -0.76416 |
| C | 3.042944 | -0.56722 | 0.544845 |
| C | 3.466936 | 0.752152 | 0.325077 |

| | | | |
|---|---|---|---|
| C | 3.839506 | -1.61166 | 0.104338 |
| C | 5.042295 | -1.35645 | -0.56293 |
| C | 5.465093 | -0.05343 | -0.78379 |
| C | 4.661956 | 1.020499 | -0.32438 |
| O | -5.45772 | 1.886874 | 0.648248 |
| O | -6.50855 | 0.340462 | -1.31925 |
| O | 6.614148 | 0.298564 | -1.4113 |
| O | 5.150659 | 2.261669 | -0.56794 |
| C | -5.40948 | 2.976849 | -0.27547 |
| C | -7.09422 | -0.47638 | -2.32363 |
| C | 4.384329 | 3.372478 | -0.12699 |
| C | 7.452099 | -0.7437 | -1.88765 |
| H | 1.690448 | -1.87611 | 1.549575 |
| H | 0.695703 | 0.202139 | -0.41085 |
| H | 0.587687 | -2.599 | -0.50163 |
| H | -0.67355 | -1.56675 | -1.21208 |
| H | -1.97324 | -1.50563 | 2.298668 |
| H | -0.99014 | 0.886327 | 1.105767 |
| H | -0.00302 | -0.96708 | 3.265525 |
| H | -0.0576 | 0.812168 | 3.30632 |
| H | -2.98352 | -2.51775 | -0.7102 |
| H | -3.25019 | 1.061064 | 1.645576 |
| H | -5.06254 | -1.90202 | -1.86465 |
| H | 2.850112 | 1.563566 | 0.689874 |
| H | 3.537187 | -2.63957 | 0.277107 |
| H | 5.647721 | -2.18846 | -0.89984 |
| H | -5.96337 | 3.794702 | 0.185626 |
| H | -4.37428 | 3.291991 | -0.44667 |
| H | -5.87695 | 2.710591 | -1.22647 |
| H | -7.34232 | -1.46896 | -1.93371 |
| H | -8.00889 | 0.031692 | -2.62452 |
| H | -6.43366 | -0.57854 | -3.1909 |
| H | 4.260751 | 3.366357 | 0.961271 |
| H | 4.946863 | 4.257233 | -0.42084 |
| H | 3.399219 | 3.393548 | -0.60515 |
| H | 8.304629 | -0.25126 | -2.35271 |
| H | 7.803716 | -1.38002 | -1.06846 |
| H | 6.938341 | -1.36009 | -2.6332 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 6** – E = −1304.713989 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.251953 | 0.074719 | 1.788081 |
| C | 1.612233 | -0.66202 | 0.622288 |
| C | 0.691974 | -0.09594 | -0.47823 |

| | | | |
|---|---|---|---|
| C | 0.262197 | -1.07631 | -1.57811 |
| O | -1.15101 | -1.24974 | -1.45568 |
| C | -1.50968 | -0.97621 | -0.10329 |
| C | -0.60222 | 0.204528 | 0.295776 |
| C | -0.1647 | 0.261719 | 1.766136 |
| C | -2.98868 | -0.72185 | -0.00761 |
| C | -3.75795 | -1.31842 | 0.983534 |
| C | -3.61857 | 0.149479 | -0.90363 |
| C | -4.97366 | 0.416357 | -0.81643 |
| C | -5.12433 | -1.05501 | 1.092976 |
| C | -5.74836 | -0.19289 | 0.194947 |
| C | 3.088007 | -0.5352 | 0.36223 |
| C | 3.720188 | 0.710695 | 0.48992 |
| C | 3.834473 | -1.62957 | -0.04382 |
| C | 5.195085 | -1.49343 | -0.33841 |
| C | 5.824602 | -0.26279 | -0.21608 |
| C | 5.070566 | 0.858542 | 0.212032 |
| O | -5.56007 | 1.225736 | -1.75418 |
| O | -7.06994 | 0.105897 | 0.195692 |
| O | 7.136078 | -0.02826 | -0.46746 |
| O | 5.761108 | 2.020596 | 0.319603 |
| C | -5.94259 | 2.518007 | -1.27717 |
| C | -7.88981 | -0.4968 | 1.187964 |
| C | 5.054592 | 3.17264 | 0.754018 |
| C | 7.932666 | -1.12279 | -0.89492 |
| H | 1.373256 | -1.72749 | 0.770583 |
| H | 1.138363 | 0.810932 | -0.89067 |
| H | 0.769429 | -2.04463 | -1.46627 |
| H | 0.460201 | -0.70161 | -2.58383 |
| H | -1.26082 | -1.8442 | 0.528075 |
| H | -1.06144 | 1.139675 | -0.03028 |
| H | -0.65479 | -0.52533 | 2.35587 |
| H | -0.37595 | 1.223273 | 2.236998 |
| H | -3.29797 | -2.0089 | 1.683766 |
| H | -3.05602 | 0.620649 | -1.7024 |
| H | -5.69689 | -1.54232 | 1.872099 |
| H | 3.137507 | 1.557264 | 0.830127 |
| H | 3.368718 | -2.60574 | -0.13335 |
| H | 5.757429 | -2.36275 | -0.65513 |
| H | -6.68541 | 2.441841 | -0.47936 |
| H | -5.06811 | 3.071214 | -0.91751 |
| H | -6.37611 | 3.043394 | -2.1282 |
| H | -8.89763 | -0.12811 | 1.004993 |
| H | -7.88138 | -1.58806 | 1.100576 |
| H | -7.57459 | -0.20721 | 2.195708 |
| H | 4.643271 | 3.033314 | 1.759444 |

| | | | |
|---|---|---|---|
| H | 5.784968 | 3.980014 | 0.772014 |
| H | 4.245809 | 3.43091 | 0.062109 |
| H | 7.568235 | -1.53701 | -1.84113 |
| H | 8.935126 | -0.72294 | -1.03905 |
| H | 7.96357 | -1.91423 | -0.13842 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 7** – E = −1304.713962 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.432541 | 0.685254 | 2.112336 |
| C | 1.667455 | -0.44654 | 1.278102 |
| C | 0.49054 | -0.43626 | 0.275892 |
| C | -0.06071 | -1.81443 | -0.06122 |
| O | -1.00526 | -2.09924 | 0.970516 |
| C | -1.70177 | -0.88726 | 1.249776 |
| C | -0.65282 | 0.235409 | 1.074187 |
| C | 0.037348 | 0.683566 | 2.376859 |
| C | -2.94777 | -0.72466 | 0.39223 |
| C | -3.40162 | -1.75573 | -0.42023 |
| C | -3.68763 | 0.462181 | 0.468653 |
| C | -4.85973 | 0.625681 | -0.26489 |
| C | -4.57668 | -1.5985 | -1.15549 |
| C | -5.30975 | -0.42549 | -1.09146 |
| C | 3.036733 | -0.37215 | 0.664946 |
| C | 3.493348 | 0.833829 | 0.111395 |
| C | 3.849651 | -1.49218 | 0.600609 |
| C | 5.102194 | -1.42767 | -0.0189 |
| C | 5.557461 | -0.23795 | -0.56892 |
| C | 4.736056 | 0.91528 | -0.49787 |
| O | -5.62226 | 1.746697 | -0.26207 |
| O | -6.42833 | -0.27802 | -1.87006 |
| O | 6.754844 | -0.06981 | -1.18175 |
| O | 5.25657 | 2.03833 | -1.05162 |
| C | -5.20892 | 2.838181 | 0.548196 |
| C | -7.66625 | -0.333 | -1.15762 |
| C | 4.470731 | 3.220032 | -1.01333 |
| C | 7.611664 | -1.19759 | -1.27807 |
| H | 1.594658 | -1.363 | 1.88513 |
| H | 0.762751 | 0.129906 | -0.61649 |
| H | 0.691317 | -2.60665 | -0.04679 |
| H | -0.54856 | -1.81292 | -1.04401 |
| H | -2.01875 | -0.95866 | 2.296507 |
| H | -1.06872 | 1.09006 | 0.541031 |
| H | -0.18886 | -0.02141 | 3.19061 |
| H | -0.24432 | 1.687714 | 2.69772 |

| | | | |
|---|---|---|---|
| H | -2.8452 | -2.68372 | -0.46992 |
| H | -3.3417 | 1.264579 | 1.109885 |
| H | -4.93964 | -2.39155 | -1.80113 |
| H | 2.862567 | 1.710954 | 0.182102 |
| H | 3.520841 | -2.43069 | 1.035247 |
| H | 5.720264 | -2.31576 | -0.05801 |
| H | -4.22585 | 3.210772 | 0.24228 |
| H | -5.95273 | 3.618669 | 0.397191 |
| H | -5.1831 | 2.562294 | 1.607502 |
| H | -7.73563 | 0.471819 | -0.42152 |
| H | -8.45461 | -0.21382 | -1.90109 |
| H | -7.78242 | -1.30157 | -0.65895 |
| H | 4.267369 | 3.531753 | 0.016711 |
| H | 5.062001 | 3.986608 | -1.51168 |
| H | 3.523811 | 3.087666 | -1.54753 |
| H | 8.503309 | -0.85038 | -1.79767 |
| H | 7.892143 | -1.57241 | -0.2879 |
| H | 7.147014 | -2.00435 | -1.85507 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 8** – E = −1304.713893 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.4067 | 0.074905 | 2.395601 |
| C | 1.615219 | -0.79064 | 1.282984 |
| C | 0.403228 | -0.53553 | 0.354771 |
| C | -0.18477 | -1.7931 | -0.2742 |
| O | -1.12924 | -2.28117 | 0.678352 |
| C | -1.79448 | -1.14425 | 1.225684 |
| C | -0.70293 | -0.05675 | 1.32704 |
| C | 0.019455 | -0.00372 | 2.6854 |
| C | -3.01403 | -0.74203 | 0.41089 |
| C | -3.49794 | -1.5494 | -0.60476 |
| C | -3.71242 | 0.433486 | 0.72867 |
| C | -4.85781 | 0.800256 | 0.035867 |
| C | -4.64576 | -1.18859 | -1.31797 |
| C | -5.33289 | -0.0224 | -1.01457 |
| C | 2.961536 | -0.5317 | 0.668305 |
| C | 3.39647 | 0.778115 | 0.43683 |
| C | 3.788632 | -1.5793 | 0.282301 |
| C | 5.021049 | -1.3383 | -0.32674 |
| C | 5.453866 | -0.03322 | -0.54724 |
| C | 4.620401 | 1.037072 | -0.15544 |
| O | -5.58894 | 1.916136 | 0.281804 |
| O | -6.45066 | 0.414402 | -1.64765 |
| O | 6.642736 | 0.307126 | -1.10152 |

| | | | |
|---|---|---|---|
| O | 5.03435 | 2.335647 | -0.29828 |
| C | -5.15854 | 2.77564 | 1.32588 |
| C | -6.95553 | -0.37642 | -2.71252 |
| C | 5.032662 | 2.824989 | -1.64154 |
| C | 7.512605 | -0.74019 | -1.50942 |
| H | 1.571483 | -1.83629 | 1.627381 |
| H | 0.653888 | 0.21921 | -0.39221 |
| H | 0.547814 | -2.58504 | -0.44628 |
| H | -0.67913 | -1.56135 | -1.22571 |
| H | -2.13104 | -1.44728 | 2.223882 |
| H | -1.08435 | 0.926016 | 1.051353 |
| H | -0.19143 | -0.91612 | 3.263282 |
| H | -0.24722 | 0.863544 | 3.291408 |
| H | -2.98418 | -2.47211 | -0.84623 |
| H | -3.35531 | 1.063554 | 1.534952 |
| H | -4.9968 | -1.83415 | -2.1134 |
| H | 2.786004 | 1.622205 | 0.738717 |
| H | 3.482114 | -2.60538 | 0.460604 |
| H | 5.644859 | -2.17713 | -0.60895 |
| H | -5.16056 | 2.262322 | 2.293453 |
| H | -4.15884 | 3.177043 | 1.127788 |
| H | -5.87603 | 3.594283 | 1.351939 |
| H | -7.83601 | 0.147519 | -3.08129 |
| H | -6.2239 | -0.47025 | -3.52232 |
| H | -7.24626 | -1.37452 | -2.36736 |
| H | 4.022365 | 2.790169 | -2.06366 |
| H | 5.366141 | 3.861532 | -1.59059 |
| H | 5.716965 | 2.252802 | -2.27262 |
| H | 8.391305 | -0.2515 | -1.92677 |
| H | 7.812848 | -1.36124 | -0.65922 |
| H | 7.047505 | -1.36835 | -2.27608 |

B3PW91/PCM(MeCN)6-311G(d,p)
(7*S*,8*R*,7'*S*,8'*R*)-**3**
**Conf 9** – E = −1304.713864 Hartree

| Symbol | X | Y | Z |
|---|---|---|---|
| O | 1.210673 | -1.52707 | -1.34885 |
| C | 1.629817 | -0.31389 | -0.73166 |
| C | 0.669269 | -0.14827 | 0.464146 |
| C | 0.307215 | 1.290505 | 0.860448 |
| O | -1.09735 | 1.44152 | 0.646268 |
| C | -1.48018 | 0.522708 | -0.37431 |
| C | -0.64387 | -0.7378 | -0.07772 |
| C | -0.21574 | -1.57425 | -1.29189 |
| C | -2.97138 | 0.331036 | -0.36061 |

| | | | |
|---|---|---|---|
| C | -3.70515 | 0.327589 | -1.54034 |
| C | -3.65081 | 0.12387 | 0.845125 |
| C | -5.01713 | -0.09661 | 0.873469 |
| C | -5.082 | 0.099002 | -1.53266 |
| C | -5.75224 | -0.12029 | -0.33189 |
| C | 3.092098 | -0.39011 | -0.38254 |
| C | 3.904051 | 0.741302 | -0.53728 |
| C | 3.650495 | -1.55408 | 0.125585 |
| C | 5.000159 | -1.59472 | 0.480866 |
| C | 5.807485 | -0.4725 | 0.339386 |
| C | 5.246147 | 0.718012 | -0.17888 |
| O | -5.6301 | -0.34882 | 2.072858 |
| O | -7.07948 | -0.36851 | -0.21776 |
| O | 7.125259 | -0.41457 | 0.655435 |
| O | 6.097609 | 1.767331 | -0.29494 |
| C | -6.46566 | 0.705633 | 2.557075 |
| C | -7.85733 | -0.39858 | -1.40695 |
| C | 5.585117 | 2.984844 | -0.81451 |
| C | 7.734383 | -1.5895 | 1.168824 |
| H | 1.475607 | 0.526007 | -1.42887 |
| H | 1.050316 | -0.72188 | 1.310999 |
| H | 0.858024 | 2.020115 | 0.25066 |
| H | 0.503049 | 1.506418 | 1.91202 |
| H | -1.18463 | 0.920079 | -1.35859 |
| H | -1.15557 | -1.34134 | 0.674213 |
| H | -0.64085 | -1.16889 | -2.22076 |
| H | -0.50578 | -2.62328 | -1.21255 |
| H | -3.20699 | 0.504003 | -2.48865 |
| H | -3.11612 | 0.135926 | 1.788688 |
| H | -5.62306 | 0.093936 | -2.47052 |
| H | 3.474791 | 1.646102 | -0.95115 |
| H | 3.040011 | -2.44281 | 0.234708 |
| H | 5.416996 | -2.51552 | 0.869443 |
| H | -6.86776 | 0.364561 | 3.511118 |
| H | -5.88136 | 1.618513 | 2.715919 |
| H | -7.2879 | 0.908071 | 1.86655 |
| H | -7.51527 | -1.18676 | -2.08553 |
| H | -8.87663 | -0.61255 | -1.09024 |
| H | -7.83239 | 0.56637 | -1.92361 |
| H | 6.421108 | 3.68249 | -0.81598 |
| H | 5.216782 | 2.859769 | -1.83843 |
| H | 4.782749 | 3.382848 | -0.18401 |
| H | 8.776089 | -1.3295 | 1.350222 |
| H | 7.270233 | -1.90247 | 2.110267 |
| H | 7.687135 | -2.41282 | 0.447935 |