

Supporting Information

The Role of Ethynylene Bond on the Optical and Electronic Properties of Diketopyrrolopyrrole Copolymers

Pichaya Pattanasattayavong,^a Maria Sygletou,^b Emmanuel Kymakis,^c Emmanuel Stratakis,^b Feng Yan,^d Vasilis G. Gregoriou,^{e,f} Thomas D. Anthopoulos,^a Christos L. Chochos^{f*}

^a Department of Physics and Centre for Plastic Electronics, Imperial College London, Exhibition Road, South Kensington, London SW7 2AZ, UK

^b Institute of Electronic Structure and Laser (IESL), Foundation for Research and Technology-Hellas (FORTH), Heraklion, 71110 Crete, Greece

^c Center of Materials Technology & Photonics and Electrical Engineering Department, Technological Educational Institute (TEI) of Crete, Heraklion, 71004 Crete, Greece

^d Department of Applied Physics and Materials Research Centre, The Hong Kong Polytechnic University, Hong Kong, China

^e National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece.

^f Advent Technologies SA, Patras Science Park, Stadiou Street, Platani-Rio, 26504, Patra, Greece

Corresponding author Email: cchochos@advent-energy.com

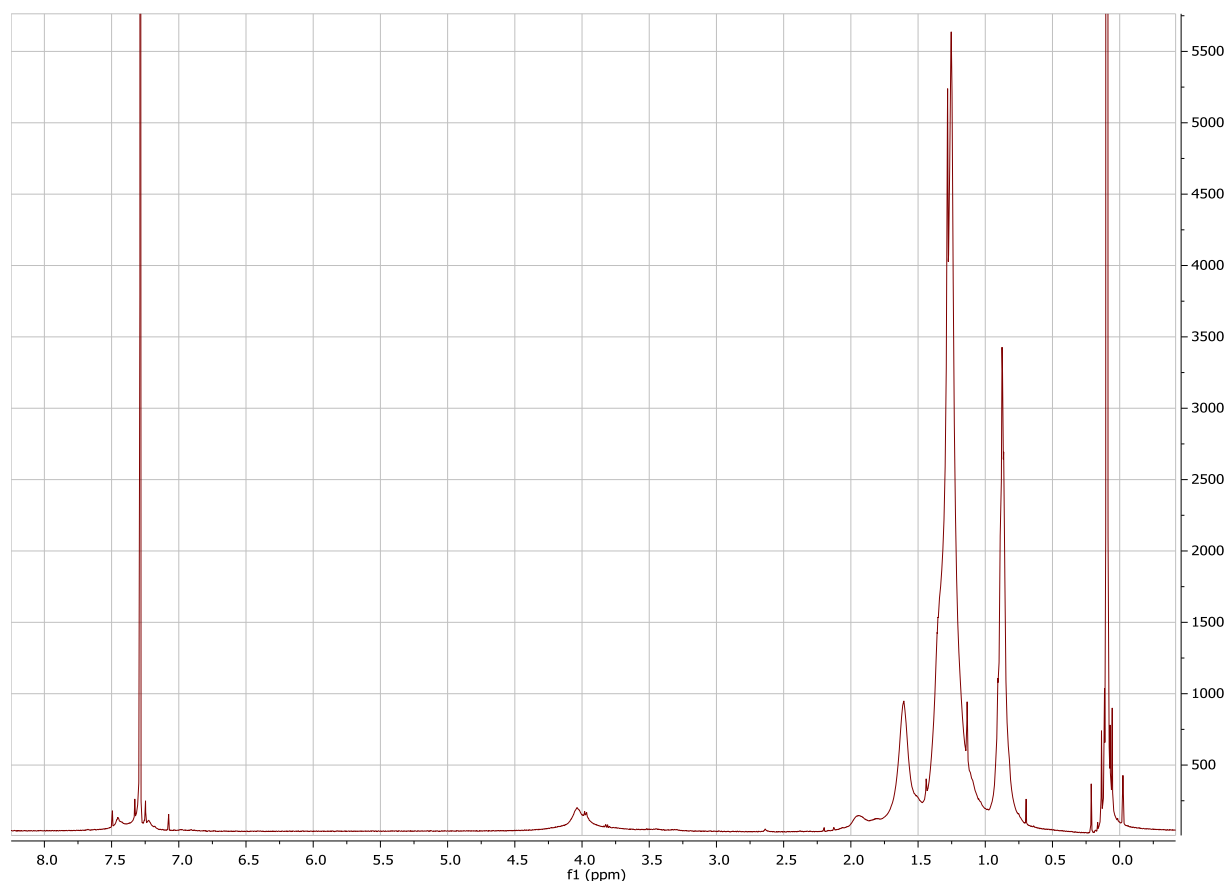


Fig. 1S ¹H-NMR spectrum of TDPPTTB

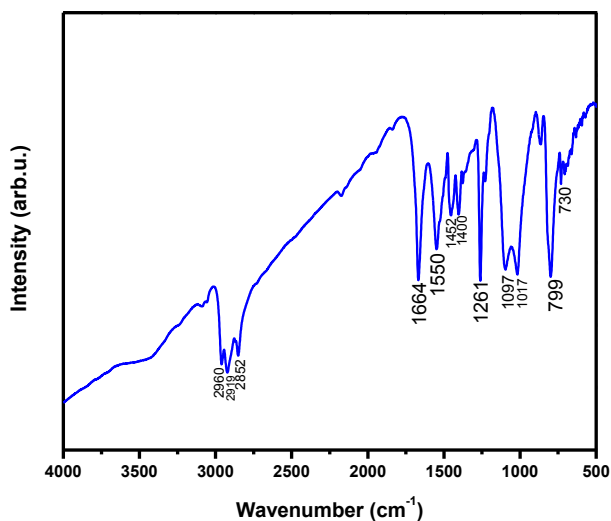


Fig. 2S FT-IR spectrum of powder TDPPTTB in transmission mode

Table S1. FT-IR analysis

| Wavenumber | Assignment |
|-----------------------|-------------------------------|
| 2960 cm^{-1} | C-H stretch alkanes |
| 2919 cm^{-1} | C-H stretch alkanes |
| 2852 cm^{-1} | C-H stretch alkanes |
| 1664 cm^{-1} | C=O stretch ketones |
| 1550 cm^{-1} | N-O asymmetric stretch |
| 1452 cm^{-1} | C-C stretch (in ring) |
| 1400 cm^{-1} | C-C stretch (in ring) |
| 1261 cm^{-1} | C-N stretch (aromatic amines) |
| 1097 cm^{-1} | C-O stretch alcohol |
| 1017 cm^{-1} | C-O stretch alcohol |
| 799 cm^{-1} | C-H aromatic |
| 730 cm^{-1} | C-H alkanes |

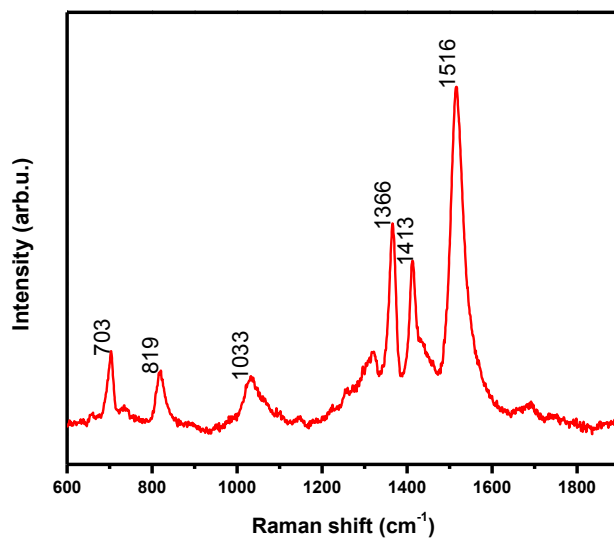


Fig. 3S Raman spectrum of TDPPTTB deposited on Si wafer from chloroform solution

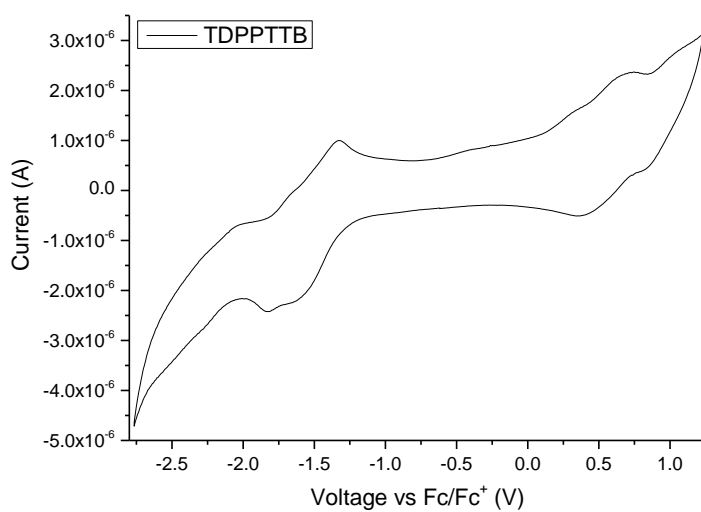


Fig. 4S Cyclic voltammogram of TDPPTTB in *o*-DCB solution

Standard orientation: tetramer TDPPTTB

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | | |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | -18.161601 | -1.297740 | 0.005518 |
| 2 | 6 | 0 | -18.794756 | -0.061609 | -0.008339 |
| 3 | 6 | 0 | -20.206866 | -0.153491 | -0.010127 |
| 4 | 6 | 0 | -20.660511 | -1.447553 | 0.002242 |
| 5 | 16 | 0 | -19.364355 | -2.588184 | 0.016341 |
| 6 | 6 | 0 | -16.734852 | -1.486966 | 0.010303 |
| 7 | 6 | 0 | -15.755497 | -0.490987 | 0.002427 |
| 8 | 6 | 0 | -14.470943 | -1.094900 | 0.010807 |
| 9 | 6 | 0 | -14.642258 | -2.530237 | 0.024698 |
| 10 | 7 | 0 | -16.066423 | -2.708264 | 0.023624 |
| 11 | 6 | 0 | -15.586193 | 0.944297 | -0.011595 |
| 12 | 7 | 0 | -14.163172 | 1.123520 | -0.010757 |
| 13 | 6 | 0 | -13.491798 | -0.098440 | 0.002538 |
| 14 | 6 | 0 | -12.068592 | -0.286782 | 0.006588 |
| 15 | 6 | 0 | -11.435045 | -1.528993 | 0.020629 |
| 16 | 6 | 0 | -10.034672 | -1.450016 | 0.021208 |
| 17 | 6 | 0 | -9.548725 | -0.147334 | 0.007640 |
| 18 | 16 | 0 | -10.872136 | 1.004785 | -0.006008 |
| 19 | 6 | 0 | -8.222322 | 0.289104 | 0.003924 |
| 20 | 6 | 0 | -13.612432 | 2.467200 | -0.022855 |
| 21 | 6 | 0 | -16.618895 | -4.051245 | 0.035765 |
| 22 | 8 | 0 | -13.857557 | -3.475868 | 0.035625 |
| 23 | 8 | 0 | -16.372244 | 1.888994 | -0.022407 |
| 24 | 6 | 0 | -7.070907 | 0.699835 | 0.000176 |
| 25 | 6 | 0 | -5.749573 | 1.151051 | -0.004224 |
| 26 | 16 | 0 | -4.408294 | 0.020351 | 0.007882 |
| 27 | 6 | 0 | -3.232734 | 1.332031 | -0.005802 |
| 28 | 6 | 0 | -3.886784 | 2.564043 | -0.018910 |
| 29 | 6 | 0 | -5.284934 | 2.462028 | -0.017998 |
| 30 | 6 | 0 | -1.807669 | 1.169451 | -0.004396 |
| 31 | 6 | 0 | -0.847049 | 2.186612 | -0.017170 |
| 32 | 6 | 0 | 0.447293 | 1.610536 | -0.011699 |
| 33 | 6 | 0 | 0.306532 | 0.169957 | 0.006208 |
| 34 | 7 | 0 | -1.114274 | -0.038291 | 0.009490 |
| 35 | 6 | 0 | -0.704549 | 3.624729 | -0.036009 |
| 36 | 7 | 0 | 0.712712 | 3.832697 | -0.041896 |
| 37 | 6 | 0 | 1.411646 | 2.620210 | -0.027712 |
| 38 | 6 | 0 | 2.843097 | 2.497164 | -0.031102 |
| 39 | 6 | 0 | 3.828237 | 3.486037 | -0.059458 |
| 40 | 6 | 0 | 5.139749 | 2.990763 | -0.054374 |
| 41 | 6 | 0 | 5.199155 | 1.602463 | -0.021587 |
| 42 | 16 | 0 | 3.595052 | 0.900143 | 0.002023 |
| 43 | 6 | 0 | 6.341138 | 0.796642 | -0.008475 |
| 44 | 6 | 0 | 7.330656 | 0.080088 | 0.003556 |
| 45 | 6 | 0 | 8.486268 | -0.706436 | 0.014764 |
| 46 | 6 | 0 | -1.637478 | -1.392789 | 0.028099 |
| 47 | 6 | 0 | 1.222827 | 5.191025 | -0.054852 |
| 48 | 16 | 0 | 10.072435 | 0.034440 | -0.025682 |
| 49 | 6 | 0 | 10.862840 | -1.542833 | 0.010756 |

| | | | | | |
|-----|----|---|------------|-----------|-----------|
| 50 | 6 | 0 | 9.903297 | -2.555326 | 0.057542 |
| 51 | 6 | 0 | 8.579383 | -2.092417 | 0.060057 |
| 52 | 6 | 0 | 12.297725 | -1.629473 | -0.004710 |
| 53 | 6 | 0 | 13.233055 | -0.593910 | 0.014571 |
| 54 | 6 | 0 | 14.543604 | -1.133645 | 0.000328 |
| 55 | 6 | 0 | 14.440620 | -2.575983 | -0.041073 |
| 56 | 7 | 0 | 13.026195 | -2.822469 | -0.038001 |
| 57 | 6 | 0 | 13.336029 | 0.847615 | 0.060947 |
| 58 | 7 | 0 | 14.750573 | 1.093205 | 0.083529 |
| 59 | 6 | 0 | 15.478185 | -0.099573 | 0.047998 |
| 60 | 6 | 0 | 16.915563 | -0.184432 | 0.065955 |
| 61 | 6 | 0 | 17.868905 | 0.821420 | 0.209058 |
| 62 | 6 | 0 | 19.196670 | 0.359257 | 0.180820 |
| 63 | 6 | 0 | 19.290274 | -1.012071 | 0.014729 |
| 64 | 16 | 0 | 17.711193 | -1.749586 | -0.100226 |
| 65 | 6 | 0 | 20.459331 | -1.796825 | -0.057135 |
| 66 | 6 | 0 | 21.458401 | -2.479137 | -0.121060 |
| 67 | 6 | 0 | 12.553087 | -4.191671 | -0.114992 |
| 68 | 6 | 0 | 15.224090 | 2.464462 | 0.081605 |
| 69 | 8 | 0 | 1.114946 | -0.750860 | 0.018090 |
| 70 | 8 | 0 | -1.511491 | 4.552487 | -0.045322 |
| 71 | 8 | 0 | 15.274349 | -3.473261 | -0.083393 |
| 72 | 8 | 0 | 12.502765 | 1.747017 | 0.070736 |
| 73 | 1 | 0 | -18.234782 | 0.868316 | -0.016748 |
| 74 | 1 | 0 | -20.864309 | 0.707738 | -0.020194 |
| 75 | 1 | 0 | -21.682294 | -1.801443 | 0.003885 |
| 76 | 1 | 0 | -11.998985 | -2.456559 | 0.029898 |
| 77 | 1 | 0 | -9.377739 | -2.310930 | 0.031091 |
| 78 | 1 | 0 | -14.468709 | 3.143496 | -0.030190 |
| 79 | 1 | 0 | -13.010805 | 2.664120 | 0.869347 |
| 80 | 1 | 0 | -13.008876 | 2.647317 | -0.917318 |
| 81 | 1 | 0 | -15.764169 | -4.729321 | 0.043684 |
| 82 | 1 | 0 | -17.224023 | -4.228898 | 0.929558 |
| 83 | 1 | 0 | -17.221219 | -4.246161 | -0.856310 |
| 84 | 1 | 0 | -3.337731 | 3.500696 | -0.028982 |
| 85 | 1 | 0 | -5.956320 | 3.311673 | -0.027055 |
| 86 | 1 | 0 | 3.615132 | 4.542919 | -0.084673 |
| 87 | 1 | 0 | 6.026051 | 3.612737 | -0.073906 |
| 88 | 1 | 0 | -0.767455 | -2.051534 | 0.036577 |
| 89 | 1 | 0 | -2.235530 | -1.581442 | 0.924485 |
| 90 | 1 | 0 | -2.236350 | -1.605724 | -0.862276 |
| 91 | 1 | 0 | 0.347211 | 5.841564 | -0.050476 |
| 92 | 1 | 0 | 1.827105 | 5.401770 | 0.832618 |
| 93 | 1 | 0 | 1.809511 | 5.392173 | -0.956397 |
| 94 | 1 | 0 | 10.143483 | -3.606245 | 0.096355 |
| 95 | 1 | 0 | 7.709008 | -2.735833 | 0.095122 |
| 96 | 1 | 0 | 17.626181 | 1.864075 | 0.341449 |
| 97 | 1 | 0 | 20.065540 | 0.998111 | 0.279663 |
| 98 | 1 | 0 | 22.339662 | -3.075503 | -0.175793 |
| 99 | 1 | 0 | 12.005398 | -4.482391 | 0.787021 |
| 100 | 1 | 0 | 11.922899 | -4.348917 | -0.995266 |
| 101 | 1 | 0 | 13.445480 | -4.813893 | -0.198598 |
| 102 | 1 | 0 | 15.874029 | 2.661445 | -0.775763 |
| 103 | 1 | 0 | 14.333349 | 3.090323 | 0.008393 |

| | | | | | |
|-----------------------------|---|---|-----------|-----------|-----------|
| 104 | 1 | 0 | 15.751386 | 2.713067 | 1.008165 |
| ----- | | | | | |
| Rotational constants (GHZ): | | | 0.1115676 | 0.0031317 | 0.0030467 |

Standard orientation: tetramer TDPPTT

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | | |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | 18.422022 | 4.746930 | -0.183873 |
| 2 | 6 | 0 | 19.573407 | 3.996089 | 0.013740 |
| 3 | 6 | 0 | 20.760198 | 4.766551 | -0.022171 |
| 4 | 6 | 0 | 20.528526 | 6.099471 | -0.245205 |
| 5 | 16 | 0 | 18.845031 | 6.443645 | -0.417167 |
| 6 | 6 | 0 | 17.085518 | 4.211765 | -0.194432 |
| 7 | 6 | 0 | 16.712921 | 2.878159 | -0.013988 |
| 8 | 6 | 0 | 15.299477 | 2.769831 | -0.095596 |
| 9 | 6 | 0 | 14.754349 | 4.085606 | -0.336949 |
| 10 | 7 | 0 | 15.910894 | 4.934316 | -0.387957 |
| 11 | 6 | 0 | 17.258959 | 1.562147 | 0.227488 |
| 12 | 7 | 0 | 16.103701 | 0.713205 | 0.277995 |
| 13 | 6 | 0 | 14.926455 | 1.435293 | 0.084675 |
| 14 | 6 | 0 | 13.594087 | 0.904301 | 0.074078 |
| 15 | 6 | 0 | 12.440316 | 1.658727 | -0.120084 |
| 16 | 6 | 0 | 11.258250 | 0.901594 | -0.083242 |
| 17 | 6 | 0 | 11.459867 | -0.452847 | 0.138791 |
| 18 | 16 | 0 | 13.170269 | -0.792946 | 0.302177 |
| 19 | 6 | 0 | 10.485978 | -1.506754 | 0.236588 |
| 20 | 16 | 0 | 8.779437 | -1.184939 | -0.028401 |
| 21 | 6 | 0 | 8.349388 | -2.859823 | 0.272685 |
| 22 | 6 | 0 | 9.486768 | -3.602533 | 0.547187 |
| 23 | 6 | 0 | 10.676621 | -2.848412 | 0.524765 |
| 24 | 6 | 0 | 6.988927 | -3.329837 | 0.217053 |
| 25 | 6 | 0 | 6.551281 | -4.647123 | 0.173882 |
| 26 | 6 | 0 | 5.155603 | -4.784003 | 0.130928 |
| 27 | 6 | 0 | 4.472788 | -3.569565 | 0.134660 |
| 28 | 16 | 0 | 5.624156 | -2.236205 | 0.208905 |
| 29 | 6 | 0 | 3.046897 | -3.432941 | 0.089527 |
| 30 | 7 | 0 | 2.330228 | -2.238539 | 0.090626 |
| 31 | 6 | 0 | 0.914180 | -2.472743 | 0.041628 |
| 32 | 6 | 0 | 0.800909 | -3.915022 | 0.008060 |
| 33 | 6 | 0 | 2.106156 | -4.467227 | 0.038336 |
| 34 | 6 | 0 | -0.142661 | -4.943208 | -0.047021 |
| 35 | 7 | 0 | 0.580727 | -6.141543 | -0.049960 |
| 36 | 6 | 0 | 1.992818 | -5.906633 | 0.002772 |
| 37 | 6 | 0 | -1.574330 | -4.850843 | -0.092976 |
| 38 | 16 | 0 | -2.357377 | -3.266841 | -0.052916 |
| 39 | 6 | 0 | -3.948702 | -3.986282 | -0.133636 |
| 40 | 6 | 0 | -3.861654 | -5.369500 | -0.192597 |

| | | | | | |
|----|----|---|------------|-----------|-----------|
| 41 | 6 | 0 | -2.542830 | -5.850358 | -0.169792 |
| 42 | 6 | 0 | -5.128855 | -3.162027 | -0.132111 |
| 43 | 6 | 0 | -5.223811 | -1.783173 | -0.047298 |
| 44 | 6 | 0 | -6.548002 | -1.300788 | -0.069650 |
| 45 | 6 | 0 | -7.504777 | -2.296453 | -0.172596 |
| 46 | 16 | 0 | -6.732177 | -3.873176 | -0.243554 |
| 47 | 6 | 0 | -8.937999 | -2.168135 | -0.220381 |
| 48 | 16 | 0 | -9.696997 | -0.596610 | -0.117846 |
| 49 | 6 | 0 | -11.311386 | -1.303109 | -0.243781 |
| 50 | 6 | 0 | -11.210334 | -2.688618 | -0.350758 |
| 51 | 6 | 0 | -9.890864 | -3.169141 | -0.337334 |
| 52 | 6 | 0 | -12.470355 | -0.455183 | -0.214444 |
| 53 | 6 | 0 | -12.540379 | 0.924372 | -0.015707 |
| 54 | 6 | 0 | -13.895224 | 1.343292 | -0.043808 |
| 55 | 6 | 0 | -14.724422 | 0.184124 | -0.286217 |
| 56 | 7 | 0 | -13.786633 | -0.899062 | -0.378288 |
| 57 | 6 | 0 | -11.711912 | 2.082182 | 0.236490 |
| 58 | 7 | 0 | -12.651529 | 3.159767 | 0.362939 |
| 59 | 6 | 0 | -13.967091 | 2.716591 | 0.196367 |
| 60 | 6 | 0 | -15.128040 | 3.558827 | 0.277789 |
| 61 | 6 | 0 | -15.244082 | 4.900514 | 0.630522 |
| 62 | 6 | 0 | -16.563539 | 5.385590 | 0.610174 |
| 63 | 6 | 0 | -17.497047 | 4.431954 | 0.239630 |
| 64 | 16 | 0 | -16.725971 | 2.900811 | -0.090401 |
| 65 | 6 | 0 | -18.930263 | 4.576502 | 0.118056 |
| 66 | 16 | 0 | -19.691440 | 6.158929 | 0.196562 |
| 67 | 6 | 0 | -21.267527 | 5.468443 | -0.010045 |
| 68 | 6 | 0 | -21.212162 | 4.106982 | -0.138782 |
| 69 | 6 | 0 | -19.886961 | 3.598359 | -0.066146 |
| 70 | 6 | 0 | -12.152521 | 4.506029 | 0.568069 |
| 71 | 6 | 0 | -14.279371 | -2.230967 | -0.671503 |
| 72 | 6 | 0 | 2.827129 | -0.874984 | 0.134596 |
| 73 | 6 | 0 | 0.095801 | -7.507998 | -0.086269 |
| 74 | 6 | 0 | 16.273050 | -0.709690 | 0.511229 |
| 75 | 6 | 0 | 15.742667 | 6.357638 | -0.620801 |
| 76 | 8 | 0 | 13.611632 | 4.515085 | -0.482583 |
| 77 | 8 | 0 | 18.401591 | 1.133490 | 0.373791 |
| 78 | 8 | 0 | 0.089876 | -1.565271 | 0.036043 |
| 79 | 8 | 0 | 2.817672 | -6.819383 | 0.011333 |
| 80 | 8 | 0 | -15.934203 | 0.029708 | -0.417248 |
| 81 | 8 | 0 | -10.499331 | 2.242047 | 0.329037 |
| 82 | 1 | 0 | 19.536641 | 2.923684 | 0.177695 |
| 83 | 1 | 0 | 21.750920 | 4.348855 | 0.112495 |
| 84 | 1 | 0 | 21.247660 | 6.903590 | -0.319234 |
| 85 | 1 | 0 | 12.479737 | 2.731695 | -0.280600 |
| 86 | 1 | 0 | 10.272653 | 1.334833 | -0.210927 |
| 87 | 1 | 0 | 9.454069 | -4.659980 | 0.780132 |
| 88 | 1 | 0 | 11.653591 | -3.271708 | 0.729001 |
| 89 | 1 | 0 | 7.231925 | -5.489712 | 0.153757 |
| 90 | 1 | 0 | 4.629852 | -5.733137 | 0.088852 |
| 91 | 1 | 0 | -4.729063 | -6.017407 | -0.248571 |
| 92 | 1 | 0 | -2.315884 | -6.904110 | -0.210080 |
| 93 | 1 | 0 | -4.355378 | -1.138935 | 0.030896 |
| 94 | 1 | 0 | -6.800634 | -0.248137 | -0.011093 |

| | | | | | |
|-----|---|---|------------|-----------|-----------|
| 95 | 1 | 0 | -12.061239 | -3.347207 | -0.427502 |
| 96 | 1 | 0 | -9.641173 | -4.221616 | -0.410216 |
| 97 | 1 | 0 | -14.408253 | 5.519737 | 0.916694 |
| 98 | 1 | 0 | -16.827670 | 6.403105 | 0.874873 |
| 99 | 1 | 0 | -22.136984 | 6.110493 | -0.025493 |
| 100 | 1 | 0 | -22.088828 | 3.485093 | -0.276613 |
| 101 | 1 | 0 | -19.643356 | 2.544065 | -0.134735 |
| 102 | 1 | 0 | -12.502460 | 5.185056 | -0.214758 |
| 103 | 1 | 0 | -12.436499 | 4.899667 | 1.549508 |
| 104 | 1 | 0 | -11.064737 | 4.434105 | 0.523136 |
| 105 | 1 | 0 | -13.828569 | -2.633016 | -1.583685 |
| 106 | 1 | 0 | -14.103562 | -2.921202 | 0.159999 |
| 107 | 1 | 0 | -15.355638 | -2.127809 | -0.818529 |
| 108 | 1 | 0 | 1.945116 | -0.232525 | 0.117887 |
| 109 | 1 | 0 | 3.391460 | -0.680643 | 1.051507 |
| 110 | 1 | 0 | 3.451511 | -0.645193 | -0.733812 |
| 111 | 1 | 0 | 0.981951 | -8.143326 | -0.052209 |
| 112 | 1 | 0 | -0.537400 | -7.732555 | 0.777450 |
| 113 | 1 | 0 | -0.454298 | -7.716096 | -1.009272 |
| 114 | 1 | 0 | 17.347346 | -0.872371 | 0.612005 |
| 115 | 1 | 0 | 15.776323 | -1.028706 | 1.432301 |
| 116 | 1 | 0 | 15.900104 | -1.302854 | -0.328998 |
| 117 | 1 | 0 | 14.668722 | 6.521887 | -0.721625 |
| 118 | 1 | 0 | 16.117418 | 6.949594 | 0.219345 |
| 119 | 1 | 0 | 16.240806 | 6.676007 | -1.541229 |

Rotational constants (GHZ): 0.0297886 0.0026084 0.0024007

Standard orientation: tetramer TDPPTPh

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | | |
|------------------|------------------|----------------|-------------------------|----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | 19.024606 | 3.942373 | 0.276681 |
| 2 | 6 | 0 | 19.749499 | 3.285147 | 1.261793 |
| 3 | 6 | 0 | 21.051980 | 3.808387 | 1.445014 |
| 4 | 6 | 0 | 21.330785 | 4.859367 | 0.609785 |
| 5 | 16 | 0 | 19.999646 | 5.234361 | -0.424593 |
| 6 | 6 | 0 | 17.676960 | 3.612085 | -0.108511 |
| 7 | 6 | 0 | 16.875395 | 2.600268 | 0.422512 |
| 8 | 6 | 0 | 15.613717 | 2.608198 | -0.230353 |
| 9 | 6 | 0 | 15.616446 | 3.665292 | -1.214702 |
| 10 | 7 | 0 | 16.921758 | 4.249702 | -1.089815 |
| 11 | 6 | 0 | 16.872782 | 1.543765 | 1.408140 |
| 12 | 7 | 0 | 15.566914 | 0.961194 | 1.285969 |
| 13 | 6 | 0 | 14.810167 | 1.598651 | 0.304203 |

| | | | | | |
|----|----|---|------------|-----------|-----------|
| 14 | 6 | 0 | 13.463060 | 1.276113 | -0.076401 |
| 15 | 6 | 0 | 12.742285 | 1.932729 | -1.068069 |
| 16 | 6 | 0 | 11.441162 | 1.427964 | -1.245015 |
| 17 | 6 | 0 | 11.120229 | 0.375920 | -0.404737 |
| 18 | 16 | 0 | 12.472550 | 0.008653 | 0.642138 |
| 19 | 6 | 0 | 9.867619 | -0.370617 | -0.325298 |
| 20 | 6 | 0 | 15.201015 | -0.156513 | 2.137328 |
| 21 | 6 | 0 | 17.288361 | 5.366261 | -1.942473 |
| 22 | 8 | 0 | 14.784544 | 4.072683 | -2.023068 |
| 23 | 8 | 0 | 17.706233 | 1.135515 | 2.214019 |
| 24 | 6 | 0 | 8.673794 | 0.183027 | -0.829655 |
| 25 | 6 | 0 | 7.478457 | -0.516734 | -0.775198 |
| 26 | 6 | 0 | 7.406766 | -1.801565 | -0.201240 |
| 27 | 6 | 0 | 8.597703 | -2.349718 | 0.315495 |
| 28 | 6 | 0 | 9.796144 | -1.655500 | 0.248472 |
| 29 | 6 | 0 | 6.154571 | -2.550294 | -0.136970 |
| 30 | 16 | 0 | 4.606571 | -1.744927 | -0.251041 |
| 31 | 6 | 0 | 3.726710 | -3.263846 | -0.104492 |
| 32 | 6 | 0 | 4.624079 | -4.317571 | 0.034030 |
| 33 | 6 | 0 | 5.971772 | -3.913983 | 0.016375 |
| 34 | 6 | 0 | 2.297300 | -3.401944 | -0.125640 |
| 35 | 6 | 0 | 1.567928 | -4.590453 | -0.034226 |
| 36 | 6 | 0 | 0.180505 | -4.297728 | -0.101550 |
| 37 | 6 | 0 | 0.021776 | -2.865042 | -0.231819 |
| 38 | 7 | 0 | 1.370935 | -2.368939 | -0.245393 |
| 39 | 6 | 0 | 1.726414 | -6.021844 | 0.078469 |
| 40 | 7 | 0 | 0.383196 | -6.520901 | 0.057503 |
| 41 | 6 | 0 | -0.549745 | -5.484535 | -0.053920 |
| 42 | 6 | 0 | -1.973915 | -5.674494 | -0.112667 |
| 43 | 6 | 0 | -2.720213 | -6.839685 | -0.263958 |
| 44 | 6 | 0 | -4.110665 | -6.625515 | -0.289133 |
| 45 | 6 | 0 | -4.471123 | -5.295480 | -0.156610 |
| 46 | 16 | 0 | -3.055422 | -4.287368 | -0.002167 |
| 47 | 6 | 0 | -5.816040 | -4.723184 | -0.146527 |
| 48 | 6 | 0 | -6.048400 | -3.366771 | -0.445538 |
| 49 | 6 | 0 | -7.331036 | -2.838413 | -0.438830 |
| 50 | 6 | 0 | -8.448596 | -3.638484 | -0.131993 |
| 51 | 6 | 0 | -8.215380 | -4.994435 | 0.174781 |
| 52 | 6 | 0 | -6.933798 | -5.522498 | 0.167792 |
| 53 | 6 | 0 | -9.806204 | -3.096661 | -0.124596 |
| 54 | 16 | 0 | -10.097076 | -1.384237 | 0.040602 |
| 55 | 6 | 0 | -11.842515 | -1.605163 | -0.049545 |
| 56 | 6 | 0 | -12.137615 | -2.956399 | -0.202692 |
| 57 | 6 | 0 | -11.001067 | -3.785307 | -0.245238 |
| 58 | 6 | 0 | -12.718482 | -0.466414 | 0.022622 |
| 59 | 6 | 0 | -12.400087 | 0.888515 | -0.041693 |
| 60 | 6 | 0 | -13.588769 | 1.661180 | 0.041102 |
| 61 | 6 | 0 | -14.709290 | 0.758555 | 0.191456 |
| 62 | 7 | 0 | -14.107009 | -0.545229 | 0.164150 |
| 63 | 6 | 0 | -11.282532 | 1.789795 | -0.221803 |
| 64 | 7 | 0 | -11.891351 | 3.089833 | -0.262415 |
| 65 | 6 | 0 | -13.277999 | 3.011964 | -0.105787 |
| 66 | 6 | 0 | -14.160953 | 4.147539 | -0.117297 |
| 67 | 6 | 0 | -13.917734 | 5.468401 | -0.478966 |

| | | | | | |
|-----|----|---|------------|-----------|-----------|
| 68 | 6 | 0 | -15.046533 | 6.303870 | -0.373595 |
| 69 | 6 | 0 | -16.180829 | 5.649629 | 0.071326 |
| 70 | 16 | 0 | -15.846884 | 3.963449 | 0.361440 |
| 71 | 6 | 0 | -17.518708 | 6.209469 | 0.288128 |
| 72 | 6 | 0 | -17.676730 | 7.581722 | 0.560707 |
| 73 | 6 | 0 | -18.942237 | 8.128089 | 0.753789 |
| 74 | 6 | 0 | -20.077643 | 7.317268 | 0.690559 |
| 75 | 6 | 0 | -19.934766 | 5.953298 | 0.429974 |
| 76 | 6 | 0 | -18.671303 | 5.404302 | 0.227280 |
| 77 | 6 | 0 | -14.938837 | -1.710882 | 0.394164 |
| 78 | 6 | 0 | -11.042351 | 4.264292 | -0.330245 |
| 79 | 6 | 0 | 0.154602 | -7.941840 | 0.239980 |
| 80 | 6 | 0 | 1.602572 | -0.939216 | -0.343989 |
| 81 | 8 | 0 | -0.955855 | -2.130348 | -0.306924 |
| 82 | 8 | 0 | 2.705589 | -6.758523 | 0.185923 |
| 83 | 8 | 0 | -15.913963 | 0.931283 | 0.340889 |
| 84 | 8 | 0 | -10.071365 | 1.619488 | -0.305843 |
| 85 | 1 | 0 | 19.331926 | 2.454032 | 1.821413 |
| 86 | 1 | 0 | 21.757966 | 3.420388 | 2.169713 |
| 87 | 1 | 0 | 22.241140 | 5.438548 | 0.538836 |
| 88 | 1 | 0 | 13.170110 | 2.749530 | -1.640942 |
| 89 | 1 | 0 | 10.758720 | 1.809257 | -1.995116 |
| 90 | 1 | 0 | 16.073850 | -0.358883 | 2.760145 |
| 91 | 1 | 0 | 14.352151 | 0.088843 | 2.782368 |
| 92 | 1 | 0 | 14.966066 | -1.049324 | 1.550437 |
| 93 | 1 | 0 | 16.419094 | 5.562603 | -2.572075 |
| 94 | 1 | 0 | 17.515064 | 6.262187 | -1.357096 |
| 95 | 1 | 0 | 18.143265 | 5.122387 | -2.579974 |
| 96 | 1 | 0 | 8.682681 | 1.179734 | -1.257780 |
| 97 | 1 | 0 | 6.584961 | -0.063260 | -1.193715 |
| 98 | 1 | 0 | 8.579016 | -3.326881 | 0.786388 |
| 99 | 1 | 0 | 10.695568 | -2.121326 | 0.639923 |
| 100 | 1 | 0 | 4.288285 | -5.345300 | 0.132748 |
| 101 | 1 | 0 | 6.796908 | -4.612794 | 0.085062 |
| 102 | 1 | 0 | -2.284134 | -7.819611 | -0.385517 |
| 103 | 1 | 0 | -4.829091 | -7.423112 | -0.436228 |
| 104 | 1 | 0 | -5.216027 | -2.723040 | -0.713350 |
| 105 | 1 | 0 | -7.471121 | -1.794256 | -0.701636 |
| 106 | 1 | 0 | -9.047560 | -5.632146 | 0.454502 |
| 107 | 1 | 0 | -6.789787 | -6.562475 | 0.442088 |
| 108 | 1 | 0 | -13.140071 | -3.341611 | -0.313641 |
| 109 | 1 | 0 | -11.055988 | -4.856941 | -0.395676 |
| 110 | 1 | 0 | -12.965507 | 5.824017 | -0.842926 |
| 111 | 1 | 0 | -15.037908 | 7.351148 | -0.651496 |
| 112 | 1 | 0 | -16.799488 | 8.215549 | 0.643190 |
| 113 | 1 | 0 | -19.041500 | 9.188700 | 0.965470 |
| 114 | 1 | 0 | -21.063772 | 7.744346 | 0.845682 |
| 115 | 1 | 0 | -20.810878 | 5.314047 | 0.375299 |
| 116 | 1 | 0 | -18.577019 | 4.346593 | -0.000212 |
| 117 | 1 | 0 | -15.041529 | -2.324119 | -0.507506 |
| 118 | 1 | 0 | -14.544997 | -2.323976 | 1.209343 |
| 119 | 1 | 0 | -15.924864 | -1.330841 | 0.666230 |
| 120 | 1 | 0 | -11.276222 | 4.967809 | 0.473213 |
| 121 | 1 | 0 | -10.018036 | 3.905863 | -0.216541 |

| | | | | | |
|-----|---|---|------------|-----------|-----------|
| 122 | 1 | 0 | -11.124842 | 4.772893 | -1.296720 |
| 123 | 1 | 0 | 1.125855 | -8.377795 | 0.478219 |
| 124 | 1 | 0 | -0.541416 | -8.127708 | 1.062438 |
| 125 | 1 | 0 | -0.222760 | -8.415257 | -0.672646 |
| 126 | 1 | 0 | 0.614898 | -0.477485 | -0.392772 |
| 127 | 1 | 0 | 2.133316 | -0.555341 | 0.532196 |
| 128 | 1 | 0 | 2.160553 | -0.682509 | -1.249298 |

Rotational constants (GHZ): 0.0257849 0.0027054 0.0024622

Standard orientation: monomer TDPPTTB

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | | |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | -3.517282 | -0.529701 | 0.000002 |
| 2 | 6 | 0 | -4.491630 | -1.521433 | 0.000008 |
| 3 | 6 | 0 | -5.814790 | -1.020853 | 0.000000 |
| 4 | 6 | 0 | -5.856926 | 0.350002 | -0.000007 |
| 5 | 16 | 0 | -4.287391 | 1.060482 | 0.000008 |
| 6 | 6 | 0 | -2.078899 | -0.635312 | -0.000001 |
| 7 | 6 | 0 | -1.127918 | 0.384014 | -0.000004 |
| 8 | 6 | 0 | 0.175367 | -0.179267 | -0.000004 |
| 9 | 6 | 0 | 0.047394 | -1.619002 | -0.000004 |
| 10 | 7 | 0 | -1.372383 | -1.840179 | -0.000001 |
| 11 | 6 | 0 | -0.999353 | 1.823835 | -0.000006 |
| 12 | 7 | 0 | 0.420689 | 2.044212 | 0.000000 |
| 13 | 6 | 0 | 1.127332 | 0.838113 | -0.000004 |
| 14 | 6 | 0 | 2.564296 | 0.727596 | -0.000004 |
| 15 | 6 | 0 | 3.538439 | 1.723053 | -0.000004 |
| 16 | 6 | 0 | 4.857289 | 1.233857 | 0.000003 |
| 17 | 6 | 0 | 4.922865 | -0.148634 | 0.000003 |
| 18 | 16 | 0 | 3.328352 | -0.862284 | -0.000015 |
| 19 | 6 | 0 | 6.075577 | -0.960637 | 0.000009 |
| 20 | 8 | 0 | -1.814324 | 2.739793 | 0.000001 |
| 21 | 8 | 0 | 0.863824 | -2.533390 | 0.000004 |
| 22 | 6 | 0 | -1.869087 | -3.202964 | 0.000000 |
| 23 | 6 | 0 | 0.917251 | 3.406921 | 0.000005 |
| 24 | 6 | 0 | 7.060485 | -1.666185 | 0.000014 |
| 25 | 1 | 0 | -4.274681 | -2.578035 | 0.000011 |
| 26 | 1 | 0 | -6.695855 | -1.651649 | -0.000004 |
| 27 | 1 | 0 | -6.730652 | 0.987664 | -0.000015 |
| 28 | 1 | 0 | 3.318139 | 2.778821 | -0.000002 |
| 29 | 1 | 0 | 5.739059 | 1.862652 | 0.000010 |
| 30 | 1 | 0 | -0.986400 | -3.844312 | 0.000002 |
| 31 | 1 | 0 | -2.462852 | -3.415049 | 0.894344 |
| 32 | 1 | 0 | -2.462851 | -3.415051 | -0.894344 |
| 33 | 1 | 0 | 0.034061 | 4.047642 | -0.000002 |
| 34 | 1 | 0 | 1.510640 | 3.619961 | 0.894480 |
| 35 | 1 | 0 | 1.510654 | 3.619962 | -0.894460 |
| 36 | 1 | 0 | 7.928760 | -2.283649 | 0.000020 |

 Rotational constants (GHZ): 0.5061670 0.1129880 0.0924781

Standard orientation: monomer TDPPTT

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | | |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | 4.553616 | -0.712895 | 0.000952 |
| 2 | 6 | 0 | 5.438921 | -1.784641 | 0.006735 |
| 3 | 6 | 0 | 6.800583 | -1.399982 | 0.005727 |
| 4 | 6 | 0 | 6.961259 | -0.038174 | -0.000803 |
| 5 | 16 | 0 | 5.457988 | 0.804882 | -0.005526 |
| 6 | 6 | 0 | 3.111223 | -0.694700 | 0.000142 |
| 7 | 6 | 0 | 2.249816 | 0.400797 | -0.000823 |
| 8 | 6 | 0 | 0.902879 | -0.049415 | -0.000613 |
| 9 | 6 | 0 | 0.907842 | -1.493790 | -0.000179 |
| 10 | 7 | 0 | 2.303764 | -1.834966 | 0.000369 |
| 11 | 6 | 0 | 2.244551 | 1.846449 | -0.000468 |
| 12 | 7 | 0 | 0.849395 | 2.187919 | 0.000395 |
| 13 | 6 | 0 | 0.040606 | 1.047338 | 0.000398 |
| 14 | 6 | 0 | -1.396729 | 1.064431 | 0.001463 |
| 15 | 6 | 0 | -2.286332 | 2.134974 | 0.005549 |
| 16 | 6 | 0 | -3.640048 | 1.754856 | 0.005454 |
| 17 | 6 | 0 | -3.829195 | 0.383048 | 0.001340 |
| 18 | 16 | 0 | -2.297695 | -0.456012 | -0.002395 |
| 19 | 6 | 0 | -5.073180 | -0.353351 | 0.000195 |
| 20 | 16 | 0 | -6.621138 | 0.480206 | -0.000262 |
| 21 | 6 | 0 | -7.488362 | -1.020430 | -0.001408 |
| 22 | 6 | 0 | -6.641622 | -2.095588 | -0.001621 |
| 23 | 6 | 0 | -5.271000 | -1.719706 | -0.000704 |
| 24 | 8 | 0 | 3.135117 | 2.689209 | -0.001208 |
| 25 | 8 | 0 | 0.017505 | -2.337967 | -0.000685 |
| 26 | 6 | 0 | 2.681963 | -3.234878 | -0.001206 |
| 27 | 6 | 0 | 0.470749 | 3.587548 | -0.000675 |
| 28 | 1 | 0 | 5.131586 | -2.818589 | 0.012065 |
| 29 | 1 | 0 | 7.623801 | -2.104674 | 0.009792 |
| 30 | 1 | 0 | 7.886611 | 0.521880 | -0.002886 |
| 31 | 1 | 0 | -1.981039 | 3.169587 | 0.009000 |
| 32 | 1 | 0 | -4.457090 | 2.467373 | 0.008637 |
| 33 | 1 | 0 | -8.569263 | -1.015509 | -0.001913 |
| 34 | 1 | 0 | -6.983680 | -3.123837 | -0.002311 |
| 35 | 1 | 0 | -4.453484 | -2.431940 | -0.000454 |
| 36 | 1 | 0 | 1.747126 | -3.797583 | -0.005523 |
| 37 | 1 | 0 | 3.258530 | -3.495660 | -0.894000 |
| 38 | 1 | 0 | 3.252148 | -3.499704 | 0.894552 |
| 39 | 1 | 0 | 1.405273 | 4.150811 | -0.003764 |
| 40 | 1 | 0 | -0.104981 | 3.848922 | -0.893975 |
| 41 | 1 | 0 | -0.100355 | 3.851750 | 0.894795 |

 Rotational constants (GHZ): 0.4460396 0.0677354 0.0588494

Standard orientation: monomer TDPPTPh

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | | |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | 4.486017 | -0.768187 | 0.009673 |
| 2 | 6 | 0 | 5.338688 | -1.848988 | 0.198363 |
| 3 | 6 | 0 | 6.711080 | -1.506552 | 0.150860 |
| 4 | 6 | 0 | 6.910625 | -0.168698 | -0.075087 |
| 5 | 16 | 0 | 5.431579 | 0.704457 | -0.220435 |
| 6 | 6 | 0 | 3.044540 | -0.713057 | -0.003140 |
| 7 | 6 | 0 | 2.211104 | 0.402107 | -0.017852 |
| 8 | 6 | 0 | 0.853053 | -0.016762 | 0.001289 |
| 9 | 6 | 0 | 0.823728 | -1.462119 | 0.005790 |
| 10 | 7 | 0 | 2.211994 | -1.834982 | 0.009653 |
| 11 | 6 | 0 | 2.240962 | 1.847969 | -0.001368 |
| 12 | 7 | 0 | 0.854938 | 2.221314 | 0.051464 |
| 13 | 6 | 0 | 0.020907 | 1.099578 | 0.054043 |
| 14 | 6 | 0 | -1.415949 | 1.156011 | 0.112792 |
| 15 | 6 | 0 | -2.261864 | 2.231430 | 0.362528 |
| 16 | 6 | 0 | -3.629247 | 1.894038 | 0.352953 |
| 17 | 6 | 0 | -3.868319 | 0.556705 | 0.095364 |
| 18 | 16 | 0 | -2.370518 | -0.304545 | -0.137154 |
| 19 | 6 | 0 | -5.161736 | -0.129936 | 0.016548 |
| 20 | 8 | 0 | 3.149530 | 2.669949 | -0.042850 |
| 21 | 8 | 0 | -0.084632 | -2.285599 | -0.012900 |
| 22 | 6 | 0 | 2.561818 | -3.240146 | -0.073747 |
| 23 | 6 | 0 | 0.501728 | 3.626579 | -0.013768 |
| 24 | 6 | 0 | -6.325798 | 0.588688 | -0.316178 |
| 25 | 6 | 0 | -7.561756 | -0.048120 | -0.381294 |
| 26 | 6 | 0 | -7.663532 | -1.417597 | -0.126982 |
| 27 | 6 | 0 | -6.515943 | -2.144060 | 0.195482 |
| 28 | 6 | 0 | -5.278936 | -1.509093 | 0.270464 |
| 29 | 1 | 0 | 4.998360 | -2.856279 | 0.383210 |
| 30 | 1 | 0 | 7.514126 | -2.222281 | 0.281753 |
| 31 | 1 | 0 | 7.851567 | 0.358533 | -0.156081 |
| 32 | 1 | 0 | -1.913816 | 3.230245 | 0.578253 |
| 33 | 1 | 0 | -4.417702 | 2.606542 | 0.564744 |
| 34 | 1 | 0 | 1.623137 | -3.776526 | -0.221365 |
| 35 | 1 | 0 | 3.229379 | -3.434175 | -0.917774 |
| 36 | 1 | 0 | 3.026000 | -3.600449 | 0.850363 |
| 37 | 1 | 0 | 1.432062 | 4.164082 | -0.204087 |
| 38 | 1 | 0 | -0.205256 | 3.820444 | -0.825053 |
| 39 | 1 | 0 | 0.081091 | 3.986199 | 0.931365 |
| 40 | 1 | 0 | -6.253749 | 1.646847 | -0.546626 |
| 41 | 1 | 0 | -8.446726 | 0.524727 | -0.642520 |

| | | | | | |
|-----------------------------|---|---|-----------|-----------|-----------|
| 42 | 1 | 0 | -8.627653 | -1.913886 | -0.182354 |
| 43 | 1 | 0 | -6.583881 | -3.208721 | 0.398216 |
| 44 | 1 | 0 | -4.398662 | -2.081757 | 0.547147 |
| ----- | | | | | |
| Rotational constants (GHZ): | | | 0.4317165 | 0.0692116 | 0.0598794 |