SUPPORTING INFORMATION (2 of 2)

# Origin of the Second-Order Proton Catalysis of Ferriin Reduction in Belousov-Zhabotinsky Reactions: Density Functional Studies of Ferroin and Ferriin Aggregates with Outer Sphere Ligands Sulfate, Bisulfate, and Sulfuric Acid

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Structures of Ferriin $[Fe(phen)_3]^{3+}$ and its Aggregates

**Structures of TC-0-000**

TC2-0-000, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.000287 | 0.000490 | -0.001048 |
| 2 | 7 | 0 | -0.000730 | -0.000080 | 1.948122 |
| 3 | 7 | 0 | 0.064367 | -0.000501 | -1.949261 |
| 4 | 6 | 0 | 0.888220 | -0.891155 | 2.448115 |
| 5 | 6 | 0 | -0.747519 | 0.704858 | 2.787169 |
| 6 | 7 | 0 | -1.484950 | -1.257696 | 0.103732 |
| 7 | 7 | 0 | 1.374192 | -1.367877 | 0.197582 |
| 8 | 7 | 0 | 1.455410 | 1.288757 | -0.152427 |
| 9 | 7 | 0 | -1.406764 | 1.340908 | -0.154635 |
| 10 | 6 | 0 | 1.017520 | 0.839529 | -2.418450 |
| 11 | 6 | 0 | -0.692332 | -0.663232 | -2.813477 |
| 12 | 6 | 0 | 1.077196 | -1.102628 | 3.823655 |
| 13 | 6 | 0 | 1.638535 | -1.625241 | 1.500712 |
| 14 | 6 | 0 | -0.630356 | 0.560691 | 4.174683 |
| 15 | 1 | 0 | -1.447345 | 1.406962 | 2.352064 |
| 16 | 6 | 0 | -2.680923 | -0.626759 | 0.027256 |
| 17 | 6 | 0 | -1.460063 | -2.574047 | 0.262763 |
| 18 | 6 | 0 | 2.058954 | -2.011594 | -0.738010 |
| 19 | 6 | 0 | 1.776104 | 1.530819 | -1.445820 |
| 20 | 6 | 0 | 2.144266 | 1.893237 | 0.806090 |
| 21 | 6 | 0 | -2.638490 | 0.778754 | -0.121210 |
| 22 | 6 | 0 | -1.301805 | 2.653597 | -0.311001 |
| 23 | 6 | 0 | 1.263095 | 1.039679 | -3.786734 |
| 24 | 6 | 0 | -0.521593 | -0.526497 | -4.196164 |
| 25 | 1 | 0 | -1.444172 | -1.325073 | -2.402700 |
| 26 | 6 | 0 | 0.278581 | -0.337310 | 4.696968 |
| 27 | 6 | 0 | 2.054248 | -2.062341 | 4.240181 |
| 28 | 6 | 0 | 2.599101 | -2.558887 | 1.922743 |
| 29 | 1 | 0 | -1.257515 | 1.161829 | 4.823666 |
| 30 | 6 | 0 | -3.912597 | -1.298574 | 0.092160 |
| 31 | 6 | 0 | -2.637202 | -3.327794 | 0.339541 |
| 32 | 1 | 0 | -0.486698 | -3.044435 | 0.320438 |
| 33 | 6 | 0 | 3.037114 | -2.958733 | -0.412625 |
| 34 | 1 | 0 | 1.821263 | -1.780302 | -1.768561 |
| 35 | 6 | 0 | 2.800551 | 2.409373 | -1.834715 |
| 36 | 6 | 0 | 3.183819 | 2.784237 | 0.514376 |
| 37 | 1 | 0 | 1.860710 | 1.675563 | 1.827973 |
| 38 | 6 | 0 | -3.827092 | 1.519147 | -0.229011 |
| 39 | 6 | 0 | -2.430916 | 3.472722 | -0.428592 |
| 40 | 1 | 0 | -0.301944 | 3.068060 | -0.333737 |
| 41 | 6 | 0 | 0.452443 | 0.319493 | -4.686986 |
| 42 | 6 | 0 | 2.305141 | 1.943465 | -4.169527 |
| 43 | 1 | 0 | -1.159360 | -1.092222 | -4.866309 |
| 44 | 1 | 0 | 0.379969 | -0.456537 | 5.771815 |
| 45 | 6 | 0 | 2.786939 | -2.759334 | 3.327646 |
| 46 | 1 | 0 | 2.204360 | -2.226364 | 5.302729 |

| | | | | | |
|---|---|---|---|---|---|
| 47 | 6 | 0 | 3.309397 | -3.236809 | 0.911716 |
| 48 | 6 | 0 | -3.862341 | -2.697756 | 0.253273 |
| 49 | 6 | 0 | -5.116557 | -0.531200 | -0.011713 |
| 50 | 1 | 0 | -2.569605 | -4.402877 | 0.464069 |
| 51 | 1 | 0 | 3.568819 | -3.465358 | -1.210438 |
| 52 | 6 | 0 | 3.514165 | 3.046681 | -0.799913 |
| 53 | 6 | 0 | 3.045168 | 2.598811 | -3.232376 |
| 54 | 1 | 0 | 3.716745 | 3.260388 | 1.329942 |
| 55 | 6 | 0 | -3.692030 | 2.913119 | -0.386734 |
| 56 | 6 | 0 | -5.075471 | 0.821197 | -0.168833 |
| 57 | 1 | 0 | -2.298187 | 4.542140 | -0.549464 |
| 58 | 1 | 0 | 0.595652 | 0.432450 | -5.757748 |
| 59 | 1 | 0 | 2.498930 | 2.098591 | -5.226332 |
| 60 | 1 | 0 | 3.527001 | -3.481998 | 3.657060 |
| 61 | 1 | 0 | 4.064713 | -3.971079 | 1.176556 |
| 62 | 1 | 0 | -4.782513 | -3.272154 | 0.309389 |
| 63 | 1 | 0 | -6.070121 | -1.047854 | 0.035597 |
| 64 | 1 | 0 | 4.317484 | 3.737645 | -1.038753 |
| 65 | 1 | 0 | 3.834717 | 3.279055 | -3.536239 |
| 66 | 1 | 0 | -4.575646 | 3.538597 | -0.475042 |
| 67 | 1 | 0 | -5.995994 | 1.390904 | -0.249611 |

Rotational constants (GHZ): 0.1037363 0.1036708

TC2-0-000, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.008540 | -0.000054 | 0.000219 |
| 2 | 7 | 0 | -0.118833 | -1.605832 | -1.057680 |
| 3 | 7 | 0 | -1.473053 | -0.978375 | 1.159017 |
| 4 | 7 | 0 | -0.114713 | 1.606058 | 1.057945 |
| 5 | 7 | 0 | -1.471814 | 0.981222 | -1.157587 |
| 6 | 7 | 0 | 1.637596 | -0.864124 | 1.040216 |
| 7 | 7 | 0 | 1.639230 | 0.860132 | -1.040343 |
| 8 | 6 | 0 | 0.590407 | -1.879416 | -2.142228 |
| 9 | 1 | 0 | 1.333495 | -1.154241 | -2.444825 |
| 10 | 6 | 0 | 0.375223 | -3.050649 | -2.873662 |
| 11 | 1 | 0 | 0.973563 | -3.232841 | -3.758018 |
| 12 | 6 | 0 | -0.586255 | -3.944908 | -2.458233 |
| 13 | 1 | 0 | -0.768604 | -4.861013 | -3.010912 |
| 14 | 6 | 0 | -1.341468 | -3.671900 | -1.301901 |
| 15 | 6 | 0 | -1.071981 | -2.471356 | -0.627778 |
| 16 | 6 | 0 | -1.787537 | -2.141638 | 0.552472 |
| 17 | 6 | 0 | -2.351193 | -4.542439 | -0.784359 |
| 18 | 1 | 0 | -2.553486 | -5.465657 | -1.317471 |
| 19 | 6 | 0 | -3.036184 | -4.227399 | 0.348107 |
| 20 | 1 | 0 | -3.797325 | -4.893892 | 0.740536 |
| 21 | 6 | 0 | -2.766640 | -3.013037 | 1.052218 |
| 22 | 6 | 0 | -3.417281 | -2.620233 | 2.238875 |
| 23 | 1 | 0 | -4.181940 | -3.261587 | 2.665570 |
| 24 | 6 | 0 | -3.075343 | -1.432011 | 2.846952 |
| 25 | 1 | 0 | -3.557432 | -1.109629 | 3.762187 |
| 26 | 6 | 0 | -2.085151 | -0.623869 | 2.273336 |
| 27 | 1 | 0 | -1.785796 | 0.315302 | 2.723409 |
| 28 | 6 | 0 | 0.595852 | 1.878140 | 2.142007 |
| 29 | 1 | 0 | 1.336755 | 1.150805 | 2.444776 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 6 | 0 | 0.384648 | 3.050559 | 2.872698 |
| 31 | 1 | 0 | 0.983914 | 3.231509 | 3.756681 |
| 32 | 6 | 0 | -0.574190 | 3.947546 | 2.457029 |
| 33 | 1 | 0 | -0.753376 | 4.864629 | 3.009115 |
| 34 | 6 | 0 | -1.330865 | 3.676038 | 1.301296 |
| 35 | 6 | 0 | -1.065437 | 2.474173 | 0.627937 |
| 36 | 6 | 0 | -1.782640 | 2.145773 | -0.551661 |
| 37 | 6 | 0 | -2.338197 | 4.549273 | 0.783624 |
| 38 | 1 | 0 | -2.537322 | 5.473547 | 1.316092 |
| 39 | 6 | 0 | -3.024881 | 4.235393 | -0.348142 |
| 40 | 1 | 0 | -3.784213 | 4.903912 | -0.740632 |
| 41 | 6 | 0 | -2.759498 | 3.019650 | -1.051448 |
| 42 | 6 | 0 | -3.411995 | 2.627852 | -2.237422 |
| 43 | 1 | 0 | -4.175017 | 3.271123 | -2.664165 |
| 44 | 6 | 0 | -3.073864 | 1.438195 | -2.844827 |
| 45 | 1 | 0 | -3.557435 | 1.116539 | -3.759537 |
| 46 | 6 | 0 | -2.085585 | 0.627659 | -2.271288 |
| 47 | 1 | 0 | -1.789174 | -0.312675 | -2.720894 |
| 48 | 6 | 0 | 1.585827 | -1.715485 | 2.048173 |
| 49 | 1 | 0 | 0.600925 | -1.996925 | 2.402660 |
| 50 | 6 | 0 | 2.749515 | -2.226222 | 2.634813 |
| 51 | 1 | 0 | 2.667159 | -2.922422 | 3.461066 |
| 52 | 6 | 0 | 3.976169 | -1.827661 | 2.151109 |
| 53 | 1 | 0 | 4.895206 | -2.203994 | 2.589247 |
| 54 | 6 | 0 | 4.044493 | -0.920131 | 1.076496 |
| 55 | 6 | 0 | 2.824771 | -0.464124 | 0.545277 |
| 56 | 6 | 0 | 2.825655 | 0.457295 | -0.545914 |
| 57 | 6 | 0 | 5.271931 | -0.447704 | 0.516191 |
| 58 | 1 | 0 | 6.203372 | -0.809976 | 0.939169 |
| 59 | 6 | 0 | 5.272776 | 0.434889 | -0.517982 |
| 60 | 1 | 0 | 6.204914 | 0.794881 | -0.941371 |
| 61 | 6 | 0 | 4.046237 | 0.910292 | -1.077732 |
| 62 | 6 | 0 | 3.979619 | 1.817889 | -2.152387 |
| 63 | 1 | 0 | 4.899366 | 2.191966 | -2.590967 |
| 64 | 6 | 0 | 2.753713 | 2.219352 | -2.635597 |
| 65 | 1 | 0 | 2.672675 | 2.915661 | -3.461889 |
| 66 | 6 | 0 | 1.589061 | 1.711470 | -2.048394 |
| 67 | 1 | 0 | 0.604670 | 1.995273 | -2.402418 |

Rotational constants (GHZ): 0.1015894 0.0959939

**Structures of TC-1-100**

TC2-1-100, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.719316 | 0.000808 | 0.051229 |
| 2 | 7 | 0 | 2.168178 | 0.458540 | -1.159526 |
| 3 | 7 | 0 | 2.076760 | -1.056171 | 0.957290 |
| 4 | 7 | 0 | -0.684817 | -0.515817 | 1.286301 |
| 5 | 7 | 0 | 0.210329 | -1.607991 | -0.901487 |
| 6 | 7 | 0 | 1.110794 | 1.634489 | 1.022809 |
| 7 | 7 | 0 | -0.577170 | 1.094984 | -0.887749 |
| 8 | 6 | 0 | 2.144271 | 1.243724 | -2.223810 |
| 9 | 1 | 0 | 1.198375 | 1.697062 | -2.487795 |
| 10 | 6 | 0 | 3.295744 | 1.472290 | -2.985818 |
| 11 | 1 | 0 | 3.228368 | 2.120563 | -3.851310 |
| 12 | 6 | 0 | 4.486502 | 0.876852 | -2.630386 |
| 13 | 1 | 0 | 5.388096 | 1.045629 | -3.210467 |
| 14 | 6 | 0 | 4.529679 | 0.040617 | -1.499633 |
| 15 | 6 | 0 | 3.328545 | -0.132979 | -0.799833 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | 3.278571 | -0.956243 | 0.347298 |
| 17 | 6 | 0 | 5.698062 | -0.635266 | -1.026089 |
| 18 | 1 | 0 | 6.626946 | -0.498745 | -1.570255 |
| 19 | 6 | 0 | 5.649852 | -1.430183 | 0.078323 |
| 20 | 1 | 0 | 6.539617 | -1.940307 | 0.432735 |
| 21 | 6 | 0 | 4.429226 | -1.614021 | 0.801517 |
| 22 | 6 | 0 | 4.288150 | -2.410326 | 1.953110 |
| 23 | 1 | 0 | 5.148000 | -2.940760 | 2.349575 |
| 24 | 6 | 0 | 3.056199 | -2.504824 | 2.563055 |
| 25 | 1 | 0 | 2.914030 | -3.108183 | 3.451644 |
| 26 | 6 | 0 | 1.960131 | -1.810665 | 2.037725 |
| 27 | 1 | 0 | 0.986286 | -1.866184 | 2.505056 |
| 28 | 6 | 0 | -1.070766 | 0.071996 | 2.407503 |
| 29 | 1 | 0 | -0.538441 | 0.961160 | 2.716193 |
| 30 | 6 | 0 | -2.118834 | -0.443113 | 3.176250 |
| 31 | 1 | 0 | -2.397846 | 0.071463 | 4.087970 |
| 32 | 6 | 0 | -2.787302 | -1.573216 | 2.759151 |
| 33 | 1 | 0 | -3.613328 | -1.976988 | 3.335206 |
| 34 | 6 | 0 | -2.387529 | -2.211108 | 1.573242 |
| 35 | 6 | 0 | -1.320448 | -1.633586 | 0.876792 |
| 36 | 6 | 0 | -0.833843 | -2.226409 | -0.309551 |
| 37 | 6 | 0 | -2.988617 | -3.393096 | 1.040054 |
| 38 | 1 | 0 | -3.828016 | -3.826851 | 1.573166 |
| 39 | 6 | 0 | -2.523544 | -3.963252 | -0.104190 |
| 40 | 1 | 0 | -2.984880 | -4.860605 | -0.503343 |
| 41 | 6 | 0 | -1.418861 | -3.395297 | -0.813585 |
| 42 | 6 | 0 | -0.870140 | -3.914590 | -1.999097 |
| 43 | 1 | 0 | -1.289448 | -4.814172 | -2.438194 |
| 44 | 6 | 0 | 0.195295 | -3.270899 | -2.593096 |
| 45 | 1 | 0 | 0.638707 | -3.645473 | -3.507921 |
| 46 | 6 | 0 | 0.719232 | -2.110334 | -2.015575 |
| 47 | 1 | 0 | 1.547728 | -1.580530 | -2.466366 |
| 48 | 6 | 0 | 2.000768 | 1.841761 | 1.979361 |
| 49 | 1 | 0 | 2.628931 | 1.008169 | 2.263984 |
| 50 | 6 | 0 | 2.114900 | 3.085624 | 2.610254 |
| 51 | 1 | 0 | 2.855603 | 3.209184 | 3.391271 |
| 52 | 6 | 0 | 1.289701 | 4.124365 | 2.236687 |
| 53 | 1 | 0 | 1.364556 | 5.094548 | 2.717316 |
| 54 | 6 | 0 | 0.339595 | 3.922148 | 1.218670 |
| 55 | 6 | 0 | 0.294026 | 2.643558 | 0.645347 |
| 56 | 6 | 0 | -0.621769 | 2.351764 | -0.388534 |
| 57 | 6 | 0 | -0.567174 | 4.915853 | 0.735340 |
| 58 | 1 | 0 | -0.536490 | 5.903310 | 1.184241 |
| 59 | 6 | 0 | -1.444323 | 4.634468 | -0.268306 |
| 60 | 1 | 0 | -2.125481 | 5.395179 | -0.635979 |
| 61 | 6 | 0 | -1.489530 | 3.337731 | -0.869122 |
| 62 | 6 | 0 | -2.335773 | 2.971236 | -1.934785 |
| 63 | 1 | 0 | -3.029763 | 3.698008 | -2.344429 |
| 64 | 6 | 0 | -2.268166 | 1.696292 | -2.440691 |
| 65 | 1 | 0 | -2.905179 | 1.379464 | -3.256268 |
| 66 | 6 | 0 | -1.379017 | 0.766845 | -1.884177 |
| 67 | 1 | 0 | -1.310579 | -0.237133 | -2.271264 |
| 68 | 16 | 0 | -4.441305 | -0.053110 | -0.385278 |
| 69 | 8 | 0 | -5.301566 | -0.912986 | 0.504247 |
| 70 | 8 | 0 | -3.584448 | 0.841120 | 0.464945 |
| 71 | 8 | 0 | -3.584556 | -0.939188 | -1.247872 |
| 72 | 8 | 0 | -5.318495 | 0.795855 | -1.268338 |

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Rotational constants (GHZ): 0.1019834 0.0698727

TC4-1-100, ferriin quartet

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.736836 | 0.015540 | 0.054237 |
| 2 | 7 | 0 | 2.170804 | 0.301025 | -1.242114 |
| 3 | 7 | 0 | 2.091286 | -0.970297 | 1.059904 |
| 4 | 7 | 0 | -0.706408 | -0.508974 | 1.283155 |
| 5 | 7 | 0 | 0.102577 | -1.832880 | -0.912015 |
| 6 | 7 | 0 | 1.198881 | 1.894700 | 1.058378 |
| 7 | 7 | 0 | -0.513638 | 1.200338 | -0.893313 |
| 8 | 6 | 0 | 2.143367 | 0.947937 | -2.397067 |
| 9 | 1 | 0 | 1.212801 | 1.421883 | -2.678645 |
| 10 | 6 | 0 | 3.272983 | 1.016800 | -3.218908 |
| 11 | 1 | 0 | 3.207029 | 1.558238 | -4.154824 |
| 12 | 6 | 0 | 4.442053 | 0.399755 | -2.829751 |
| 13 | 1 | 0 | 5.327643 | 0.442727 | -3.455651 |
| 14 | 6 | 0 | 4.488357 | -0.295982 | -1.606285 |
| 15 | 6 | 0 | 3.311303 | -0.314757 | -0.847034 |
| 16 | 6 | 0 | 3.270281 | -0.992005 | 0.393253 |
| 17 | 6 | 0 | 5.642237 | -0.972391 | -1.100009 |
| 18 | 1 | 0 | 6.550149 | -0.956243 | -1.693901 |
| 19 | 6 | 0 | 5.604831 | -1.618513 | 0.097368 |
| 20 | 1 | 0 | 6.482835 | -2.127774 | 0.480903 |
| 21 | 6 | 0 | 4.409701 | -1.643902 | 0.882430 |
| 22 | 6 | 0 | 4.287362 | -2.281211 | 2.132082 |
| 23 | 1 | 0 | 5.142056 | -2.799021 | 2.555453 |
| 24 | 6 | 0 | 3.084772 | -2.238293 | 2.803505 |
| 25 | 1 | 0 | 2.961256 | -2.716472 | 3.767717 |
| 26 | 6 | 0 | 1.994629 | -1.570187 | 2.236355 |
| 27 | 1 | 0 | 1.039554 | -1.526802 | 2.742011 |
| 28 | 6 | 0 | -1.061293 | 0.160899 | 2.368106 |
| 29 | 1 | 0 | -0.505244 | 1.060069 | 2.596655 |
| 30 | 6 | 0 | -2.099551 | -0.277950 | 3.193098 |
| 31 | 1 | 0 | -2.353775 | 0.303273 | 4.071205 |
| 32 | 6 | 0 | -2.785593 | -1.423902 | 2.861842 |
| 33 | 1 | 0 | -3.607179 | -1.779450 | 3.475140 |
| 34 | 6 | 0 | -2.416381 | -2.147405 | 1.715363 |
| 35 | 6 | 0 | -1.353531 | -1.646570 | 0.947611 |
| 36 | 6 | 0 | -0.920001 | -2.354628 | -0.210681 |
| 37 | 6 | 0 | -3.067419 | -3.349839 | 1.300695 |
| 38 | 1 | 0 | -3.900794 | -3.710251 | 1.894669 |
| 39 | 6 | 0 | -2.656896 | -4.024964 | 0.195544 |
| 40 | 1 | 0 | -3.153851 | -4.938269 | -0.115638 |
| 41 | 6 | 0 | -1.561851 | -3.545982 | -0.587458 |
| 42 | 6 | 0 | -1.081141 | -4.188169 | -1.743766 |
| 43 | 1 | 0 | -1.548444 | -5.110907 | -2.073540 |
| 44 | 6 | 0 | -0.030843 | -3.638421 | -2.447832 |
| 45 | 1 | 0 | 0.355411 | -4.111281 | -3.343145 |
| 46 | 6 | 0 | 0.540348 | -2.441967 | -1.998930 |
| 47 | 1 | 0 | 1.359069 | -1.968888 | -2.529469 |
| 48 | 6 | 0 | 2.063807 | 2.183346 | 2.012393 |
| 49 | 1 | 0 | 2.683063 | 1.370600 | 2.375713 |
| 50 | 6 | 0 | 2.174218 | 3.478155 | 2.535926 |
| 51 | 1 | 0 | 2.896755 | 3.676707 | 3.318700 |
| 52 | 6 | 0 | 1.355856 | 4.473421 | 2.047866 |
| 53 | 1 | 0 | 1.417225 | 5.484506 | 2.438300 |
| 54 | 6 | 0 | 0.426334 | 4.180979 | 1.030582 |
| 55 | 6 | 0 | 0.392052 | 2.855071 | 0.565799 |
| 56 | 6 | 0 | -0.520057 | 2.484121 | -0.462919 |
| 57 | 6 | 0 | -0.464350 | 5.141593 | 0.460947 |
| 58 | 1 | 0 | -0.431696 | 6.161315 | 0.830977 |
| 59 | 6 | 0 | -1.331208 | 4.785666 | -0.525245 |
| 60 | 1 | 0 | -2.005850 | 5.515471 | -0.961434 |

| | | | | | |
|---|---|---|---|---|---|
| 61 | 6 | 0 | -1.377699 | 3.445256 | -1.019892 |
| 62 | 6 | 0 | -2.235931 | 3.025796 | -2.056107 |
| 63 | 1 | 0 | -2.914441 | 3.741805 | -2.508625 |
| 64 | 6 | 0 | -2.205957 | 1.719381 | -2.476332 |
| 65 | 1 | 0 | -2.856421 | 1.359391 | -3.262649 |
| 66 | 6 | 0 | -1.327715 | 0.819663 | -1.861607 |
| 67 | 1 | 0 | -1.281603 | -0.214191 | -2.166726 |
| 68 | 16 | 0 | -4.414361 | -0.041866 | -0.411918 |
| 69 | 8 | 0 | -5.286092 | -0.867836 | 0.497981 |
| 70 | 8 | 0 | -3.539334 | 0.856634 | 0.414706 |
| 71 | 8 | 0 | -3.575104 | -0.961180 | -1.257814 |
| 72 | 8 | 0 | -5.280774 | 0.802031 | -1.310658 |

Rotational constants (GHZ): 0.0951506 0.0693620

**Structures of TC-1-010**

TC2-1-010, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.719966 | -0.004265 | 0.038214 |
| 2 | 7 | 0 | 2.182313 | 0.482350 | -1.144780 |
| 3 | 7 | 0 | 2.074859 | -1.051945 | 0.957686 |
| 4 | 7 | 0 | -0.695538 | -0.549205 | 1.248134 |
| 5 | 7 | 0 | 0.242503 | -1.609059 | -0.937952 |
| 6 | 7 | 0 | 1.076982 | 1.625642 | 1.028947 |
| 7 | 7 | 0 | -0.573739 | 1.083318 | -0.911668 |
| 8 | 6 | 0 | 2.166146 | 1.275303 | -2.203530 |
| 9 | 1 | 0 | 1.218020 | 1.713295 | -2.484541 |
| 10 | 6 | 0 | 3.328930 | 1.531573 | -2.938932 |
| 11 | 1 | 0 | 3.267744 | 2.185780 | -3.800407 |
| 12 | 6 | 0 | 4.522765 | 0.955260 | -2.563015 |
| 13 | 1 | 0 | 5.433223 | 1.145812 | -3.122164 |
| 14 | 6 | 0 | 4.557377 | 0.109480 | -1.439189 |
| 15 | 6 | 0 | 3.345432 | -0.091842 | -0.766082 |
| 16 | 6 | 0 | 3.286522 | -0.926445 | 0.372185 |
| 17 | 6 | 0 | 5.727527 | -0.550571 | -0.948355 |
| 18 | 1 | 0 | 6.664778 | -0.392413 | -1.471956 |
| 19 | 6 | 0 | 5.670579 | -1.357256 | 0.146989 |
| 20 | 1 | 0 | 6.561585 | -1.855449 | 0.514933 |
| 21 | 6 | 0 | 4.438925 | -1.569338 | 0.842971 |
| 22 | 6 | 0 | 4.288956 | -2.379367 | 1.983776 |
| 23 | 1 | 0 | 5.149815 | -2.898844 | 2.392297 |
| 24 | 6 | 0 | 3.047105 | -2.500376 | 2.568328 |
| 25 | 1 | 0 | 2.897637 | -3.114573 | 3.448237 |
| 26 | 6 | 0 | 1.950186 | -1.819228 | 2.028348 |
| 27 | 1 | 0 | 0.968720 | -1.896097 | 2.476312 |
| 28 | 6 | 0 | -1.103985 | 0.021750 | 2.368786 |
| 29 | 1 | 0 | -0.595980 | 0.921805 | 2.686566 |
| 30 | 6 | 0 | -2.143717 | -0.523527 | 3.128758 |
| 31 | 1 | 0 | -2.439486 | -0.021842 | 4.042339 |
| 32 | 6 | 0 | -2.779671 | -1.667920 | 2.703395 |
| 33 | 1 | 0 | -3.596833 | -2.097017 | 3.273622 |
| 34 | 6 | 0 | -2.361525 | -2.285553 | 1.511570 |
| 35 | 6 | 0 | -1.303222 | -1.678159 | 0.825748 |
| 36 | 6 | 0 | -0.801127 | -2.247363 | -0.365356 |
| 37 | 6 | 0 | -2.943774 | -3.467696 | 0.957194 |
| 38 | 1 | 0 | -3.776634 | -3.924030 | 1.481767 |
| 39 | 6 | 0 | -2.470938 | -4.007457 | -0.199089 |
| 40 | 1 | 0 | -2.919257 | -4.903331 | -0.615941 |
| 41 | 6 | 0 | -1.370244 | -3.413432 | -0.892872 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 6 | 0 | -0.805983 | -3.908463 | -2.082281 |
| 43 | 1 | 0 | -1.212196 | -4.805122 | -2.539178 |
| 44 | 6 | 0 | 0.259528 | -3.246572 | -2.654480 |
| 45 | 1 | 0 | 0.716324 | -3.603064 | -3.569932 |
| 46 | 6 | 0 | 0.767425 | -2.090159 | -2.053322 |
| 47 | 1 | 0 | 1.595792 | -1.546491 | -2.487395 |
| 48 | 6 | 0 | 1.947506 | 1.835126 | 2.002796 |
| 49 | 1 | 0 | 2.581238 | 1.006898 | 2.290922 |
| 50 | 6 | 0 | 2.035753 | 3.074927 | 2.645778 |
| 51 | 1 | 0 | 2.761078 | 3.200352 | 3.440763 |
| 52 | 6 | 0 | 1.205360 | 4.107296 | 2.266391 |
| 53 | 1 | 0 | 1.260022 | 5.074129 | 2.756266 |
| 54 | 6 | 0 | 0.276240 | 3.902583 | 1.229698 |
| 55 | 6 | 0 | 0.255890 | 2.628772 | 0.645669 |
| 56 | 6 | 0 | -0.638877 | 2.335078 | -0.406464 |
| 57 | 6 | 0 | -0.633193 | 4.890616 | 0.738530 |
| 58 | 1 | 0 | -0.620936 | 5.874431 | 1.196147 |
| 59 | 6 | 0 | -1.489417 | 4.608767 | -0.282418 |
| 60 | 1 | 0 | -2.172325 | 5.364850 | -0.656179 |
| 61 | 6 | 0 | -1.509537 | 3.316294 | -0.894075 |
| 62 | 6 | 0 | -2.333564 | 2.949394 | -1.975168 |
| 63 | 1 | 0 | -3.027936 | 3.671662 | -2.392055 |
| 64 | 6 | 0 | -2.242142 | 1.677936 | -2.490730 |
| 65 | 1 | 0 | -2.858184 | 1.362413 | -3.323558 |
| 66 | 6 | 0 | -1.351814 | 0.755769 | -1.927146 |
| 67 | 1 | 0 | -1.267802 | -0.246422 | -2.318930 |
| 68 | 16 | 0 | -4.289324 | -0.100273 | -0.234793 |
| 69 | 8 | 0 | -5.218920 | -0.828360 | 0.645802 |
| 70 | 8 | 0 | -3.390410 | 0.819734 | 0.462693 |
| 71 | 8 | 0 | -3.641824 | -0.970146 | -1.229923 |
| 72 | 8 | 0 | -5.218367 | 0.941952 | -1.102384 |
| 73 | 1 | 0 | -5.846361 | 0.454170 | -1.653318 |

Rotational constants (GHZ): 0.1020202 0.0704239

TC4-1-010, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.750981 | 0.032074 | 0.051457 |
| 2 | 7 | 0 | 2.195257 | 0.381124 | -1.215059 |
| 3 | 7 | 0 | 2.121610 | -0.911949 | 1.075213 |
| 4 | 7 | 0 | -0.699585 | -0.542667 | 1.252970 |
| 5 | 7 | 0 | 0.196304 | -1.835922 | -0.929095 |
| 6 | 7 | 0 | 1.102368 | 1.929870 | 1.064407 |
| 7 | 7 | 0 | -0.526329 | 1.157847 | -0.929993 |
| 8 | 6 | 0 | 2.164334 | 1.035829 | -2.365559 |
| 9 | 1 | 0 | 1.223329 | 1.479977 | -2.659699 |
| 10 | 6 | 0 | 3.304139 | 1.150312 | -3.167776 |
| 11 | 1 | 0 | 3.234757 | 1.697033 | -4.100362 |
| 12 | 6 | 0 | 4.487253 | 0.570451 | -2.764192 |
| 13 | 1 | 0 | 5.380808 | 0.648957 | -3.375094 |
| 14 | 6 | 0 | 4.537560 | -0.133541 | -1.545622 |
| 15 | 6 | 0 | 3.349898 | -0.198210 | -0.805671 |
| 16 | 6 | 0 | 3.311505 | -0.888178 | 0.427462 |
| 17 | 6 | 0 | 5.704749 | -0.777265 | -1.027478 |
| 18 | 1 | 0 | 6.620775 | -0.725554 | -1.606673 |
| 19 | 6 | 0 | 5.669330 | -1.437093 | 0.162451 |
| 20 | 1 | 0 | 6.557010 | -1.922165 | 0.554845 |
| 21 | 6 | 0 | 4.463266 | -1.508987 | 0.927783 |
| 22 | 6 | 0 | 4.341394 | -2.164650 | 2.167945 |

| | | | | | |
|---|---|---|---|---|---|
| 23 | 1 | 0 | 5.205303 | -2.660105 | 2.599223 |
| 24 | 6 | 0 | 3.127479 | -2.168523 | 2.819915 |
| 25 | 1 | 0 | 3.003944 | -2.662229 | 3.776243 |
| 26 | 6 | 0 | 2.025614 | -1.528984 | 2.242838 |
| 27 | 1 | 0 | 1.061746 | -1.522918 | 2.733146 |
| 28 | 6 | 0 | -1.102148 | 0.112149 | 2.329862 |
| 29 | 1 | 0 | -0.589966 | 1.034130 | 2.568937 |
| 30 | 6 | 0 | -2.133808 | -0.368563 | 3.139564 |
| 31 | 1 | 0 | -2.425299 | 0.202693 | 4.012589 |
| 32 | 6 | 0 | -2.762317 | -1.544486 | 2.803346 |
| 33 | 1 | 0 | -3.575012 | -1.936262 | 3.406229 |
| 34 | 6 | 0 | -2.347441 | -2.251077 | 1.660720 |
| 35 | 6 | 0 | -1.295392 | -1.705589 | 0.907075 |
| 36 | 6 | 0 | -0.822473 | -2.392305 | -0.248576 |
| 37 | 6 | 0 | -2.949264 | -3.474518 | 1.232911 |
| 38 | 1 | 0 | -3.773666 | -3.869482 | 1.817432 |
| 39 | 6 | 0 | -2.504873 | -4.125074 | 0.125844 |
| 40 | 1 | 0 | -2.965159 | -5.053592 | -0.196408 |
| 41 | 6 | 0 | -1.418765 | -3.602013 | -0.641003 |
| 42 | 6 | 0 | -0.898431 | -4.222806 | -1.792601 |
| 43 | 1 | 0 | -1.330302 | -5.158368 | -2.134132 |
| 44 | 6 | 0 | 0.147811 | -3.638541 | -2.473702 |
| 45 | 1 | 0 | 0.565887 | -4.095473 | -3.362909 |
| 46 | 6 | 0 | 0.674364 | -2.427476 | -2.008490 |
| 47 | 1 | 0 | 1.489530 | -1.928239 | -2.520632 |
| 48 | 6 | 0 | 1.928770 | 2.257647 | 2.039747 |
| 49 | 1 | 0 | 2.583682 | 1.476742 | 2.410157 |
| 50 | 6 | 0 | 1.953646 | 3.551822 | 2.575950 |
| 51 | 1 | 0 | 2.646734 | 3.784114 | 3.375865 |
| 52 | 6 | 0 | 1.089730 | 4.503211 | 2.078834 |
| 53 | 1 | 0 | 1.084449 | 5.512151 | 2.479345 |
| 54 | 6 | 0 | 0.200049 | 4.167637 | 1.039279 |
| 55 | 6 | 0 | 0.252692 | 2.847052 | 0.562364 |
| 56 | 6 | 0 | -0.613337 | 2.434410 | -0.490848 |
| 57 | 6 | 0 | -0.732730 | 5.081078 | 0.458791 |
| 58 | 1 | 0 | -0.767696 | 6.096722 | 0.839594 |
| 59 | 6 | 0 | -1.553973 | 4.687391 | -0.551462 |
| 60 | 1 | 0 | -2.258821 | 5.382000 | -0.997053 |
| 61 | 6 | 0 | -1.510064 | 3.352303 | -1.060830 |
| 62 | 6 | 0 | -2.312665 | 2.898073 | -2.124872 |
| 63 | 1 | 0 | -3.018601 | 3.579461 | -2.588730 |
| 64 | 6 | 0 | -2.189999 | 1.601941 | -2.564222 |
| 65 | 1 | 0 | -2.788572 | 1.219282 | -3.381298 |
| 66 | 6 | 0 | -1.281820 | 0.746563 | -1.932847 |
| 67 | 1 | 0 | -1.162347 | -0.278870 | -2.250669 |
| 68 | 16 | 0 | -4.246613 | -0.167231 | -0.280726 |
| 69 | 8 | 0 | -5.190064 | -0.852526 | 0.619265 |
| 70 | 8 | 0 | -3.381603 | 0.809727 | 0.381804 |
| 71 | 8 | 0 | -3.559844 | -1.087645 | -1.201470 |
| 72 | 8 | 0 | -5.165739 | 0.803324 | -1.238080 |
| 73 | 1 | 0 | -5.756072 | 0.270663 | -1.789046 |

Rotational constants (GHZ): 0.0954292 0.0699081

**Structures of TC-1-001**

TC2-1-001, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.721458 | 0.022934 | 0.038001 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 7 | 0 | 2.204412 | 0.558005 | -1.110691 |
| 3 | 7 | 0 | 2.087201 | -1.013458 | 0.973707 |
| 4 | 7 | 0 | -0.708538 | -0.564409 | 1.220792 |
| 5 | 7 | 0 | 0.305649 | -1.599392 | -0.951938 |
| 6 | 7 | 0 | 1.018981 | 1.661458 | 1.042958 |
| 7 | 7 | 0 | -0.585789 | 1.084261 | -0.932361 |
| 8 | 6 | 0 | 2.208479 | 1.396475 | -2.137914 |
| 9 | 1 | 0 | 1.260621 | 1.840389 | -2.413625 |
| 10 | 6 | 0 | 3.380667 | 1.688040 | -2.845378 |
| 11 | 1 | 0 | 3.335707 | 2.375807 | -3.682472 |
| 12 | 6 | 0 | 4.571445 | 1.098301 | -2.472908 |
| 13 | 1 | 0 | 5.487186 | 1.313937 | -3.015693 |
| 14 | 6 | 0 | 4.592876 | 0.212800 | -1.377049 |
| 15 | 6 | 0 | 3.369217 | -0.015844 | -0.726506 |
| 16 | 6 | 0 | 3.303702 | -0.874944 | 0.394988 |
| 17 | 6 | 0 | 5.760949 | -0.458447 | -0.893526 |
| 18 | 1 | 0 | 6.707252 | -0.286293 | -1.396782 |
| 19 | 6 | 0 | 5.694715 | -1.299137 | 0.175844 |
| 20 | 1 | 0 | 6.587382 | -1.804628 | 0.530841 |
| 21 | 6 | 0 | 4.456525 | -1.532269 | 0.855120 |
| 22 | 6 | 0 | 4.299765 | -2.379298 | 1.970204 |
| 23 | 1 | 0 | 5.155571 | -2.914677 | 2.371008 |
| 24 | 6 | 0 | 3.052884 | -2.520851 | 2.544110 |
| 25 | 1 | 0 | 2.903015 | -3.166242 | 3.402462 |
| 26 | 6 | 0 | 1.960704 | -1.821008 | 2.017647 |
| 27 | 1 | 0 | 0.974261 | -1.909792 | 2.454191 |
| 28 | 6 | 0 | -1.177581 | 0.005643 | 2.320646 |
| 29 | 1 | 0 | -0.726569 | 0.940558 | 2.624672 |
| 30 | 6 | 0 | -2.202474 | -0.579414 | 3.071511 |
| 31 | 1 | 0 | -2.541749 | -0.084612 | 3.974553 |
| 32 | 6 | 0 | -2.765073 | -1.767118 | 2.654546 |
| 33 | 1 | 0 | -3.561907 | -2.233258 | 3.226276 |
| 34 | 6 | 0 | -2.301040 | -2.376492 | 1.473235 |
| 35 | 6 | 0 | -1.257153 | -1.726172 | 0.797885 |
| 36 | 6 | 0 | -0.719286 | -2.277780 | -0.386601 |
| 37 | 6 | 0 | -2.822794 | -3.588447 | 0.922386 |
| 38 | 1 | 0 | -3.639400 | -4.084702 | 1.436721 |
| 39 | 6 | 0 | -2.314392 | -4.112006 | -0.226020 |
| 40 | 1 | 0 | -2.720412 | -5.031344 | -0.635932 |
| 41 | 6 | 0 | -1.233743 | -3.473100 | -0.911704 |
| 42 | 6 | 0 | -0.630417 | -3.957706 | -2.087892 |
| 43 | 1 | 0 | -0.988857 | -4.875808 | -2.544177 |
| 44 | 6 | 0 | 0.421292 | -3.261513 | -2.650054 |
| 45 | 1 | 0 | 0.907510 | -3.616078 | -3.552065 |
| 46 | 6 | 0 | 0.871026 | -2.079906 | -2.051053 |
| 47 | 1 | 0 | 1.690309 | -1.510439 | -2.471711 |
| 48 | 6 | 0 | 1.889606 | 1.906283 | 2.011934 |
| 49 | 1 | 0 | 2.558373 | 1.100281 | 2.286879 |
| 50 | 6 | 0 | 1.934739 | 3.145198 | 2.662060 |
| 51 | 1 | 0 | 2.659877 | 3.302034 | 3.452840 |
| 52 | 6 | 0 | 1.059029 | 4.146092 | 2.291434 |
| 53 | 1 | 0 | 1.083001 | 5.110776 | 2.789988 |
| 54 | 6 | 0 | 0.135263 | 3.911812 | 1.253452 |
| 55 | 6 | 0 | 0.163382 | 2.638991 | 0.660469 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 6 | 0 | -0.705978 | 2.325967 | -0.409205 |
| 57 | 6 | 0 | -0.808739 | 4.870651 | 0.766256 |
| 58 | 1 | 0 | -0.841766 | 5.852061 | 1.228898 |
| 59 | 6 | 0 | -1.643572 | 4.568964 | -0.266823 |
| 60 | 1 | 0 | -2.347256 | 5.309194 | -0.634560 |
| 61 | 6 | 0 | -1.605027 | 3.285056 | -0.897328 |
| 62 | 6 | 0 | -2.389386 | 2.909361 | -2.004893 |
| 63 | 1 | 0 | -3.099603 | 3.611395 | -2.431179 |
| 64 | 6 | 0 | -2.239056 | 1.649817 | -2.543909 |
| 65 | 1 | 0 | -2.819128 | 1.335835 | -3.403980 |
| 66 | 6 | 0 | -1.334187 | 0.748301 | -1.971506 |
| 67 | 1 | 0 | -1.223849 | -0.254312 | -2.359903 |
| 68 | 16 | 0 | -4.162025 | -0.092669 | -0.323857 |
| 69 | 8 | 0 | -3.362637 | 0.853693 | 0.405064 |
| 70 | 8 | 0 | -3.543990 | -1.119010 | -1.117759 |
| 71 | 8 | 0 | -5.151531 | 0.785578 | -1.207985 |
| 72 | 1 | 0 | -5.730462 | 0.254091 | -1.777603 |
| 73 | 8 | 0 | -5.150927 | -0.863404 | 0.660446 |
| 74 | 1 | 0 | -5.673532 | -0.265672 | 1.217939 |

Rotational constants (GHZ): 0.1011969 0.0709208

TC4-1-001, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.777460 | 0.004261 | 0.035797 |
| 2 | 7 | 0 | 2.229173 | 0.384342 | -1.211429 |
| 3 | 7 | 0 | 2.150611 | -0.917732 | 1.072450 |
| 4 | 7 | 0 | -0.678859 | -0.576749 | 1.234405 |
| 5 | 7 | 0 | 0.231566 | -1.864079 | -0.945539 |
| 6 | 7 | 0 | 1.086178 | 1.907744 | 1.051090 |
| 7 | 7 | 0 | -0.509544 | 1.111915 | -0.960260 |
| 8 | 6 | 0 | 2.199590 | 1.038663 | -2.362286 |
| 9 | 1 | 0 | 1.250991 | 1.451040 | -2.676845 |
| 10 | 6 | 0 | 3.351549 | 1.194595 | -3.139560 |
| 11 | 1 | 0 | 3.282595 | 1.739789 | -4.073062 |
| 12 | 6 | 0 | 4.546121 | 0.658398 | -2.710155 |
| 13 | 1 | 0 | 5.449713 | 0.771866 | -3.300464 |
| 14 | 6 | 0 | 4.594842 | -0.046337 | -1.491903 |
| 15 | 6 | 0 | 3.394323 | -0.155724 | -0.778705 |
| 16 | 6 | 0 | 3.352919 | -0.851651 | 0.450568 |
| 17 | 6 | 0 | 5.772503 | -0.649283 | -0.949075 |
| 18 | 1 | 0 | 6.699102 | -0.561205 | -1.506667 |
| 19 | 6 | 0 | 5.733777 | -1.315986 | 0.236928 |
| 20 | 1 | 0 | 6.629050 | -1.771004 | 0.647511 |
| 21 | 6 | 0 | 4.513759 | -1.435244 | 0.973630 |
| 22 | 6 | 0 | 4.386211 | -2.103626 | 2.206380 |
| 23 | 1 | 0 | 5.256602 | -2.572053 | 2.654414 |
| 24 | 6 | 0 | 3.158334 | -2.155048 | 2.829544 |
| 25 | 1 | 0 | 3.029851 | -2.660961 | 3.778796 |
| 26 | 6 | 0 | 2.049023 | -1.547612 | 2.232930 |
| 27 | 1 | 0 | 1.075073 | -1.577817 | 2.701752 |
| 28 | 6 | 0 | -1.084470 | 0.069370 | 2.315443 |
| 29 | 1 | 0 | -0.568130 | 0.984876 | 2.569296 |
| 30 | 6 | 0 | -2.128390 | -0.409789 | 3.111439 |
| 31 | 1 | 0 | -2.421184 | 0.155109 | 3.988113 |
| 32 | 6 | 0 | -2.763847 | -1.577044 | 2.759429 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 1 | 0 | -3.585051 | -1.967663 | 3.351531 |
| 34 | 6 | 0 | -2.345788 | -2.276142 | 1.612189 |
| 35 | 6 | 0 | -1.280473 | -1.733451 | 0.873707 |
| 36 | 6 | 0 | -0.804050 | -2.413507 | -0.284328 |
| 37 | 6 | 0 | -2.955930 | -3.489244 | 1.166914 |
| 38 | 1 | 0 | -3.787432 | -3.883548 | 1.741670 |
| 39 | 6 | 0 | -2.509498 | -4.131105 | 0.055313 |
| 40 | 1 | 0 | -2.976170 | -5.051492 | -0.280578 |
| 41 | 6 | 0 | -1.411212 | -3.611268 | -0.696007 |
| 42 | 6 | 0 | -0.884083 | -4.228126 | -1.847302 |
| 43 | 1 | 0 | -1.324212 | -5.154156 | -2.203729 |
| 44 | 6 | 0 | 0.180513 | -3.652929 | -2.506425 |
| 45 | 1 | 0 | 0.605823 | -4.107682 | -3.393267 |
| 46 | 6 | 0 | 0.717785 | -2.453549 | -2.022086 |
| 47 | 1 | 0 | 1.547982 | -1.962363 | -2.517431 |
| 48 | 6 | 0 | 1.898081 | 2.247784 | 2.034465 |
| 49 | 1 | 0 | 2.567455 | 1.479314 | 2.404952 |
| 50 | 6 | 0 | 1.889409 | 3.538785 | 2.578934 |
| 51 | 1 | 0 | 2.571564 | 3.781614 | 3.385058 |
| 52 | 6 | 0 | 1.007254 | 4.473268 | 2.082097 |
| 53 | 1 | 0 | 0.975851 | 5.479224 | 2.488759 |
| 54 | 6 | 0 | 0.133259 | 4.124006 | 1.033647 |
| 55 | 6 | 0 | 0.219655 | 2.808472 | 0.548845 |
| 56 | 6 | 0 | -0.627249 | 2.383529 | -0.515278 |
| 57 | 6 | 0 | -0.815128 | 5.020529 | 0.451567 |
| 58 | 1 | 0 | -0.876141 | 6.032196 | 0.839565 |
| 59 | 6 | 0 | -1.617381 | 4.616886 | -0.569620 |
| 60 | 1 | 0 | -2.332921 | 5.298812 | -1.017544 |
| 61 | 6 | 0 | -1.537478 | 3.287260 | -1.088742 |
| 62 | 6 | 0 | -2.317159 | 2.825397 | -2.165138 |
| 63 | 1 | 0 | -3.031993 | 3.494942 | -2.632455 |
| 64 | 6 | 0 | -2.158582 | 1.535520 | -2.616383 |
| 65 | 1 | 0 | -2.735004 | 1.149093 | -3.448041 |
| 66 | 6 | 0 | -1.240496 | 0.694719 | -1.980466 |
| 67 | 1 | 0 | -1.095907 | -0.325991 | -2.305648 |
| 68 | 16 | 0 | -4.168851 | -0.061616 | -0.311661 |
| 69 | 8 | 0 | -3.286320 | 0.815453 | 0.408564 |
| 70 | 8 | 0 | -3.662401 | -1.091217 | -1.181154 |
| 71 | 8 | 0 | -5.141706 | 0.906106 | -1.110963 |
| 72 | 1 | 0 | -5.737941 | 0.437398 | -1.718773 |
| 73 | 8 | 0 | -5.136169 | -0.820614 | 0.693633 |
| 74 | 1 | 0 | -5.439178 | -0.263284 | 1.430226 |

Rotational constants (GHZ): 0.0963135 0.0693810

**Structures of TC-2-110**

TC2-2-110, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.018399 | 0.675887 | 0.110459 |
| 2 | 7 | 0 | -1.589486 | 0.839635 | -1.018077 |
| 3 | 7 | 0 | -0.658764 | 2.321180 | 0.913421 |
| 4 | 7 | 0 | 1.562871 | 0.566434 | 1.235696 |
| 5 | 7 | 0 | 1.112541 | 1.745871 | -1.042219 |
| 6 | 7 | 0 | -1.049306 | -0.446233 | 1.307067 |
| 7 | 7 | 0 | 0.507113 | -0.997435 | -0.710355 |
| 8 | 6 | 0 | -1.985751 | 0.071187 | -2.016517 |
| 9 | 1 | 0 | -1.349275 | -0.754682 | -2.295224 |
| 10 | 6 | 0 | -3.179694 | 0.323843 | -2.703280 |
| 11 | 1 | 0 | -3.459820 | -0.334269 | -3.516370 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 6 | 0 | -3.977098 | 1.380342 | -2.331083 |
| 13 | 1 | 0 | -4.911298 | 1.582640 | -2.845090 |
| 14 | 6 | 0 | -3.569700 | 2.210769 | -1.269632 |
| 15 | 6 | 0 | -2.354824 | 1.891504 | -0.651973 |
| 16 | 6 | 0 | -1.848561 | 2.696098 | 0.392831 |
| 17 | 6 | 0 | -4.293339 | 3.351245 | -0.799994 |
| 18 | 1 | 0 | -5.239440 | 3.590824 | -1.274760 |
| 19 | 6 | 0 | -3.808590 | 4.124993 | 0.210424 |
| 20 | 1 | 0 | -4.360293 | 4.992243 | 0.558461 |
| 21 | 6 | 0 | -2.558062 | 3.821438 | 0.833797 |
| 22 | 6 | 0 | -1.971005 | 4.572580 | 1.868776 |
| 23 | 1 | 0 | -2.480322 | 5.451759 | 2.250352 |
| 24 | 6 | 0 | -0.753539 | 4.182138 | 2.383165 |
| 25 | 1 | 0 | -0.274816 | 4.740486 | 3.178687 |
| 26 | 6 | 0 | -0.116309 | 3.041669 | 1.880893 |
| 27 | 1 | 0 | 0.833905 | 2.708820 | 2.276475 |
| 28 | 6 | 0 | 1.719040 | -0.027059 | 2.408494 |
| 29 | 1 | 0 | 0.855335 | -0.507633 | 2.847057 |
| 30 | 6 | 0 | 2.952497 | -0.027535 | 3.066878 |
| 31 | 1 | 0 | 3.031190 | -0.527305 | 4.024855 |
| 32 | 6 | 0 | 4.042202 | 0.585078 | 2.488382 |
| 33 | 1 | 0 | 5.009594 | 0.581935 | 2.979407 |
| 34 | 6 | 0 | 3.892187 | 1.225562 | 1.247361 |
| 35 | 6 | 0 | 2.619921 | 1.182776 | 0.666073 |
| 36 | 6 | 0 | 2.374753 | 1.825184 | -0.568142 |
| 37 | 6 | 0 | 4.938124 | 1.905493 | 0.549975 |
| 38 | 1 | 0 | 5.927887 | 1.917211 | 0.994156 |
| 39 | 6 | 0 | 4.703491 | 2.523007 | -0.639518 |
| 40 | 1 | 0 | 5.501306 | 3.039129 | -1.163548 |
| 41 | 6 | 0 | 3.401690 | 2.508816 | -1.231919 |
| 42 | 6 | 0 | 3.063983 | 3.127908 | -2.448526 |
| 43 | 1 | 0 | 3.823182 | 3.665579 | -3.007602 |
| 44 | 6 | 0 | 1.769653 | 3.043901 | -2.916284 |
| 45 | 1 | 0 | 1.478118 | 3.511411 | -3.849271 |
| 46 | 6 | 0 | 0.807555 | 2.340316 | -2.184393 |
| 47 | 1 | 0 | -0.212033 | 2.251157 | -2.534294 |
| 48 | 6 | 0 | -1.813611 | -0.098103 | 2.327702 |
| 49 | 1 | 0 | -1.925137 | 0.957923 | 2.532339 |
| 50 | 6 | 0 | -2.439721 | -1.056689 | 3.130967 |
| 51 | 1 | 0 | -3.049855 | -0.723258 | 3.961874 |
| 52 | 6 | 0 | -2.285902 | -2.395167 | 2.848127 |
| 53 | 1 | 0 | -2.774122 | -3.152457 | 3.452757 |
| 54 | 6 | 0 | -1.486902 | -2.782850 | 1.757780 |
| 55 | 6 | 0 | -0.881850 | -1.755532 | 1.022863 |
| 56 | 6 | 0 | -0.046124 | -2.054652 | -0.075162 |
| 57 | 6 | 0 | -1.264392 | -4.133481 | 1.348235 |
| 58 | 1 | 0 | -1.744449 | -4.927339 | 1.910971 |
| 59 | 6 | 0 | -0.478380 | -4.419494 | 0.274127 |
| 60 | 1 | 0 | -0.319779 | -5.447082 | -0.036922 |
| 61 | 6 | 0 | 0.159047 | -3.380072 | -0.472429 |
| 62 | 6 | 0 | 0.972944 | -3.583008 | -1.603196 |
| 63 | 1 | 0 | 1.161084 | -4.592050 | -1.955671 |
| 64 | 6 | 0 | 1.521513 | -2.497421 | -2.243633 |
| 65 | 1 | 0 | 2.158343 | -2.617433 | -3.110769 |
| 66 | 6 | 0 | 1.277050 | -1.204961 | -1.763674 |
| 67 | 1 | 0 | 1.691777 | -0.339772 | -2.257437 |
| 68 | 16 | 0 | 4.475896 | -1.926698 | -0.409628 |
| 69 | 8 | 0 | 5.690067 | -1.577320 | 0.410924 |
| 70 | 8 | 0 | 3.315346 | -2.188595 | 0.508123 |
| 71 | 8 | 0 | 4.163316 | -0.786745 | -1.340776 |
| 72 | 8 | 0 | 4.753149 | -3.163734 | -1.222924 |
| 73 | 16 | 0 | -4.137881 | -2.118839 | -0.317727 |
| 74 | 8 | 0 | -5.396146 | -1.821364 | -1.334014 |

| | | | | | |
|---|---|---|---|---|---|
| 75 | 1 | 0 | -5.601191 | -2.609094 | -1.856549 |
| 76 | 8 | 0 | -3.940349 | -0.804193 | 0.293116 |
| 77 | 8 | 0 | -4.609989 | -3.157346 | 0.614354 |
| 78 | 8 | 0 | -3.038936 | -2.579241 | -1.181536 |

Rotational constants (GHZ): 0.0832272 0.0568638

TC4-2-110, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.038886 | 0.670220 | 0.080253 |
| 2 | 7 | 0 | -1.688122 | 0.912185 | -1.076824 |
| 3 | 7 | 0 | -0.766468 | 2.515908 | 0.882670 |
| 4 | 7 | 0 | 1.685054 | 0.669633 | 1.318568 |
| 5 | 7 | 0 | 1.198914 | 1.645807 | -1.104053 |
| 6 | 7 | 0 | -0.940086 | -0.502903 | 1.285075 |
| 7 | 7 | 0 | 0.508158 | -1.202923 | -0.857563 |
| 8 | 6 | 0 | -2.093079 | 0.107397 | -2.039236 |
| 9 | 1 | 0 | -1.436384 | -0.707504 | -2.307977 |
| 10 | 6 | 0 | -3.315606 | 0.303488 | -2.692914 |
| 11 | 1 | 0 | -3.609457 | -0.382571 | -3.477613 |
| 12 | 6 | 0 | -4.119428 | 1.352389 | -2.315456 |
| 13 | 1 | 0 | -5.076562 | 1.523282 | -2.798182 |
| 14 | 6 | 0 | -3.697089 | 2.221026 | -1.289978 |
| 15 | 6 | 0 | -2.453439 | 1.953467 | -0.693425 |
| 16 | 6 | 0 | -1.960715 | 2.811268 | 0.335273 |
| 17 | 6 | 0 | -4.456120 | 3.347834 | -0.845238 |
| 18 | 1 | 0 | -5.417133 | 3.536384 | -1.313381 |
| 19 | 6 | 0 | -3.985932 | 4.168118 | 0.132354 |
| 20 | 1 | 0 | -4.562427 | 5.025891 | 0.463920 |
| 21 | 6 | 0 | -2.719284 | 3.921479 | 0.746302 |
| 22 | 6 | 0 | -2.168309 | 4.730950 | 1.758782 |
| 23 | 1 | 0 | -2.720743 | 5.598590 | 2.106166 |
| 24 | 6 | 0 | -0.939808 | 4.415836 | 2.297437 |
| 25 | 1 | 0 | -0.493548 | 5.021830 | 3.077129 |
| 26 | 6 | 0 | -0.261595 | 3.282729 | 1.831905 |
| 27 | 1 | 0 | 0.699594 | 2.988441 | 2.238219 |
| 28 | 6 | 0 | 1.860864 | 0.152462 | 2.520953 |
| 29 | 1 | 0 | 1.007122 | -0.319486 | 2.990273 |
| 30 | 6 | 0 | 3.104803 | 0.211545 | 3.158039 |
| 31 | 1 | 0 | 3.213772 | -0.228417 | 4.142096 |
| 32 | 6 | 0 | 4.168257 | 0.813938 | 2.521520 |
| 33 | 1 | 0 | 5.143789 | 0.860509 | 2.994387 |
| 34 | 6 | 0 | 3.990384 | 1.374388 | 1.243910 |
| 35 | 6 | 0 | 2.713213 | 1.265742 | 0.681009 |
| 36 | 6 | 0 | 2.451337 | 1.794520 | -0.606757 |
| 37 | 6 | 0 | 5.020710 | 2.021581 | 0.494683 |
| 38 | 1 | 0 | 6.010709 | 2.089857 | 0.933306 |
| 39 | 6 | 0 | 4.769566 | 2.533638 | -0.739405 |
| 40 | 1 | 0 | 5.553464 | 3.022610 | -1.308486 |
| 41 | 6 | 0 | 3.468850 | 2.436199 | -1.326244 |
| 42 | 6 | 0 | 3.139620 | 2.922068 | -2.603675 |
| 43 | 1 | 0 | 3.898967 | 3.420875 | -3.197596 |
| 44 | 6 | 0 | 1.860771 | 2.754251 | -3.093604 |
| 45 | 1 | 0 | 1.581002 | 3.114750 | -4.076091 |
| 46 | 6 | 0 | 0.903787 | 2.104282 | -2.313276 |
| 47 | 1 | 0 | -0.106956 | 1.950097 | -2.665099 |
| 48 | 6 | 0 | -1.647977 | -0.112448 | 2.331643 |
| 49 | 1 | 0 | -1.727863 | 0.951282 | 2.507698 |
| 50 | 6 | 0 | -2.258853 | -1.033446 | 3.186243 |

| | | | | | |
|---|---|---|---|---|---|
| 51 | 1 | 0 | -2.829135 | -0.665748 | 4.030656 |
| 52 | 6 | 0 | -2.132217 | -2.379032 | 2.931845 |
| 53 | 1 | 0 | -2.603195 | -3.114853 | 3.575482 |
| 54 | 6 | 0 | -1.382560 | -2.809337 | 1.822722 |
| 55 | 6 | 0 | -0.795159 | -1.821416 | 1.016030 |
| 56 | 6 | 0 | -0.018211 | -2.195193 | -0.113703 |
| 57 | 6 | 0 | -1.199920 | -4.183294 | 1.476355 |
| 58 | 1 | 0 | -1.672058 | -4.935044 | 2.100391 |
| 59 | 6 | 0 | -0.455034 | -4.540304 | 0.396288 |
| 60 | 1 | 0 | -0.316870 | -5.585518 | 0.138194 |
| 61 | 6 | 0 | 0.162326 | -3.549614 | -0.427069 |
| 62 | 6 | 0 | 0.944240 | -3.839649 | -1.562935 |
| 63 | 1 | 0 | 1.116096 | -4.874821 | -1.840960 |
| 64 | 6 | 0 | 1.478094 | -2.812681 | -2.305406 |
| 65 | 1 | 0 | 2.085785 | -3.006402 | -3.180630 |
| 66 | 6 | 0 | 1.235641 | -1.487626 | -1.919199 |
| 67 | 1 | 0 | 1.622944 | -0.654484 | -2.488594 |
| 68 | 16 | 0 | 4.369508 | -1.828320 | -0.364574 |
| 69 | 8 | 0 | 5.597620 | -1.427818 | 0.411493 |
| 70 | 8 | 0 | 3.253984 | -2.130941 | 0.596250 |
| 71 | 8 | 0 | 3.979736 | -0.707420 | -1.287455 |
| 72 | 8 | 0 | 4.668485 | -3.058623 | -1.181014 |
| 73 | 16 | 0 | -4.091665 | -2.168746 | -0.208470 |
| 74 | 8 | 0 | -5.378595 | -1.881588 | -1.191211 |
| 75 | 1 | 0 | -5.580278 | -2.665643 | -1.720470 |
| 76 | 8 | 0 | -3.892356 | -0.853624 | 0.401740 |
| 77 | 8 | 0 | -4.529358 | -3.213937 | 0.732959 |
| 78 | 8 | 0 | -3.011028 | -2.616031 | -1.101570 |

Rotational constants (GHZ): 0.0803022 0.0561046

**Structures of TC-2-020**

TC2-2-020, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.010726 | 0.669632 | 0.095572 |
| 2 | 7 | 0 | -1.593826 | 0.864324 | -1.010337 |
| 3 | 7 | 0 | -0.617677 | 2.317658 | 0.920086 |
| 4 | 7 | 0 | 1.583069 | 0.539757 | 1.200518 |
| 5 | 7 | 0 | 1.117976 | 1.728920 | -1.070210 |
| 6 | 7 | 0 | -1.040187 | -0.446151 | 1.299459 |
| 7 | 7 | 0 | 0.483119 | -1.005941 | -0.739335 |
| 8 | 6 | 0 | -2.013435 | 0.109667 | -2.009789 |
| 9 | 1 | 0 | -1.392813 | -0.723257 | -2.302695 |
| 10 | 6 | 0 | -3.211705 | 0.384954 | -2.679942 |
| 11 | 1 | 0 | -3.511135 | -0.262324 | -3.494855 |
| 12 | 6 | 0 | -3.989356 | 1.449520 | -2.289298 |
| 13 | 1 | 0 | -4.926951 | 1.669221 | -2.789774 |
| 14 | 6 | 0 | -3.557102 | 2.265405 | -1.226478 |
| 15 | 6 | 0 | -2.338834 | 1.924674 | -0.627171 |
| 16 | 6 | 0 | -1.808975 | 2.712952 | 0.418220 |
| 17 | 6 | 0 | -4.259801 | 3.410759 | -0.737387 |
| 18 | 1 | 0 | -5.208379 | 3.667113 | -1.198157 |
| 19 | 6 | 0 | -3.753045 | 4.167691 | 0.274898 |
| 20 | 1 | 0 | -4.289460 | 5.038034 | 0.638755 |
| 21 | 6 | 0 | -2.499283 | 3.841855 | 0.880113 |
| 22 | 6 | 0 | -1.892059 | 4.573254 | 1.917604 |
| 23 | 1 | 0 | -2.386443 | 5.453684 | 2.315487 |
| 24 | 6 | 0 | -0.674431 | 4.161088 | 2.414287 |
| 25 | 1 | 0 | -0.180621 | 4.702741 | 3.212115 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 6 | 0 | -0.056885 | 3.019265 | 1.891183 |
| 27 | 1 | 0 | 0.892296 | 2.669392 | 2.273925 |
| 28 | 6 | 0 | 1.747901 | -0.058619 | 2.368235 |
| 29 | 1 | 0 | 0.890756 | -0.552135 | 2.805274 |
| 30 | 6 | 0 | 2.980341 | -0.044403 | 3.029431 |
| 31 | 1 | 0 | 3.063292 | -0.544277 | 3.986994 |
| 32 | 6 | 0 | 4.062155 | 0.583111 | 2.454765 |
| 33 | 1 | 0 | 5.028661 | 0.592801 | 2.947433 |
| 34 | 6 | 0 | 3.907272 | 1.218258 | 1.210137 |
| 35 | 6 | 0 | 2.634146 | 1.166247 | 0.630210 |
| 36 | 6 | 0 | 2.383972 | 1.804215 | -0.605116 |
| 37 | 6 | 0 | 4.950836 | 1.894813 | 0.505474 |
| 38 | 1 | 0 | 5.940839 | 1.913922 | 0.948986 |
| 39 | 6 | 0 | 4.713545 | 2.498361 | -0.690861 |
| 40 | 1 | 0 | 5.509938 | 3.010005 | -1.221366 |
| 41 | 6 | 0 | 3.409652 | 2.480385 | -1.278222 |
| 42 | 6 | 0 | 3.067883 | 3.093342 | -2.497108 |
| 43 | 1 | 0 | 3.826126 | 3.624928 | -3.063197 |
| 44 | 6 | 0 | 1.770620 | 3.012545 | -2.956249 |
| 45 | 1 | 0 | 1.475299 | 3.476196 | -3.889937 |
| 46 | 6 | 0 | 0.809215 | 2.318538 | -2.213769 |
| 47 | 1 | 0 | -0.213089 | 2.233373 | -2.556714 |
| 48 | 6 | 0 | -1.790794 | -0.094444 | 2.329109 |
| 49 | 1 | 0 | -1.889763 | 0.961666 | 2.539330 |
| 50 | 6 | 0 | -2.418470 | -1.049831 | 3.134941 |
| 51 | 1 | 0 | -3.017504 | -0.713377 | 3.972655 |
| 52 | 6 | 0 | -2.279894 | -2.388782 | 2.846668 |
| 53 | 1 | 0 | -2.769252 | -3.143482 | 3.453567 |
| 54 | 6 | 0 | -1.494957 | -2.780037 | 1.747442 |
| 55 | 6 | 0 | -0.889097 | -1.756010 | 1.009255 |
| 56 | 6 | 0 | -0.069169 | -2.059397 | -0.099728 |
| 57 | 6 | 0 | -1.288334 | -4.131750 | 1.332139 |
| 58 | 1 | 0 | -1.770155 | -4.922624 | 1.897522 |
| 59 | 6 | 0 | -0.515144 | -4.422428 | 0.250303 |
| 60 | 1 | 0 | -0.368398 | -5.450485 | -0.064825 |
| 61 | 6 | 0 | 0.122289 | -3.386213 | -0.500857 |
| 62 | 6 | 0 | 0.921692 | -3.593002 | -1.640294 |
| 63 | 1 | 0 | 1.099542 | -4.602667 | -1.996357 |
| 64 | 6 | 0 | 1.464663 | -2.508646 | -2.290050 |
| 65 | 1 | 0 | 2.083069 | -2.631459 | -3.170569 |
| 66 | 6 | 0 | 1.231084 | -1.215874 | -1.807581 |
| 67 | 1 | 0 | 1.643423 | -0.351665 | -2.306539 |
| 68 | 16 | 0 | 4.323015 | -1.818901 | -0.285182 |
| 69 | 8 | 0 | 5.552094 | -1.593504 | 0.495372 |
| 70 | 8 | 0 | 3.131481 | -2.075188 | 0.524366 |
| 71 | 8 | 0 | 4.143865 | -0.837068 | -1.366818 |
| 72 | 8 | 0 | 4.528751 | -3.267773 | -1.034670 |
| 73 | 1 | 0 | 5.285636 | -3.232245 | -1.636266 |
| 74 | 16 | 0 | -4.150910 | -2.082847 | -0.308898 |
| 75 | 8 | 0 | -5.413216 | -1.773751 | -1.316259 |
| 76 | 1 | 0 | -5.625434 | -2.558142 | -1.841099 |
| 77 | 8 | 0 | -3.944472 | -0.773558 | 0.310593 |
| 78 | 8 | 0 | -4.621630 | -3.126309 | 0.618300 |
| 79 | 8 | 0 | -3.058195 | -2.541120 | -1.181836 |

Rotational constants (GHZ): 0.0833108 0.0574722

TC4-2-020, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.003861 | 0.705808 | 0.074800 |
| 2 | 7 | 0 | -1.737203 | 0.895596 | -1.066895 |
| 3 | 7 | 0 | -0.852538 | 2.518206 | 0.895168 |
| 4 | 7 | 0 | 1.665296 | 0.736017 | 1.292104 |
| 5 | 7 | 0 | 1.131686 | 1.699108 | -1.127897 |
| 6 | 7 | 0 | -0.920875 | -0.511754 | 1.275497 |
| 7 | 7 | 0 | 0.541711 | -1.143797 | -0.879072 |
| 8 | 6 | 0 | -2.122072 | 0.085386 | -2.033272 |
| 9 | 1 | 0 | -1.440993 | -0.705251 | -2.313760 |
| 10 | 6 | 0 | -3.355725 | 0.244837 | -2.675682 |
| 11 | 1 | 0 | -3.631957 | -0.444153 | -3.464161 |
| 12 | 6 | 0 | -4.192327 | 1.261727 | -2.282171 |
| 13 | 1 | 0 | -5.159008 | 1.403069 | -2.755255 |
| 14 | 6 | 0 | -3.792008 | 2.135646 | -1.252447 |
| 15 | 6 | 0 | -2.534581 | 1.907026 | -0.668470 |
| 16 | 6 | 0 | -2.062884 | 2.773662 | 0.362522 |
| 17 | 6 | 0 | -4.586926 | 3.230536 | -0.791006 |
| 18 | 1 | 0 | -5.558316 | 3.388409 | -1.248864 |
| 19 | 6 | 0 | -4.137540 | 4.058107 | 0.190152 |
| 20 | 1 | 0 | -4.741470 | 4.891327 | 0.535208 |
| 21 | 6 | 0 | -2.857215 | 3.851950 | 0.790336 |
| 22 | 6 | 0 | -2.326454 | 4.672552 | 1.804591 |
| 23 | 1 | 0 | -2.906822 | 5.516309 | 2.164950 |
| 24 | 6 | 0 | -1.081984 | 4.398219 | 2.328739 |
| 25 | 1 | 0 | -0.650532 | 5.013606 | 3.109395 |
| 26 | 6 | 0 | -0.366955 | 3.295303 | 1.846424 |
| 27 | 1 | 0 | 0.609149 | 3.034456 | 2.239799 |
| 28 | 6 | 0 | 1.862566 | 0.235058 | 2.496442 |
| 29 | 1 | 0 | 1.021867 | -0.246363 | 2.979791 |
| 30 | 6 | 0 | 3.111196 | 0.324882 | 3.122768 |
| 31 | 1 | 0 | 3.235249 | -0.097531 | 4.112673 |
| 32 | 6 | 0 | 4.158819 | 0.931855 | 2.467370 |
| 33 | 1 | 0 | 5.138353 | 1.000136 | 2.929129 |
| 34 | 6 | 0 | 3.961267 | 1.467694 | 1.180330 |
| 35 | 6 | 0 | 2.677143 | 1.340761 | 0.635588 |
| 36 | 6 | 0 | 2.394093 | 1.851063 | -0.654972 |
| 37 | 6 | 0 | 4.979309 | 2.102801 | 0.404781 |
| 38 | 1 | 0 | 5.974491 | 2.184215 | 0.829169 |
| 39 | 6 | 0 | 4.709824 | 2.588421 | -0.836641 |
| 40 | 1 | 0 | 5.484484 | 3.067328 | -1.426426 |
| 41 | 6 | 0 | 3.400822 | 2.478611 | -1.401459 |
| 42 | 6 | 0 | 3.049422 | 2.949140 | -2.680082 |
| 43 | 1 | 0 | 3.799629 | 3.436972 | -3.294297 |
| 44 | 6 | 0 | 1.760560 | 2.784007 | -3.141482 |
| 45 | 1 | 0 | 1.462516 | 3.135817 | -4.121697 |
| 46 | 6 | 0 | 0.815143 | 2.147536 | -2.334454 |
| 47 | 1 | 0 | -0.203388 | 1.995439 | -2.664494 |
| 48 | 6 | 0 | -1.633225 | -0.154678 | 2.330858 |
| 49 | 1 | 0 | -1.746781 | 0.904215 | 2.517719 |
| 50 | 6 | 0 | -2.206760 | -1.103633 | 3.180727 |
| 51 | 1 | 0 | -2.782460 | -0.763105 | 4.032798 |
| 52 | 6 | 0 | -2.037847 | -2.441731 | 2.912138 |
| 53 | 1 | 0 | -2.479480 | -3.199048 | 3.551592 |
| 54 | 6 | 0 | -1.281721 | -2.836136 | 1.794000 |
| 55 | 6 | 0 | -0.733578 | -1.821833 | 0.992994 |
| 56 | 6 | 0 | 0.049314 | -2.159013 | -0.144444 |
| 57 | 6 | 0 | -1.054464 | -4.200289 | 1.434336 |
| 58 | 1 | 0 | -1.497348 | -4.972877 | 2.054289 |
| 59 | 6 | 0 | -0.304280 | -4.522916 | 0.347498 |
| 60 | 1 | 0 | -0.132220 | -5.560424 | 0.079228 |
| 61 | 6 | 0 | 0.274504 | -3.504370 | -0.470135 |
| 62 | 6 | 0 | 1.060062 | -3.757839 | -1.611360 |
| 63 | 1 | 0 | 1.265941 | -4.783975 | -1.899408 |

| | | | | | |
|---|---|---|---|---|---|
| 64 | 6 | 0 | 1.554331 | -2.706150 | -2.348664 |
| 65 | 1 | 0 | 2.161728 | -2.872029 | -3.230198 |
| 66 | 6 | 0 | 1.270803 | -1.394543 | -1.948148 |
| 67 | 1 | 0 | 1.634935 | -0.542141 | -2.506989 |
| 68 | 16 | 0 | 4.338488 | -1.652272 | -0.198387 |
| 69 | 8 | 0 | 5.572090 | -1.363935 | 0.553495 |
| 70 | 8 | 0 | 3.164742 | -1.898853 | 0.640575 |
| 71 | 8 | 0 | 4.120095 | -0.727017 | -1.321274 |
| 72 | 8 | 0 | 4.568629 | -3.128441 | -0.884650 |
| 73 | 1 | 0 | 5.301234 | -3.095916 | -1.515816 |
| 74 | 16 | 0 | -4.027265 | -2.272905 | -0.206134 |
| 75 | 8 | 0 | -5.326654 | -2.013617 | -1.179631 |
| 76 | 1 | 0 | -5.507053 | -2.796053 | -1.718677 |
| 77 | 8 | 0 | -3.860342 | -0.956602 | 0.411187 |
| 78 | 8 | 0 | -4.430737 | -3.335860 | 0.730679 |
| 79 | 8 | 0 | -2.939329 | -2.685190 | -1.107468 |

Rotational constants (GHZ): 0.0804334 0.0561551

**Structures of TC-2-011**

TC2-2-011, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.039249 | 0.693203 | 0.093059 |
| 2 | 7 | 0 | -1.630954 | 0.865007 | -1.002186 |
| 3 | 7 | 0 | -0.668700 | 2.324254 | 0.929078 |
| 4 | 7 | 0 | 1.564236 | 0.579129 | 1.190781 |
| 5 | 7 | 0 | 1.069020 | 1.774787 | -1.072374 |
| 6 | 7 | 0 | -1.038469 | -0.450372 | 1.295437 |
| 7 | 7 | 0 | 0.482197 | -0.969332 | -0.756540 |
| 8 | 6 | 0 | -2.043917 | 0.106755 | -2.001926 |
| 9 | 1 | 0 | -1.411046 | -0.713699 | -2.303222 |
| 10 | 6 | 0 | -3.253096 | 0.361373 | -2.660258 |
| 11 | 1 | 0 | -3.546588 | -0.287939 | -3.475692 |
| 12 | 6 | 0 | -4.048344 | 1.408626 | -2.257996 |
| 13 | 1 | 0 | -4.994137 | 1.612052 | -2.749831 |
| 14 | 6 | 0 | -3.623210 | 2.228227 | -1.195185 |
| 15 | 6 | 0 | -2.393847 | 1.908347 | -0.607342 |
| 16 | 6 | 0 | -1.870210 | 2.701386 | 0.437260 |
| 17 | 6 | 0 | -4.342927 | 3.358346 | -0.695480 |
| 18 | 1 | 0 | -5.299971 | 3.598808 | -1.147199 |
| 19 | 6 | 0 | -3.841273 | 4.121081 | 0.315004 |
| 20 | 1 | 0 | -4.390362 | 4.980247 | 0.686381 |
| 21 | 6 | 0 | -2.576733 | 3.816060 | 0.908719 |
| 22 | 6 | 0 | -1.973840 | 4.554484 | 1.943680 |
| 23 | 1 | 0 | -2.480118 | 5.424884 | 2.348587 |
| 24 | 6 | 0 | -0.745084 | 4.162079 | 2.428978 |
| 25 | 1 | 0 | -0.254278 | 4.710084 | 3.224304 |
| 26 | 6 | 0 | -0.111848 | 3.032787 | 1.897647 |
| 27 | 1 | 0 | 0.846521 | 2.698969 | 2.271768 |
| 28 | 6 | 0 | 1.743365 | -0.017482 | 2.357257 |
| 29 | 1 | 0 | 0.892823 | -0.513386 | 2.804282 |
| 30 | 6 | 0 | 2.984055 | -0.001367 | 3.004533 |
| 31 | 1 | 0 | 3.078544 | -0.500590 | 3.961324 |
| 32 | 6 | 0 | 4.057330 | 0.630967 | 2.419286 |
| 33 | 1 | 0 | 5.029387 | 0.643262 | 2.901038 |
| 34 | 6 | 0 | 3.886822 | 1.266935 | 1.175896 |
| 35 | 6 | 0 | 2.606410 | 1.212442 | 0.610139 |
| 36 | 6 | 0 | 2.340883 | 1.850488 | -0.622174 |
| 37 | 6 | 0 | 4.920535 | 1.948264 | 0.461059 |

| | | | | | |
|---|---|---|---|---|---|
| 38 | 1 | 0 | 5.914731 | 1.972296 | 0.894747 |
| 39 | 6 | 0 | 4.667743 | 2.551141 | -0.732605 |
| 40 | 1 | 0 | 5.456308 | 3.066911 | -1.270661 |
| 41 | 6 | 0 | 3.357522 | 2.529777 | -1.305389 |
| 42 | 6 | 0 | 3.000161 | 3.147574 | -2.517869 |
| 43 | 1 | 0 | 3.750972 | 3.681995 | -3.091045 |
| 44 | 6 | 0 | 1.697153 | 3.069314 | -2.959686 |
| 45 | 1 | 0 | 1.389087 | 3.538063 | -3.886641 |
| 46 | 6 | 0 | 0.745423 | 2.370835 | -2.208302 |
| 47 | 1 | 0 | -0.280986 | 2.287295 | -2.538921 |
| 48 | 6 | 0 | -1.793315 | -0.119943 | 2.329156 |
| 49 | 1 | 0 | -1.920021 | 0.932888 | 2.541165 |
| 50 | 6 | 0 | -2.391661 | -1.092885 | 3.136452 |
| 51 | 1 | 0 | -2.995800 | -0.773393 | 3.977100 |
| 52 | 6 | 0 | -2.218507 | -2.427260 | 2.846371 |
| 53 | 1 | 0 | -2.684684 | -3.195553 | 3.454388 |
| 54 | 6 | 0 | -1.428604 | -2.795976 | 1.742855 |
| 55 | 6 | 0 | -0.854504 | -1.755588 | 1.002946 |
| 56 | 6 | 0 | -0.035988 | -2.036765 | -0.113505 |
| 57 | 6 | 0 | -1.188395 | -4.141864 | 1.325504 |
| 58 | 1 | 0 | -1.645342 | -4.945064 | 1.894068 |
| 59 | 6 | 0 | -0.416272 | -4.412192 | 0.238029 |
| 60 | 1 | 0 | -0.245436 | -5.435773 | -0.079208 |
| 61 | 6 | 0 | 0.185578 | -3.358715 | -0.518503 |
| 62 | 6 | 0 | 0.974567 | -3.543637 | -1.667598 |
| 63 | 1 | 0 | 1.174806 | -4.547758 | -2.027257 |
| 64 | 6 | 0 | 1.475441 | -2.443405 | -2.328117 |
| 65 | 1 | 0 | 2.078949 | -2.549679 | -3.221456 |
| 66 | 6 | 0 | 1.214929 | -1.158123 | -1.840795 |
| 67 | 1 | 0 | 1.598798 | -0.282284 | -2.344169 |
| 68 | 16 | 0 | 4.221370 | -1.808262 | -0.336073 |
| 69 | 8 | 0 | 3.088325 | -1.992806 | 0.529426 |
| 70 | 8 | 0 | 4.225757 | -0.809057 | -1.372372 |
| 71 | 8 | 0 | 4.498251 | -3.244389 | -0.955686 |
| 72 | 1 | 0 | 5.182854 | -3.243628 | -1.646252 |
| 73 | 16 | 0 | -4.096721 | -2.168438 | -0.313477 |
| 74 | 8 | 0 | -5.370217 | -1.877555 | -1.311633 |
| 75 | 1 | 0 | -5.566663 | -2.659895 | -1.845506 |
| 76 | 8 | 0 | -3.917061 | -0.861074 | 0.318261 |
| 77 | 8 | 0 | -4.538335 | -3.232144 | 0.604991 |
| 78 | 8 | 0 | -2.997398 | -2.592185 | -1.195664 |
| 79 | 8 | 0 | 5.525162 | -1.509456 | 0.520880 |
| 80 | 1 | 0 | 5.552505 | -2.002680 | 1.357934 |

Rotational constants (GHZ): 0.0829111 0.0576912

TC4-2-011, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.015073 | 0.716482 | 0.102654 |
| 2 | 7 | 0 | -1.567804 | 0.961014 | -1.046354 |
| 3 | 7 | 0 | -0.658068 | 2.318514 | 1.010101 |
| 4 | 7 | 0 | 1.645271 | 0.625668 | 1.167975 |
| 5 | 7 | 0 | 1.315264 | 1.846491 | -1.200701 |
| 6 | 7 | 0 | -1.141989 | -0.554165 | 1.466787 |
| 7 | 7 | 0 | 0.398510 | -1.035647 | -0.684098 |
| 8 | 6 | 0 | -1.949078 | 0.267320 | -2.105409 |
| 9 | 1 | 0 | -1.307575 | -0.535589 | -2.435588 |
| 10 | 6 | 0 | -3.136574 | 0.566504 | -2.782405 |
| 11 | 1 | 0 | -3.409089 | -0.030309 | -3.643802 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 6 | 0 | -3.941534 | 1.587835 | -2.335125 |
| 13 | 1 | 0 | -4.874253 | 1.821919 | -2.838161 |
| 14 | 6 | 0 | -3.547913 | 2.342526 | -1.212315 |
| 15 | 6 | 0 | -2.337268 | 1.986814 | -0.608278 |
| 16 | 6 | 0 | -1.849533 | 2.714961 | 0.499313 |
| 17 | 6 | 0 | -4.289618 | 3.436412 | -0.667424 |
| 18 | 1 | 0 | -5.232657 | 3.701159 | -1.134521 |
| 19 | 6 | 0 | -3.825282 | 4.133141 | 0.406343 |
| 20 | 1 | 0 | -4.389947 | 4.964177 | 0.816055 |
| 21 | 6 | 0 | -2.578919 | 3.792926 | 1.018046 |
| 22 | 6 | 0 | -2.015780 | 4.467072 | 2.118523 |
| 23 | 1 | 0 | -2.542662 | 5.307826 | 2.558324 |
| 24 | 6 | 0 | -0.802413 | 4.052646 | 2.624307 |
| 25 | 1 | 0 | -0.344475 | 4.553203 | 3.468806 |
| 26 | 6 | 0 | -0.142803 | 2.963920 | 2.045096 |
| 27 | 1 | 0 | 0.808329 | 2.616071 | 2.424715 |
| 28 | 6 | 0 | 1.763737 | 0.030283 | 2.342929 |
| 29 | 1 | 0 | 0.872483 | -0.418942 | 2.758432 |
| 30 | 6 | 0 | 2.982020 | -0.011134 | 3.027006 |
| 31 | 1 | 0 | 3.027725 | -0.508984 | 3.987898 |
| 32 | 6 | 0 | 4.093337 | 0.568293 | 2.461136 |
| 33 | 1 | 0 | 5.054866 | 0.540913 | 2.963240 |
| 34 | 6 | 0 | 3.984890 | 1.202659 | 1.209641 |
| 35 | 6 | 0 | 2.721119 | 1.211612 | 0.595839 |
| 36 | 6 | 0 | 2.549650 | 1.854026 | -0.664080 |
| 37 | 6 | 0 | 5.088173 | 1.816217 | 0.539543 |
| 38 | 1 | 0 | 6.059467 | 1.787090 | 1.022211 |
| 39 | 6 | 0 | 4.927488 | 2.417285 | -0.668983 |
| 40 | 1 | 0 | 5.767918 | 2.880525 | -1.175740 |
| 41 | 6 | 0 | 3.646180 | 2.458113 | -1.300136 |
| 42 | 6 | 0 | 3.400066 | 3.070505 | -2.544436 |
| 43 | 1 | 0 | 4.218087 | 3.548811 | -3.073884 |
| 44 | 6 | 0 | 2.128470 | 3.056345 | -3.075354 |
| 45 | 1 | 0 | 1.912180 | 3.520793 | -4.030327 |
| 46 | 6 | 0 | 1.098060 | 2.423977 | -2.367765 |
| 47 | 1 | 0 | 0.085688 | 2.379973 | -2.753715 |
| 48 | 6 | 0 | -1.914745 | -0.261921 | 2.494835 |
| 49 | 1 | 0 | -1.992477 | 0.783652 | 2.771548 |
| 50 | 6 | 0 | -2.600793 | -1.254435 | 3.204983 |
| 51 | 1 | 0 | -3.226989 | -0.973233 | 4.043450 |
| 52 | 6 | 0 | -2.471007 | -2.568841 | 2.817304 |
| 53 | 1 | 0 | -2.995126 | -3.359844 | 3.344099 |
| 54 | 6 | 0 | -1.651540 | -2.896002 | 1.720423 |
| 55 | 6 | 0 | -1.006341 | -1.832398 | 1.070527 |
| 56 | 6 | 0 | -0.176341 | -2.087068 | -0.059414 |
| 57 | 6 | 0 | -1.465446 | -4.226349 | 1.235693 |
| 58 | 1 | 0 | -1.978799 | -5.036884 | 1.742708 |
| 59 | 6 | 0 | -0.668213 | -4.470109 | 0.162552 |
| 60 | 1 | 0 | -0.527881 | -5.480171 | -0.208679 |
| 61 | 6 | 0 | -0.002168 | -3.403826 | -0.517385 |
| 62 | 6 | 0 | 0.802702 | -3.593906 | -1.654408 |
| 63 | 1 | 0 | 0.959895 | -4.597936 | -2.035256 |
| 64 | 6 | 0 | 1.370148 | -2.505540 | -2.276740 |
| 65 | 1 | 0 | 1.988911 | -2.613010 | -3.159277 |
| 66 | 6 | 0 | 1.143900 | -1.227674 | -1.760202 |
| 67 | 1 | 0 | 1.566734 | -0.351904 | -2.231234 |
| 68 | 16 | 0 | 4.153173 | -1.927590 | -0.277633 |
| 69 | 8 | 0 | 3.014118 | -2.081632 | 0.585988 |
| 70 | 8 | 0 | 4.186488 | -0.929388 | -1.314348 |
| 71 | 8 | 0 | 4.393645 | -3.370243 | -0.897473 |
| 72 | 1 | 0 | 5.083777 | -3.386801 | -1.582508 |
| 73 | 16 | 0 | -4.159650 | -1.933158 | -0.476585 |
| 74 | 8 | 0 | -5.354254 | -1.567017 | -1.544895 |

| | | | | | |
|---|---|---|---|---|---|
| 75 | 1 | 0 | -5.525865 | -2.318204 | -2.129525 |
| 76 | 8 | 0 | -3.991955 | -0.657366 | 0.220756 |
| 77 | 8 | 0 | -4.691459 | -3.021398 | 0.361052 |
| 78 | 8 | 0 | -3.011919 | -2.349038 | -1.298694 |
| 79 | 8 | 0 | 5.463137 | -1.663784 | 0.581382 |
| 80 | 1 | 0 | 5.476750 | -2.158217 | 1.418013 |

Rotational constants (GHZ): 0.0815772 0.0558250

**Structures of TC-2-002**

TC2-2-002, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.014708 | 0.713390 | 0.089387 |
| 2 | 7 | 0 | -1.605499 | 0.893401 | -1.011287 |
| 3 | 7 | 0 | -0.635334 | 2.350823 | 0.916973 |
| 4 | 7 | 0 | 1.584040 | 0.586838 | 1.190151 |
| 5 | 7 | 0 | 1.106232 | 1.774752 | -1.079226 |
| 6 | 7 | 0 | -1.032416 | -0.413883 | 1.296556 |
| 7 | 7 | 0 | 0.487350 | -0.960319 | -0.751456 |
| 8 | 6 | 0 | -2.012492 | 0.148598 | -2.025075 |
| 9 | 1 | 0 | -1.374531 | -0.665113 | -2.337279 |
| 10 | 6 | 0 | -3.223983 | 0.403489 | -2.678201 |
| 11 | 1 | 0 | -3.513248 | -0.234368 | -3.504659 |
| 12 | 6 | 0 | -4.027147 | 1.440221 | -2.259125 |
| 13 | 1 | 0 | -4.975376 | 1.642806 | -2.746467 |
| 14 | 6 | 0 | -3.602135 | 2.252632 | -1.191788 |
| 15 | 6 | 0 | -2.369104 | 1.932736 | -0.609574 |
| 16 | 6 | 0 | -1.841635 | 2.724675 | 0.434399 |
| 17 | 6 | 0 | -4.323570 | 3.377902 | -0.683465 |
| 18 | 1 | 0 | -5.283421 | 3.617173 | -1.129586 |
| 19 | 6 | 0 | -3.817802 | 4.138571 | 0.326184 |
| 20 | 1 | 0 | -4.366822 | 4.995319 | 0.703097 |
| 21 | 6 | 0 | -2.548134 | 3.836409 | 0.911157 |
| 22 | 6 | 0 | -1.940015 | 4.576456 | 1.942079 |
| 23 | 1 | 0 | -2.446017 | 5.445045 | 2.351057 |
| 24 | 6 | 0 | -0.706223 | 4.188040 | 2.417508 |
| 25 | 1 | 0 | -0.210998 | 4.737696 | 3.208912 |
| 26 | 6 | 0 | -0.073214 | 3.060798 | 1.881418 |
| 27 | 1 | 0 | 0.888891 | 2.729710 | 2.248061 |
| 28 | 6 | 0 | 1.754156 | -0.005138 | 2.360517 |
| 29 | 1 | 0 | 0.896794 | -0.485972 | 2.810895 |
| 30 | 6 | 0 | 2.995061 | -0.003503 | 3.007442 |
| 31 | 1 | 0 | 3.082069 | -0.497892 | 3.967422 |
| 32 | 6 | 0 | 4.077854 | 0.608619 | 2.418131 |
| 33 | 1 | 0 | 5.050015 | 0.609154 | 2.899783 |
| 34 | 6 | 0 | 3.917049 | 1.239035 | 1.170681 |
| 35 | 6 | 0 | 2.635942 | 1.200509 | 0.605552 |
| 36 | 6 | 0 | 2.379580 | 1.834142 | -0.630562 |
| 37 | 6 | 0 | 4.960852 | 1.899269 | 0.450734 |
| 38 | 1 | 0 | 5.955488 | 1.911016 | 0.883879 |
| 39 | 6 | 0 | 4.716797 | 2.497670 | -0.747022 |
| 40 | 1 | 0 | 5.512866 | 2.997498 | -1.289019 |
| 41 | 6 | 0 | 3.406089 | 2.492818 | -1.319039 |
| 42 | 6 | 0 | 3.057225 | 3.107673 | -2.535462 |
| 43 | 1 | 0 | 3.815704 | 3.626083 | -3.113194 |
| 44 | 6 | 0 | 1.752526 | 3.047123 | -2.975319 |
| 45 | 1 | 0 | 1.450822 | 3.514704 | -3.904946 |
| 46 | 6 | 0 | 0.790597 | 2.368954 | -2.218541 |
| 47 | 1 | 0 | -0.237526 | 2.301060 | -2.547256 |

| | | | | | |
|---|---|---|---|---|---|
| 48 | 6 | 0 | -1.784474 | -0.070995 | 2.328559 |
| 49 | 1 | 0 | -1.894267 | 0.983538 | 2.541243 |
| 50 | 6 | 0 | -2.402881 | -1.033748 | 3.133783 |
| 51 | 1 | 0 | -3.003685 | -0.703652 | 3.972643 |
| 52 | 6 | 0 | -2.250236 | -2.370857 | 2.845459 |
| 53 | 1 | 0 | -2.731269 | -3.131082 | 3.451987 |
| 54 | 6 | 0 | -1.464060 | -2.753366 | 1.742993 |
| 55 | 6 | 0 | -0.866884 | -1.722895 | 1.005925 |
| 56 | 6 | 0 | -0.052974 | -2.018461 | -0.110296 |
| 57 | 6 | 0 | -1.252700 | -4.103387 | 1.322416 |
| 58 | 1 | 0 | -1.726537 | -4.898187 | 1.889075 |
| 59 | 6 | 0 | -0.483927 | -4.386576 | 0.235392 |
| 60 | 1 | 0 | -0.333287 | -5.412601 | -0.083992 |
| 61 | 6 | 0 | 0.141900 | -3.344017 | -0.516698 |
| 62 | 6 | 0 | 0.931587 | -3.543964 | -1.663289 |
| 63 | 1 | 0 | 1.112493 | -4.551571 | -2.023232 |
| 64 | 6 | 0 | 1.458011 | -2.453628 | -2.319551 |
| 65 | 1 | 0 | 2.063472 | -2.570997 | -3.210135 |
| 66 | 6 | 0 | 1.220764 | -1.163380 | -1.832423 |
| 67 | 1 | 0 | 1.623012 | -0.295212 | -2.334794 |
| 68 | 16 | 0 | 4.203103 | -1.856491 | -0.313133 |
| 69 | 8 | 0 | 3.062892 | -2.024426 | 0.546571 |
| 70 | 8 | 0 | 4.224732 | -0.859969 | -1.351820 |
| 71 | 8 | 0 | 4.465298 | -3.297180 | -0.928313 |
| 72 | 1 | 0 | 5.154965 | -3.306212 | -1.613926 |
| 73 | 16 | 0 | -4.067012 | -2.062279 | -0.393180 |
| 74 | 8 | 0 | -5.367414 | -1.854326 | -1.278603 |
| 75 | 1 | 0 | -5.503991 | -2.550370 | -1.942654 |
| 76 | 8 | 0 | -3.909473 | -0.832856 | 0.328822 |
| 77 | 8 | 0 | -4.512611 | -3.146349 | 0.679764 |
| 78 | 8 | 0 | -3.004435 | -2.609419 | -1.203465 |
| 79 | 8 | 0 | 5.505900 | -1.571569 | 0.549454 |
| 80 | 1 | 0 | 5.525093 | -2.065389 | 1.386369 |
| 81 | 1 | 0 | -4.289892 | -4.057072 | 0.423006 |

Rotational constants (GHZ): 0.0828605 0.0576063

TC4-2-002, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.007846 | 0.747247 | 0.090932 |
| 2 | 7 | 0 | -1.545519 | 0.995186 | -1.060840 |
| 3 | 7 | 0 | -0.635774 | 2.347986 | 0.999178 |
| 4 | 7 | 0 | 1.660764 | 0.644428 | 1.163316 |
| 5 | 7 | 0 | 1.351647 | 1.857965 | -1.211871 |
| 6 | 7 | 0 | -1.146613 | -0.507922 | 1.454507 |
| 7 | 7 | 0 | 0.404606 | -1.014939 | -0.684706 |
| 8 | 6 | 0 | -1.917445 | 0.314078 | -2.132533 |
| 9 | 1 | 0 | -1.266865 | -0.478499 | -2.473083 |
| 10 | 6 | 0 | -3.111573 | 0.605112 | -2.800416 |
| 11 | 1 | 0 | -3.378375 | 0.019425 | -3.671655 |
| 12 | 6 | 0 | -3.930505 | 1.609469 | -2.334140 |
| 13 | 1 | 0 | -4.868471 | 1.836597 | -2.830488 |
| 14 | 6 | 0 | -3.540656 | 2.357176 | -1.206411 |
| 15 | 6 | 0 | -2.322282 | 2.009270 | -0.611149 |
| 16 | 6 | 0 | -1.834414 | 2.735538 | 0.498397 |
| 17 | 6 | 0 | -4.290810 | 3.439366 | -0.649337 |
| 18 | 1 | 0 | -5.239115 | 3.697808 | -1.108985 |
| 19 | 6 | 0 | -3.825260 | 4.134124 | 0.424844 |
| 20 | 1 | 0 | -4.394750 | 4.957569 | 0.843023 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 6 | 0 | -2.570854 | 3.803457 | 1.026310 |
| 22 | 6 | 0 | -2.006675 | 4.479169 | 2.125563 |
| 23 | 1 | 0 | -2.538704 | 5.312835 | 2.572446 |
| 24 | 6 | 0 | -0.785481 | 4.075107 | 2.620328 |
| 25 | 1 | 0 | -0.326026 | 4.577270 | 3.463027 |
| 26 | 6 | 0 | -0.119346 | 2.994632 | 2.032873 |
| 27 | 1 | 0 | 0.837857 | 2.655009 | 2.404662 |
| 28 | 6 | 0 | 1.767445 | 0.055562 | 2.342807 |
| 29 | 1 | 0 | 0.868157 | -0.374712 | 2.761108 |
| 30 | 6 | 0 | 2.984423 | -0.002706 | 3.027736 |
| 31 | 1 | 0 | 3.020797 | -0.494687 | 3.992020 |
| 32 | 6 | 0 | 4.106294 | 0.552432 | 2.458140 |
| 33 | 1 | 0 | 5.067123 | 0.510458 | 2.960531 |
| 34 | 6 | 0 | 4.009650 | 1.181187 | 1.202829 |
| 35 | 6 | 0 | 2.746568 | 1.208818 | 0.588343 |
| 36 | 6 | 0 | 2.586221 | 1.847013 | -0.674906 |
| 37 | 6 | 0 | 5.123885 | 1.770276 | 0.528951 |
| 38 | 1 | 0 | 6.094552 | 1.726298 | 1.011701 |
| 39 | 6 | 0 | 4.973848 | 2.367020 | -0.683074 |
| 40 | 1 | 0 | 5.822342 | 2.811975 | -1.192747 |
| 41 | 6 | 0 | 3.693380 | 2.427451 | -1.314327 |
| 42 | 6 | 0 | 3.458374 | 3.036923 | -2.562152 |
| 43 | 1 | 0 | 4.284812 | 3.497614 | -3.094119 |
| 44 | 6 | 0 | 2.186838 | 3.042303 | -3.093280 |
| 45 | 1 | 0 | 1.978892 | 3.505131 | -4.050874 |
| 46 | 6 | 0 | 1.145230 | 2.432260 | -2.382682 |
| 47 | 1 | 0 | 0.132672 | 2.404389 | -2.769356 |
| 48 | 6 | 0 | -1.921048 | -0.204977 | 2.478273 |
| 49 | 1 | 0 | -1.997271 | 0.842748 | 2.746688 |
| 50 | 6 | 0 | -2.612534 | -1.189389 | 3.195648 |
| 51 | 1 | 0 | -3.238926 | -0.898639 | 4.030608 |
| 52 | 6 | 0 | -2.485563 | -2.507287 | 2.820483 |
| 53 | 1 | 0 | -3.013259 | -3.292190 | 3.352722 |
| 54 | 6 | 0 | -1.666827 | -2.846456 | 1.725598 |
| 55 | 6 | 0 | -1.012330 | -1.790955 | 1.070210 |
| 56 | 6 | 0 | -0.182684 | -2.058333 | -0.057182 |
| 57 | 6 | 0 | -1.493151 | -4.180923 | 1.246976 |
| 58 | 1 | 0 | -2.012362 | -4.984752 | 1.758769 |
| 59 | 6 | 0 | -0.699765 | -4.435656 | 0.173022 |
| 60 | 1 | 0 | -0.569349 | -5.448312 | -0.194542 |
| 61 | 6 | 0 | -0.023468 | -3.378432 | -0.510542 |
| 62 | 6 | 0 | 0.780071 | -3.581849 | -1.646699 |
| 63 | 1 | 0 | 0.926073 | -4.588883 | -2.023821 |
| 64 | 6 | 0 | 1.360992 | -2.502371 | -2.271033 |
| 65 | 1 | 0 | 1.979976 | -2.619565 | -3.152122 |
| 66 | 6 | 0 | 1.149581 | -1.219933 | -1.758364 |
| 67 | 1 | 0 | 1.584086 | -0.351278 | -2.231915 |
| 68 | 16 | 0 | 4.126472 | -1.974698 | -0.243965 |
| 69 | 8 | 0 | 2.978984 | -2.111054 | 0.611624 |
| 70 | 8 | 0 | 4.179706 | -0.979650 | -1.282938 |
| 71 | 8 | 0 | 4.352120 | -3.421726 | -0.858920 |
| 72 | 1 | 0 | 5.046157 | -3.448343 | -1.539790 |
| 73 | 16 | 0 | -4.100428 | -1.857661 | -0.557911 |
| 74 | 8 | 0 | -5.351825 | -1.594721 | -1.497180 |
| 75 | 1 | 0 | -5.496140 | -2.290574 | -2.159902 |
| 76 | 8 | 0 | -3.951191 | -0.651571 | 0.204478 |
| 77 | 8 | 0 | -4.625994 | -2.965422 | 0.452917 |
| 78 | 8 | 0 | -3.009573 | -2.404754 | -1.330042 |
| 79 | 8 | 0 | 5.433734 | -1.725576 | 0.622939 |
| 80 | 1 | 0 | 5.439237 | -2.222424 | 1.458196 |
| 81 | 1 | 0 | -4.356052 | -3.866925 | 0.208993 |

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Rotational constants (GHZ): 0.0814457 0.0558268

**Structures of TC-3-030**

TC2-3-030, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.111567 | 0.603035 | 0.020894 |
| 2 | 7 | 0 | -1.332321 | 1.845161 | -0.830790 |
| 3 | 7 | 0 | 0.892166 | 2.204441 | 0.459227 |
| 4 | 7 | 0 | 1.180450 | -0.597856 | 0.847353 |
| 5 | 7 | 0 | 0.997010 | 0.386234 | -1.556444 |
| 6 | 7 | 0 | -1.198856 | 0.687263 | 1.623425 |
| 7 | 7 | 0 | -1.197388 | -0.956794 | -0.396338 |
| 8 | 6 | 0 | -2.451809 | 1.586032 | -1.482030 |
| 9 | 1 | 0 | -2.754156 | 0.553583 | -1.573587 |
| 10 | 6 | 0 | -3.222415 | 2.613868 | -2.041309 |
| 11 | 1 | 0 | -4.136056 | 2.353466 | -2.561637 |
| 12 | 6 | 0 | -2.816347 | 3.923655 | -1.921345 |
| 13 | 1 | 0 | -3.402369 | 4.730906 | -2.349046 |
| 14 | 6 | 0 | -1.621085 | 4.216097 | -1.235710 |
| 15 | 6 | 0 | -0.917448 | 3.126228 | -0.709555 |
| 16 | 6 | 0 | 0.294075 | 3.320973 | -0.013657 |
| 17 | 6 | 0 | -1.081575 | 5.527095 | -1.046819 |
| 18 | 1 | 0 | -1.627126 | 6.371666 | -1.455244 |
| 19 | 6 | 0 | 0.086691 | 5.715773 | -0.371746 |
| 20 | 1 | 0 | 0.489168 | 6.713700 | -0.230723 |
| 21 | 6 | 0 | 0.812055 | 4.608831 | 0.170314 |
| 22 | 6 | 0 | 2.015695 | 4.706594 | 0.894706 |
| 23 | 1 | 0 | 2.462107 | 5.680661 | 1.067929 |
| 24 | 6 | 0 | 2.606300 | 3.561784 | 1.380626 |
| 25 | 1 | 0 | 3.529055 | 3.602815 | 1.946695 |
| 26 | 6 | 0 | 2.015715 | 2.313455 | 1.145232 |
| 27 | 1 | 0 | 2.461893 | 1.407032 | 1.525973 |
| 28 | 6 | 0 | 1.246542 | -1.027256 | 2.096917 |
| 29 | 1 | 0 | 0.500657 | -0.662605 | 2.790471 |
| 30 | 6 | 0 | 2.250469 | -1.906018 | 2.514981 |
| 31 | 1 | 0 | 2.268113 | -2.221823 | 3.551119 |
| 32 | 6 | 0 | 3.184436 | -2.361721 | 1.612269 |
| 33 | 1 | 0 | 3.964969 | -3.050890 | 1.916777 |
| 34 | 6 | 0 | 3.126538 | -1.919552 | 0.280435 |
| 35 | 6 | 0 | 2.100398 | -1.025087 | -0.042502 |
| 36 | 6 | 0 | 1.990591 | -0.504110 | -1.350174 |
| 37 | 6 | 0 | 4.032289 | -2.318846 | -0.749928 |
| 38 | 1 | 0 | 4.818094 | -3.022551 | -0.496921 |
| 39 | 6 | 0 | 3.916250 | -1.832097 | -2.014352 |
| 40 | 1 | 0 | 4.608006 | -2.138119 | -2.792273 |
| 41 | 6 | 0 | 2.890695 | -0.894889 | -2.349764 |
| 42 | 6 | 0 | 2.717231 | -0.314255 | -3.617329 |
| 43 | 1 | 0 | 3.384624 | -0.584428 | -4.429423 |
| 44 | 6 | 0 | 1.702905 | 0.599789 | -3.811869 |
| 45 | 1 | 0 | 1.546068 | 1.068886 | -4.775932 |
| 46 | 6 | 0 | 0.851955 | 0.932733 | -2.754050 |
| 47 | 1 | 0 | 0.042663 | 1.638331 | -2.885323 |
| 48 | 6 | 0 | -1.166680 | 1.576216 | 2.603620 |
| 49 | 1 | 0 | -0.486900 | 2.410832 | 2.498824 |
| 50 | 6 | 0 | -1.967699 | 1.433354 | 3.740918 |
| 51 | 1 | 0 | -1.908029 | 2.184226 | 4.519853 |
| 52 | 6 | 0 | -2.809901 | 0.347980 | 3.856666 |
| 53 | 1 | 0 | -3.436346 | 0.221704 | 4.733957 |
| 54 | 6 | 0 | -2.861408 | -0.601176 | 2.821283 |
| 55 | 6 | 0 | -2.026149 | -0.376163 | 1.718956 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 6 | 0 | -2.033240 | -1.261837 | 0.620196 |
| 57 | 6 | 0 | -3.712782 | -1.748425 | 2.807026 |
| 58 | 1 | 0 | -4.359223 | -1.921012 | 3.661288 |
| 59 | 6 | 0 | -3.728120 | -2.594668 | 1.741283 |
| 60 | 1 | 0 | -4.389295 | -3.454857 | 1.727555 |
| 61 | 6 | 0 | -2.888108 | -2.369172 | 0.607317 |
| 62 | 6 | 0 | -2.871764 | -3.168007 | -0.550160 |
| 63 | 1 | 0 | -3.521722 | -4.034432 | -0.615387 |
| 64 | 6 | 0 | -2.037519 | -2.829658 | -1.588694 |
| 65 | 1 | 0 | -2.002976 | -3.416897 | -2.497740 |
| 66 | 6 | 0 | -1.196203 | -1.716420 | -1.476882 |
| 67 | 1 | 0 | -0.530593 | -1.440862 | -2.281655 |
| 68 | 16 | 0 | 0.871833 | -4.375422 | -0.389542 |
| 69 | 8 | 0 | 0.218712 | -3.607672 | 0.670673 |
| 70 | 8 | 0 | 1.062207 | -3.654346 | -1.658032 |
| 71 | 8 | 0 | -0.260398 | -5.526195 | -0.705158 |
| 72 | 1 | 0 | 0.022408 | -6.084827 | -1.442429 |
| 73 | 16 | 0 | -5.404779 | -0.066894 | -0.419318 |
| 74 | 8 | 0 | -6.394021 | 1.093317 | -1.033125 |
| 75 | 1 | 0 | -6.965457 | 0.721783 | -1.720027 |
| 76 | 8 | 0 | -4.588014 | 0.711743 | 0.514754 |
| 77 | 8 | 0 | -6.287808 | -1.056676 | 0.215645 |
| 78 | 8 | 0 | -4.670958 | -0.605071 | -1.577748 |
| 79 | 16 | 0 | 5.252206 | 1.087606 | 0.689791 |
| 80 | 8 | 0 | 6.282485 | -0.114978 | 0.267773 |
| 81 | 1 | 0 | 6.896675 | -0.303642 | 0.991116 |
| 82 | 8 | 0 | 4.400117 | 1.184732 | -0.498318 |
| 83 | 8 | 0 | 6.091058 | 2.273644 | 0.932836 |
| 84 | 8 | 0 | 4.564584 | 0.613808 | 1.903064 |
| 85 | 8 | 0 | 2.075470 | -5.106300 | 0.043061 |

Rotational constants (GHZ): 0.0641025 0.0462994

TC4-3-030, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.245950 | -0.327547 | 0.212859 |
| 2 | 7 | 0 | -1.965576 | -0.984696 | 1.394628 |
| 3 | 7 | 0 | -0.192903 | -2.243384 | -0.171548 |
| 4 | 7 | 0 | 1.532052 | 0.263225 | -0.912439 |
| 5 | 7 | 0 | 1.116432 | -0.549021 | 1.606226 |
| 6 | 7 | 0 | -1.353096 | 0.050710 | -1.344958 |
| 7 | 7 | 0 | -0.612221 | 1.519335 | 0.704390 |
| 8 | 6 | 0 | -2.818632 | -0.316829 | 2.144175 |
| 9 | 1 | 0 | -2.598453 | 0.726497 | 2.331331 |
| 10 | 6 | 0 | -3.957980 | -0.927395 | 2.686174 |
| 11 | 1 | 0 | -4.635816 | -0.340155 | 3.293900 |
| 12 | 6 | 0 | -4.198054 | -2.257005 | 2.428641 |
| 13 | 1 | 0 | -5.075249 | -2.753311 | 2.831878 |
| 14 | 6 | 0 | -3.294662 | -2.987019 | 1.630838 |
| 15 | 6 | 0 | -2.186024 | -2.286687 | 1.130913 |
| 16 | 6 | 0 | -1.230499 | -2.959098 | 0.318175 |
| 17 | 6 | 0 | -3.441610 | -4.373401 | 1.316863 |
| 18 | 1 | 0 | -4.305307 | -4.902443 | 1.707112 |
| 19 | 6 | 0 | -2.518464 | -5.018547 | 0.553442 |
| 20 | 1 | 0 | -2.627690 | -6.073135 | 0.321568 |
| 21 | 6 | 0 | -1.381481 | -4.326273 | 0.032394 |
| 22 | 6 | 0 | -0.393511 | -4.932196 | -0.768129 |
| 23 | 1 | 0 | -0.475986 | -5.987496 | -1.008496 |
| 24 | 6 | 0 | 0.659691 | -4.181296 | -1.239816 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | 1 | 0 | 1.435145 | -4.616917 | -1.858667 |
| 26 | 6 | 0 | 0.726070 | -2.819841 | -0.926402 |
| 27 | 1 | 0 | 1.519012 | -2.189521 | -1.304323 |
| 28 | 6 | 0 | 1.684846 | 0.658337 | -2.161712 |
| 29 | 1 | 0 | 0.816048 | 0.594679 | -2.807213 |
| 30 | 6 | 0 | 2.911418 | 1.135102 | -2.638285 |
| 31 | 1 | 0 | 2.995033 | 1.447033 | -3.672715 |
| 32 | 6 | 0 | 3.987809 | 1.197826 | -1.782539 |
| 33 | 1 | 0 | 4.950942 | 1.562994 | -2.124203 |
| 34 | 6 | 0 | 3.840530 | 0.781891 | -0.447541 |
| 35 | 6 | 0 | 2.572706 | 0.321899 | -0.064039 |
| 36 | 6 | 0 | 2.352223 | -0.119506 | 1.271542 |
| 37 | 6 | 0 | 4.894710 | 0.805188 | 0.515546 |
| 38 | 1 | 0 | 5.867803 | 1.171693 | 0.205542 |
| 39 | 6 | 0 | 4.687769 | 0.371573 | 1.785924 |
| 40 | 1 | 0 | 5.491111 | 0.380843 | 2.515637 |
| 41 | 6 | 0 | 3.407424 | -0.111735 | 2.198395 |
| 42 | 6 | 0 | 3.134657 | -0.590968 | 3.490913 |
| 43 | 1 | 0 | 3.925476 | -0.599983 | 4.234604 |
| 44 | 6 | 0 | 1.871742 | -1.048933 | 3.799220 |
| 45 | 1 | 0 | 1.632080 | -1.431802 | 4.783978 |
| 46 | 6 | 0 | 0.873567 | -1.010188 | 2.823742 |
| 47 | 1 | 0 | -0.136308 | -1.340324 | 3.029173 |
| 48 | 6 | 0 | -1.688234 | -0.738128 | -2.352766 |
| 49 | 1 | 0 | -1.338589 | -1.761056 | -2.324038 |
| 50 | 6 | 0 | -2.460247 | -0.269061 | -3.419258 |
| 51 | 1 | 0 | -2.709665 | -0.949774 | -4.224092 |
| 52 | 6 | 0 | -2.900585 | 1.035727 | -3.422280 |
| 53 | 1 | 0 | -3.511495 | 1.414168 | -4.235332 |
| 54 | 6 | 0 | -2.557426 | 1.887915 | -2.356515 |
| 55 | 6 | 0 | -1.769786 | 1.338413 | -1.338026 |
| 56 | 6 | 0 | -1.379651 | 2.125446 | -0.231739 |
| 57 | 6 | 0 | -2.973116 | 3.249798 | -2.241131 |
| 58 | 1 | 0 | -3.591517 | 3.667048 | -3.028960 |
| 59 | 6 | 0 | -2.611664 | 4.002259 | -1.166375 |
| 60 | 1 | 0 | -2.936154 | 5.033942 | -1.077415 |
| 61 | 6 | 0 | -1.800112 | 3.455049 | -0.124631 |
| 62 | 6 | 0 | -1.400187 | 4.154160 | 1.030080 |
| 63 | 1 | 0 | -1.700391 | 5.188851 | 1.160967 |
| 64 | 6 | 0 | -0.637237 | 3.517009 | 1.981611 |
| 65 | 1 | 0 | -0.315324 | 4.028052 | 2.880395 |
| 66 | 6 | 0 | -0.248279 | 2.188051 | 1.785441 |
| 67 | 1 | 0 | 0.350262 | 1.665055 | 2.517129 |
| 68 | 16 | 0 | 2.518421 | 3.860206 | 0.371501 |
| 69 | 8 | 0 | 1.531466 | 3.415302 | -0.612858 |
| 70 | 8 | 0 | 2.568018 | 3.066748 | 1.609966 |
| 71 | 8 | 0 | 1.904614 | 5.321377 | 0.812937 |
| 72 | 1 | 0 | 2.430348 | 5.705447 | 1.528411 |
| 73 | 16 | 0 | -5.074048 | 0.459640 | -0.471597 |
| 74 | 8 | 0 | -6.314195 | -0.117740 | 0.440447 |
| 75 | 1 | 0 | -6.891047 | 0.607434 | 0.718642 |
| 76 | 8 | 0 | -4.281228 | -0.750670 | -0.691476 |
| 77 | 8 | 0 | -5.694797 | 1.008777 | -1.689623 |
| 78 | 8 | 0 | -4.426450 | 1.489652 | 0.356281 |
| 79 | 16 | 0 | 4.324340 | -2.787634 | -1.155950 |
| 80 | 8 | 0 | 5.733287 | -1.957365 | -1.061951 |
| 81 | 1 | 0 | 6.178675 | -1.949199 | -1.920795 |
| 82 | 8 | 0 | 3.779266 | -2.614207 | 0.193407 |
| 83 | 8 | 0 | 4.692357 | -4.173490 | -1.490144 |
| 84 | 8 | 0 | 3.546457 | -2.127860 | -2.218828 |
| 85 | 8 | 0 | 3.852855 | 4.139450 | -0.186006 |

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Rotational constants (GHZ): 0.0645448 0.0462281

**Structures of TC-3-021**

TC2-3-021a, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.116169 | 0.628804 | 0.016958 |
| 2 | 7 | 0 | -1.333131 | 1.887502 | -0.814006 |
| 3 | 7 | 0 | 0.882555 | 2.220751 | 0.494171 |
| 4 | 7 | 0 | 1.172917 | -0.590010 | 0.828302 |
| 5 | 7 | 0 | 1.000766 | 0.441754 | -1.557807 |
| 6 | 7 | 0 | -1.207959 | 0.662042 | 1.616688 |
| 7 | 7 | 0 | -1.193317 | -0.927307 | -0.446302 |
| 8 | 6 | 0 | -2.450864 | 1.641336 | -1.473636 |
| 9 | 1 | 0 | -2.755234 | 0.611353 | -1.584089 |
| 10 | 6 | 0 | -3.217844 | 2.679552 | -2.017988 |
| 11 | 1 | 0 | -4.130299 | 2.429002 | -2.545246 |
| 12 | 6 | 0 | -2.809784 | 3.986560 | -1.875358 |
| 13 | 1 | 0 | -3.392915 | 4.801640 | -2.292014 |
| 14 | 6 | 0 | -1.616548 | 4.265513 | -1.180825 |
| 15 | 6 | 0 | -0.917342 | 3.165862 | -0.669349 |
| 16 | 6 | 0 | 0.290361 | 3.346574 | 0.036161 |
| 17 | 6 | 0 | -1.074948 | 5.572077 | -0.968231 |
| 18 | 1 | 0 | -1.616691 | 6.424395 | -1.365478 |
| 19 | 6 | 0 | 0.090559 | 5.747038 | -0.284721 |
| 20 | 1 | 0 | 0.494783 | 6.741578 | -0.125944 |
| 21 | 6 | 0 | 0.810634 | 4.629860 | 0.243502 |
| 22 | 6 | 0 | 2.010947 | 4.712432 | 0.975190 |
| 23 | 1 | 0 | 2.459556 | 5.682174 | 1.166048 |
| 24 | 6 | 0 | 2.595641 | 3.558088 | 1.445819 |
| 25 | 1 | 0 | 3.515695 | 3.587329 | 2.016996 |
| 26 | 6 | 0 | 2.002799 | 2.315383 | 1.187773 |
| 27 | 1 | 0 | 2.444861 | 1.401786 | 1.555903 |
| 28 | 6 | 0 | 1.236505 | -1.041595 | 2.069870 |
| 29 | 1 | 0 | 0.494507 | -0.684182 | 2.771048 |
| 30 | 6 | 0 | 2.232796 | -1.937287 | 2.472119 |
| 31 | 1 | 0 | 2.248161 | -2.270535 | 3.502751 |
| 32 | 6 | 0 | 3.164905 | -2.382156 | 1.562461 |
| 33 | 1 | 0 | 3.940478 | -3.082314 | 1.854517 |
| 34 | 6 | 0 | 3.109261 | -1.916999 | 0.237286 |
| 35 | 6 | 0 | 2.090951 | -1.006800 | -0.069173 |
| 36 | 6 | 0 | 1.983248 | -0.464860 | -1.368519 |
| 37 | 6 | 0 | 4.009132 | -2.308778 | -0.801192 |
| 38 | 1 | 0 | 4.790214 | -3.022014 | -0.560646 |
| 39 | 6 | 0 | 3.892211 | -1.803555 | -2.058375 |
| 40 | 1 | 0 | 4.578864 | -2.104580 | -2.842689 |
| 41 | 6 | 0 | 2.875180 | -0.851267 | -2.376621 |
| 42 | 6 | 0 | 2.706890 | -0.247638 | -3.634518 |
| 43 | 1 | 0 | 3.368634 | -0.513740 | -4.452488 |
| 44 | 6 | 0 | 1.706160 | 0.684398 | -3.810699 |
| 45 | 1 | 0 | 1.554046 | 1.172542 | -4.765968 |
| 46 | 6 | 0 | 0.862073 | 1.011242 | -2.745150 |
| 47 | 1 | 0 | 0.061898 | 1.729540 | -2.862868 |
| 48 | 6 | 0 | -1.185846 | 1.525703 | 2.619551 |
| 49 | 1 | 0 | -0.523556 | 2.376102 | 2.531346 |
| 50 | 6 | 0 | -1.973923 | 1.335803 | 3.759075 |
| 51 | 1 | 0 | -1.923124 | 2.066817 | 4.557263 |
| 52 | 6 | 0 | -2.791955 | 0.230122 | 3.852978 |
| 53 | 1 | 0 | -3.407120 | 0.067262 | 4.732172 |
| 54 | 6 | 0 | -2.833635 | -0.691470 | 2.792490 |
| 55 | 6 | 0 | -2.012658 | -0.420237 | 1.690682 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 6 | 0 | -2.014039 | -1.275266 | 0.567250 |
| 57 | 6 | 0 | -3.664826 | -1.853356 | 2.753426 |
| 58 | 1 | 0 | -4.299628 | -2.061257 | 3.608548 |
| 59 | 6 | 0 | -3.676696 | -2.669208 | 1.664373 |
| 60 | 1 | 0 | -4.323848 | -3.539375 | 1.631420 |
| 61 | 6 | 0 | -2.852503 | -2.395500 | 0.529285 |
| 62 | 6 | 0 | -2.837874 | -3.156733 | -0.652133 |
| 63 | 1 | 0 | -3.474280 | -4.031285 | -0.737755 |
| 64 | 6 | 0 | -2.025303 | -2.768749 | -1.693007 |
| 65 | 1 | 0 | -1.999315 | -3.322422 | -2.623640 |
| 66 | 6 | 0 | -1.200767 | -1.646101 | -1.555739 |
| 67 | 1 | 0 | -0.550641 | -1.332839 | -2.360794 |
| 68 | 16 | 0 | 0.741767 | -4.292231 | -0.421217 |
| 69 | 8 | 0 | 0.186376 | -3.486064 | 0.630969 |
| 70 | 8 | 0 | 1.097618 | -3.730711 | -1.698114 |
| 71 | 8 | 0 | -0.295069 | -5.480271 | -0.613705 |
| 72 | 1 | 0 | -0.104393 | -6.037771 | -1.386287 |
| 73 | 16 | 0 | -5.369341 | -0.055907 | -0.398643 |
| 74 | 8 | 0 | -6.355999 | 1.115714 | -0.993334 |
| 75 | 1 | 0 | -6.926301 | 0.757107 | -1.688087 |
| 76 | 8 | 0 | -4.545526 | 0.706403 | 0.542742 |
| 77 | 8 | 0 | -6.252754 | -1.051288 | 0.226825 |
| 78 | 8 | 0 | -4.641344 | -0.581106 | -1.566750 |
| 79 | 16 | 0 | 5.222081 | 1.063859 | 0.689750 |
| 80 | 8 | 0 | 6.253691 | -0.132913 | 0.254450 |
| 81 | 1 | 0 | 6.873116 | -0.323283 | 0.972875 |
| 82 | 8 | 0 | 4.369372 | 1.173077 | -0.496809 |
| 83 | 8 | 0 | 6.059932 | 2.247688 | 0.945897 |
| 84 | 8 | 0 | 4.534835 | 0.575436 | 1.897593 |
| 85 | 8 | 0 | 2.059558 | -5.021944 | 0.085283 |
| 86 | 1 | 0 | 2.015110 | -5.278717 | 1.021888 |

Rotational constants (GHZ): 0.0640016 0.0467689

TC2-3-021b, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.039994 | -0.448039 | 0.242871 |
| 2 | 7 | 0 | 0.620449 | -2.000441 | -0.706104 |
| 3 | 7 | 0 | -1.348975 | -1.688868 | 0.965383 |
| 4 | 7 | 0 | -0.817290 | 1.063703 | 1.181809 |
| 5 | 7 | 0 | -1.296219 | 0.019160 | -1.158045 |
| 6 | 7 | 0 | 1.245916 | -0.794500 | 1.651699 |
| 7 | 7 | 0 | 1.329116 | 0.752541 | -0.440004 |
| 8 | 6 | 0 | 1.637447 | -2.083796 | -1.545886 |
| 9 | 1 | 0 | 2.189636 | -1.177320 | -1.743504 |
| 10 | 6 | 0 | 1.965676 | -3.289918 | -2.174974 |
| 11 | 1 | 0 | 2.809196 | -3.311638 | -2.855063 |
| 12 | 6 | 0 | 1.215141 | -4.419005 | -1.928699 |
| 13 | 1 | 0 | 1.453430 | -5.361580 | -2.411212 |
| 14 | 6 | 0 | 0.122031 | -4.344810 | -1.044931 |
| 15 | 6 | 0 | -0.128562 | -3.097342 | -0.458680 |
| 16 | 6 | 0 | -1.200701 | -2.927004 | 0.444230 |
| 17 | 6 | 0 | -0.739004 | -5.436835 | -0.711400 |
| 18 | 1 | 0 | -0.548672 | -6.401620 | -1.170383 |
| 19 | 6 | 0 | -1.769722 | -5.274156 | 0.164051 |

| | | | | | |
|---|---|---|---|---|---|
| 20 | 1 | 0 | -2.415640 | -6.108326 | 0.418222 |
| 21 | 6 | 0 | -2.025756 | -4.007653 | 0.777506 |
| 22 | 6 | 0 | -3.041630 | -3.759367 | 1.719841 |
| 23 | 1 | 0 | -3.710491 | -4.561204 | 2.015260 |
| 24 | 6 | 0 | -3.165931 | -2.500377 | 2.260007 |
| 25 | 1 | 0 | -3.931359 | -2.275372 | 2.992361 |
| 26 | 6 | 0 | -2.302465 | -1.474998 | 1.854221 |
| 27 | 1 | 0 | -2.388335 | -0.481741 | 2.267682 |
| 28 | 6 | 0 | -0.541313 | 1.531828 | 2.387839 |
| 29 | 1 | 0 | 0.240617 | 1.039672 | 2.949834 |
| 30 | 6 | 0 | -1.246817 | 2.609194 | 2.931079 |
| 31 | 1 | 0 | -0.989769 | 2.953032 | 3.925834 |
| 32 | 6 | 0 | -2.239820 | 3.219476 | 2.197475 |
| 33 | 1 | 0 | -2.791142 | 4.063395 | 2.599035 |
| 34 | 6 | 0 | -2.539635 | 2.740161 | 0.911165 |
| 35 | 6 | 0 | -1.793075 | 1.647170 | 0.455563 |
| 36 | 6 | 0 | -2.043860 | 1.089219 | -0.817662 |
| 37 | 6 | 0 | -3.538859 | 3.289971 | 0.049407 |
| 38 | 1 | 0 | -4.110684 | 4.140959 | 0.404651 |
| 39 | 6 | 0 | -3.763545 | 2.767165 | -1.185861 |
| 40 | 1 | 0 | -4.519537 | 3.191740 | -1.838363 |
| 41 | 6 | 0 | -3.014767 | 1.645206 | -1.658168 |
| 42 | 6 | 0 | -3.176771 | 1.049210 | -2.919591 |
| 43 | 1 | 0 | -3.910581 | 1.447389 | -3.612767 |
| 44 | 6 | 0 | -2.400970 | -0.037210 | -3.258081 |
| 45 | 1 | 0 | -2.501856 | -0.523274 | -4.221058 |
| 46 | 6 | 0 | -1.471486 | -0.540687 | -2.343963 |
| 47 | 1 | 0 | -0.857064 | -1.395661 | -2.589757 |
| 48 | 6 | 0 | 1.160575 | -1.639329 | 2.666733 |
| 49 | 1 | 0 | 0.293284 | -2.284286 | 2.708478 |
| 50 | 6 | 0 | 2.147667 | -1.688731 | 3.656454 |
| 51 | 1 | 0 | 2.035964 | -2.394470 | 4.470957 |
| 52 | 6 | 0 | 3.235314 | -0.844802 | 3.586036 |
| 53 | 1 | 0 | 4.007851 | -0.868229 | 4.348217 |
| 54 | 6 | 0 | 3.347518 | 0.049266 | 2.507092 |
| 55 | 6 | 0 | 2.313583 | 0.027700 | 1.562155 |
| 56 | 6 | 0 | 2.362246 | 0.861552 | 0.423652 |
| 57 | 6 | 0 | 4.440518 | 0.946446 | 2.299509 |
| 58 | 1 | 0 | 5.237698 | 0.967129 | 3.035519 |
| 59 | 6 | 0 | 4.490287 | 1.744697 | 1.198231 |
| 60 | 1 | 0 | 5.330789 | 2.411195 | 1.036190 |
| 61 | 6 | 0 | 3.452843 | 1.712813 | 0.214659 |
| 62 | 6 | 0 | 3.458021 | 2.452584 | -0.982238 |
| 63 | 1 | 0 | 4.286203 | 3.119139 | -1.199412 |
| 64 | 6 | 0 | 2.412878 | 2.311849 | -1.864203 |
| 65 | 1 | 0 | 2.385221 | 2.861547 | -2.796726 |
| 66 | 6 | 0 | 1.346889 | 1.457637 | -1.556690 |
| 67 | 1 | 0 | 0.513822 | 1.340344 | -2.233817 |
| 68 | 16 | 0 | 0.097364 | 4.523066 | -0.344299 |
| 69 | 8 | 0 | 0.776535 | 3.681178 | 0.640672 |
| 70 | 8 | 0 | -0.485245 | 3.803178 | -1.488077 |
| 71 | 8 | 0 | 1.353828 | 5.383637 | -0.965233 |
| 72 | 1 | 0 | 1.049666 | 5.943259 | -1.693431 |
| 73 | 16 | 0 | 5.122061 | -1.157074 | -1.026052 |

| | | | | | |
|---|---|---|---|---|---|
| 74 | 8 | 0 | 6.005121 | -2.410332 | -1.438881 |
| 75 | 1 | 0 | 6.535404 | -2.263936 | -2.240287 |
| 76 | 8 | 0 | 4.349774 | -1.606931 | 0.101027 |
| 77 | 8 | 0 | 6.192432 | -0.076553 | -0.578561 |
| 78 | 8 | 0 | 4.485522 | -0.588894 | -2.186517 |
| 79 | 16 | 0 | -5.021273 | -0.925858 | -0.143164 |
| 80 | 8 | 0 | -5.788509 | -0.119952 | -1.352611 |
| 81 | 1 | 0 | -6.403869 | 0.529711 | -0.985116 |
| 82 | 8 | 0 | -3.960407 | -1.621300 | -0.873662 |
| 83 | 8 | 0 | -6.028530 | -1.822828 | 0.449853 |
| 84 | 8 | 0 | -4.565295 | 0.118755 | 0.787288 |
| 85 | 8 | 0 | -0.821537 | 5.517491 | 0.236255 |
| 86 | 1 | 0 | 6.555450 | -0.236484 | 0.309416 |

Rotational constants (GHZ): 0.0640537 0.0480393

TC4-3-021, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.263013 | -0.350404 | 0.219748 |
| 2 | 7 | 0 | -1.996418 | -0.988419 | 1.387246 |
| 3 | 7 | 0 | -0.238675 | -2.259213 | -0.186948 |
| 4 | 7 | 0 | 1.523894 | 0.242676 | -0.895553 |
| 5 | 7 | 0 | 1.095142 | -0.606100 | 1.610784 |
| 6 | 7 | 0 | -1.353767 | 0.068176 | -1.338902 |
| 7 | 7 | 0 | -0.598159 | 1.498066 | 0.732817 |
| 8 | 6 | 0 | -2.840340 | -0.315295 | 2.142464 |
| 9 | 1 | 0 | -2.603352 | 0.721472 | 2.344120 |
| 10 | 6 | 0 | -3.991990 | -0.913046 | 2.672425 |
| 11 | 1 | 0 | -4.661719 | -0.322023 | 3.285438 |
| 12 | 6 | 0 | -4.254166 | -2.234837 | 2.396794 |
| 13 | 1 | 0 | -5.141365 | -2.720907 | 2.790473 |
| 14 | 6 | 0 | -3.360337 | -2.970512 | 1.593430 |
| 15 | 6 | 0 | -2.237857 | -2.283334 | 1.106661 |
| 16 | 6 | 0 | -1.290410 | -2.962575 | 0.290292 |
| 17 | 6 | 0 | -3.529502 | -4.350343 | 1.262124 |
| 18 | 1 | 0 | -4.403829 | -4.869132 | 1.642298 |
| 19 | 6 | 0 | -2.613912 | -5.002295 | 0.495328 |
| 20 | 1 | 0 | -2.739979 | -6.052083 | 0.250685 |
| 21 | 6 | 0 | -1.462854 | -4.323499 | -0.012363 |
| 22 | 6 | 0 | -0.481024 | -4.936388 | -0.815157 |
| 23 | 1 | 0 | -0.579796 | -5.987353 | -1.068008 |
| 24 | 6 | 0 | 0.587091 | -4.197996 | -1.273168 |
| 25 | 1 | 0 | 1.358325 | -4.639523 | -1.893108 |
| 26 | 6 | 0 | 0.674674 | -2.841505 | -0.944091 |
| 27 | 1 | 0 | 1.479415 | -2.219795 | -1.311692 |
| 28 | 6 | 0 | 1.683537 | 0.657881 | -2.137044 |
| 29 | 1 | 0 | 0.816394 | 0.613537 | -2.786277 |
| 30 | 6 | 0 | 2.915537 | 1.133485 | -2.602819 |
| 31 | 1 | 0 | 3.003937 | 1.462223 | -3.631567 |
| 32 | 6 | 0 | 3.990777 | 1.169959 | -1.744724 |
| 33 | 1 | 0 | 4.958171 | 1.532113 | -2.077617 |
| 34 | 6 | 0 | 3.836077 | 0.734426 | -0.415731 |
| 35 | 6 | 0 | 2.563209 | 0.277725 | -0.042929 |
| 36 | 6 | 0 | 2.334449 | -0.177429 | 1.286747 |
| 37 | 6 | 0 | 4.886940 | 0.738500 | 0.551292 |
| 38 | 1 | 0 | 5.864359 | 1.099440 | 0.248617 |
| 39 | 6 | 0 | 4.670749 | 0.294391 | 1.816577 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 1 | 0 | 5.470964 | 0.289886 | 2.549689 |
| 41 | 6 | 0 | 3.385173 | -0.183798 | 2.218356 |
| 42 | 6 | 0 | 3.104920 | -0.677488 | 3.504316 |
| 43 | 1 | 0 | 3.892505 | -0.698150 | 4.251130 |
| 44 | 6 | 0 | 1.839924 | -1.136443 | 3.800562 |
| 45 | 1 | 0 | 1.594660 | -1.531827 | 4.778932 |
| 46 | 6 | 0 | 0.846049 | -1.082548 | 2.820935 |
| 47 | 1 | 0 | -0.165659 | -1.412422 | 3.017961 |
| 48 | 6 | 0 | -1.701517 | -0.702657 | -2.356196 |
| 49 | 1 | 0 | -1.378595 | -1.734624 | -2.334308 |
| 50 | 6 | 0 | -2.453414 | -0.203502 | -3.423690 |
| 51 | 1 | 0 | -2.714601 | -0.870082 | -4.236567 |
| 52 | 6 | 0 | -2.859908 | 1.112109 | -3.417798 |
| 53 | 1 | 0 | -3.454875 | 1.513747 | -4.231473 |
| 54 | 6 | 0 | -2.503170 | 1.945021 | -2.341046 |
| 55 | 6 | 0 | -1.738404 | 1.365622 | -1.322488 |
| 56 | 6 | 0 | -1.340378 | 2.131846 | -0.203666 |
| 57 | 6 | 0 | -2.886733 | 3.315773 | -2.214995 |
| 58 | 1 | 0 | -3.487629 | 3.755659 | -3.004010 |
| 59 | 6 | 0 | -2.518145 | 4.048696 | -1.129541 |
| 60 | 1 | 0 | -2.819059 | 5.086680 | -1.032410 |
| 61 | 6 | 0 | -1.731031 | 3.470616 | -0.085655 |
| 62 | 6 | 0 | -1.328469 | 4.146585 | 1.080617 |
| 63 | 1 | 0 | -1.604755 | 5.186716 | 1.220333 |
| 64 | 6 | 0 | -0.595284 | 3.478549 | 2.037221 |
| 65 | 1 | 0 | -0.277274 | 3.970693 | 2.948272 |
| 66 | 6 | 0 | -0.237892 | 2.142741 | 1.830746 |
| 67 | 1 | 0 | 0.340425 | 1.596733 | 2.563109 |
| 68 | 16 | 0 | 2.455068 | 3.787541 | 0.420695 |
| 69 | 8 | 0 | 1.538929 | 3.302128 | -0.575104 |
| 70 | 8 | 0 | 2.676728 | 3.078157 | 1.653739 |
| 71 | 8 | 0 | 1.979484 | 5.273358 | 0.723364 |
| 72 | 1 | 0 | 2.445303 | 5.681048 | 1.472906 |
| 73 | 16 | 0 | -5.052719 | 0.537262 | -0.480242 |
| 74 | 8 | 0 | -6.308610 | -0.020050 | 0.422105 |
| 75 | 1 | 0 | -6.865610 | 0.715912 | 0.712155 |
| 76 | 8 | 0 | -4.288573 | -0.689148 | -0.711473 |
| 77 | 8 | 0 | -5.655844 | 1.114962 | -1.693909 |
| 78 | 8 | 0 | -4.382504 | 1.542109 | 0.360702 |
| 79 | 16 | 0 | 4.281404 | -2.813922 | -1.167619 |
| 80 | 8 | 0 | 5.695531 | -1.992459 | -1.071787 |
| 81 | 1 | 0 | 6.138870 | -1.981700 | -1.931675 |
| 82 | 8 | 0 | 3.743682 | -2.651808 | 0.186077 |
| 83 | 8 | 0 | 4.640136 | -4.197915 | -1.518560 |
| 84 | 8 | 0 | 3.502102 | -2.137872 | -2.219250 |
| 85 | 8 | 0 | 3.902654 | 3.977340 | -0.204816 |
| 86 | 1 | 0 | 3.885019 | 4.262842 | -1.133742 |

Rotational constants (GHZ): 0.0646088 0.0463579

**Structures of TC-3-012**

TC2-3-012a, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.004733 | -0.471943 | 0.263003 |
| 2 | 7 | 0 | 0.619679 | -2.058359 | -0.649400 |
| 3 | 7 | 0 | -1.345963 | -1.661012 | 1.003556 |
| 4 | 7 | 0 | -0.744119 | 1.078958 | 1.170672 |
| 5 | 7 | 0 | -1.240439 | -0.005260 | -1.153204 |
| 6 | 7 | 0 | 1.281771 | -0.808284 | 1.677555 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 7 | 0 | 1.396417 | 0.692323 | -0.442640 |
| 8 | 6 | 0 | 1.649271 | -2.187337 | -1.467357 |
| 9 | 1 | 0 | 2.258527 | -1.314473 | -1.650735 |
| 10 | 6 | 0 | 1.935927 | -3.411875 | -2.083636 |
| 11 | 1 | 0 | 2.794740 | -3.473510 | -2.741260 |
| 12 | 6 | 0 | 1.132780 | -4.505789 | -1.849453 |
| 13 | 1 | 0 | 1.339928 | -5.460296 | -2.322908 |
| 14 | 6 | 0 | 0.028394 | -4.381361 | -0.984224 |
| 15 | 6 | 0 | -0.177572 | -3.122754 | -0.407331 |
| 16 | 6 | 0 | -1.248907 | -2.905185 | 0.485554 |
| 17 | 6 | 0 | -0.881660 | -5.435095 | -0.656855 |
| 18 | 1 | 0 | -0.726284 | -6.408956 | -1.109858 |
| 19 | 6 | 0 | -1.913746 | -5.227673 | 0.207630 |
| 20 | 1 | 0 | -2.595684 | -6.033605 | 0.458394 |
| 21 | 6 | 0 | -2.121014 | -3.950208 | 0.816276 |
| 22 | 6 | 0 | -3.130702 | -3.656935 | 1.751268 |
| 23 | 1 | 0 | -3.836317 | -4.427885 | 2.043259 |
| 24 | 6 | 0 | -3.200068 | -2.393378 | 2.293983 |
| 25 | 1 | 0 | -3.956022 | -2.136199 | 3.025873 |
| 26 | 6 | 0 | -2.289143 | -1.408062 | 1.894467 |
| 27 | 1 | 0 | -2.333191 | -0.411512 | 2.308600 |
| 28 | 6 | 0 | -0.465618 | 1.564573 | 2.368940 |
| 29 | 1 | 0 | 0.304090 | 1.068036 | 2.943932 |
| 30 | 6 | 0 | -1.151610 | 2.667769 | 2.887812 |
| 31 | 1 | 0 | -0.891760 | 3.025822 | 3.876705 |
| 32 | 6 | 0 | -2.130701 | 3.281447 | 2.139314 |
| 33 | 1 | 0 | -2.667299 | 4.143680 | 2.521467 |
| 34 | 6 | 0 | -2.434321 | 2.783164 | 0.859567 |
| 35 | 6 | 0 | -1.707131 | 1.666423 | 0.428518 |
| 36 | 6 | 0 | -1.959188 | 1.093825 | -0.838530 |
| 37 | 6 | 0 | -3.416484 | 3.339368 | -0.017473 |
| 38 | 1 | 0 | -3.974032 | 4.206633 | 0.320340 |
| 39 | 6 | 0 | -3.641937 | 2.802661 | -1.246914 |
| 40 | 1 | 0 | -4.383842 | 3.231913 | -1.912169 |
| 41 | 6 | 0 | -2.913091 | 1.657609 | -1.695019 |
| 42 | 6 | 0 | -3.088222 | 1.037446 | -2.944937 |
| 43 | 1 | 0 | -3.810234 | 1.439324 | -3.648127 |
| 44 | 6 | 0 | -2.342920 | -0.077595 | -3.255076 |
| 45 | 1 | 0 | -2.454858 | -0.582843 | -4.206781 |
| 46 | 6 | 0 | -1.427456 | -0.584955 | -2.327287 |
| 47 | 1 | 0 | -0.834039 | -1.459694 | -2.554823 |
| 48 | 6 | 0 | 1.181539 | -1.633260 | 2.707980 |
| 49 | 1 | 0 | 0.309175 | -2.271157 | 2.754066 |
| 50 | 6 | 0 | 2.159061 | -1.668490 | 3.707223 |
| 51 | 1 | 0 | 2.036141 | -2.357636 | 4.534193 |
| 52 | 6 | 0 | 3.251691 | -0.830967 | 3.631194 |
| 53 | 1 | 0 | 4.016033 | -0.843043 | 4.401848 |
| 54 | 6 | 0 | 3.380298 | 0.039860 | 2.535366 |
| 55 | 6 | 0 | 2.357124 | 0.002918 | 1.580208 |
| 56 | 6 | 0 | 2.421249 | 0.814973 | 0.427150 |
| 57 | 6 | 0 | 4.478935 | 0.928709 | 2.321562 |
| 58 | 1 | 0 | 5.270173 | 0.956870 | 3.063693 |
| 59 | 6 | 0 | 4.543379 | 1.707071 | 1.207315 |
| 60 | 1 | 0 | 5.388084 | 2.367424 | 1.041816 |
| 61 | 6 | 0 | 3.512658 | 1.665807 | 0.217471 |
| 62 | 6 | 0 | 3.521384 | 2.398715 | -0.981832 |
| 63 | 1 | 0 | 4.346493 | 3.069419 | -1.197705 |
| 64 | 6 | 0 | 2.486762 | 2.239617 | -1.875699 |
| 65 | 1 | 0 | 2.468034 | 2.776232 | -2.816459 |
| 66 | 6 | 0 | 1.426825 | 1.377678 | -1.572953 |
| 67 | 1 | 0 | 0.602359 | 1.246613 | -2.259371 |
| 68 | 16 | 0 | 0.296361 | 4.437545 | -0.417856 |
| 69 | 8 | 0 | 0.862962 | 3.623377 | 0.622533 |

| | | | | | |
|---|---|---|---|---|---|
| 70 | 8 | 0 | -0.419321 | 3.857011 | -1.523629 |
| 71 | 8 | 0 | 1.502480 | 5.325208 | -0.947359 |
| 72 | 1 | 0 | 1.274739 | 5.853611 | -1.731000 |
| 73 | 16 | 0 | 5.082096 | -1.219240 | -1.042499 |
| 74 | 8 | 0 | 5.650623 | -2.616266 | -1.692649 |
| 75 | 1 | 0 | 6.142531 | -2.434788 | -2.505969 |
| 76 | 8 | 0 | 4.312058 | -1.720781 | 0.098353 |
| 77 | 8 | 0 | 6.266199 | -0.424832 | -0.684378 |
| 78 | 8 | 0 | 4.269730 | -0.597826 | -2.103330 |
| 79 | 16 | 0 | -4.909157 | -0.727115 | -0.199646 |
| 80 | 8 | 0 | -5.723991 | -0.054578 | -1.385590 |
| 81 | 1 | 0 | -6.331752 | 0.642344 | -1.085602 |
| 82 | 8 | 0 | -3.903526 | -1.526410 | -0.846076 |
| 83 | 8 | 0 | -5.979231 | -1.659578 | 0.512941 |
| 84 | 8 | 0 | -4.567357 | 0.262013 | 0.788400 |
| 85 | 8 | 0 | -0.708474 | 5.502663 | 0.199620 |
| 86 | 1 | 0 | -0.397809 | 5.883353 | 1.038535 |
| 87 | 1 | 0 | -6.213183 | -2.445046 | -0.009833 |

Rotational constants (GHZ): 0.0637279 0.0487204

TC2-3-012b, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.025419 | -0.446803 | 0.247767 |
| 2 | 7 | 0 | 0.622338 | -2.004774 | -0.699565 |
| 3 | 7 | 0 | -1.342684 | -1.679223 | 0.974408 |
| 4 | 7 | 0 | -0.794729 | 1.071388 | 1.184294 |
| 5 | 7 | 0 | -1.286766 | 0.020613 | -1.152069 |
| 6 | 7 | 0 | 1.260843 | -0.793393 | 1.654033 |
| 7 | 7 | 0 | 1.346078 | 0.744656 | -0.442778 |
| 8 | 6 | 0 | 1.639434 | -2.096423 | -1.538511 |
| 9 | 1 | 0 | 2.201583 | -1.195436 | -1.732861 |
| 10 | 6 | 0 | 1.955175 | -3.304283 | -2.170623 |
| 11 | 1 | 0 | 2.799629 | -3.333077 | -2.849257 |
| 12 | 6 | 0 | 1.191722 | -4.425694 | -1.929321 |
| 13 | 1 | 0 | 1.420300 | -5.369267 | -2.414510 |
| 14 | 6 | 0 | 0.098123 | -4.342069 | -1.046902 |
| 15 | 6 | 0 | -0.138671 | -3.094342 | -0.456510 |
| 16 | 6 | 0 | -1.209320 | -2.915855 | 0.447063 |
| 17 | 6 | 0 | -0.775797 | -5.425803 | -0.718698 |
| 18 | 1 | 0 | -0.595409 | -6.390750 | -1.181295 |
| 19 | 6 | 0 | -1.805613 | -5.255734 | 0.156139 |
| 20 | 1 | 0 | -2.460821 | -6.083667 | 0.406577 |
| 21 | 6 | 0 | -2.047060 | -3.989119 | 0.775448 |
| 22 | 6 | 0 | -3.059749 | -3.733732 | 1.718474 |
| 23 | 1 | 0 | -3.739090 | -4.528433 | 2.009151 |
| 24 | 6 | 0 | -3.165843 | -2.476491 | 2.269856 |
| 25 | 1 | 0 | -3.925096 | -2.248005 | 3.007828 |
| 26 | 6 | 0 | -2.287964 | -1.460849 | 1.872158 |
| 27 | 1 | 0 | -2.358986 | -0.468909 | 2.293576 |
| 28 | 6 | 0 | -0.515353 | 1.541041 | 2.388628 |
| 29 | 1 | 0 | 0.265901 | 1.047622 | 2.950393 |
| 30 | 6 | 0 | -1.217027 | 2.621598 | 2.931648 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 1 | 0 | -0.956723 | 2.966081 | 3.925287 |
| 32 | 6 | 0 | -2.209512 | 3.233475 | 2.199582 |
| 33 | 1 | 0 | -2.757579 | 4.079735 | 2.600473 |
| 34 | 6 | 0 | -2.512586 | 2.753171 | 0.913875 |
| 35 | 6 | 0 | -1.769817 | 1.657694 | 0.458699 |
| 36 | 6 | 0 | -2.023415 | 1.100358 | -0.814265 |
| 37 | 6 | 0 | -3.509816 | 3.307126 | 0.052748 |
| 38 | 1 | 0 | -4.076897 | 4.161263 | 0.407817 |
| 39 | 6 | 0 | -3.739070 | 2.784682 | -1.181957 |
| 40 | 1 | 0 | -4.493800 | 3.211788 | -1.834109 |
| 41 | 6 | 0 | -2.996520 | 1.657845 | -1.653192 |
| 42 | 6 | 0 | -3.172540 | 1.052379 | -2.909507 |
| 43 | 1 | 0 | -3.909246 | 1.450075 | -3.599777 |
| 44 | 6 | 0 | -2.408592 | -0.043528 | -3.243747 |
| 45 | 1 | 0 | -2.520884 | -0.537157 | -4.201525 |
| 46 | 6 | 0 | -1.474177 | -0.545733 | -2.333075 |
| 47 | 1 | 0 | -0.867791 | -1.406546 | -2.578177 |
| 48 | 6 | 0 | 1.174915 | -1.635956 | 2.671091 |
| 49 | 1 | 0 | 0.306722 | -2.279536 | 2.715266 |
| 50 | 6 | 0 | 2.162927 | -1.684717 | 3.659781 |
| 51 | 1 | 0 | 2.050752 | -2.388305 | 4.476060 |
| 52 | 6 | 0 | 3.252187 | -0.843046 | 3.586235 |
| 53 | 1 | 0 | 4.025337 | -0.866162 | 4.347791 |
| 54 | 6 | 0 | 3.365444 | 0.047768 | 2.504748 |
| 55 | 6 | 0 | 2.330486 | 0.025969 | 1.561074 |
| 56 | 6 | 0 | 2.380096 | 0.855333 | 0.419717 |
| 57 | 6 | 0 | 4.460386 | 0.941561 | 2.292949 |
| 58 | 1 | 0 | 5.258438 | 0.962768 | 3.027972 |
| 59 | 6 | 0 | 4.510880 | 1.735980 | 1.188895 |
| 60 | 1 | 0 | 5.352936 | 2.399667 | 1.023539 |
| 61 | 6 | 0 | 3.472562 | 1.702905 | 0.206274 |
| 62 | 6 | 0 | 3.478585 | 2.437265 | -0.993919 |
| 63 | 1 | 0 | 4.308073 | 3.100984 | -1.214701 |
| 64 | 6 | 0 | 2.432831 | 2.294424 | -1.874877 |
| 65 | 1 | 0 | 2.406109 | 2.839547 | -2.810094 |
| 66 | 6 | 0 | 1.365081 | 1.444065 | -1.563101 |
| 67 | 1 | 0 | 0.532110 | 1.325391 | -2.240056 |
| 68 | 16 | 0 | 0.121735 | 4.510516 | -0.357108 |
| 69 | 8 | 0 | 0.795398 | 3.667262 | 0.630472 |
| 70 | 8 | 0 | -0.463955 | 3.790078 | -1.499078 |
| 71 | 8 | 0 | 1.382725 | 5.362926 | -0.978995 |
| 72 | 1 | 0 | 1.082227 | 5.923103 | -1.708299 |
| 73 | 16 | 0 | 5.131373 | -1.179780 | -1.023516 |
| 74 | 8 | 0 | 6.012596 | -2.435980 | -1.430880 |
| 75 | 1 | 0 | 6.544714 | -2.293205 | -2.231744 |
| 76 | 8 | 0 | 4.357662 | -1.623831 | 0.104961 |
| 77 | 8 | 0 | 6.203042 | -0.099063 | -0.580125 |
| 78 | 8 | 0 | 4.495617 | -0.615338 | -2.186295 |
| 79 | 16 | 0 | -4.935234 | -0.800343 | -0.189971 |
| 80 | 8 | 0 | -5.764571 | -0.128403 | -1.366063 |
| 81 | 1 | 0 | -6.374414 | 0.563359 | -1.058452 |
| 82 | 8 | 0 | -3.925150 | -1.584334 | -0.848295 |
| 83 | 8 | 0 | -5.990980 | -1.749416 | 0.522551 |
| 84 | 8 | 0 | -4.598532 | 0.184437 | 0.803982 |

| | | | | | |
|---|---|---|---|---|---|
| 85 | 8 | 0 | -0.793056 | 5.510576 | 0.220250 |
| 86 | 1 | 0 | -6.225725 | -2.529985 | -0.007011 |
| 87 | 1 | 0 | 6.566254 | -0.256131 | 0.308316 |

Rotational constants (GHZ): 0.0641915 0.0479529

TC4-3-012, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.181597 | -0.218828 | 0.054937 |
| 2 | 7 | 0 | 1.521389 | -1.394785 | -1.190628 |
| 3 | 7 | 0 | -0.160806 | -1.995167 | 0.816261 |
| 4 | 7 | 0 | -1.304518 | 0.828450 | 1.261863 |
| 5 | 7 | 0 | -1.383056 | -0.404737 | -1.121495 |
| 6 | 7 | 0 | 1.564172 | 0.185671 | 1.362900 |
| 7 | 7 | 0 | 0.743611 | 1.440059 | -0.794634 |
| 8 | 6 | 0 | 2.348910 | -1.041445 | -2.153191 |
| 9 | 1 | 0 | 2.333795 | -0.004075 | -2.459301 |
| 10 | 6 | 0 | 3.206881 | -1.968086 | -2.760824 |
| 11 | 1 | 0 | 3.877213 | -1.636349 | -3.544523 |
| 12 | 6 | 0 | 3.179801 | -3.280934 | -2.350083 |
| 13 | 1 | 0 | 3.831983 | -4.020044 | -2.804775 |
| 14 | 6 | 0 | 2.292042 | -3.676212 | -1.329164 |
| 15 | 6 | 0 | 1.482315 | -2.673796 | -0.772493 |
| 16 | 6 | 0 | 0.567628 | -2.995510 | 0.271199 |
| 17 | 6 | 0 | 2.169871 | -5.017004 | -0.849856 |
| 18 | 1 | 0 | 2.799863 | -5.782814 | -1.291149 |
| 19 | 6 | 0 | 1.282347 | -5.327759 | 0.132851 |
| 20 | 1 | 0 | 1.186993 | -6.346482 | 0.494558 |
| 21 | 6 | 0 | 0.458803 | -4.321012 | 0.725975 |
| 22 | 6 | 0 | -0.452265 | -4.574767 | 1.768088 |
| 23 | 1 | 0 | -0.565757 | -5.587490 | 2.141625 |
| 24 | 6 | 0 | -1.177322 | -3.537248 | 2.308352 |
| 25 | 1 | 0 | -1.879165 | -3.695224 | 3.118073 |
| 26 | 6 | 0 | -1.000006 | -2.244434 | 1.807201 |
| 27 | 1 | 0 | -1.539115 | -1.402826 | 2.217688 |
| 28 | 6 | 0 | -1.210096 | 1.426452 | 2.433341 |
| 29 | 1 | 0 | -0.256582 | 1.358571 | 2.944492 |
| 30 | 6 | 0 | -2.291603 | 2.114587 | 2.997302 |
| 31 | 1 | 0 | -2.173596 | 2.592890 | 3.962467 |
| 32 | 6 | 0 | -3.483883 | 2.171108 | 2.311149 |
| 33 | 1 | 0 | -4.339235 | 2.697828 | 2.722257 |
| 34 | 6 | 0 | -3.598520 | 1.540029 | 1.057675 |
| 35 | 6 | 0 | -2.458562 | 0.879266 | 0.573900 |
| 36 | 6 | 0 | -2.499272 | 0.222669 | -0.689500 |
| 37 | 6 | 0 | -4.791024 | 1.539550 | 0.271891 |
| 38 | 1 | 0 | -5.664245 | 2.054629 | 0.658937 |
| 39 | 6 | 0 | -4.831395 | 0.907667 | -0.930620 |
| 40 | 1 | 0 | -5.737958 | 0.903207 | -1.526911 |
| 41 | 6 | 0 | -3.682227 | 0.232235 | -1.446275 |
| 42 | 6 | 0 | -3.667043 | -0.441411 | -2.681032 |
| 43 | 1 | 0 | -4.563321 | -0.453803 | -3.292634 |
| 44 | 6 | 0 | -2.520814 | -1.080662 | -3.093245 |
| 45 | 1 | 0 | -2.476227 | -1.615982 | -4.033824 |
| 46 | 6 | 0 | -1.386431 | -1.046127 | -2.278308 |
| 47 | 1 | 0 | -0.467580 | -1.535284 | -2.572446 |
| 48 | 6 | 0 | 1.937633 | -0.496950 | 2.432915 |
| 49 | 1 | 0 | 1.440772 | -1.439072 | 2.621402 |
| 50 | 6 | 0 | 2.933650 | -0.019631 | 3.289526 |
| 51 | 1 | 0 | 3.208037 | -0.611639 | 4.154229 |

| | | | | | |
|---|---|---|---|---|---|
| 52 | 6 | 0 | 3.555927 | 1.177789 | 3.014931 |
| 53 | 1 | 0 | 4.339971 | 1.558519 | 3.661267 |
| 54 | 6 | 0 | 3.173111 | 1.915431 | 1.879125 |
| 55 | 6 | 0 | 2.161051 | 1.367567 | 1.083362 |
| 56 | 6 | 0 | 1.720682 | 2.041609 | -0.077957 |
| 57 | 6 | 0 | 3.757203 | 3.158732 | 1.484517 |
| 58 | 1 | 0 | 4.549321 | 3.572265 | 2.099822 |
| 59 | 6 | 0 | 3.337150 | 3.805159 | 0.363456 |
| 60 | 1 | 0 | 3.786549 | 4.746274 | 0.063897 |
| 61 | 6 | 0 | 2.299748 | 3.258926 | -0.454458 |
| 62 | 6 | 0 | 1.822358 | 3.846900 | -1.639970 |
| 63 | 1 | 0 | 2.236972 | 4.792496 | -1.974049 |
| 64 | 6 | 0 | 0.839867 | 3.211784 | -2.368525 |
| 65 | 1 | 0 | 0.456472 | 3.637102 | -3.287903 |
| 66 | 6 | 0 | 0.314163 | 1.998660 | -1.914963 |
| 67 | 1 | 0 | -0.458664 | 1.480995 | -2.465364 |
| 68 | 16 | 0 | -1.901696 | 4.202341 | -0.448314 |
| 69 | 8 | 0 | -0.930958 | 3.709173 | 0.490242 |
| 70 | 8 | 0 | -2.415287 | 3.372558 | -1.506692 |
| 71 | 8 | 0 | -1.249095 | 5.522515 | -1.044177 |
| 72 | 1 | 0 | -1.765498 | 5.919786 | -1.764887 |
| 73 | 16 | 0 | 5.080626 | -0.163066 | -0.113251 |
| 74 | 8 | 0 | 6.013256 | -1.101009 | -1.089275 |
| 75 | 1 | 0 | 6.624925 | -0.553621 | -1.600776 |
| 76 | 8 | 0 | 4.182759 | -1.159011 | 0.473799 |
| 77 | 8 | 0 | 6.004327 | 0.462879 | 0.848328 |
| 78 | 8 | 0 | 4.434101 | 0.812003 | -1.005764 |
| 79 | 16 | 0 | -3.997086 | -2.809732 | 0.243061 |
| 80 | 8 | 0 | -5.206787 | -2.643264 | -0.772219 |
| 81 | 1 | 0 | -6.006552 | -2.278858 | -0.356644 |
| 82 | 8 | 0 | -2.849686 | -3.071401 | -0.583776 |
| 83 | 8 | 0 | -4.375501 | -4.106448 | 1.079344 |
| 84 | 8 | 0 | -4.009831 | -1.737643 | 1.203270 |
| 85 | 8 | 0 | -3.192560 | 4.731957 | 0.310605 |
| 86 | 1 | 0 | -2.988322 | 5.206703 | 1.134171 |
| 87 | 1 | 0 | -4.269582 | -4.934570 | 0.580913 |

Rotational constants (GHZ): 0.0619418 0.0504199

**Structures of TC-3-003**

TC2-3-003, ferriin doublet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.030988 | -0.466721 | 0.243640 |
| 2 | 7 | 0 | 0.609230 | -2.033472 | -0.691625 |
| 3 | 7 | 0 | -1.350640 | -1.686624 | 0.982008 |
| 4 | 7 | 0 | -0.791385 | 1.065570 | 1.170001 |
| 5 | 7 | 0 | -1.292800 | -0.004401 | -1.158036 |
| 6 | 7 | 0 | 1.256917 | -0.799960 | 1.650339 |
| 7 | 7 | 0 | 1.343335 | 0.717134 | -0.461755 |
| 8 | 6 | 0 | 1.625943 | -2.136254 | -1.530030 |
| 9 | 1 | 0 | 2.193502 | -1.240264 | -1.731072 |
| 10 | 6 | 0 | 1.935503 | -3.350159 | -2.153226 |
| 11 | 1 | 0 | 2.780138 | -3.387816 | -2.831185 |
| 12 | 6 | 0 | 1.166155 | -4.465960 | -1.904343 |
| 13 | 1 | 0 | 1.390065 | -5.413950 | -2.383027 |
| 14 | 6 | 0 | 0.072991 | -4.370589 | -1.022656 |
| 15 | 6 | 0 | -0.156856 | -3.117762 | -0.440591 |
| 16 | 6 | 0 | -1.225650 | -2.927406 | 0.462263 |
| 17 | 6 | 0 | -0.807162 | -5.447061 | -0.687179 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | 1 | 0 | -0.632361 | -6.416105 | -1.143292 |
| 19 | 6 | 0 | -1.836154 | -5.265207 | 0.186301 |
| 20 | 1 | 0 | -2.496318 | -6.087555 | 0.441952 |
| 21 | 6 | 0 | -2.070071 | -3.993204 | 0.797442 |
| 22 | 6 | 0 | -3.081248 | -3.725107 | 1.738499 |
| 23 | 1 | 0 | -3.765931 | -4.513370 | 2.034068 |
| 24 | 6 | 0 | -3.178978 | -2.463755 | 2.282156 |
| 25 | 1 | 0 | -3.936738 | -2.225684 | 3.018612 |
| 26 | 6 | 0 | -2.294356 | -1.456484 | 1.878615 |
| 27 | 1 | 0 | -2.359174 | -0.461675 | 2.294024 |
| 28 | 6 | 0 | -0.508074 | 1.545374 | 2.369571 |
| 29 | 1 | 0 | 0.266682 | 1.049565 | 2.938079 |
| 30 | 6 | 0 | -1.195529 | 2.642639 | 2.898742 |
| 31 | 1 | 0 | -0.931042 | 2.995991 | 3.888091 |
| 32 | 6 | 0 | -2.181990 | 3.256277 | 2.160020 |
| 33 | 1 | 0 | -2.720036 | 4.113865 | 2.550429 |
| 34 | 6 | 0 | -2.491641 | 2.763524 | 0.879603 |
| 35 | 6 | 0 | -1.761479 | 1.653263 | 0.437273 |
| 36 | 6 | 0 | -2.017460 | 1.087649 | -0.831771 |
| 37 | 6 | 0 | -3.482859 | 3.319032 | 0.012472 |
| 38 | 1 | 0 | -4.042876 | 4.181230 | 0.359042 |
| 39 | 6 | 0 | -3.714553 | 2.787215 | -1.217935 |
| 40 | 1 | 0 | -4.464342 | 3.215173 | -1.875114 |
| 41 | 6 | 0 | -2.982072 | 1.649105 | -1.677595 |
| 42 | 6 | 0 | -3.164317 | 1.033104 | -2.928501 |
| 43 | 1 | 0 | -3.895156 | 1.433141 | -3.623553 |
| 44 | 6 | 0 | -2.415256 | -0.076350 | -3.249468 |
| 45 | 1 | 0 | -2.533514 | -0.579362 | -4.201587 |
| 46 | 6 | 0 | -1.487795 | -0.581143 | -2.332434 |
| 47 | 1 | 0 | -0.893126 | -1.452616 | -2.568402 |
| 48 | 6 | 0 | 1.172052 | -1.633671 | 2.674781 |
| 49 | 1 | 0 | 0.306041 | -2.279902 | 2.723081 |
| 50 | 6 | 0 | 2.158526 | -1.669268 | 3.665653 |
| 51 | 1 | 0 | 2.047611 | -2.365840 | 4.488061 |
| 52 | 6 | 0 | 3.244753 | -0.824353 | 3.586412 |
| 53 | 1 | 0 | 4.016741 | -0.837871 | 4.349331 |
| 54 | 6 | 0 | 3.356898 | 0.056381 | 2.496445 |
| 55 | 6 | 0 | 2.323700 | 0.022397 | 1.552064 |
| 56 | 6 | 0 | 2.374363 | 0.839735 | 0.401535 |
| 57 | 6 | 0 | 4.451101 | 0.949738 | 2.276909 |
| 58 | 1 | 0 | 5.247834 | 0.979286 | 3.013031 |
| 59 | 6 | 0 | 4.503764 | 1.731966 | 1.164551 |
| 60 | 1 | 0 | 5.345865 | 2.393812 | 0.992797 |
| 61 | 6 | 0 | 3.467467 | 1.685907 | 0.180146 |
| 62 | 6 | 0 | 3.477049 | 2.403683 | -1.028995 |
| 63 | 1 | 0 | 4.306324 | 3.065340 | -1.256345 |
| 64 | 6 | 0 | 2.436129 | 2.243509 | -1.915482 |
| 65 | 1 | 0 | 2.416191 | 2.770804 | -2.861436 |
| 66 | 6 | 0 | 1.369222 | 1.395465 | -1.596298 |
| 67 | 1 | 0 | 0.538370 | 1.266188 | -2.275354 |
| 68 | 16 | 0 | 0.238651 | 4.427316 | -0.401722 |
| 69 | 8 | 0 | 0.820531 | 3.603374 | 0.622624 |
| 70 | 8 | 0 | -0.486752 | 3.855854 | -1.505961 |
| 71 | 8 | 0 | 1.435630 | 5.324563 | -0.935630 |
| 72 | 1 | 0 | 1.198152 | 5.858199 | -1.712831 |
| 73 | 16 | 0 | 5.118064 | -1.213895 | -1.009841 |
| 74 | 8 | 0 | 5.983827 | -2.483116 | -1.408557 |
| 75 | 1 | 0 | 6.508022 | -2.357941 | -2.217578 |
| 76 | 8 | 0 | 4.339920 | -1.640417 | 0.122430 |
| 77 | 8 | 0 | 6.201069 | -0.141546 | -0.573767 |
| 78 | 8 | 0 | 4.487754 | -0.650633 | -2.176247 |
| 79 | 16 | 0 | -4.938836 | -0.771394 | -0.177794 |
| 80 | 8 | 0 | -5.766495 | -0.098250 | -1.354318 |

| | | | | | |
|---|---|---|---|---|---|
| 81 | 1 | 0 | -6.375573 | 0.594502 | -1.047386 |
| 82 | 8 | 0 | -3.935336 | -1.563942 | -0.836002 |
| 83 | 8 | 0 | -5.998517 | -1.710882 | 0.540802 |
| 84 | 8 | 0 | -4.592047 | 0.215179 | 0.811055 |
| 85 | 8 | 0 | -0.762725 | 5.480685 | 0.239815 |
| 86 | 1 | 0 | -0.448315 | 5.844451 | 1.084847 |
| 87 | 1 | 0 | -6.238368 | -2.492448 | 0.014827 |
| 88 | 1 | 0 | 6.560786 | -0.294883 | 0.316806 |

Rotational constants (GHZ): 0.0640604 0.0480454

TC4-3-003, ferriin quartet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.169210 | -0.201873 | 0.010175 |
| 2 | 7 | 0 | 1.587120 | -1.288938 | -1.250653 |
| 3 | 7 | 0 | -0.069177 | -2.010593 | 0.741135 |
| 4 | 7 | 0 | -1.361902 | 0.752196 | 1.243430 |
| 5 | 7 | 0 | -1.389164 | -0.448984 | -1.161921 |
| 6 | 7 | 0 | 1.535494 | 0.258106 | 1.332052 |
| 7 | 7 | 0 | 0.665025 | 1.490481 | -0.823291 |
| 8 | 6 | 0 | 2.392459 | -0.886502 | -2.217079 |
| 9 | 1 | 0 | 2.308309 | 0.149550 | -2.523327 |
| 10 | 6 | 0 | 3.321746 | -1.747925 | -2.813139 |
| 11 | 1 | 0 | 3.959650 | -1.380733 | -3.608888 |
| 12 | 6 | 0 | 3.406917 | -3.051811 | -2.375603 |
| 13 | 1 | 0 | 4.121589 | -3.737523 | -2.820960 |
| 14 | 6 | 0 | 2.555357 | -3.501381 | -1.347249 |
| 15 | 6 | 0 | 1.656546 | -2.561899 | -0.812673 |
| 16 | 6 | 0 | 0.759732 | -2.949049 | 0.224765 |
| 17 | 6 | 0 | 2.549928 | -4.839099 | -0.844063 |
| 18 | 1 | 0 | 3.248498 | -5.557691 | -1.261239 |
| 19 | 6 | 0 | 1.680227 | -5.213026 | 0.132324 |
| 20 | 1 | 0 | 1.675777 | -6.233166 | 0.503326 |
| 21 | 6 | 0 | 0.756951 | -4.276349 | 0.693636 |
| 22 | 6 | 0 | -0.163675 | -4.600904 | 1.710036 |
| 23 | 1 | 0 | -0.197840 | -5.614387 | 2.099368 |
| 24 | 6 | 0 | -1.009850 | -3.632266 | 2.203490 |
| 25 | 1 | 0 | -1.734265 | -3.851764 | 2.979405 |
| 26 | 6 | 0 | -0.928781 | -2.331867 | 1.695064 |
| 27 | 1 | 0 | -1.574849 | -1.545071 | 2.057388 |
| 28 | 6 | 0 | -1.299093 | 1.341904 | 2.424363 |
| 29 | 1 | 0 | -0.338786 | 1.324441 | 2.928118 |
| 30 | 6 | 0 | -2.413416 | 1.954717 | 3.006567 |
| 31 | 1 | 0 | -2.324290 | 2.414600 | 3.984388 |
| 32 | 6 | 0 | -3.610585 | 1.953716 | 2.322736 |
| 33 | 1 | 0 | -4.493074 | 2.417229 | 2.753771 |
| 34 | 6 | 0 | -3.692579 | 1.348902 | 1.054880 |
| 35 | 6 | 0 | -2.520235 | 0.756463 | 0.557350 |
| 36 | 6 | 0 | -2.531666 | 0.121380 | -0.717864 |
| 37 | 6 | 0 | -4.881745 | 1.315965 | 0.265144 |
| 38 | 1 | 0 | -5.778123 | 1.789921 | 0.652365 |
| 39 | 6 | 0 | -4.891323 | 0.711893 | -0.951004 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 1 | 0 | -5.795395 | 0.694718 | -1.551562 |
| 41 | 6 | 0 | -3.716259 | 0.088822 | -1.474134 |
| 42 | 6 | 0 | -3.675505 | -0.571610 | -2.715001 |
| 43 | 1 | 0 | -4.569525 | -0.618395 | -3.329215 |
| 44 | 6 | 0 | -2.506857 | -1.168563 | -3.133533 |
| 45 | 1 | 0 | -2.450524 | -1.702252 | -4.075167 |
| 46 | 6 | 0 | -1.374714 | -1.091647 | -2.320593 |
| 47 | 1 | 0 | -0.436808 | -1.547141 | -2.610247 |
| 48 | 6 | 0 | 1.950465 | -0.418916 | 2.392816 |
| 49 | 1 | 0 | 1.513708 | -1.395262 | 2.555045 |
| 50 | 6 | 0 | 2.908850 | 0.103513 | 3.265835 |
| 51 | 1 | 0 | 3.212661 | -0.479417 | 4.127921 |
| 52 | 6 | 0 | 3.455461 | 1.344805 | 3.013793 |
| 53 | 1 | 0 | 4.204950 | 1.762932 | 3.679275 |
| 54 | 6 | 0 | 3.045349 | 2.071933 | 1.879603 |
| 55 | 6 | 0 | 2.066488 | 1.477138 | 1.069901 |
| 56 | 6 | 0 | 1.608961 | 2.132827 | -0.095796 |
| 57 | 6 | 0 | 3.572650 | 3.344316 | 1.498074 |
| 58 | 1 | 0 | 4.332795 | 3.802017 | 2.122843 |
| 59 | 6 | 0 | 3.142494 | 3.967143 | 0.367950 |
| 60 | 1 | 0 | 3.556247 | 4.928577 | 0.080776 |
| 61 | 6 | 0 | 2.145398 | 3.372491 | -0.466274 |
| 62 | 6 | 0 | 1.663343 | 3.938097 | -1.661308 |
| 63 | 1 | 0 | 2.044330 | 4.897569 | -1.998027 |
| 64 | 6 | 0 | 0.711061 | 3.266403 | -2.399345 |
| 65 | 1 | 0 | 0.325888 | 3.677628 | -3.325216 |
| 66 | 6 | 0 | 0.221192 | 2.038933 | -1.944955 |
| 67 | 1 | 0 | -0.545389 | 1.502411 | -2.486832 |
| 68 | 16 | 0 | -2.014449 | 4.079374 | -0.405725 |
| 69 | 8 | 0 | -0.930473 | 3.740222 | 0.473697 |
| 70 | 8 | 0 | -2.535684 | 3.126673 | -1.346226 |
| 71 | 8 | 0 | -1.543779 | 5.404339 | -1.156698 |
| 72 | 1 | 0 | -2.189045 | 5.718031 | -1.809632 |
| 73 | 16 | 0 | 4.950103 | -0.145490 | -0.120177 |
| 74 | 8 | 0 | 6.006710 | -0.874295 | -1.061642 |
| 75 | 1 | 0 | 6.589742 | -0.255031 | -1.528314 |
| 76 | 8 | 0 | 4.140583 | -1.196556 | 0.429827 |
| 77 | 8 | 0 | 5.871847 | 0.495938 | 1.014362 |
| 78 | 8 | 0 | 4.355527 | 0.974560 | -0.796256 |
| 79 | 16 | 0 | -3.976390 | -2.871798 | 0.296877 |
| 80 | 8 | 0 | -5.299178 | -2.682878 | -0.572473 |
| 81 | 1 | 0 | -6.086622 | -2.532747 | -0.026548 |
| 82 | 8 | 0 | -2.916824 | -3.044761 | -0.657165 |
| 83 | 8 | 0 | -4.252413 | -4.230444 | 1.079547 |
| 84 | 8 | 0 | -3.899558 | -1.860360 | 1.315033 |
| 85 | 8 | 0 | -3.277240 | 4.577860 | 0.430420 |
| 86 | 1 | 0 | -3.044790 | 5.239813 | 1.099857 |
| 87 | 1 | 0 | -4.303680 | -5.001938 | 0.494105 |
| 88 | 1 | 0 | 6.361494 | -0.171137 | 1.520119 |

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Rotational constants (GHZ): 0.0627753 0.0500972

Structures of Ferroin $[Fe(phen)_3]^{2+}$ and its Aggregates

**Structures of DC-0-000**

DC1-0-000, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.005121 | 0.003597 | -0.004074 |
| 2 | 7 | 0 | 1.527272 | 0.551012 | 1.057656 |
| 3 | 7 | 0 | 0.402814 | 1.593104 | -1.044940 |
| 4 | 7 | 0 | -1.573015 | -0.432986 | -1.065317 |
| 5 | 7 | 0 | -1.258133 | 1.046794 | 1.050981 |
| 6 | 7 | 0 | 1.174347 | -1.129155 | -1.054643 |
| 7 | 7 | 0 | -0.297754 | -1.611330 | 1.036825 |
| 8 | 6 | 0 | 2.061041 | -0.020292 | 2.124729 |
| 9 | 1 | 0 | 1.580870 | -0.918710 | 2.490837 |
| 10 | 6 | 0 | 3.189106 | 0.507409 | 2.766555 |
| 11 | 1 | 0 | 3.584581 | -0.002509 | 3.637581 |
| 12 | 6 | 0 | 3.773572 | 1.660145 | 2.289319 |
| 13 | 1 | 0 | 4.646244 | 2.086979 | 2.773613 |
| 14 | 6 | 0 | 3.222216 | 2.288100 | 1.157400 |
| 15 | 6 | 0 | 2.095097 | 1.681625 | 0.581883 |
| 16 | 6 | 0 | 1.476649 | 2.254805 | -0.558436 |
| 17 | 6 | 0 | 3.729225 | 3.490347 | 0.569541 |
| 18 | 1 | 0 | 4.601152 | 3.956052 | 1.018223 |
| 19 | 6 | 0 | 3.134873 | 4.041413 | -0.524155 |
| 20 | 1 | 0 | 3.524305 | 4.953911 | -0.964848 |
| 21 | 6 | 0 | 1.984976 | 3.435039 | -1.122611 |
| 22 | 6 | 0 | 1.316543 | 3.937853 | -2.254019 |
| 23 | 1 | 0 | 1.668081 | 4.848090 | -2.729686 |
| 24 | 6 | 0 | 0.221261 | 3.258813 | -2.741162 |
| 25 | 1 | 0 | -0.317553 | 3.615048 | -3.611763 |
| 26 | 6 | 0 | -0.208281 | 2.083573 | -2.110830 |
| 27 | 1 | 0 | -1.059727 | 1.530262 | -2.485696 |
| 28 | 6 | 0 | -1.677816 | -1.196487 | -2.140518 |
| 29 | 1 | 0 | -0.766081 | -1.645438 | -2.513143 |
| 30 | 6 | 0 | -2.904056 | -1.415812 | -2.781791 |
| 31 | 1 | 0 | -2.931253 | -2.050922 | -3.659879 |
| 32 | 6 | 0 | -4.048785 | -0.823696 | -2.294808 |
| 33 | 1 | 0 | -5.008632 | -0.978661 | -2.777695 |
| 34 | 6 | 0 | -3.962667 | -0.005296 | -1.153413 |
| 35 | 6 | 0 | -2.691293 | 0.151191 | -0.580266 |
| 36 | 6 | 0 | -2.518255 | 0.964118 | 0.568922 |
| 37 | 6 | 0 | -5.072798 | 0.669606 | -0.553061 |
| 38 | 1 | 0 | -6.054330 | 0.545058 | -0.999895 |
| 39 | 6 | 0 | -4.906771 | 1.449409 | 0.550322 |
| 40 | 1 | 0 | -5.753388 | 1.957846 | 1.001120 |
| 41 | 6 | 0 | -3.616815 | 1.618991 | 1.146363 |
| 42 | 6 | 0 | -3.362623 | 2.400661 | 2.288322 |
| 43 | 1 | 0 | -4.177491 | 2.927631 | 2.774720 |
| 44 | 6 | 0 | -2.074815 | 2.481299 | 2.771263 |
| 45 | 1 | 0 | -1.841358 | 3.072035 | 3.649715 |
| 46 | 6 | 0 | -1.043024 | 1.786870 | 2.126179 |
| 47 | 1 | 0 | -0.026653 | 1.829236 | 2.495834 |
| 48 | 6 | 0 | 1.905481 | -0.831168 | -2.116043 |
| 49 | 1 | 0 | 1.839611 | 0.183431 | -2.487107 |
| 50 | 6 | 0 | 2.725278 | -1.776803 | -2.745861 |
| 51 | 1 | 0 | 3.302788 | -1.477004 | -3.612910 |
| 52 | 6 | 0 | 2.782863 | -3.065583 | -2.262233 |
| 53 | 1 | 0 | 3.409085 | -3.814705 | -2.736646 |
| 54 | 6 | 0 | 2.011668 | -3.407903 | -1.136256 |
| 55 | 6 | 0 | 1.225634 | -2.390956 | -0.572697 |

| | | | | | |
|---|---|---|---|---|---|
| 56 | 6 | 0 | 0.415159 | -2.656369 | 0.560548 |
| 57 | 6 | 0 | 1.974795 | -4.710270 | -0.544360 |
| 58 | 1 | 0 | 2.584659 | -5.493347 | -0.984171 |
| 59 | 6 | 0 | 1.193352 | -4.966449 | 0.540398 |
| 60 | 1 | 0 | 1.168423 | -5.957559 | 0.982615 |
| 61 | 6 | 0 | 0.386457 | -3.940268 | 1.126690 |
| 62 | 6 | 0 | -0.445164 | -4.123064 | 2.246767 |
| 63 | 1 | 0 | -0.504912 | -5.097152 | 2.722009 |
| 64 | 6 | 0 | -1.172523 | -3.053823 | 2.721918 |
| 65 | 1 | 0 | -1.823229 | -3.156428 | 3.582797 |
| 66 | 6 | 0 | -1.071858 | -1.806479 | 2.091884 |
| 67 | 1 | 0 | -1.626971 | -0.952025 | 2.457467 |

Rotational constants (GHZ): 0.1032396 0.1025596

DC3-0-000, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.000059 | 0.030605 | 0.000000 |
| 2 | 7 | 0 | -1.613400 | 0.053123 | -1.075459 |
| 3 | 7 | 0 | -0.897681 | 1.435243 | 1.009522 |
| 4 | 7 | 0 | 1.613543 | 0.051273 | 1.075441 |
| 5 | 7 | 0 | 0.899179 | 1.434569 | -1.009220 |
| 6 | 7 | 0 | -0.813748 | -1.386074 | 1.020489 |
| 7 | 7 | 0 | 0.812376 | -1.386712 | -1.020781 |
| 8 | 6 | 0 | -1.913964 | -0.692895 | -2.125422 |
| 9 | 1 | 0 | -1.157074 | -1.384985 | -2.470094 |
| 10 | 6 | 0 | -3.153080 | -0.577728 | -2.767325 |
| 11 | 1 | 0 | -3.357268 | -1.205709 | -3.626486 |
| 12 | 6 | 0 | -4.087654 | 0.324488 | -2.306264 |
| 13 | 1 | 0 | -5.052276 | 0.424770 | -2.793464 |
| 14 | 6 | 0 | -3.782078 | 1.124800 | -1.189433 |
| 15 | 6 | 0 | -2.518561 | 0.941348 | -0.612759 |
| 16 | 6 | 0 | -2.127162 | 1.697119 | 0.516244 |
| 17 | 6 | 0 | -4.658376 | 2.098014 | -0.613006 |
| 18 | 1 | 0 | -5.636363 | 2.239730 | -1.061720 |
| 19 | 6 | 0 | -4.280528 | 2.829208 | 0.472157 |
| 20 | 1 | 0 | -4.951510 | 3.564119 | 0.905115 |
| 21 | 6 | 0 | -2.994973 | 2.646449 | 1.072945 |
| 22 | 6 | 0 | -2.526391 | 3.342668 | 2.202484 |
| 23 | 1 | 0 | -3.157804 | 4.087448 | 2.676456 |
| 24 | 6 | 0 | -1.269318 | 3.065303 | 2.695141 |
| 25 | 1 | 0 | -0.881362 | 3.581605 | 3.565212 |
| 26 | 6 | 0 | -0.472295 | 2.097554 | 2.071660 |
| 27 | 1 | 0 | 0.513964 | 1.855604 | 2.446265 |
| 28 | 6 | 0 | 1.913380 | -0.695277 | 2.125237 |
| 29 | 1 | 0 | 1.155824 | -1.386716 | 2.469753 |
| 30 | 6 | 0 | 3.152596 | -0.581448 | 2.767181 |
| 31 | 1 | 0 | 3.356168 | -1.209819 | 3.626202 |
| 32 | 6 | 0 | 4.088045 | 0.319974 | 2.306340 |
| 33 | 1 | 0 | 5.052753 | 0.419217 | 2.793579 |
| 34 | 6 | 0 | 3.783259 | 1.120829 | 1.189683 |
| 35 | 6 | 0 | 2.519573 | 0.938725 | 0.612949 |
| 36 | 6 | 0 | 2.128907 | 1.695143 | -0.515873 |
| 37 | 6 | 0 | 4.660497 | 2.093337 | 0.613497 |
| 38 | 1 | 0 | 5.638616 | 2.234008 | 1.062251 |
| 39 | 6 | 0 | 4.283358 | 2.825153 | -0.471493 |
| 40 | 1 | 0 | 4.955050 | 3.559524 | -0.904268 |
| 41 | 6 | 0 | 2.997635 | 2.643773 | -1.072337 |
| 42 | 6 | 0 | 2.529737 | 3.340713 | -2.201713 |

| | | | | | |
|---|---|---|---|---|---|
| 43 | 1 | 0 | 3.161870 | 4.084992 | -2.675513 |
| 44 | 6 | 0 | 1.272400 | 3.064676 | -2.694445 |
| 45 | 1 | 0 | 0.884948 | 3.581558 | -3.564397 |
| 46 | 6 | 0 | 0.474435 | 2.097554 | -2.071195 |
| 47 | 1 | 0 | -0.512067 | 1.856663 | -2.445848 |
| 48 | 6 | 0 | -1.700453 | -1.329116 | 2.024242 |
| 49 | 1 | 0 | -1.968481 | -0.343482 | 2.384433 |
| 50 | 6 | 0 | -2.230458 | -2.465716 | 2.603208 |
| 51 | 1 | 0 | -2.929770 | -2.362440 | 3.424772 |
| 52 | 6 | 0 | -1.840900 | -3.737674 | 2.135404 |
| 53 | 1 | 0 | -2.240271 | -4.640214 | 2.587832 |
| 54 | 6 | 0 | -0.937808 | -3.827394 | 1.085663 |
| 55 | 6 | 0 | -0.444765 | -2.617313 | 0.531441 |
| 56 | 6 | 0 | 0.441984 | -2.617668 | -0.532078 |
| 57 | 6 | 0 | -0.449414 | -5.051887 | 0.512078 |
| 58 | 1 | 0 | -0.811114 | -5.989780 | 0.924042 |
| 59 | 6 | 0 | 0.443899 | -5.052252 | -0.513343 |
| 60 | 1 | 0 | 0.804552 | -5.990443 | -0.925547 |
| 61 | 6 | 0 | 0.933692 | -3.828156 | -1.086591 |
| 62 | 6 | 0 | 1.836965 | -3.739182 | -2.136239 |
| 63 | 1 | 0 | 2.235348 | -4.642050 | -2.588880 |
| 64 | 6 | 0 | 2.228029 | -2.467531 | -2.603647 |
| 65 | 1 | 0 | 2.927539 | -2.364827 | -3.425114 |
| 66 | 6 | 0 | 1.699265 | -1.330491 | -2.024427 |
| 67 | 1 | 0 | 1.968457 | -0.345065 | -2.384316 |

Rotational constants (GHZ): 0.1058329 0.1023620

**Structures of DC-1-100**

DC1-1-100, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.772959 | -0.011550 | 0.066665 |
| 2 | 7 | 0 | 2.158515 | -0.997817 | 0.964203 |
| 3 | 7 | 0 | 2.290057 | 0.457398 | -1.232080 |
| 4 | 7 | 0 | -0.589737 | 1.144903 | -0.950421 |
| 5 | 7 | 0 | 1.084080 | 1.638802 | 1.032030 |
| 6 | 7 | 0 | 0.220395 | -1.610554 | -0.870573 |
| 7 | 7 | 0 | -0.714259 | -0.568152 | 1.367190 |
| 8 | 6 | 0 | 2.055602 | -1.729973 | 2.062563 |
| 9 | 1 | 0 | 1.079815 | -1.772376 | 2.528110 |
| 10 | 6 | 0 | 3.147389 | -2.413805 | 2.610918 |
| 11 | 1 | 0 | 3.003172 | -2.997170 | 3.513157 |
| 12 | 6 | 0 | 4.380669 | -2.331048 | 2.003440 |
| 13 | 1 | 0 | 5.243154 | -2.848432 | 2.411933 |
| 14 | 6 | 0 | 4.516955 | -1.560509 | 0.834170 |
| 15 | 6 | 0 | 3.365297 | -0.914294 | 0.354417 |
| 16 | 6 | 0 | 3.436922 | -0.119463 | -0.822766 |
| 17 | 6 | 0 | 5.748284 | -1.398743 | 0.122552 |
| 18 | 1 | 0 | 6.631414 | -1.902463 | 0.503281 |
| 19 | 6 | 0 | 5.816352 | -0.632815 | -1.000052 |
| 20 | 1 | 0 | 6.754274 | -0.512977 | -1.533510 |
| 21 | 6 | 0 | 4.655012 | 0.030929 | -1.506537 |
| 22 | 6 | 0 | 4.640113 | 0.833269 | -2.663014 |
| 23 | 1 | 0 | 5.556328 | 0.981229 | -3.226357 |
| 24 | 6 | 0 | 3.459313 | 1.420119 | -3.064269 |
| 25 | 1 | 0 | 3.415346 | 2.042812 | -3.950507 |
| 26 | 6 | 0 | 2.291895 | 1.206428 | -2.318271 |
| 27 | 1 | 0 | 1.345233 | 1.645161 | -2.609926 |
| 28 | 6 | 0 | -1.373177 | 0.853779 | -1.968392 |

| | | | | | |
|---|---|---|---|---|---|
| 29 | 1 | 0 | -1.296703 | -0.145690 | -2.374533 |
| 30 | 6 | 0 | -2.266662 | 1.789802 | -2.508726 |
| 31 | 1 | 0 | -2.896580 | 1.499376 | -3.340703 |
| 32 | 6 | 0 | -2.342730 | 3.048395 | -1.960932 |
| 33 | 1 | 0 | -3.035186 | 3.787737 | -2.351426 |
| 34 | 6 | 0 | -1.511810 | 3.379054 | -0.872372 |
| 35 | 6 | 0 | -0.642575 | 2.378473 | -0.409719 |
| 36 | 6 | 0 | 0.256083 | 2.644801 | 0.659988 |
| 37 | 6 | 0 | -1.496636 | 4.656741 | -0.230704 |
| 38 | 1 | 0 | -2.178326 | 5.422547 | -0.588057 |
| 39 | 6 | 0 | -0.645894 | 4.911084 | 0.800577 |
| 40 | 1 | 0 | -0.635955 | 5.882876 | 1.284472 |
| 41 | 6 | 0 | 0.262058 | 3.910783 | 1.271213 |
| 42 | 6 | 0 | 1.177138 | 4.113633 | 2.320710 |
| 43 | 1 | 0 | 1.214734 | 5.074680 | 2.824161 |
| 44 | 6 | 0 | 2.013785 | 3.083975 | 2.689247 |
| 45 | 1 | 0 | 2.732380 | 3.202641 | 3.492202 |
| 46 | 6 | 0 | 1.937175 | 1.856190 | 2.020142 |
| 47 | 1 | 0 | 2.580581 | 1.031526 | 2.298823 |
| 48 | 6 | 0 | 0.711006 | -2.104840 | -1.996333 |
| 49 | 1 | 0 | 1.544143 | -1.573546 | -2.438263 |
| 50 | 6 | 0 | 0.184287 | -3.252100 | -2.601295 |
| 51 | 1 | 0 | 0.624895 | -3.610929 | -3.524475 |
| 52 | 6 | 0 | -0.882354 | -3.901080 | -2.019101 |
| 53 | 1 | 0 | -1.310727 | -4.790297 | -2.471103 |
| 54 | 6 | 0 | -1.421398 | -3.396668 | -0.822157 |
| 55 | 6 | 0 | -0.827931 | -2.239865 | -0.289440 |
| 56 | 6 | 0 | -1.333891 | -1.674289 | 0.913543 |
| 57 | 6 | 0 | -2.530897 | -3.984105 | -0.135765 |
| 58 | 1 | 0 | -2.986770 | -4.872364 | -0.561992 |
| 59 | 6 | 0 | -3.009677 | -3.443552 | 1.016318 |
| 60 | 1 | 0 | -3.856018 | -3.889907 | 1.528696 |
| 61 | 6 | 0 | -2.417750 | -2.270007 | 1.577013 |
| 62 | 6 | 0 | -2.855670 | -1.653365 | 2.762099 |
| 63 | 1 | 0 | -3.696735 | -2.071551 | 3.305979 |
| 64 | 6 | 0 | -2.212279 | -0.521802 | 3.212419 |
| 65 | 1 | 0 | -2.526861 | -0.020012 | 4.120354 |
| 66 | 6 | 0 | -1.136416 | -0.001834 | 2.481557 |
| 67 | 1 | 0 | -0.608378 | 0.884507 | 2.812217 |
| 68 | 16 | 0 | -4.554780 | -0.083742 | -0.430445 |
| 69 | 8 | 0 | -3.657098 | 0.774467 | 0.416588 |
| 70 | 8 | 0 | -3.738962 | -0.983645 | -1.317870 |
| 71 | 8 | 0 | -5.425262 | -0.928850 | 0.463706 |
| 72 | 8 | 0 | -5.421999 | 0.800645 | -1.288600 |

Rotational constants (GHZ): 0.1004302 0.0668455

DC3-1-100, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.722934 | 0.026897 | 0.066062 |
| 2 | 7 | 0 | 2.384321 | -1.021030 | 0.980414 |
| 3 | 7 | 0 | 2.404699 | 0.596413 | -1.179329 |
| 4 | 7 | 0 | -0.693395 | 1.191839 | -1.031826 |
| 5 | 7 | 0 | 0.914762 | 1.675212 | 1.041018 |
| 6 | 7 | 0 | 0.270575 | -1.592541 | -0.870335 |
| 7 | 7 | 0 | -0.749226 | -0.710397 | 1.431116 |
| 8 | 6 | 0 | 2.334064 | -1.820892 | 2.028258 |
| 9 | 1 | 0 | 1.361715 | -1.946730 | 2.493157 |
| 10 | 6 | 0 | 3.470757 | -2.471880 | 2.526621 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 1 | 0 | 3.381807 | -3.120495 | 3.390727 |
| 12 | 6 | 0 | 4.683586 | -2.267514 | 1.906288 |
| 13 | 1 | 0 | 5.585108 | -2.752216 | 2.268847 |
| 14 | 6 | 0 | 4.757028 | -1.417190 | 0.786456 |
| 15 | 6 | 0 | 3.558355 | -0.814432 | 0.356111 |
| 16 | 6 | 0 | 3.571590 | 0.055740 | -0.783392 |
| 17 | 6 | 0 | 5.973848 | -1.142513 | 0.086559 |
| 18 | 1 | 0 | 6.887046 | -1.615273 | 0.435061 |
| 19 | 6 | 0 | 5.988244 | -0.309040 | -0.987189 |
| 20 | 1 | 0 | 6.913156 | -0.100231 | -1.516316 |
| 21 | 6 | 0 | 4.785735 | 0.310698 | -1.451216 |
| 22 | 6 | 0 | 4.739581 | 1.172890 | -2.563244 |
| 23 | 1 | 0 | 5.653934 | 1.395015 | -3.105298 |
| 24 | 6 | 0 | 3.536174 | 1.720713 | -2.949297 |
| 25 | 1 | 0 | 3.467511 | 2.387117 | -3.801705 |
| 26 | 6 | 0 | 2.380284 | 1.401792 | -2.223834 |
| 27 | 1 | 0 | 1.411582 | 1.804549 | -2.500177 |
| 28 | 6 | 0 | -1.455027 | 0.908387 | -2.067925 |
| 29 | 1 | 0 | -1.301875 | -0.056547 | -2.535148 |
| 30 | 6 | 0 | -2.412028 | 1.809448 | -2.556137 |
| 31 | 1 | 0 | -3.019437 | 1.530990 | -3.408720 |
| 32 | 6 | 0 | -2.578680 | 3.019769 | -1.925359 |
| 33 | 1 | 0 | -3.322861 | 3.731056 | -2.270348 |
| 34 | 6 | 0 | -1.777254 | 3.340134 | -0.811578 |
| 35 | 6 | 0 | -0.836443 | 2.377665 | -0.407624 |
| 36 | 6 | 0 | 0.022359 | 2.638137 | 0.699660 |
| 37 | 6 | 0 | -1.865213 | 4.571341 | -0.090658 |
| 38 | 1 | 0 | -2.600306 | 5.304829 | -0.407684 |
| 39 | 6 | 0 | -1.045891 | 4.821472 | 0.966236 |
| 40 | 1 | 0 | -1.112581 | 5.758000 | 1.511259 |
| 41 | 6 | 0 | -0.073227 | 3.861154 | 1.387787 |
| 42 | 6 | 0 | 0.805989 | 4.066184 | 2.467494 |
| 43 | 1 | 0 | 0.762186 | 4.996004 | 3.026087 |
| 44 | 6 | 0 | 1.710106 | 3.081174 | 2.797005 |
| 45 | 1 | 0 | 2.403265 | 3.204753 | 3.621147 |
| 46 | 6 | 0 | 1.732518 | 1.892038 | 2.059249 |
| 47 | 1 | 0 | 2.422329 | 1.093985 | 2.302167 |
| 48 | 6 | 0 | 0.799045 | -2.009751 | -2.010624 |
| 49 | 1 | 0 | 1.613750 | -1.418860 | -2.409505 |
| 50 | 6 | 0 | 0.331537 | -3.146509 | -2.678489 |
| 51 | 1 | 0 | 0.801008 | -3.443098 | -3.609455 |
| 52 | 6 | 0 | -0.719557 | -3.860778 | -2.146979 |
| 53 | 1 | 0 | -1.108253 | -4.741308 | -2.649140 |
| 54 | 6 | 0 | -1.299039 | -3.436657 | -0.937580 |
| 55 | 6 | 0 | -0.759905 | -2.288560 | -0.331496 |
| 56 | 6 | 0 | -1.309826 | -1.810026 | 0.894028 |
| 57 | 6 | 0 | -2.405414 | -4.097432 | -0.315939 |
| 58 | 1 | 0 | -2.817995 | -4.975206 | -0.803688 |
| 59 | 6 | 0 | -2.933548 | -3.636014 | 0.848342 |
| 60 | 1 | 0 | -3.779143 | -4.135548 | 1.310414 |
| 61 | 6 | 0 | -2.392388 | -2.479585 | 1.489333 |
| 62 | 6 | 0 | -2.886261 | -1.947809 | 2.693648 |
| 63 | 1 | 0 | -3.727883 | -2.426327 | 3.184528 |
| 64 | 6 | 0 | -2.299517 | -0.823607 | 3.232409 |
| 65 | 1 | 0 | -2.660978 | -0.388588 | 4.157158 |
| 66 | 6 | 0 | -1.225091 | -0.225193 | 2.561646 |
| 67 | 1 | 0 | -0.743078 | 0.665503 | 2.950824 |
| 68 | 16 | 0 | -4.504082 | -0.180125 | -0.442416 |
| 69 | 8 | 0 | -3.643273 | 0.682690 | 0.437011 |
| 70 | 8 | 0 | -3.653331 | -1.046945 | -1.329911 |
| 71 | 8 | 0 | -5.370617 | -1.059613 | 0.422582 |
| 72 | 8 | 0 | -5.378040 | 0.698210 | -1.299928 |

Rotational constants (GHZ): 0.0993640 0.0648212

**Structures of DC-1-010**

DC1-1-010, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.796908 | -0.008313 | 0.058663 |
| 2 | 7 | 0 | 2.201344 | -0.938987 | 0.984812 |
| 3 | 7 | 0 | 2.311280 | 0.480076 | -1.235744 |
| 4 | 7 | 0 | -0.591569 | 1.088912 | -0.988695 |
| 5 | 7 | 0 | 1.045496 | 1.664569 | 1.002485 |
| 6 | 7 | 0 | 0.287513 | -1.631517 | -0.859322 |
| 7 | 7 | 0 | -0.688090 | -0.580102 | 1.356381 |
| 8 | 6 | 0 | 2.109142 | -1.653950 | 2.095248 |
| 9 | 1 | 0 | 1.130534 | -1.716552 | 2.552491 |
| 10 | 6 | 0 | 3.214931 | -2.296112 | 2.665352 |
| 11 | 1 | 0 | 3.079182 | -2.867273 | 3.576653 |
| 12 | 6 | 0 | 4.450904 | -2.188861 | 2.067255 |
| 13 | 1 | 0 | 5.323909 | -2.673916 | 2.492653 |
| 14 | 6 | 0 | 4.576115 | -1.435352 | 0.885723 |
| 15 | 6 | 0 | 3.410941 | -0.831346 | 0.384354 |
| 16 | 6 | 0 | 3.470620 | -0.055532 | -0.805998 |
| 17 | 6 | 0 | 5.808970 | -1.249821 | 0.182577 |
| 18 | 1 | 0 | 6.702698 | -1.720627 | 0.580241 |
| 19 | 6 | 0 | 5.865445 | -0.501907 | -0.952751 |
| 20 | 1 | 0 | 6.804566 | -0.363714 | -1.479624 |
| 21 | 6 | 0 | 4.690122 | 0.118563 | -1.481397 |
| 22 | 6 | 0 | 4.662579 | 0.899936 | -2.651929 |
| 23 | 1 | 0 | 5.579440 | 1.065251 | -3.209388 |
| 24 | 6 | 0 | 3.468852 | 1.444066 | -3.074560 |
| 25 | 1 | 0 | 3.415082 | 2.049315 | -3.972238 |
| 26 | 6 | 0 | 2.301161 | 1.209060 | -2.335476 |
| 27 | 1 | 0 | 1.344833 | 1.614121 | -2.643719 |
| 28 | 6 | 0 | -1.347210 | 0.762702 | -2.017395 |
| 29 | 1 | 0 | -1.216541 | -0.230972 | -2.426481 |
| 30 | 6 | 0 | -2.280821 | 1.654338 | -2.564183 |
| 31 | 1 | 0 | -2.882629 | 1.337765 | -3.407700 |
| 32 | 6 | 0 | -2.430090 | 2.904083 | -2.009400 |
| 33 | 1 | 0 | -3.156953 | 3.607591 | -2.403587 |
| 34 | 6 | 0 | -1.625948 | 3.273435 | -0.913832 |
| 35 | 6 | 0 | -0.708756 | 2.317684 | -0.448216 |
| 36 | 6 | 0 | 0.168647 | 2.627230 | 0.627735 |
| 37 | 6 | 0 | -1.683140 | 4.547358 | -0.267006 |
| 38 | 1 | 0 | -2.402150 | 5.277408 | -0.625990 |
| 39 | 6 | 0 | -0.853268 | 4.842077 | 0.770381 |
| 40 | 1 | 0 | -0.897614 | 5.811014 | 1.258003 |
| 41 | 6 | 0 | 0.104837 | 3.889881 | 1.241949 |
| 42 | 6 | 0 | 1.003564 | 4.138054 | 2.295798 |
| 43 | 1 | 0 | 0.987494 | 5.097970 | 2.802488 |
| 44 | 6 | 0 | 1.893873 | 3.154181 | 2.663746 |
| 45 | 1 | 0 | 2.603064 | 3.309362 | 3.468757 |
| 46 | 6 | 0 | 1.884217 | 1.925194 | 1.992511 |
| 47 | 1 | 0 | 2.569162 | 1.134819 | 2.271677 |
| 48 | 6 | 0 | 0.800313 | -2.132241 | -1.971980 |
| 49 | 1 | 0 | 1.639897 | -1.601729 | -2.402384 |
| 50 | 6 | 0 | 0.288058 | -3.285469 | -2.578605 |
| 51 | 1 | 0 | 0.747050 | -3.649398 | -3.490745 |
| 52 | 6 | 0 | -0.787475 | -3.933383 | -2.012307 |
| 53 | 1 | 0 | -1.204854 | -4.826889 | -2.466044 |
| 54 | 6 | 0 | -1.348701 | -3.423441 | -0.827619 |

| | | | | | |
|---|---|---|---|---|---|
| 55 | 6 | 0 | -0.768591 | -2.261265 | -0.292459 |
| 56 | 6 | 0 | -1.293456 | -1.693356 | 0.901031 |
| 57 | 6 | 0 | -2.465584 | -4.012977 | -0.155060 |
| 58 | 1 | 0 | -2.911107 | -4.905267 | -0.583804 |
| 59 | 6 | 0 | -2.961751 | -3.471540 | 0.989446 |
| 60 | 1 | 0 | -3.811137 | -3.921496 | 1.493632 |
| 61 | 6 | 0 | -2.380414 | -2.294732 | 1.555353 |
| 62 | 6 | 0 | -2.832483 | -1.679138 | 2.736521 |
| 63 | 1 | 0 | -3.675140 | -2.102513 | 3.273844 |
| 64 | 6 | 0 | -2.197193 | -0.546025 | 3.193687 |
| 65 | 1 | 0 | -2.519487 | -0.047996 | 4.100945 |
| 66 | 6 | 0 | -1.120547 | -0.018396 | 2.469083 |
| 67 | 1 | 0 | -0.601396 | 0.871798 | 2.803389 |
| 68 | 16 | 0 | -4.405862 | -0.189871 | -0.319334 |
| 69 | 8 | 0 | -3.560754 | 0.769276 | 0.405387 |
| 70 | 8 | 0 | -3.702700 | -1.051956 | -1.273329 |
| 71 | 8 | 0 | -5.349732 | -0.906614 | 0.555698 |
| 72 | 8 | 0 | -5.332853 | 0.721650 | -1.327393 |
| 73 | 1 | 0 | -5.794398 | 1.408518 | -0.826745 |

Rotational constants (GHZ): 0.1014396 0.0668370

DC3-1-010, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.714511 | 0.056043 | 0.038679 |
| 2 | 7 | 0 | 2.356044 | -1.006923 | 0.981405 |
| 3 | 7 | 0 | 2.417809 | 0.621897 | -1.170357 |
| 4 | 7 | 0 | -0.698106 | 1.227519 | -1.060723 |
| 5 | 7 | 0 | 0.889820 | 1.694876 | 1.031785 |
| 6 | 7 | 0 | 0.276429 | -1.557529 | -0.913648 |
| 7 | 7 | 0 | -0.753310 | -0.702178 | 1.393110 |
| 8 | 6 | 0 | 2.287215 | -1.809961 | 2.025840 |
| 9 | 1 | 0 | 1.308336 | -1.932725 | 2.477418 |
| 10 | 6 | 0 | 3.413219 | -2.468567 | 2.538249 |
| 11 | 1 | 0 | 3.308352 | -3.119286 | 3.398992 |
| 12 | 6 | 0 | 4.635765 | -2.268567 | 1.936076 |
| 13 | 1 | 0 | 5.529583 | -2.758898 | 2.309979 |
| 14 | 6 | 0 | 4.729474 | -1.414835 | 0.820380 |
| 15 | 6 | 0 | 3.540172 | -0.804410 | 0.374932 |
| 16 | 6 | 0 | 3.575063 | 0.070839 | -0.760277 |
| 17 | 6 | 0 | 5.957866 | -1.144212 | 0.139553 |
| 18 | 1 | 0 | 6.863256 | -1.623102 | 0.499857 |
| 19 | 6 | 0 | 5.992436 | -0.306785 | -0.930602 |
| 20 | 1 | 0 | 6.926084 | -0.100938 | -1.445326 |
| 21 | 6 | 0 | 4.800271 | 0.321783 | -1.409141 |
| 22 | 6 | 0 | 4.775733 | 1.189906 | -2.517188 |
| 23 | 1 | 0 | 5.699297 | 1.408790 | -3.044735 |
| 24 | 6 | 0 | 3.581786 | 1.748025 | -2.917680 |
| 25 | 1 | 0 | 3.530047 | 2.419379 | -3.767380 |
| 26 | 6 | 0 | 2.413556 | 1.433328 | -2.210530 |
| 27 | 1 | 0 | 1.451430 | 1.844227 | -2.497846 |
| 28 | 6 | 0 | -1.445507 | 0.953862 | -2.110010 |
| 29 | 1 | 0 | -1.273982 | 0.000499 | -2.595178 |
| 30 | 6 | 0 | -2.414826 | 1.848323 | -2.585332 |
| 31 | 1 | 0 | -3.009182 | 1.579922 | -3.450706 |
| 32 | 6 | 0 | -2.603673 | 3.044585 | -1.931809 |
| 33 | 1 | 0 | -3.354766 | 3.752071 | -2.269723 |
| 34 | 6 | 0 | -1.812678 | 3.356447 | -0.808950 |
| 35 | 6 | 0 | -0.860940 | 2.399389 | -0.416431 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 6 | 0 | -0.012553 | 2.651963 | 0.701061 |
| 37 | 6 | 0 | -1.921480 | 4.574087 | -0.067846 |
| 38 | 1 | 0 | -2.663972 | 5.303293 | -0.377234 |
| 39 | 6 | 0 | -1.111166 | 4.816559 | 0.997451 |
| 40 | 1 | 0 | -1.192436 | 5.743075 | 1.557362 |
| 41 | 6 | 0 | -0.128245 | 3.861806 | 1.408532 |
| 42 | 6 | 0 | 0.742431 | 4.060795 | 2.496228 |
| 43 | 1 | 0 | 0.683371 | 4.980719 | 3.069548 |
| 44 | 6 | 0 | 1.657949 | 3.082574 | 2.814116 |
| 45 | 1 | 0 | 2.345359 | 3.201833 | 3.643665 |
| 46 | 6 | 0 | 1.699652 | 1.905823 | 2.057595 |
| 47 | 1 | 0 | 2.398267 | 1.112838 | 2.291526 |
| 48 | 6 | 0 | 0.805150 | -1.957360 | -2.060032 |
| 49 | 1 | 0 | 1.605386 | -1.348028 | -2.460498 |
| 50 | 6 | 0 | 0.356384 | -3.099938 | -2.730959 |
| 51 | 1 | 0 | 0.824864 | -3.381228 | -3.667143 |
| 52 | 6 | 0 | -0.673038 | -3.841075 | -2.194047 |
| 53 | 1 | 0 | -1.044645 | -4.728918 | -2.696239 |
| 54 | 6 | 0 | -1.250886 | -3.436595 | -0.977060 |
| 55 | 6 | 0 | -0.735854 | -2.277275 | -0.371966 |
| 56 | 6 | 0 | -1.284381 | -1.818498 | 0.861454 |
| 57 | 6 | 0 | -2.330619 | -4.130677 | -0.344806 |
| 58 | 1 | 0 | -2.724670 | -5.017638 | -0.831251 |
| 59 | 6 | 0 | -2.854077 | -3.691734 | 0.830399 |
| 60 | 1 | 0 | -3.676405 | -4.219420 | 1.303170 |
| 61 | 6 | 0 | -2.336817 | -2.523316 | 1.470283 |
| 62 | 6 | 0 | -2.826793 | -2.011422 | 2.685820 |
| 63 | 1 | 0 | -3.644591 | -2.518545 | 3.188281 |
| 64 | 6 | 0 | -2.264568 | -0.873853 | 3.221792 |
| 65 | 1 | 0 | -2.621384 | -0.456722 | 4.156515 |
| 66 | 6 | 0 | -1.221926 | -0.238394 | 2.534631 |
| 67 | 1 | 0 | -0.761052 | 0.664953 | 2.920186 |
| 68 | 16 | 0 | -4.318456 | -0.312719 | -0.341223 |
| 69 | 8 | 0 | -3.531447 | 0.645885 | 0.446291 |
| 70 | 8 | 0 | -3.562172 | -1.085120 | -1.330557 |
| 71 | 8 | 0 | -5.235161 | -1.122787 | 0.479644 |
| 72 | 8 | 0 | -5.280235 | 0.604765 | -1.311383 |
| 73 | 1 | 0 | -5.781803 | 1.238922 | -0.780656 |

Rotational constants (GHZ): 0.0987622 0.0656988

**Structures of DC-1-001**

DC1-1-001, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.759320 | 0.012050 | 0.034374 |
| 2 | 7 | 0 | 2.213548 | 0.477429 | -1.165703 |
| 3 | 7 | 0 | 2.139114 | -0.947186 | 1.010304 |
| 4 | 7 | 0 | -0.646565 | -0.556664 | 1.256493 |
| 5 | 7 | 0 | 0.307832 | -1.616583 | -0.920426 |
| 6 | 7 | 0 | 1.034032 | 1.670304 | 1.005573 |
| 7 | 7 | 0 | -0.547327 | 1.049892 | -0.965617 |
| 8 | 6 | 0 | 2.199663 | 1.221736 | -2.259379 |
| 9 | 1 | 0 | 1.244477 | 1.631541 | -2.560971 |
| 10 | 6 | 0 | 3.358288 | 1.470901 | -3.006492 |
| 11 | 1 | 0 | 3.287820 | 2.087783 | -3.895102 |
| 12 | 6 | 0 | 4.561427 | 0.930878 | -2.607815 |
| 13 | 1 | 0 | 5.470688 | 1.109421 | -3.173345 |
| 14 | 6 | 0 | 4.602586 | 0.137360 | -1.446862 |
| 15 | 6 | 0 | 3.391025 | -0.051626 | -0.764092 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | 3.348428 | -0.837333 | 0.415718 |
| 17 | 6 | 0 | 5.784827 | -0.481649 | -0.930359 |
| 18 | 1 | 0 | 6.719051 | -0.332595 | -1.462939 |
| 19 | 6 | 0 | 5.743394 | -1.239304 | 0.199743 |
| 20 | 1 | 0 | 6.643991 | -1.706091 | 0.586419 |
| 21 | 6 | 0 | 4.516840 | -1.437894 | 0.909835 |
| 22 | 6 | 0 | 4.392798 | -2.195469 | 2.088817 |
| 23 | 1 | 0 | 5.265759 | -2.680834 | 2.513982 |
| 24 | 6 | 0 | 3.156242 | -2.305301 | 2.686055 |
| 25 | 1 | 0 | 3.021953 | -2.878956 | 3.596024 |
| 26 | 6 | 0 | 2.047410 | -1.664183 | 2.118484 |
| 27 | 1 | 0 | 1.070435 | -1.733618 | 2.578966 |
| 28 | 6 | 0 | -1.075146 | 0.001855 | 2.375487 |
| 29 | 1 | 0 | -0.574758 | 0.905385 | 2.698032 |
| 30 | 6 | 0 | -2.123286 | -0.541067 | 3.129664 |
| 31 | 1 | 0 | -2.431124 | -0.037321 | 4.038812 |
| 32 | 6 | 0 | -2.748012 | -1.691511 | 2.705119 |
| 33 | 1 | 0 | -3.569264 | -2.125076 | 3.266837 |
| 34 | 6 | 0 | -2.308097 | -2.308391 | 1.519894 |
| 35 | 6 | 0 | -1.246169 | -1.693171 | 0.839819 |
| 36 | 6 | 0 | -0.730073 | -2.267542 | -0.349479 |
| 37 | 6 | 0 | -2.875786 | -3.500992 | 0.971077 |
| 38 | 1 | 0 | -3.707318 | -3.963001 | 1.493814 |
| 39 | 6 | 0 | -2.389552 | -4.044594 | -0.177594 |
| 40 | 1 | 0 | -2.826336 | -4.948956 | -0.589569 |
| 41 | 6 | 0 | -1.290508 | -3.444172 | -0.869576 |
| 42 | 6 | 0 | -0.721151 | -3.951172 | -2.051756 |
| 43 | 1 | 0 | -1.119328 | -4.856552 | -2.499040 |
| 44 | 6 | 0 | 0.340912 | -3.284711 | -2.623120 |
| 45 | 1 | 0 | 0.806280 | -3.646813 | -3.532740 |
| 46 | 6 | 0 | 0.830883 | -2.114653 | -2.028803 |
| 47 | 1 | 0 | 1.655403 | -1.568748 | -2.469083 |
| 48 | 6 | 0 | 1.876507 | 1.942688 | 1.988516 |
| 49 | 1 | 0 | 2.553648 | 1.152252 | 2.286454 |
| 50 | 6 | 0 | 1.893149 | 3.187262 | 2.631811 |
| 51 | 1 | 0 | 2.603359 | 3.355100 | 3.433364 |
| 52 | 6 | 0 | 1.009186 | 4.170890 | 2.245349 |
| 53 | 1 | 0 | 1.000881 | 5.140091 | 2.734129 |
| 54 | 6 | 0 | 0.108845 | 3.908022 | 1.196532 |
| 55 | 6 | 0 | 0.170814 | 2.633652 | 0.611644 |
| 56 | 6 | 0 | -0.692906 | 2.294427 | -0.460804 |
| 57 | 6 | 0 | -0.848916 | 4.846136 | 0.696276 |
| 58 | 1 | 0 | -0.899058 | 5.827442 | 1.157793 |
| 59 | 6 | 0 | -1.672205 | 4.522748 | -0.338562 |
| 60 | 1 | 0 | -2.390442 | 5.242204 | -0.719601 |
| 61 | 6 | 0 | -1.607910 | 3.234683 | -0.957865 |
| 62 | 6 | 0 | -2.395189 | 2.838237 | -2.054168 |
| 63 | 1 | 0 | -3.121252 | 3.526097 | -2.475903 |
| 64 | 6 | 0 | -2.222060 | 1.577333 | -2.578818 |
| 65 | 1 | 0 | -2.803646 | 1.237462 | -3.427979 |
| 66 | 6 | 0 | -1.288348 | 0.704820 | -2.004120 |
| 67 | 1 | 0 | -1.145366 | -0.291113 | -2.400983 |
| 68 | 16 | 0 | -4.224454 | -0.105957 | -0.308939 |
| 69 | 8 | 0 | -3.353676 | 0.749184 | 0.448751 |
| 70 | 8 | 0 | -3.718775 | -1.080234 | -1.239804 |
| 71 | 8 | 0 | -5.226296 | 0.884514 | -1.046497 |
| 72 | 1 | 0 | -5.811757 | 0.436582 | -1.679643 |
| 73 | 8 | 0 | -5.169337 | -0.932001 | 0.667061 |
| 74 | 1 | 0 | -5.442354 | -0.425080 | 1.450056 |

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Rotational constants (GHZ): 0.1019073 0.0693165

DC3-1-001, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.816227 | -0.190653 | 0.033833 |
| 2 | 7 | 0 | -2.268663 | 0.158016 | 1.252265 |
| 3 | 7 | 0 | -2.394602 | -1.090503 | -1.101542 |
| 4 | 7 | 0 | 0.567926 | -0.688339 | -1.216632 |
| 5 | 7 | 0 | -0.077527 | -1.922389 | 1.060138 |
| 6 | 7 | 0 | -1.145225 | 1.764074 | -0.851869 |
| 7 | 7 | 0 | 0.632400 | 1.066183 | 1.068738 |
| 8 | 6 | 0 | -2.173810 | 0.743953 | 2.435935 |
| 9 | 1 | 0 | -1.179877 | 1.029433 | 2.754452 |
| 10 | 6 | 0 | -3.291707 | 0.994101 | 3.239768 |
| 11 | 1 | 0 | -3.153281 | 1.478373 | 4.199593 |
| 12 | 6 | 0 | -4.542679 | 0.629497 | 2.795253 |
| 13 | 1 | 0 | -5.428445 | 0.820589 | 3.393027 |
| 14 | 6 | 0 | -4.669840 | -0.001483 | 1.543821 |
| 15 | 6 | 0 | -3.491525 | -0.225637 | 0.810288 |
| 16 | 6 | 0 | -3.558589 | -0.878637 | -0.455560 |
| 17 | 6 | 0 | -5.923408 | -0.415535 | 0.991674 |
| 18 | 1 | 0 | -6.824075 | -0.231397 | 1.569173 |
| 19 | 6 | 0 | -5.989569 | -1.018965 | -0.225222 |
| 20 | 1 | 0 | -6.943995 | -1.325350 | -0.642044 |
| 21 | 6 | 0 | -4.803087 | -1.267371 | -0.983512 |
| 22 | 6 | 0 | -4.793129 | -1.883882 | -2.249350 |
| 23 | 1 | 0 | -5.730549 | -2.197960 | -2.698351 |
| 24 | 6 | 0 | -3.595771 | -2.078864 | -2.903290 |
| 25 | 1 | 0 | -3.558739 | -2.547245 | -3.880118 |
| 26 | 6 | 0 | -2.405747 | -1.663948 | -2.289680 |
| 27 | 1 | 0 | -1.444011 | -1.801969 | -2.772052 |
| 28 | 6 | 0 | 0.830066 | -0.099002 | -2.372470 |
| 29 | 1 | 0 | 0.208856 | 0.746412 | -2.637728 |
| 30 | 6 | 0 | 1.855304 | -0.531101 | -3.220861 |
| 31 | 1 | 0 | 2.022888 | -0.006715 | -4.154529 |
| 32 | 6 | 0 | 2.638768 | -1.598578 | -2.848015 |
| 33 | 1 | 0 | 3.452956 | -1.945216 | -3.476496 |
| 34 | 6 | 0 | 2.377771 | -2.246749 | -1.626898 |
| 35 | 6 | 0 | 1.314885 | -1.756812 | -0.848382 |
| 36 | 6 | 0 | 0.988675 | -2.394463 | 0.384296 |
| 37 | 6 | 0 | 3.143889 | -3.353524 | -1.143552 |
| 38 | 1 | 0 | 3.969491 | -3.709772 | -1.751489 |
| 39 | 6 | 0 | 2.856230 | -3.938289 | 0.049212 |
| 40 | 1 | 0 | 3.447393 | -4.771028 | 0.417431 |
| 41 | 6 | 0 | 1.763334 | -3.473973 | 0.845188 |
| 42 | 6 | 0 | 1.400754 | -4.034700 | 2.084299 |
| 43 | 1 | 0 | 1.975481 | -4.864884 | 2.483681 |
| 44 | 6 | 0 | 0.321989 | -3.524995 | 2.774207 |
| 45 | 1 | 0 | 0.022186 | -3.935355 | 3.731713 |
| 46 | 6 | 0 | -0.401654 | -2.459929 | 2.220756 |
| 47 | 1 | 0 | -1.260580 | -2.035849 | 2.729467 |
| 48 | 6 | 0 | -2.035618 | 2.082034 | -1.772741 |
| 49 | 1 | 0 | -2.719766 | 1.298623 | -2.079586 |
| 50 | 6 | 0 | -2.099795 | 3.358801 | -2.346137 |
| 51 | 1 | 0 | -2.850245 | 3.570796 | -3.099087 |
| 52 | 6 | 0 | -1.196987 | 4.316322 | -1.941946 |
| 53 | 1 | 0 | -1.212161 | 5.314864 | -2.368157 |
| 54 | 6 | 0 | -0.239538 | 3.998126 | -0.960108 |
| 55 | 6 | 0 | -0.258316 | 2.688937 | -0.437372 |
| 56 | 6 | 0 | 0.685422 | 2.318074 | 0.576892 |
| 57 | 6 | 0 | 0.728925 | 4.935514 | -0.483963 |
| 58 | 1 | 0 | 0.729255 | 5.935912 | -0.905863 |

| | | | | | |
|---|---|---|---|---|---|
| 59 | 6 | 0 | 1.622819 | 4.584199 | 0.477229 |
| 60 | 1 | 0 | 2.355031 | 5.297481 | 0.843283 |
| 61 | 6 | 0 | 1.616985 | 3.269590 | 1.038184 |
| 62 | 6 | 0 | 2.503241 | 2.867085 | 2.054734 |
| 63 | 1 | 0 | 3.237054 | 3.571938 | 2.433437 |
| 64 | 6 | 0 | 2.422849 | 1.588625 | 2.555574 |
| 65 | 1 | 0 | 3.087040 | 1.244918 | 3.340107 |
| 66 | 6 | 0 | 1.467441 | 0.711250 | 2.025354 |
| 67 | 1 | 0 | 1.382980 | -0.304098 | 2.393850 |
| 68 | 16 | 0 | 4.255166 | 0.135076 | 0.008941 |
| 69 | 8 | 0 | 3.269643 | 0.918432 | -0.683881 |
| 70 | 8 | 0 | 3.891976 | -0.871666 | 0.970670 |
| 71 | 8 | 0 | 5.230948 | 1.200171 | 0.675014 |
| 72 | 1 | 0 | 5.877493 | 0.800309 | 1.280924 |
| 73 | 8 | 0 | 5.189819 | -0.621649 | -1.031028 |
| 74 | 1 | 0 | 5.406144 | -0.086686 | -1.812866 |

Rotational constants (GHZ): 0.0991659 0.0650914

**Structures of DC-2-110**

DC1-2-110, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.043974 | 0.740483 | 0.107162 |
| 2 | 7 | 0 | 1.614842 | 0.653120 | 1.225264 |
| 3 | 7 | 0 | 1.184672 | 1.704253 | -1.103944 |
| 4 | 7 | 0 | -1.626246 | 0.919400 | -1.079877 |
| 5 | 7 | 0 | -0.628875 | 2.381420 | 0.880090 |
| 6 | 7 | 0 | 0.459172 | -0.992648 | -0.658632 |
| 7 | 7 | 0 | -1.060459 | -0.396082 | 1.418809 |
| 8 | 6 | 0 | 1.775100 | 0.119636 | 2.425374 |
| 9 | 1 | 0 | 0.897259 | -0.306271 | 2.892860 |
| 10 | 6 | 0 | 3.016795 | 0.101500 | 3.072794 |
| 11 | 1 | 0 | 3.089615 | -0.353642 | 4.053946 |
| 12 | 6 | 0 | 4.121502 | 0.647212 | 2.457344 |
| 13 | 1 | 0 | 5.094900 | 0.634287 | 2.937035 |
| 14 | 6 | 0 | 3.974544 | 1.229543 | 1.186400 |
| 15 | 6 | 0 | 2.692186 | 1.200199 | 0.620791 |
| 16 | 6 | 0 | 2.455798 | 1.780013 | -0.650110 |
| 17 | 6 | 0 | 5.036158 | 1.833799 | 0.442015 |
| 18 | 1 | 0 | 6.031100 | 1.838691 | 0.875915 |
| 19 | 6 | 0 | 4.809919 | 2.389511 | -0.779581 |
| 20 | 1 | 0 | 5.620747 | 2.847078 | -1.337949 |
| 21 | 6 | 0 | 3.502414 | 2.384903 | -1.361559 |
| 22 | 6 | 0 | 3.180898 | 2.939129 | -2.613655 |
| 23 | 1 | 0 | 3.953683 | 3.415188 | -3.209218 |
| 24 | 6 | 0 | 1.879825 | 2.867239 | -3.064024 |
| 25 | 1 | 0 | 1.595471 | 3.285291 | -4.023055 |
| 26 | 6 | 0 | 0.902784 | 2.239284 | -2.281240 |
| 27 | 1 | 0 | -0.122483 | 2.159425 | -2.618961 |
| 28 | 6 | 0 | -2.056615 | 0.175285 | -2.077901 |
| 29 | 1 | 0 | -1.425933 | -0.650368 | -2.379550 |
| 30 | 6 | 0 | -3.271493 | 0.435556 | -2.727756 |
| 31 | 1 | 0 | -3.585323 | -0.210201 | -3.538915 |
| 32 | 6 | 0 | -4.050803 | 1.489059 | -2.311331 |
| 33 | 1 | 0 | -5.001745 | 1.704835 | -2.788667 |
| 34 | 6 | 0 | -3.608566 | 2.294701 | -1.244019 |
| 35 | 6 | 0 | -2.373470 | 1.961562 | -0.665390 |
| 36 | 6 | 0 | -1.837158 | 2.750360 | 0.389614 |
| 37 | 6 | 0 | -4.328331 | 3.419281 | -0.732681 |

| | | | | | |
|---|---|---|---|---|---|
| 38 | 1 | 0 | -5.288094 | 3.664156 | -1.177504 |
| 39 | 6 | 0 | -3.822302 | 4.170314 | 0.283079 |
| 40 | 1 | 0 | -4.370306 | 5.025473 | 0.666714 |
| 41 | 6 | 0 | -2.554098 | 3.860774 | 0.868317 |
| 42 | 6 | 0 | -1.965512 | 4.607388 | 1.905654 |
| 43 | 1 | 0 | -2.484946 | 5.471079 | 2.309209 |
| 44 | 6 | 0 | -0.732726 | 4.228628 | 2.388399 |
| 45 | 1 | 0 | -0.245875 | 4.781437 | 3.183716 |
| 46 | 6 | 0 | -0.092876 | 3.105586 | 1.849418 |
| 47 | 1 | 0 | 0.872767 | 2.785437 | 2.218813 |
| 48 | 6 | 0 | 1.184612 | -1.256648 | -1.731286 |
| 49 | 1 | 0 | 1.615076 | -0.412287 | -2.250411 |
| 50 | 6 | 0 | 1.397092 | -2.561196 | -2.192418 |
| 51 | 1 | 0 | 2.007251 | -2.714024 | -3.074746 |
| 52 | 6 | 0 | 0.839534 | -3.620303 | -1.515597 |
| 53 | 1 | 0 | 0.993220 | -4.642487 | -1.847486 |
| 54 | 6 | 0 | 0.051466 | -3.367036 | -0.378003 |
| 55 | 6 | 0 | -0.109659 | -2.025797 | 0.005701 |
| 56 | 6 | 0 | -0.931610 | -1.702899 | 1.120784 |
| 57 | 6 | 0 | -0.604814 | -4.388070 | 0.378933 |
| 58 | 1 | 0 | -0.473360 | -5.420502 | 0.069702 |
| 59 | 6 | 0 | -1.382698 | -4.078088 | 1.450483 |
| 60 | 1 | 0 | -1.886496 | -4.856712 | 2.014605 |
| 61 | 6 | 0 | -1.567787 | -2.719465 | 1.851416 |
| 62 | 6 | 0 | -2.368662 | -2.320186 | 2.935792 |
| 63 | 1 | 0 | -2.886652 | -3.070063 | 3.525485 |
| 64 | 6 | 0 | -2.488586 | -0.979962 | 3.229239 |
| 65 | 1 | 0 | -3.100430 | -0.637607 | 4.056032 |
| 66 | 6 | 0 | -1.815086 | -0.038504 | 2.440260 |
| 67 | 1 | 0 | -1.887755 | 1.021946 | 2.650471 |
| 68 | 16 | 0 | -4.390879 | -2.182303 | -0.491579 |
| 69 | 8 | 0 | -4.157941 | -0.888913 | 0.238535 |
| 70 | 8 | 0 | -3.143738 | -2.611082 | -1.216616 |
| 71 | 8 | 0 | -4.776641 | -3.249827 | 0.500522 |
| 72 | 8 | 0 | -5.504257 | -1.994764 | -1.488898 |
| 73 | 16 | 0 | 4.427856 | -1.893652 | -0.291739 |
| 74 | 8 | 0 | 4.658160 | -3.284598 | -1.140682 |
| 75 | 1 | 0 | 4.725569 | -4.037988 | -0.537430 |
| 76 | 8 | 0 | 4.207513 | -0.929303 | -1.372621 |
| 77 | 8 | 0 | 3.267120 | -2.154285 | 0.570827 |
| 78 | 8 | 0 | 5.672205 | -1.672169 | 0.465526 |

Rotational constants (GHZ): 0.0817115 0.0549566

DC3-2-110, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.051501 | 0.789094 | 0.071693 |
| 2 | 7 | 0 | 1.745867 | 0.695899 | 1.315176 |
| 3 | 7 | 0 | 1.393344 | 1.891055 | -1.078626 |
| 4 | 7 | 0 | -1.753478 | 0.994308 | -1.212358 |
| 5 | 7 | 0 | -0.766661 | 2.410619 | 0.818403 |
| 6 | 7 | 0 | 0.418535 | -0.932680 | -0.656854 |
| 7 | 7 | 0 | -1.109843 | -0.426201 | 1.474130 |
| 8 | 6 | 0 | 1.888370 | 0.110132 | 2.488366 |
| 9 | 1 | 0 | 0.988715 | -0.289691 | 2.943221 |
| 10 | 6 | 0 | 3.129751 | 0.002994 | 3.129126 |
| 11 | 1 | 0 | 3.194453 | -0.491644 | 4.091659 |
| 12 | 6 | 0 | 4.245824 | 0.521884 | 2.513219 |
| 13 | 1 | 0 | 5.225542 | 0.449221 | 2.975197 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | 4.115095 | 1.156394 | 1.264621 |
| 15 | 6 | 0 | 2.825632 | 1.212656 | 0.701696 |
| 16 | 6 | 0 | 2.636864 | 1.853883 | -0.566619 |
| 17 | 6 | 0 | 5.219464 | 1.724484 | 0.557022 |
| 18 | 1 | 0 | 6.206754 | 1.656006 | 1.003256 |
| 19 | 6 | 0 | 5.039881 | 2.333823 | -0.643858 |
| 20 | 1 | 0 | 5.879545 | 2.765608 | -1.179956 |
| 21 | 6 | 0 | 3.740705 | 2.419177 | -1.234819 |
| 22 | 6 | 0 | 3.495066 | 3.036733 | -2.475479 |
| 23 | 1 | 0 | 4.320991 | 3.480197 | -3.023484 |
| 24 | 6 | 0 | 2.212714 | 3.069686 | -2.978926 |
| 25 | 1 | 0 | 1.992243 | 3.538333 | -3.931397 |
| 26 | 6 | 0 | 1.179730 | 2.476565 | -2.241888 |
| 27 | 1 | 0 | 0.157175 | 2.466262 | -2.604841 |
| 28 | 6 | 0 | -2.196052 | 0.261796 | -2.213910 |
| 29 | 1 | 0 | -1.537668 | -0.520463 | -2.571993 |
| 30 | 6 | 0 | -3.453504 | 0.477921 | -2.795283 |
| 31 | 1 | 0 | -3.779205 | -0.155740 | -3.611408 |
| 32 | 6 | 0 | -4.258890 | 1.478391 | -2.302265 |
| 33 | 1 | 0 | -5.242195 | 1.662237 | -2.724412 |
| 34 | 6 | 0 | -3.804903 | 2.272290 | -1.230822 |
| 35 | 6 | 0 | -2.529350 | 1.979438 | -0.718239 |
| 36 | 6 | 0 | -1.998323 | 2.746242 | 0.359810 |
| 37 | 6 | 0 | -4.555664 | 3.343970 | -0.654705 |
| 38 | 1 | 0 | -5.541940 | 3.558192 | -1.055128 |
| 39 | 6 | 0 | -4.045363 | 4.083141 | 0.367034 |
| 40 | 1 | 0 | -4.614863 | 4.900089 | 0.799383 |
| 41 | 6 | 0 | -2.747016 | 3.806661 | 0.900787 |
| 42 | 6 | 0 | -2.164297 | 4.538187 | 1.952560 |
| 43 | 1 | 0 | -2.710033 | 5.363453 | 2.399399 |
| 44 | 6 | 0 | -0.907116 | 4.193624 | 2.397211 |
| 45 | 1 | 0 | -0.426443 | 4.736070 | 3.203232 |
| 46 | 6 | 0 | -0.238021 | 3.115705 | 1.806355 |
| 47 | 1 | 0 | 0.744122 | 2.808857 | 2.142515 |
| 48 | 6 | 0 | 1.131534 | -1.155691 | -1.747929 |
| 49 | 1 | 0 | 1.527269 | -0.286288 | -2.253754 |
| 50 | 6 | 0 | 1.368800 | -2.443723 | -2.239512 |
| 51 | 1 | 0 | 1.965660 | -2.563894 | -3.135635 |
| 52 | 6 | 0 | 0.851225 | -3.528221 | -1.571636 |
| 53 | 1 | 0 | 1.023347 | -4.539961 | -1.925624 |
| 54 | 6 | 0 | 0.078671 | -3.318130 | -0.414707 |
| 55 | 6 | 0 | -0.113947 | -1.990260 | 0.002316 |
| 56 | 6 | 0 | -0.932164 | -1.717297 | 1.137886 |
| 57 | 6 | 0 | -0.537724 | -4.376211 | 0.324336 |
| 58 | 1 | 0 | -0.380935 | -5.396102 | -0.013319 |
| 59 | 6 | 0 | -1.311296 | -4.116084 | 1.411492 |
| 60 | 1 | 0 | -1.786864 | -4.922334 | 1.961129 |
| 61 | 6 | 0 | -1.529570 | -2.773559 | 1.847019 |
| 62 | 6 | 0 | -2.334931 | -2.428269 | 2.947103 |
| 63 | 1 | 0 | -2.823513 | -3.212118 | 3.517682 |
| 64 | 6 | 0 | -2.499553 | -1.102243 | 3.281990 |
| 65 | 1 | 0 | -3.116912 | -0.806396 | 4.122550 |
| 66 | 6 | 0 | -1.865750 | -0.119854 | 2.509818 |
| 67 | 1 | 0 | -1.976942 | 0.935024 | 2.737959 |
| 68 | 16 | 0 | -4.341367 | -2.235563 | -0.511417 |
| 69 | 8 | 0 | -4.133295 | -0.960649 | 0.257041 |
| 70 | 8 | 0 | -3.099689 | -2.589642 | -1.284031 |
| 71 | 8 | 0 | -4.662792 | -3.351435 | 0.449299 |
| 72 | 8 | 0 | -5.488414 | -2.053644 | -1.471479 |
| 73 | 16 | 0 | 4.398861 | -1.913338 | -0.367897 |
| 74 | 8 | 0 | 4.550563 | -3.280785 | -1.270899 |
| 75 | 1 | 0 | 4.602685 | -4.057851 | -0.697061 |
| 76 | 8 | 0 | 4.195133 | -0.901739 | -1.408329 |

| | | | | | |
|---|---|---|---|---|---|
| 77 | 8 | 0 | 3.247357 | -2.154525 | 0.512695 |
| 78 | 8 | 0 | 5.668442 | -1.772516 | 0.365915 |

Rotational constants (GHZ): 0.0808107 0.0530644

**Structures of DC-2-020**

DC1-2-020, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.059988 | 0.746615 | 0.093101 |
| 2 | 7 | 0 | 1.621408 | 0.658672 | 1.224450 |
| 3 | 7 | 0 | 1.210590 | 1.709976 | -1.108146 |
| 4 | 7 | 0 | -1.605517 | 0.918598 | -1.101706 |
| 5 | 7 | 0 | -0.622058 | 2.385329 | 0.861618 |
| 6 | 7 | 0 | 0.476945 | -0.986017 | -0.672950 |
| 7 | 7 | 0 | -1.053400 | -0.389525 | 1.397821 |
| 8 | 6 | 0 | 1.771596 | 0.125741 | 2.426070 |
| 9 | 1 | 0 | 0.890039 | -0.299438 | 2.887101 |
| 10 | 6 | 0 | 3.008135 | 0.106207 | 3.083164 |
| 11 | 1 | 0 | 3.072504 | -0.348301 | 4.065193 |
| 12 | 6 | 0 | 4.118443 | 0.649524 | 2.475816 |
| 13 | 1 | 0 | 5.088053 | 0.635386 | 2.963059 |
| 14 | 6 | 0 | 3.982217 | 1.231195 | 1.203381 |
| 15 | 6 | 0 | 2.704201 | 1.203730 | 0.628024 |
| 16 | 6 | 0 | 2.478328 | 1.783757 | -0.644636 |
| 17 | 6 | 0 | 5.050476 | 1.833192 | 0.466780 |
| 18 | 1 | 0 | 6.042091 | 1.836526 | 0.908238 |
| 19 | 6 | 0 | 4.834346 | 2.389108 | -0.756550 |
| 20 | 1 | 0 | 5.650101 | 2.845260 | -1.308846 |
| 21 | 6 | 0 | 3.531190 | 2.386835 | -1.348236 |
| 22 | 6 | 0 | 3.219808 | 2.941571 | -2.602676 |
| 23 | 1 | 0 | 3.997803 | 3.416400 | -3.192395 |
| 24 | 6 | 0 | 1.921992 | 2.871880 | -3.062782 |
| 25 | 1 | 0 | 1.645603 | 3.290690 | -4.023799 |
| 26 | 6 | 0 | 0.938097 | 2.245428 | -2.287371 |
| 27 | 1 | 0 | -0.085040 | 2.167650 | -2.632095 |
| 28 | 6 | 0 | -2.029593 | 0.171485 | -2.100678 |
| 29 | 1 | 0 | -1.385346 | -0.640314 | -2.412448 |
| 30 | 6 | 0 | -3.255268 | 0.410765 | -2.737776 |
| 31 | 1 | 0 | -3.561814 | -0.234157 | -3.552696 |
| 32 | 6 | 0 | -4.051755 | 1.446992 | -2.308482 |
| 33 | 1 | 0 | -5.010498 | 1.646877 | -2.777146 |
| 34 | 6 | 0 | -3.613728 | 2.258616 | -1.244366 |
| 35 | 6 | 0 | -2.367410 | 1.946003 | -0.677691 |
| 36 | 6 | 0 | -1.837293 | 2.739233 | 0.377318 |
| 37 | 6 | 0 | -4.347954 | 3.370213 | -0.725035 |
| 38 | 1 | 0 | -5.315060 | 3.600271 | -1.161706 |
| 39 | 6 | 0 | -3.845190 | 4.128147 | 0.287084 |
| 40 | 1 | 0 | -4.403226 | 4.974418 | 0.675877 |
| 41 | 6 | 0 | -2.567834 | 3.837619 | 0.862481 |
| 42 | 6 | 0 | -1.983671 | 4.591537 | 1.897052 |
| 43 | 1 | 0 | -2.513034 | 5.446991 | 2.305145 |
| 44 | 6 | 0 | -0.742424 | 4.230206 | 2.371333 |
| 45 | 1 | 0 | -0.258547 | 4.789376 | 3.163995 |
| 46 | 6 | 0 | -0.090322 | 3.116178 | 1.828252 |
| 47 | 1 | 0 | 0.881266 | 2.808471 | 2.192676 |
| 48 | 6 | 0 | 1.211524 | -1.249931 | -1.739234 |
| 49 | 1 | 0 | 1.654678 | -0.406529 | -2.248929 |
| 50 | 6 | 0 | 1.417814 | -2.553674 | -2.205959 |
| 51 | 1 | 0 | 2.036387 | -2.706368 | -3.082405 |

| | | | | | |
|---|---|---|---|---|---|
| 52 | 6 | 0 | 0.843789 | -3.611892 | -1.541966 |
| 53 | 1 | 0 | 0.992556 | -4.633401 | -1.878076 |
| 54 | 6 | 0 | 0.046471 | -3.358578 | -0.410621 |
| 55 | 6 | 0 | -0.107437 | -2.018353 | -0.020830 |
| 56 | 6 | 0 | -0.932149 | -1.695577 | 1.092194 |
| 57 | 6 | 0 | -0.622378 | -4.379007 | 0.335915 |
| 58 | 1 | 0 | -0.496757 | -5.410632 | 0.021605 |
| 59 | 6 | 0 | -1.402585 | -4.069802 | 1.405966 |
| 60 | 1 | 0 | -1.912862 | -4.848124 | 1.964659 |
| 61 | 6 | 0 | -1.576752 | -2.712189 | 1.816213 |
| 62 | 6 | 0 | -2.372614 | -2.313691 | 2.905396 |
| 63 | 1 | 0 | -2.894588 | -3.063878 | 3.491153 |
| 64 | 6 | 0 | -2.477650 | -0.975357 | 3.211335 |
| 65 | 1 | 0 | -3.081361 | -0.634251 | 4.044579 |
| 66 | 6 | 0 | -1.799898 | -0.033794 | 2.425633 |
| 67 | 1 | 0 | -1.863276 | 1.025597 | 2.644096 |
| 68 | 16 | 0 | -4.247431 | -2.142961 | -0.368128 |
| 69 | 8 | 0 | -4.093722 | -0.821379 | 0.255253 |
| 70 | 8 | 0 | -3.127414 | -2.576684 | -1.207997 |
| 71 | 8 | 0 | -4.730989 | -3.172211 | 0.568430 |
| 72 | 8 | 0 | -5.440631 | -1.958836 | -1.486908 |
| 73 | 1 | 0 | -6.233635 | -1.593752 | -1.070115 |
| 74 | 16 | 0 | 4.429099 | -1.898528 | -0.268131 |
| 75 | 8 | 0 | 4.662566 | -3.289128 | -1.116688 |
| 76 | 1 | 0 | 4.727958 | -4.042758 | -0.513494 |
| 77 | 8 | 0 | 4.219650 | -0.932501 | -1.349656 |
| 78 | 8 | 0 | 3.260852 | -2.156988 | 0.584965 |
| 79 | 8 | 0 | 5.668029 | -1.680937 | 0.499051 |

Rotational constants (GHZ): 0.0823278 0.0550478

DC3-2-020, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.049005 | 0.783998 | 0.068242 |
| 2 | 7 | 0 | 1.740352 | 0.695037 | 1.322084 |
| 3 | 7 | 0 | 1.392376 | 1.910250 | -1.062368 |
| 4 | 7 | 0 | -1.741080 | 0.984597 | -1.228647 |
| 5 | 7 | 0 | -0.786041 | 2.390820 | 0.824574 |
| 6 | 7 | 0 | 0.438367 | -0.926828 | -0.673926 |
| 7 | 7 | 0 | -1.108091 | -0.453160 | 1.452458 |
| 8 | 6 | 0 | 1.880758 | 0.099256 | 2.490481 |
| 9 | 1 | 0 | 0.981781 | -0.311860 | 2.936524 |
| 10 | 6 | 0 | 3.119274 | -0.004458 | 3.137319 |
| 11 | 1 | 0 | 3.182308 | -0.507774 | 4.095446 |
| 12 | 6 | 0 | 4.234764 | 0.528774 | 2.532753 |
| 13 | 1 | 0 | 5.212376 | 0.459272 | 2.999626 |
| 14 | 6 | 0 | 4.106155 | 1.174365 | 1.289629 |
| 15 | 6 | 0 | 2.819570 | 1.226053 | 0.719773 |
| 16 | 6 | 0 | 2.633094 | 1.878236 | -0.543254 |
| 17 | 6 | 0 | 5.210034 | 1.758361 | 0.594324 |
| 18 | 1 | 0 | 6.195169 | 1.693310 | 1.045775 |
| 19 | 6 | 0 | 5.032432 | 2.378818 | -0.601121 |
| 20 | 1 | 0 | 5.871525 | 2.823312 | -1.127610 |
| 21 | 6 | 0 | 3.736042 | 2.459795 | -1.198783 |
| 22 | 6 | 0 | 3.492437 | 3.088881 | -2.434040 |
| 23 | 1 | 0 | 4.317762 | 3.545348 | -2.972150 |
| 24 | 6 | 0 | 2.212774 | 3.116901 | -2.944536 |
| 25 | 1 | 0 | 1.993872 | 3.594539 | -3.892893 |
| 26 | 6 | 0 | 1.180584 | 2.506862 | -2.220316 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 1 | 0 | 0.160344 | 2.492218 | -2.589538 |
| 28 | 6 | 0 | -2.167092 | 0.256842 | -2.240870 |
| 29 | 1 | 0 | -1.495287 | -0.512147 | -2.603879 |
| 30 | 6 | 0 | -3.423727 | 0.462195 | -2.827256 |
| 31 | 1 | 0 | -3.734001 | -0.163281 | -3.655948 |
| 32 | 6 | 0 | -4.246088 | 1.446396 | -2.327583 |
| 33 | 1 | 0 | -5.228735 | 1.622119 | -2.754851 |
| 34 | 6 | 0 | -3.809168 | 2.235307 | -1.245962 |
| 35 | 6 | 0 | -2.531946 | 1.954874 | -0.729895 |
| 36 | 6 | 0 | -2.018710 | 2.715650 | 0.361193 |
| 37 | 6 | 0 | -4.579016 | 3.288914 | -0.661587 |
| 38 | 1 | 0 | -5.565857 | 3.493839 | -1.065371 |
| 39 | 6 | 0 | -4.085388 | 4.022220 | 0.372349 |
| 40 | 1 | 0 | -4.669093 | 4.825332 | 0.811586 |
| 41 | 6 | 0 | -2.786270 | 3.757759 | 0.910668 |
| 42 | 6 | 0 | -2.221328 | 4.483742 | 1.975925 |
| 43 | 1 | 0 | -2.781947 | 5.295125 | 2.429638 |
| 44 | 6 | 0 | -0.962458 | 4.151233 | 2.424829 |
| 45 | 1 | 0 | -0.495084 | 4.689830 | 3.241156 |
| 46 | 6 | 0 | -0.274215 | 3.090280 | 1.825247 |
| 47 | 1 | 0 | 0.709295 | 2.792303 | 2.165308 |
| 48 | 6 | 0 | 1.158904 | -1.133427 | -1.763206 |
| 49 | 1 | 0 | 1.552756 | -0.256224 | -2.256945 |
| 50 | 6 | 0 | 1.406503 | -2.414639 | -2.267759 |
| 51 | 1 | 0 | 2.008850 | -2.521089 | -3.161914 |
| 52 | 6 | 0 | 0.892995 | -3.509619 | -1.614250 |
| 53 | 1 | 0 | 1.074259 | -4.516397 | -1.977649 |
| 54 | 6 | 0 | 0.114248 | -3.316982 | -0.458257 |
| 55 | 6 | 0 | -0.090857 | -1.994959 | -0.029218 |
| 56 | 6 | 0 | -0.913807 | -1.739575 | 1.106897 |
| 57 | 6 | 0 | -0.493755 | -4.387561 | 0.269608 |
| 58 | 1 | 0 | -0.326405 | -5.402918 | -0.076584 |
| 59 | 6 | 0 | -1.270330 | -4.144948 | 1.358693 |
| 60 | 1 | 0 | -1.736904 | -4.960685 | 1.902071 |
| 61 | 6 | 0 | -1.501360 | -2.808274 | 1.806605 |
| 62 | 6 | 0 | -2.309495 | -2.480475 | 2.910877 |
| 63 | 1 | 0 | -2.787623 | -3.274561 | 3.476108 |
| 64 | 6 | 0 | -2.487529 | -1.159436 | 3.257177 |
| 65 | 1 | 0 | -3.105394 | -0.877222 | 4.102010 |
| 66 | 6 | 0 | -1.866655 | -0.164165 | 2.490727 |
| 67 | 1 | 0 | -1.990744 | 0.887445 | 2.727154 |
| 68 | 16 | 0 | -4.179990 | -2.190005 | -0.394309 |
| 69 | 8 | 0 | -4.076250 | -0.873974 | 0.250491 |
| 70 | 8 | 0 | -3.043480 | -2.566288 | -1.239772 |
| 71 | 8 | 0 | -4.624829 | -3.252828 | 0.523729 |
| 72 | 8 | 0 | -5.378545 | -2.033158 | -1.511638 |
| 73 | 1 | 0 | -6.181361 | -1.692057 | -1.093360 |
| 74 | 16 | 0 | 4.418189 | -1.880220 | -0.370573 |
| 75 | 8 | 0 | 4.585152 | -3.239952 | -1.282503 |
| 76 | 1 | 0 | 4.636278 | -4.020904 | -0.713797 |
| 77 | 8 | 0 | 4.211407 | -0.862406 | -1.404369 |
| 78 | 8 | 0 | 3.264346 | -2.137336 | 0.502419 |
| 79 | 8 | 0 | 5.682871 | -1.734232 | 0.370594 |

Rotational constants (GHZ): 0.0813731 0.0532153

**Structures of DC-2-011**

DC1-2-011, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.004423 | 0.723048 | 0.094377 |
| 2 | 7 | 0 | -1.590482 | 0.923895 | -1.013910 |
| 3 | 7 | 0 | -0.617568 | 2.369037 | 0.918835 |
| 4 | 7 | 0 | 1.596983 | 0.623643 | 1.195965 |
| 5 | 7 | 0 | 1.132962 | 1.720183 | -1.117170 |
| 6 | 7 | 0 | -1.012984 | -0.382338 | 1.337601 |
| 7 | 7 | 0 | 0.452761 | -0.976272 | -0.730515 |
| 8 | 6 | 0 | -2.022858 | 0.182531 | -2.018208 |
| 9 | 1 | 0 | -1.397262 | -0.644470 | -2.322510 |
| 10 | 6 | 0 | -3.235638 | 0.440077 | -2.670774 |
| 11 | 1 | 0 | -3.540343 | -0.207936 | -3.484041 |
| 12 | 6 | 0 | -4.022381 | 1.492595 | -2.264294 |
| 13 | 1 | 0 | -4.970732 | 1.704629 | -2.748167 |
| 14 | 6 | 0 | -3.580249 | 2.304078 | -1.202771 |
| 15 | 6 | 0 | -2.349384 | 1.970194 | -0.618587 |
| 16 | 6 | 0 | -1.815510 | 2.762377 | 0.429362 |
| 17 | 6 | 0 | -4.290987 | 3.439739 | -0.700886 |
| 18 | 1 | 0 | -5.247990 | 3.687852 | -1.149692 |
| 19 | 6 | 0 | -3.780529 | 4.199186 | 0.307136 |
| 20 | 1 | 0 | -4.322768 | 5.063193 | 0.678808 |
| 21 | 6 | 0 | -2.516231 | 3.884741 | 0.898342 |
| 22 | 6 | 0 | -1.911657 | 4.627266 | 1.929279 |
| 23 | 1 | 0 | -2.413078 | 5.502811 | 2.329892 |
| 24 | 6 | 0 | -0.684225 | 4.227694 | 2.411070 |
| 25 | 1 | 0 | -0.186456 | 4.777202 | 3.201904 |
| 26 | 6 | 0 | -0.064581 | 3.087882 | 1.881977 |
| 27 | 1 | 0 | 0.893118 | 2.750191 | 2.256494 |
| 28 | 6 | 0 | 1.777150 | 0.076796 | 2.386247 |
| 29 | 1 | 0 | 0.912527 | -0.372132 | 2.857293 |
| 30 | 6 | 0 | 3.022674 | 0.072666 | 3.027366 |
| 31 | 1 | 0 | 3.108977 | -0.391243 | 4.003252 |
| 32 | 6 | 0 | 4.112619 | 0.644461 | 2.411179 |
| 33 | 1 | 0 | 5.089780 | 0.644160 | 2.883529 |
| 34 | 6 | 0 | 3.947291 | 1.234945 | 1.145220 |
| 35 | 6 | 0 | 2.659743 | 1.195935 | 0.589093 |
| 36 | 6 | 0 | 2.407913 | 1.789582 | -0.673884 |
| 37 | 6 | 0 | 4.998493 | 1.854924 | 0.399270 |
| 38 | 1 | 0 | 5.995572 | 1.867847 | 0.828095 |
| 39 | 6 | 0 | 4.759234 | 2.414596 | -0.817716 |
| 40 | 1 | 0 | 5.561798 | 2.883193 | -1.378782 |
| 41 | 6 | 0 | 3.446953 | 2.405584 | -1.387932 |
| 42 | 6 | 0 | 3.114322 | 2.974440 | -2.630704 |
| 43 | 1 | 0 | 3.881984 | 3.458792 | -3.226177 |
| 44 | 6 | 0 | 1.809809 | 2.908309 | -3.069863 |
| 45 | 1 | 0 | 1.515842 | 3.338753 | -4.020416 |
| 46 | 6 | 0 | 0.841005 | 2.270779 | -2.284225 |
| 47 | 1 | 0 | -0.187147 | 2.197505 | -2.614821 |
| 48 | 6 | 0 | -1.746089 | -0.030895 | 2.380617 |
| 49 | 1 | 0 | -1.825830 | 1.027494 | 2.592106 |
| 50 | 6 | 0 | -2.389703 | -0.972430 | 3.193533 |
| 51 | 1 | 0 | -2.978663 | -0.624786 | 4.034611 |
| 52 | 6 | 0 | -2.274573 | -2.314412 | 2.909276 |
| 53 | 1 | 0 | -2.771783 | -3.062021 | 3.519140 |
| 54 | 6 | 0 | -1.497874 | -2.714054 | 1.807628 |
| 55 | 6 | 0 | -0.888137 | -1.697806 | 1.057230 |
| 56 | 6 | 0 | -0.085494 | -2.021480 | -0.066197 |
| 57 | 6 | 0 | -1.304829 | -4.073221 | 1.407336 |
| 58 | 1 | 0 | -1.787977 | -4.853951 | 1.986380 |
| 59 | 6 | 0 | -0.541373 | -4.383490 | 0.324857 |
| 60 | 1 | 0 | -0.403316 | -5.416968 | 0.022375 |
| 61 | 6 | 0 | 0.090908 | -3.359779 | -0.448600 |
| 62 | 6 | 0 | 0.869667 | -3.596854 | -1.595148 |
| 63 | 1 | 0 | 1.038418 | -4.614600 | -1.932935 |

| | | | | | |
|---|---|---|---|---|---|
| 64 | 6 | 0 | 1.398991 | -2.524161 | -2.277082 |
| 65 | 1 | 0 | 1.997638 | -2.665619 | -3.169565 |
| 66 | 6 | 0 | 1.169377 | -1.222612 | -1.813528 |
| 67 | 1 | 0 | 1.576433 | -0.369505 | -2.338769 |
| 68 | 16 | 0 | 4.197600 | -1.899035 | -0.304648 |
| 69 | 8 | 0 | 3.082217 | -2.060735 | 0.586387 |
| 70 | 8 | 0 | 4.197719 | -0.925113 | -1.364078 |
| 71 | 8 | 0 | 4.456372 | -3.350251 | -0.901878 |
| 72 | 1 | 0 | 5.124873 | -3.361271 | -1.607760 |
| 73 | 16 | 0 | -4.216595 | -2.180013 | -0.345204 |
| 74 | 8 | 0 | -5.476037 | -1.904016 | -1.367277 |
| 75 | 1 | 0 | -5.658707 | -2.691864 | -1.897518 |
| 76 | 8 | 0 | -4.060042 | -0.864703 | 0.277888 |
| 77 | 8 | 0 | -4.669233 | -3.236705 | 0.576277 |
| 78 | 8 | 0 | -3.103081 | -2.607051 | -1.206474 |
| 79 | 8 | 0 | 5.521213 | -1.596123 | 0.523035 |
| 80 | 1 | 0 | 5.546196 | -2.052307 | 1.380683 |

Rotational constants (GHZ): 0.0819751 0.0566518

DC3-2-011, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.052094 | 0.809235 | 0.046193 |
| 2 | 7 | 0 | -1.763400 | 1.007145 | -1.224413 |
| 3 | 7 | 0 | -0.798714 | 2.395776 | 0.835848 |
| 4 | 7 | 0 | 1.749087 | 0.722784 | 1.285491 |
| 5 | 7 | 0 | 1.374121 | 1.949686 | -1.089042 |
| 6 | 7 | 0 | -1.077541 | -0.457320 | 1.429864 |
| 7 | 7 | 0 | 0.442320 | -0.887113 | -0.725085 |
| 8 | 6 | 0 | -2.193355 | 0.289738 | -2.242417 |
| 9 | 1 | 0 | -1.513206 | -0.458640 | -2.632113 |
| 10 | 6 | 0 | -3.464177 | 0.480290 | -2.802261 |
| 11 | 1 | 0 | -3.776973 | -0.135923 | -3.636978 |
| 12 | 6 | 0 | -4.297562 | 1.436839 | -2.268350 |
| 13 | 1 | 0 | -5.291875 | 1.599145 | -2.673197 |
| 14 | 6 | 0 | -3.857338 | 2.213427 | -1.179263 |
| 15 | 6 | 0 | -2.564855 | 1.951044 | -0.692857 |
| 16 | 6 | 0 | -2.047205 | 2.701796 | 0.402951 |
| 17 | 6 | 0 | -4.639439 | 3.236348 | -0.557897 |
| 18 | 1 | 0 | -5.638808 | 3.425884 | -0.937581 |
| 19 | 6 | 0 | -4.142371 | 3.959382 | 0.481580 |
| 20 | 1 | 0 | -4.735664 | 4.739200 | 0.949018 |
| 21 | 6 | 0 | -2.826800 | 3.714955 | 0.988365 |
| 22 | 6 | 0 | -2.256777 | 4.433091 | 2.056243 |
| 23 | 1 | 0 | -2.826442 | 5.222188 | 2.537185 |
| 24 | 6 | 0 | -0.981352 | 4.121908 | 2.472430 |
| 25 | 1 | 0 | -0.509270 | 4.655817 | 3.289113 |
| 26 | 6 | 0 | -0.282008 | 3.088415 | 1.838777 |
| 27 | 1 | 0 | 0.714827 | 2.807261 | 2.153085 |
| 28 | 6 | 0 | 1.901630 | 0.127945 | 2.452056 |
| 29 | 1 | 0 | 1.007511 | -0.282423 | 2.908189 |
| 30 | 6 | 0 | 3.146847 | 0.023858 | 3.086738 |
| 31 | 1 | 0 | 3.218762 | -0.476185 | 4.045901 |
| 32 | 6 | 0 | 4.256554 | 0.553236 | 2.469346 |
| 33 | 1 | 0 | 5.239279 | 0.482584 | 2.925318 |
| 34 | 6 | 0 | 4.116404 | 1.193320 | 1.223534 |
| 35 | 6 | 0 | 2.822561 | 1.250971 | 0.669970 |
| 36 | 6 | 0 | 2.623800 | 1.900580 | -0.592529 |
| 37 | 6 | 0 | 5.215875 | 1.762495 | 0.508986 |

| | | | | | |
|---|---|---|---|---|---|
| 38 | 1 | 0 | 6.206364 | 1.693856 | 0.948046 |
| 39 | 6 | 0 | 5.027440 | 2.373151 | -0.690036 |
| 40 | 1 | 0 | 5.863343 | 2.805316 | -1.231577 |
| 41 | 6 | 0 | 3.723089 | 2.464841 | -1.268605 |
| 42 | 6 | 0 | 3.467039 | 3.093384 | -2.501953 |
| 43 | 1 | 0 | 4.289134 | 3.536760 | -3.055656 |
| 44 | 6 | 0 | 2.179061 | 3.139176 | -2.989086 |
| 45 | 1 | 0 | 1.950013 | 3.617913 | -3.934449 |
| 46 | 6 | 0 | 1.150814 | 2.546606 | -2.244588 |
| 47 | 1 | 0 | 0.124120 | 2.546343 | -2.595648 |
| 48 | 6 | 0 | -1.821462 | -0.190922 | 2.484579 |
| 49 | 1 | 0 | -1.956439 | 0.855798 | 2.735950 |
| 50 | 6 | 0 | -2.414333 | -1.203229 | 3.250915 |
| 51 | 1 | 0 | -3.020247 | -0.938890 | 4.110033 |
| 52 | 6 | 0 | -2.225078 | -2.517542 | 2.886139 |
| 53 | 1 | 0 | -2.682099 | -3.324578 | 3.450418 |
| 54 | 6 | 0 | -1.433190 | -2.821243 | 1.763323 |
| 55 | 6 | 0 | -0.872377 | -1.736846 | 1.066271 |
| 56 | 6 | 0 | -0.065850 | -1.968441 | -0.086831 |
| 57 | 6 | 0 | -1.193428 | -4.149750 | 1.295773 |
| 58 | 1 | 0 | -1.640153 | -4.977250 | 1.837992 |
| 59 | 6 | 0 | -0.433266 | -4.370324 | 0.190821 |
| 60 | 1 | 0 | -0.259149 | -5.379203 | -0.170443 |
| 61 | 6 | 0 | 0.148050 | -3.283383 | -0.534441 |
| 62 | 6 | 0 | 0.912070 | -3.453775 | -1.702679 |
| 63 | 1 | 0 | 1.099761 | -4.453966 | -2.080524 |
| 64 | 6 | 0 | 1.400794 | -2.344363 | -2.353394 |
| 65 | 1 | 0 | 1.986752 | -2.433582 | -3.260697 |
| 66 | 6 | 0 | 1.145106 | -1.072044 | -1.830600 |
| 67 | 1 | 0 | 1.520614 | -0.184661 | -2.321499 |
| 68 | 16 | 0 | 4.194282 | -1.897450 | -0.336932 |
| 69 | 8 | 0 | 3.072951 | -2.041751 | 0.549657 |
| 70 | 8 | 0 | 4.226260 | -0.901178 | -1.375035 |
| 71 | 8 | 0 | 4.407484 | -3.343455 | -0.963892 |
| 72 | 1 | 0 | 5.086769 | -3.364154 | -1.659095 |
| 73 | 16 | 0 | -4.151509 | -2.197337 | -0.371477 |
| 74 | 8 | 0 | -5.429211 | -1.935567 | -1.374458 |
| 75 | 1 | 0 | -5.584626 | -2.710419 | -1.931760 |
| 76 | 8 | 0 | -4.034375 | -0.897439 | 0.291178 |
| 77 | 8 | 0 | -4.559865 | -3.298047 | 0.518624 |
| 78 | 8 | 0 | -3.030046 | -2.556880 | -1.253126 |
| 79 | 8 | 0 | 5.526440 | -1.657338 | 0.497149 |
| 80 | 1 | 0 | 5.530079 | -2.124771 | 1.349013 |

Rotational constants (GHZ): 0.0816933 0.0538098

**Structures of DC-2-002**

DC1-2-002, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.014470 | -0.720258 | 0.083113 |
| 2 | 7 | 0 | 1.590979 | -0.901135 | -1.041352 |
| 3 | 7 | 0 | 0.669574 | -2.343791 | 0.917125 |
| 4 | 7 | 0 | -1.574564 | -0.635916 | 1.205041 |
| 5 | 7 | 0 | -1.121947 | -1.748877 | -1.102887 |
| 6 | 7 | 0 | 1.015592 | 0.414169 | 1.305947 |
| 7 | 7 | 0 | -0.481871 | 0.962360 | -0.752789 |
| 8 | 6 | 0 | 1.990797 | -0.169590 | -2.066902 |
| 9 | 1 | 0 | 1.336140 | 0.629865 | -2.384945 |
| 10 | 6 | 0 | 3.207858 | -0.401241 | -2.721278 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 1 | 0 | 3.484537 | 0.235186 | -3.553913 |
| 12 | 6 | 0 | 4.032930 | -1.417570 | -2.295101 |
| 13 | 1 | 0 | 4.984909 | -1.608186 | -2.780636 |
| 14 | 6 | 0 | 3.621216 | -2.223109 | -1.217714 |
| 15 | 6 | 0 | 2.382871 | -1.916957 | -0.633235 |
| 16 | 6 | 0 | 1.876658 | -2.709068 | 0.428582 |
| 17 | 6 | 0 | 4.368108 | -3.328761 | -0.701233 |
| 18 | 1 | 0 | 5.330411 | -3.554901 | -1.150188 |
| 19 | 6 | 0 | 3.883115 | -4.088515 | 0.318886 |
| 20 | 1 | 0 | 4.451636 | -4.930933 | 0.700618 |
| 21 | 6 | 0 | 2.611316 | -3.803845 | 0.909650 |
| 22 | 6 | 0 | 2.031021 | -4.550848 | 1.951241 |
| 23 | 1 | 0 | 2.558575 | -5.406370 | 2.361354 |
| 24 | 6 | 0 | 0.793329 | -4.181563 | 2.430873 |
| 25 | 1 | 0 | 0.313370 | -4.736048 | 3.229177 |
| 26 | 6 | 0 | 0.139515 | -3.066542 | 1.890088 |
| 27 | 1 | 0 | -0.826684 | -2.752171 | 2.263206 |
| 28 | 6 | 0 | -1.748190 | -0.082457 | 2.393266 |
| 29 | 1 | 0 | -0.884560 | 0.381086 | 2.851697 |
| 30 | 6 | 0 | -2.986320 | -0.088953 | 3.048436 |
| 31 | 1 | 0 | -3.067364 | 0.381414 | 4.021665 |
| 32 | 6 | 0 | -4.075768 | -0.679173 | 2.449097 |
| 33 | 1 | 0 | -5.047427 | -0.687435 | 2.932559 |
| 34 | 6 | 0 | -3.917030 | -1.278071 | 1.186303 |
| 35 | 6 | 0 | -2.636475 | -1.226929 | 0.615113 |
| 36 | 6 | 0 | -2.390987 | -1.829744 | -0.644695 |
| 37 | 6 | 0 | -4.968238 | -1.918906 | 0.458341 |
| 38 | 1 | 0 | -5.960153 | -1.940561 | 0.898599 |
| 39 | 6 | 0 | -4.735082 | -2.487873 | -0.755486 |
| 40 | 1 | 0 | -5.537420 | -2.972949 | -1.302662 |
| 41 | 6 | 0 | -3.429335 | -2.467735 | -1.340123 |
| 42 | 6 | 0 | -3.102508 | -3.047179 | -2.579525 |
| 43 | 1 | 0 | -3.870172 | -3.548504 | -3.160754 |
| 44 | 6 | 0 | -1.803631 | -2.970179 | -3.033271 |
| 45 | 1 | 0 | -1.514106 | -3.409009 | -3.981336 |
| 46 | 6 | 0 | -0.835041 | -2.310461 | -2.265917 |
| 47 | 1 | 0 | 0.188770 | -2.228954 | -2.607886 |
| 48 | 6 | 0 | 1.765413 | 0.086486 | 2.344120 |
| 49 | 1 | 0 | 1.873875 | -0.968194 | 2.560875 |
| 50 | 6 | 0 | 2.392143 | 1.047376 | 3.148050 |
| 51 | 1 | 0 | 2.994488 | 0.718044 | 3.986974 |
| 52 | 6 | 0 | 2.241243 | 2.384515 | 2.859536 |
| 53 | 1 | 0 | 2.723424 | 3.147510 | 3.462491 |
| 54 | 6 | 0 | 1.448990 | 2.759659 | 1.759250 |
| 55 | 6 | 0 | 0.856464 | 1.724969 | 1.019504 |
| 56 | 6 | 0 | 0.041956 | 2.023481 | -0.102406 |
| 57 | 6 | 0 | 1.226052 | 4.111473 | 1.349331 |
| 58 | 1 | 0 | 1.693749 | 4.906741 | 1.921206 |
| 59 | 6 | 0 | 0.453805 | 4.396949 | 0.266155 |
| 60 | 1 | 0 | 0.293745 | 5.424993 | -0.043800 |
| 61 | 6 | 0 | -0.161609 | 3.354543 | -0.495669 |
| 62 | 6 | 0 | -0.952440 | 3.567084 | -1.638934 |
| 63 | 1 | 0 | -1.142410 | 4.578471 | -1.984295 |
| 64 | 6 | 0 | -1.467222 | 2.478638 | -2.306529 |
| 65 | 1 | 0 | -2.075464 | 2.600558 | -3.195347 |
| 66 | 6 | 0 | -1.210911 | 1.185728 | -1.832419 |
| 67 | 1 | 0 | -1.606803 | 0.320684 | -2.346432 |
| 68 | 16 | 0 | -4.231390 | 1.832041 | -0.295454 |
| 69 | 8 | 0 | -3.111152 | 2.009429 | 0.586557 |
| 70 | 8 | 0 | -4.229201 | 0.851901 | -1.349147 |
| 71 | 8 | 0 | -4.507068 | 3.277665 | -0.898662 |
| 72 | 1 | 0 | -5.179080 | 3.279533 | -1.601201 |
| 73 | 16 | 0 | 4.074882 | 2.063992 | -0.407271 |

| | | | | | |
|---|---|---|---|---|---|
| 74 | 8 | 0 | 5.389654 | 1.837864 | -1.272070 |
| 75 | 1 | 0 | 5.552651 | 2.546437 | -1.916584 |
| 76 | 8 | 0 | 3.899259 | 0.838187 | 0.321214 |
| 77 | 8 | 0 | 4.476684 | 3.238658 | 0.586031 |
| 78 | 8 | 0 | 3.034324 | 2.621791 | -1.230295 |
| 79 | 8 | 0 | -5.546233 | 1.521518 | 0.542827 |
| 80 | 1 | 0 | -5.572106 | 1.986320 | 1.395778 |
| 81 | 1 | 0 | 5.032798 | 2.939985 | 1.324890 |

Rotational constants (GHZ): 0.0827974 0.0569244

DC3-2-002, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.014843 | -0.925025 | 0.014328 |
| 2 | 7 | 0 | 1.600952 | -1.001666 | -1.080296 |
| 3 | 7 | 0 | 0.973658 | -2.588084 | 0.968382 |
| 4 | 7 | 0 | -1.578954 | -0.985968 | 1.098951 |
| 5 | 7 | 0 | -1.288712 | -1.880154 | -1.397937 |
| 6 | 7 | 0 | 1.060277 | 0.443717 | 1.356535 |
| 7 | 7 | 0 | -0.579024 | 1.029545 | -0.726683 |
| 8 | 6 | 0 | 1.854439 | -0.266482 | -2.150483 |
| 9 | 1 | 0 | 1.069850 | 0.403978 | -2.473507 |
| 10 | 6 | 0 | 3.073724 | -0.332598 | -2.834418 |
| 11 | 1 | 0 | 3.224898 | 0.296696 | -3.703671 |
| 12 | 6 | 0 | 4.063167 | -1.171969 | -2.376903 |
| 13 | 1 | 0 | 5.027173 | -1.225007 | -2.872695 |
| 14 | 6 | 0 | 3.813896 | -1.975211 | -1.249049 |
| 15 | 6 | 0 | 2.549869 | -1.865255 | -0.645038 |
| 16 | 6 | 0 | 2.220943 | -2.694643 | 0.466569 |
| 17 | 6 | 0 | 4.771990 | -2.883596 | -0.698362 |
| 18 | 1 | 0 | 5.748691 | -2.946428 | -1.168041 |
| 19 | 6 | 0 | 4.471534 | -3.649097 | 0.384902 |
| 20 | 1 | 0 | 5.203653 | -4.333568 | 0.802217 |
| 21 | 6 | 0 | 3.179662 | -3.578916 | 0.993322 |
| 22 | 6 | 0 | 2.791492 | -4.350253 | 2.105408 |
| 23 | 1 | 0 | 3.500334 | -5.042588 | 2.549491 |
| 24 | 6 | 0 | 1.518612 | -4.217332 | 2.616568 |
| 25 | 1 | 0 | 1.193545 | -4.796369 | 3.473393 |
| 26 | 6 | 0 | 0.629811 | -3.316755 | 2.013117 |
| 27 | 1 | 0 | -0.380379 | -3.185760 | 2.385440 |
| 28 | 6 | 0 | -1.684860 | -0.594931 | 2.358811 |
| 29 | 1 | 0 | -0.783390 | -0.221456 | 2.825878 |
| 30 | 6 | 0 | -2.892621 | -0.647767 | 3.063111 |
| 31 | 1 | 0 | -2.917191 | -0.312471 | 4.093454 |
| 32 | 6 | 0 | -4.025589 | -1.106000 | 2.431693 |
| 33 | 1 | 0 | -4.980640 | -1.140680 | 2.945992 |
| 34 | 6 | 0 | -3.939856 | -1.532145 | 1.093533 |
| 35 | 6 | 0 | -2.680902 | -1.463690 | 0.472380 |
| 36 | 6 | 0 | -2.529864 | -1.911255 | -0.872734 |
| 37 | 6 | 0 | -5.061689 | -2.008077 | 0.344922 |
| 38 | 1 | 0 | -6.028966 | -2.040500 | 0.836146 |
| 39 | 6 | 0 | -4.925847 | -2.398291 | -0.950008 |
| 40 | 1 | 0 | -5.782365 | -2.747704 | -1.518240 |
| 41 | 6 | 0 | -3.649574 | -2.363789 | -1.593436 |
| 42 | 6 | 0 | -3.430892 | -2.760045 | -2.926368 |
| 43 | 1 | 0 | -4.267492 | -3.108802 | -3.524354 |
| 44 | 6 | 0 | -2.159774 | -2.701097 | -3.455800 |
| 45 | 1 | 0 | -1.963163 | -2.996712 | -4.480033 |
| 46 | 6 | 0 | -1.103897 | -2.254255 | -2.649835 |

| | | | | | |
|---|---|---|---|---|---|
| 47 | 1 | 0 | -0.088921 | -2.198676 | -3.028240 |
| 48 | 6 | 0 | 1.871671 | 0.139584 | 2.351074 |
| 49 | 1 | 0 | 2.026904 | -0.914238 | 2.551806 |
| 50 | 6 | 0 | 2.506456 | 1.111898 | 3.134299 |
| 51 | 1 | 0 | 3.165179 | 0.804898 | 3.938627 |
| 52 | 6 | 0 | 2.278692 | 2.439385 | 2.857668 |
| 53 | 1 | 0 | 2.755060 | 3.224006 | 3.437605 |
| 54 | 6 | 0 | 1.413245 | 2.788079 | 1.804232 |
| 55 | 6 | 0 | 0.822393 | 1.737851 | 1.072101 |
| 56 | 6 | 0 | -0.054449 | 2.047196 | -0.020178 |
| 57 | 6 | 0 | 1.128399 | 4.144059 | 1.455766 |
| 58 | 1 | 0 | 1.600981 | 4.933910 | 2.031383 |
| 59 | 6 | 0 | 0.288609 | 4.436126 | 0.429566 |
| 60 | 1 | 0 | 0.070777 | 5.466045 | 0.163790 |
| 61 | 6 | 0 | -0.322310 | 3.394749 | -0.334191 |
| 62 | 6 | 0 | -1.177948 | 3.650201 | -1.421139 |
| 63 | 1 | 0 | -1.410568 | 4.676778 | -1.687307 |
| 64 | 6 | 0 | -1.699130 | 2.596088 | -2.134438 |
| 65 | 1 | 0 | -2.358380 | 2.754076 | -2.980110 |
| 66 | 6 | 0 | -1.368151 | 1.290500 | -1.750557 |
| 67 | 1 | 0 | -1.756373 | 0.440201 | -2.297658 |
| 68 | 16 | 0 | -4.267807 | 1.756948 | 0.087091 |
| 69 | 8 | 0 | -3.099660 | 1.809915 | 0.922311 |
| 70 | 8 | 0 | -4.330285 | 0.931039 | -1.089754 |
| 71 | 8 | 0 | -4.567730 | 3.270746 | -0.295117 |
| 72 | 1 | 0 | -5.271570 | 3.363710 | -0.959054 |
| 73 | 16 | 0 | 3.884844 | 2.216138 | -0.611444 |
| 74 | 8 | 0 | 5.159160 | 2.024059 | -1.542571 |
| 75 | 1 | 0 | 5.263139 | 2.725725 | -2.206220 |
| 76 | 8 | 0 | 3.831057 | 1.020223 | 0.182540 |
| 77 | 8 | 0 | 4.273111 | 3.464618 | 0.293561 |
| 78 | 8 | 0 | 2.760678 | 2.666461 | -1.388999 |
| 79 | 8 | 0 | -5.538115 | 1.331839 | 0.943927 |
| 80 | 1 | 0 | -5.523032 | 1.682638 | 1.849828 |
| 81 | 1 | 0 | 4.933106 | 3.253042 | 0.974721 |

Rotational constants (GHZ): 0.0808610 0.0542103

**Structures of DC-3-030**

DC1-3-030, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.060038 | 0.660123 | 0.007222 |
| 2 | 7 | 0 | -1.273482 | 1.913457 | -0.842923 |
| 3 | 7 | 0 | 0.985845 | 2.248360 | 0.384199 |
| 4 | 7 | 0 | 1.232486 | -0.543026 | 0.833064 |
| 5 | 7 | 0 | 0.949632 | 0.321107 | -1.599438 |
| 6 | 7 | 0 | -1.129677 | 0.831424 | 1.755015 |
| 7 | 7 | 0 | -1.251416 | -0.855732 | -0.274345 |
| 8 | 6 | 0 | -2.423433 | 1.685295 | -1.452544 |
| 9 | 1 | 0 | -2.751836 | 0.658838 | -1.520059 |
| 10 | 6 | 0 | -3.200682 | 2.720663 | -1.990272 |
| 11 | 1 | 0 | -4.140636 | 2.472718 | -2.470008 |
| 12 | 6 | 0 | -2.764667 | 4.023852 | -1.902985 |
| 13 | 1 | 0 | -3.349144 | 4.840596 | -2.315320 |
| 14 | 6 | 0 | -1.538548 | 4.291919 | -1.264461 |
| 15 | 6 | 0 | -0.838376 | 3.190340 | -0.750449 |
| 16 | 6 | 0 | 0.400680 | 3.372259 | -0.088365 |
| 17 | 6 | 0 | -0.969449 | 5.595630 | -1.108663 |
| 18 | 1 | 0 | -1.512046 | 6.446216 | -1.509847 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 6 | 0 | 0.222265 | 5.770762 | -0.472949 |
| 20 | 1 | 0 | 0.646195 | 6.763611 | -0.357343 |
| 21 | 6 | 0 | 0.943707 | 4.657088 | 0.062902 |
| 22 | 6 | 0 | 2.169560 | 4.751884 | 0.748810 |
| 23 | 1 | 0 | 2.635991 | 5.721940 | 0.890796 |
| 24 | 6 | 0 | 2.753699 | 3.603044 | 1.234027 |
| 25 | 1 | 0 | 3.695480 | 3.635501 | 1.770114 |
| 26 | 6 | 0 | 2.129119 | 2.363522 | 1.036871 |
| 27 | 1 | 0 | 2.574066 | 1.455153 | 1.415074 |
| 28 | 6 | 0 | 1.359948 | -0.923344 | 2.093918 |
| 29 | 1 | 0 | 0.677537 | -0.483242 | 2.809644 |
| 30 | 6 | 0 | 2.331499 | -1.845705 | 2.501099 |
| 31 | 1 | 0 | 2.389372 | -2.118854 | 3.548550 |
| 32 | 6 | 0 | 3.189728 | -2.391827 | 1.573249 |
| 33 | 1 | 0 | 3.947460 | -3.112015 | 1.864628 |
| 34 | 6 | 0 | 3.081869 | -1.995430 | 0.230348 |
| 35 | 6 | 0 | 2.082070 | -1.062751 | -0.077821 |
| 36 | 6 | 0 | 1.928230 | -0.590643 | -1.405086 |
| 37 | 6 | 0 | 3.920052 | -2.474848 | -0.823545 |
| 38 | 1 | 0 | 4.683800 | -3.206492 | -0.580563 |
| 39 | 6 | 0 | 3.774287 | -2.021546 | -2.097170 |
| 40 | 1 | 0 | 4.418985 | -2.384412 | -2.891661 |
| 41 | 6 | 0 | 2.772963 | -1.054040 | -2.424689 |
| 42 | 6 | 0 | 2.570421 | -0.520924 | -3.709414 |
| 43 | 1 | 0 | 3.195324 | -0.847123 | -4.535077 |
| 44 | 6 | 0 | 1.577619 | 0.416955 | -3.896851 |
| 45 | 1 | 0 | 1.395082 | 0.852912 | -4.872581 |
| 46 | 6 | 0 | 0.781467 | 0.815128 | -2.816294 |
| 47 | 1 | 0 | -0.011712 | 1.540235 | -2.945050 |
| 48 | 6 | 0 | -1.042656 | 1.721301 | 2.725577 |
| 49 | 1 | 0 | -0.332934 | 2.528524 | 2.588219 |
| 50 | 6 | 0 | -1.821395 | 1.627172 | 3.886639 |
| 51 | 1 | 0 | -1.717634 | 2.381753 | 4.658091 |
| 52 | 6 | 0 | -2.700504 | 0.575419 | 4.029528 |
| 53 | 1 | 0 | -3.313299 | 0.477608 | 4.920512 |
| 54 | 6 | 0 | -2.807267 | -0.381637 | 3.003592 |
| 55 | 6 | 0 | -1.988128 | -0.199879 | 1.876025 |
| 56 | 6 | 0 | -2.053769 | -1.110371 | 0.785346 |
| 57 | 6 | 0 | -3.694182 | -1.502016 | 3.039516 |
| 58 | 1 | 0 | -4.321282 | -1.637534 | 3.915334 |
| 59 | 6 | 0 | -3.760810 | -2.369398 | 1.994491 |
| 60 | 1 | 0 | -4.445166 | -3.211623 | 2.017201 |
| 61 | 6 | 0 | -2.947483 | -2.191653 | 0.831809 |
| 62 | 6 | 0 | -3.010822 | -3.023296 | -0.300231 |
| 63 | 1 | 0 | -3.693010 | -3.867429 | -0.310326 |
| 64 | 6 | 0 | -2.210438 | -2.740538 | -1.380492 |
| 65 | 1 | 0 | -2.233006 | -3.352239 | -2.274250 |
| 66 | 6 | 0 | -1.337166 | -1.647870 | -1.328920 |
| 67 | 1 | 0 | -0.697256 | -1.412922 | -2.168061 |
| 68 | 16 | 0 | 0.714138 | -4.450527 | -0.369424 |
| 69 | 8 | 0 | 0.154655 | -3.679356 | 0.742240 |
| 70 | 8 | 0 | 0.859206 | -3.719997 | -1.637486 |
| 71 | 8 | 0 | -0.480185 | -5.550791 | -0.636693 |
| 72 | 1 | 0 | -0.295361 | -6.057963 | -1.439149 |
| 73 | 16 | 0 | -5.481406 | -0.133002 | -0.537375 |
| 74 | 8 | 0 | -6.625340 | 0.929619 | -1.054244 |
| 75 | 1 | 0 | -7.151436 | 0.538402 | -1.765935 |
| 76 | 8 | 0 | -4.765266 | 0.672536 | 0.455022 |
| 77 | 8 | 0 | -6.217584 | -1.278231 | 0.020507 |
| 78 | 8 | 0 | -4.702168 | -0.477813 | -1.737699 |
| 79 | 16 | 0 | 5.406138 | 0.922298 | 0.640962 |
| 80 | 8 | 0 | 6.279389 | -0.427544 | 0.316006 |
| 81 | 1 | 0 | 6.832348 | -0.660964 | 1.074791 |

| | | | | | |
|---|---|---|---|---|---|
| 82 | 8 | 0 | 4.591203 | 1.052073 | -0.570261 |
| 83 | 8 | 0 | 6.387415 | 2.004522 | 0.826373 |
| 84 | 8 | 0 | 4.650989 | 0.615246 | 1.867005 |
| 85 | 8 | 0 | 1.910562 | -5.235381 | -0.017818 |

Rotational constants (GHZ): 0.0625015 0.0450395

DC3-3-030, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.008485 | -0.493137 | 0.252548 |
| 2 | 7 | 0 | 0.496286 | -2.085419 | -0.703482 |
| 3 | 7 | 0 | -1.378145 | -1.845812 | 1.174440 |
| 4 | 7 | 0 | -0.746503 | 1.049689 | 1.134457 |
| 5 | 7 | 0 | -1.336799 | 0.105730 | -1.290611 |
| 6 | 7 | 0 | 1.595108 | -0.757154 | 1.688601 |
| 7 | 7 | 0 | 1.600328 | 0.782883 | -0.520049 |
| 8 | 6 | 0 | 1.443247 | -2.176216 | -1.622336 |
| 9 | 1 | 0 | 2.063232 | -1.303426 | -1.764593 |
| 10 | 6 | 0 | 1.644572 | -3.339925 | -2.374422 |
| 11 | 1 | 0 | 2.445781 | -3.361801 | -3.104327 |
| 12 | 6 | 0 | 0.824481 | -4.427161 | -2.175628 |
| 13 | 1 | 0 | 0.953112 | -5.339406 | -2.750131 |
| 14 | 6 | 0 | -0.198664 | -4.350628 | -1.210785 |
| 15 | 6 | 0 | -0.317408 | -3.149282 | -0.490970 |
| 16 | 6 | 0 | -1.326529 | -3.014794 | 0.506378 |
| 17 | 6 | 0 | -1.111284 | -5.417703 | -0.935861 |
| 18 | 1 | 0 | -1.011437 | -6.337862 | -1.503493 |
| 19 | 6 | 0 | -2.080321 | -5.286635 | 0.010252 |
| 20 | 1 | 0 | -2.770364 | -6.099912 | 0.213358 |
| 21 | 6 | 0 | -2.209610 | -4.078435 | 0.763602 |
| 22 | 6 | 0 | -3.173927 | -3.875546 | 1.769533 |
| 23 | 1 | 0 | -3.881372 | -4.666487 | 1.999585 |
| 24 | 6 | 0 | -3.206385 | -2.678833 | 2.449350 |
| 25 | 1 | 0 | -3.937557 | -2.493508 | 3.227503 |
| 26 | 6 | 0 | -2.284840 | -1.676315 | 2.114811 |
| 27 | 1 | 0 | -2.285111 | -0.720046 | 2.624177 |
| 28 | 6 | 0 | -0.468976 | 1.473772 | 2.357894 |
| 29 | 1 | 0 | 0.295156 | 0.929610 | 2.896857 |
| 30 | 6 | 0 | -1.122282 | 2.563601 | 2.941043 |
| 31 | 1 | 0 | -0.848714 | 2.867616 | 3.944890 |
| 32 | 6 | 0 | -2.091448 | 3.231990 | 2.228066 |
| 33 | 1 | 0 | -2.611178 | 4.085929 | 2.650956 |
| 34 | 6 | 0 | -2.415299 | 2.791952 | 0.933747 |
| 35 | 6 | 0 | -1.709731 | 1.687437 | 0.429056 |
| 36 | 6 | 0 | -2.021141 | 1.183217 | -0.867854 |
| 37 | 6 | 0 | -3.424378 | 3.402987 | 0.125654 |
| 38 | 1 | 0 | -3.955545 | 4.258830 | 0.530258 |
| 39 | 6 | 0 | -3.714992 | 2.927432 | -1.113460 |
| 40 | 1 | 0 | -4.483894 | 3.393229 | -1.722216 |
| 41 | 6 | 0 | -3.016000 | 1.800124 | -1.644748 |
| 42 | 6 | 0 | -3.267290 | 1.249803 | -2.913864 |
| 43 | 1 | 0 | -4.028946 | 1.694370 | -3.547209 |
| 44 | 6 | 0 | -2.549872 | 0.151378 | -3.335322 |
| 45 | 1 | 0 | -2.724078 | -0.295866 | -4.307364 |
| 46 | 6 | 0 | -1.586082 | -0.400592 | -2.482433 |
| 47 | 1 | 0 | -1.008226 | -1.271342 | -2.773732 |
| 48 | 6 | 0 | 1.594720 | -1.579311 | 2.719677 |
| 49 | 1 | 0 | 0.742274 | -2.245249 | 2.805314 |
| 50 | 6 | 0 | 2.627185 | -1.590127 | 3.666883 |

| | | | | | |
|---|---|---|---|---|---|
| 51 | 1 | 0 | 2.586348 | -2.285584 | 4.497696 |
| 52 | 6 | 0 | 3.672214 | -0.703949 | 3.524226 |
| 53 | 1 | 0 | 4.484402 | -0.678721 | 4.244762 |
| 54 | 6 | 0 | 3.693884 | 0.175349 | 2.425949 |
| 55 | 6 | 0 | 2.619852 | 0.097403 | 1.518170 |
| 56 | 6 | 0 | 2.616490 | 0.925641 | 0.349880 |
| 57 | 6 | 0 | 4.749109 | 1.109347 | 2.188813 |
| 58 | 1 | 0 | 5.565249 | 1.158843 | 2.903329 |
| 59 | 6 | 0 | 4.740036 | 1.903299 | 1.085719 |
| 60 | 1 | 0 | 5.549748 | 2.602106 | 0.898656 |
| 61 | 6 | 0 | 3.680865 | 1.820101 | 0.129941 |
| 62 | 6 | 0 | 3.653691 | 2.572106 | -1.059361 |
| 63 | 1 | 0 | 4.455619 | 3.274373 | -1.266099 |
| 64 | 6 | 0 | 2.617010 | 2.399224 | -1.945387 |
| 65 | 1 | 0 | 2.566802 | 2.958434 | -2.872325 |
| 66 | 6 | 0 | 1.598278 | 1.489382 | -1.631392 |
| 67 | 1 | 0 | 0.762807 | 1.331645 | -2.303349 |
| 68 | 16 | 0 | 0.194252 | 4.640814 | -0.417800 |
| 69 | 8 | 0 | 0.908907 | 3.845619 | 0.582404 |
| 70 | 8 | 0 | -0.377474 | 3.879200 | -1.538347 |
| 71 | 8 | 0 | 1.421217 | 5.521816 | -1.071366 |
| 72 | 1 | 0 | 1.092281 | 6.060327 | -1.804555 |
| 73 | 16 | 0 | 4.924968 | -1.542490 | -0.944692 |
| 74 | 8 | 0 | 5.430504 | -2.870826 | -1.773188 |
| 75 | 1 | 0 | 6.002796 | -2.610632 | -2.508572 |
| 76 | 8 | 0 | 4.028177 | -2.144725 | 0.044157 |
| 77 | 8 | 0 | 6.138021 | -0.934370 | -0.375137 |
| 78 | 8 | 0 | 4.268597 | -0.688947 | -1.948679 |
| 79 | 16 | 0 | -5.022640 | -0.768972 | 0.090255 |
| 80 | 8 | 0 | -5.785676 | 0.145678 | -1.046772 |
| 81 | 1 | 0 | -5.973154 | 1.024178 | -0.688913 |
| 82 | 8 | 0 | -4.085126 | -1.558725 | -0.713020 |
| 83 | 8 | 0 | -6.078425 | -1.577155 | 0.723085 |
| 84 | 8 | 0 | -4.411447 | 0.208979 | 1.002769 |
| 85 | 8 | 0 | -0.744638 | 5.624994 | 0.148675 |

Rotational constants (GHZ): 0.0608223 0.0476785

**Structures of DC-3-021**

DC1-3-021a, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.066118 | 0.666761 | 0.004425 |
| 2 | 7 | 0 | -1.270294 | 1.947063 | -0.818567 |
| 3 | 7 | 0 | 0.985145 | 2.240588 | 0.426834 |
| 4 | 7 | 0 | 1.220219 | -0.559236 | 0.806678 |
| 5 | 7 | 0 | 0.945728 | 0.360850 | -1.607041 |
| 6 | 7 | 0 | -1.142051 | 0.793312 | 1.752091 |
| 7 | 7 | 0 | -1.258476 | -0.838546 | -0.322120 |
| 8 | 6 | 0 | -2.419852 | 1.739804 | -1.436547 |
| 9 | 1 | 0 | -2.753585 | 0.717032 | -1.530087 |
| 10 | 6 | 0 | -3.190451 | 2.792220 | -1.950101 |
| 11 | 1 | 0 | -4.130690 | 2.561387 | -2.437799 |
| 12 | 6 | 0 | -2.747932 | 4.090577 | -1.829392 |
| 13 | 1 | 0 | -3.327371 | 4.920314 | -2.222452 |
| 14 | 6 | 0 | -1.522123 | 4.336515 | -1.181629 |
| 15 | 6 | 0 | -0.828986 | 3.218958 | -0.693079 |
| 16 | 6 | 0 | 0.407914 | 3.378475 | -0.021305 |
| 17 | 6 | 0 | -0.947391 | 5.633210 | -0.991447 |
| 18 | 1 | 0 | -1.484487 | 6.496175 | -1.373115 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 6 | 0 | 0.242440 | 5.786681 | -0.346764 |
| 20 | 1 | 0 | 0.670705 | 6.774201 | -0.204529 |
| 21 | 6 | 0 | 0.956061 | 4.656592 | 0.164615 |
| 22 | 6 | 0 | 2.178529 | 4.728758 | 0.859315 |
| 23 | 1 | 0 | 2.648742 | 5.692759 | 1.027620 |
| 24 | 6 | 0 | 2.754422 | 3.565664 | 1.319562 |
| 25 | 1 | 0 | 3.693342 | 3.580082 | 1.861378 |
| 26 | 6 | 0 | 2.125099 | 2.334467 | 1.088662 |
| 27 | 1 | 0 | 2.564166 | 1.415441 | 1.447182 |
| 28 | 6 | 0 | 1.346059 | -0.967010 | 2.058425 |
| 29 | 1 | 0 | 0.661829 | -0.544715 | 2.782944 |
| 30 | 6 | 0 | 2.319120 | -1.895854 | 2.448203 |
| 31 | 1 | 0 | 2.376016 | -2.189905 | 3.489994 |
| 32 | 6 | 0 | 3.180869 | -2.419654 | 1.511608 |
| 33 | 1 | 0 | 3.940498 | -3.143431 | 1.788980 |
| 34 | 6 | 0 | 3.072173 | -1.997324 | 0.175694 |
| 35 | 6 | 0 | 2.072106 | -1.058453 | -0.114170 |
| 36 | 6 | 0 | 1.916950 | -0.562788 | -1.432757 |
| 37 | 6 | 0 | 3.907175 | -2.460062 | -0.888376 |
| 38 | 1 | 0 | 4.672429 | -3.194597 | -0.659282 |
| 39 | 6 | 0 | 3.754111 | -1.990008 | -2.155122 |
| 40 | 1 | 0 | 4.394866 | -2.342129 | -2.957563 |
| 41 | 6 | 0 | 2.754285 | -1.014683 | -2.463320 |
| 42 | 6 | 0 | 2.551133 | -0.457780 | -3.738066 |
| 43 | 1 | 0 | 3.170391 | -0.774284 | -4.571659 |
| 44 | 6 | 0 | 1.566957 | 0.492796 | -3.904482 |
| 45 | 1 | 0 | 1.385325 | 0.948676 | -4.871209 |
| 46 | 6 | 0 | 0.778763 | 0.879310 | -2.813708 |
| 47 | 1 | 0 | -0.007395 | 1.614709 | -2.926012 |
| 48 | 6 | 0 | -1.056878 | 1.655380 | 2.747615 |
| 49 | 1 | 0 | -0.351604 | 2.469858 | 2.632002 |
| 50 | 6 | 0 | -1.831528 | 1.523374 | 3.907805 |
| 51 | 1 | 0 | -1.729125 | 2.255758 | 4.700518 |
| 52 | 6 | 0 | -2.704149 | 0.462968 | 4.023327 |
| 53 | 1 | 0 | -3.312880 | 0.335340 | 4.913297 |
| 54 | 6 | 0 | -2.809308 | -0.463993 | 2.970038 |
| 55 | 6 | 0 | -1.995123 | -0.245093 | 1.845893 |
| 56 | 6 | 0 | -2.058876 | -1.124983 | 0.730055 |
| 57 | 6 | 0 | -3.689809 | -1.590128 | 2.976777 |
| 58 | 1 | 0 | -4.313229 | -1.753974 | 3.850326 |
| 59 | 6 | 0 | -3.754808 | -2.428577 | 1.908604 |
| 60 | 1 | 0 | -4.434000 | -3.275157 | 1.909756 |
| 61 | 6 | 0 | -2.945732 | -2.213315 | 0.749425 |
| 62 | 6 | 0 | -3.004399 | -3.016124 | -0.402600 |
| 63 | 1 | 0 | -3.681084 | -3.864070 | -0.434453 |
| 64 | 6 | 0 | -2.208457 | -2.698373 | -1.478185 |
| 65 | 1 | 0 | -2.233242 | -3.283329 | -2.390167 |
| 66 | 6 | 0 | -1.343749 | -1.600417 | -1.399609 |
| 67 | 1 | 0 | -0.707072 | -1.339440 | -2.234198 |
| 68 | 16 | 0 | 0.608790 | -4.310058 | -0.360357 |
| 69 | 8 | 0 | 0.130343 | -3.522588 | 0.741661 |
| 70 | 8 | 0 | 0.880263 | -3.738636 | -1.652955 |
| 71 | 8 | 0 | -0.441598 | -5.495846 | -0.503321 |
| 72 | 1 | 0 | -0.306879 | -6.028980 | -1.304475 |
| 73 | 16 | 0 | -5.468456 | -0.120076 | -0.549099 |
| 74 | 8 | 0 | -6.614562 | 0.951826 | -1.040638 |
| 75 | 1 | 0 | -7.146815 | 0.572280 | -1.754139 |
| 76 | 8 | 0 | -4.752249 | 0.663735 | 0.460498 |
| 77 | 8 | 0 | -6.202670 | -1.279011 | -0.017608 |
| 78 | 8 | 0 | -4.688691 | -0.436168 | -1.757118 |
| 79 | 16 | 0 | 5.388736 | 0.910173 | 0.618671 |
| 80 | 8 | 0 | 6.271683 | -0.423235 | 0.252607 |
| 81 | 1 | 0 | 6.825937 | -0.675289 | 1.004449 |

| | | | | | |
|---|---|---|---|---|---|
| 82 | 8 | 0 | 4.559414 | 1.060008 | -0.580312 |
| 83 | 8 | 0 | 6.361002 | 1.997793 | 0.819010 |
| 84 | 8 | 0 | 4.651186 | 0.565522 | 1.845434 |
| 85 | 8 | 0 | 1.954997 | -5.054935 | 0.043166 |
| 86 | 1 | 0 | 1.986638 | -5.303846 | 0.981922 |

Rotational constants (GHZ): 0.0629678 0.0452594

DC1-3-021b, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.007485 | -0.487172 | 0.254483 |
| 2 | 7 | 0 | 0.633846 | -2.023098 | -0.734176 |
| 3 | 7 | 0 | -1.318767 | -1.743635 | 0.955966 |
| 4 | 7 | 0 | -0.812588 | 1.009169 | 1.208005 |
| 5 | 7 | 0 | -1.238676 | 0.019318 | -1.162268 |
| 6 | 7 | 0 | 1.252471 | -0.826198 | 1.690596 |
| 7 | 7 | 0 | 1.384083 | 0.705900 | -0.405463 |
| 8 | 6 | 0 | 1.639548 | -2.107585 | -1.587471 |
| 9 | 1 | 0 | 2.197297 | -1.200873 | -1.769306 |
| 10 | 6 | 0 | 1.961629 | -3.301171 | -2.245938 |
| 11 | 1 | 0 | 2.802852 | -3.312916 | -2.930105 |
| 12 | 6 | 0 | 1.206308 | -4.431691 | -2.022058 |
| 13 | 1 | 0 | 1.433694 | -5.366409 | -2.525317 |
| 14 | 6 | 0 | 0.119817 | -4.363051 | -1.129940 |
| 15 | 6 | 0 | -0.115471 | -3.125556 | -0.510931 |
| 16 | 6 | 0 | -1.189005 | -2.969859 | 0.401640 |
| 17 | 6 | 0 | -0.749461 | -5.457033 | -0.821711 |
| 18 | 1 | 0 | -0.568217 | -6.412031 | -1.305349 |
| 19 | 6 | 0 | -1.778597 | -5.308459 | 0.057556 |
| 20 | 1 | 0 | -2.431563 | -6.144270 | 0.289554 |
| 21 | 6 | 0 | -2.023719 | -4.055702 | 0.704341 |
| 22 | 6 | 0 | -3.043669 | -3.829852 | 1.647349 |
| 23 | 1 | 0 | -3.721061 | -4.634750 | 1.914911 |
| 24 | 6 | 0 | -3.158560 | -2.583730 | 2.219361 |
| 25 | 1 | 0 | -3.928536 | -2.371133 | 2.951654 |
| 26 | 6 | 0 | -2.276731 | -1.560097 | 1.847095 |
| 27 | 1 | 0 | -2.356562 | -0.575885 | 2.286090 |
| 28 | 6 | 0 | -0.571223 | 1.466785 | 2.425676 |
| 29 | 1 | 0 | 0.190830 | 0.957478 | 3.001284 |
| 30 | 6 | 0 | -1.267878 | 2.553479 | 2.967224 |
| 31 | 1 | 0 | -1.025935 | 2.885589 | 3.970406 |
| 32 | 6 | 0 | -2.238197 | 3.184352 | 2.221022 |
| 33 | 1 | 0 | -2.786987 | 4.033135 | 2.616745 |
| 34 | 6 | 0 | -2.517498 | 2.712850 | 0.927375 |
| 35 | 6 | 0 | -1.768272 | 1.617500 | 0.473813 |
| 36 | 6 | 0 | -2.003133 | 1.075913 | -0.815475 |
| 37 | 6 | 0 | -3.505805 | 3.275291 | 0.060559 |
| 38 | 1 | 0 | -4.077947 | 4.126097 | 0.417092 |
| 39 | 6 | 0 | -3.724922 | 2.760658 | -1.178726 |
| 40 | 1 | 0 | -4.476276 | 3.192090 | -1.832862 |
| 41 | 6 | 0 | -2.972293 | 1.642735 | -1.655456 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 6 | 0 | -3.129608 | 1.066576 | -2.926775 |
| 43 | 1 | 0 | -3.866139 | 1.469049 | -3.615119 |
| 44 | 6 | 0 | -2.339866 | -0.005946 | -3.277146 |
| 45 | 1 | 0 | -2.431353 | -0.477664 | -4.248885 |
| 46 | 6 | 0 | -1.404864 | -0.507627 | -2.364417 |
| 47 | 1 | 0 | -0.776340 | -1.349523 | -2.623307 |
| 48 | 6 | 0 | 1.164096 | -1.665347 | 2.710041 |
| 49 | 1 | 0 | 0.294858 | -2.309564 | 2.740673 |
| 50 | 6 | 0 | 2.135727 | -1.719172 | 3.717131 |
| 51 | 1 | 0 | 2.011831 | -2.425601 | 4.530110 |
| 52 | 6 | 0 | 3.224004 | -0.875208 | 3.665859 |
| 53 | 1 | 0 | 3.985813 | -0.895644 | 4.439208 |
| 54 | 6 | 0 | 3.346163 | 0.017024 | 2.586269 |
| 55 | 6 | 0 | 2.326284 | -0.008672 | 1.622971 |
| 56 | 6 | 0 | 2.395242 | 0.830965 | 0.482618 |
| 57 | 6 | 0 | 4.439101 | 0.921193 | 2.402757 |
| 58 | 1 | 0 | 5.222636 | 0.943175 | 3.153997 |
| 59 | 6 | 0 | 4.503588 | 1.728023 | 1.309047 |
| 60 | 1 | 0 | 5.342315 | 2.402550 | 1.168744 |
| 61 | 6 | 0 | 3.485348 | 1.694428 | 0.304646 |
| 62 | 6 | 0 | 3.515672 | 2.446196 | -0.883822 |
| 63 | 1 | 0 | 4.340616 | 3.125869 | -1.072341 |
| 64 | 6 | 0 | 2.493984 | 2.296952 | -1.792200 |
| 65 | 1 | 0 | 2.481702 | 2.855559 | -2.720523 |
| 66 | 6 | 0 | 1.437646 | 1.418879 | -1.516680 |
| 67 | 1 | 0 | 0.622955 | 1.294777 | -2.216628 |
| 68 | 16 | 0 | 0.067979 | 4.614700 | -0.407842 |
| 69 | 8 | 0 | 0.765261 | 3.827187 | 0.610678 |
| 70 | 8 | 0 | -0.470188 | 3.845976 | -1.540154 |
| 71 | 8 | 0 | 1.304032 | 5.502709 | -1.034512 |
| 72 | 1 | 0 | 0.987922 | 6.039562 | -1.774590 |
| 73 | 16 | 0 | 5.126314 | -1.131234 | -1.040245 |
| 74 | 8 | 0 | 6.032622 | -2.346077 | -1.518471 |
| 75 | 1 | 0 | 6.526001 | -2.158031 | -2.334901 |
| 76 | 8 | 0 | 4.392187 | -1.638959 | 0.087156 |
| 77 | 8 | 0 | 6.181452 | -0.041641 | -0.575542 |
| 78 | 8 | 0 | 4.458060 | -0.540419 | -2.170634 |
| 79 | 16 | 0 | -5.125886 | -0.873206 | -0.103564 |
| 80 | 8 | 0 | -5.883837 | -0.030560 | -1.295713 |
| 81 | 1 | 0 | -6.497513 | 0.612106 | -0.913705 |
| 82 | 8 | 0 | -4.087607 | -1.578945 | -0.857386 |
| 83 | 8 | 0 | -6.148204 | -1.759930 | 0.479590 |
| 84 | 8 | 0 | -4.644525 | 0.145492 | 0.841534 |
| 85 | 8 | 0 | -0.891755 | 5.592434 | 0.133665 |
| 86 | 1 | 0 | 6.548347 | -0.212989 | 0.308376 |

Rotational constants (GHZ): 0.0628395 0.0473262

DC3-3-021, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.005866 | -0.526821 | 0.275778 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 7 | 0 | 0.443869 | -2.149625 | -0.647318 |
| 3 | 7 | 0 | -1.445588 | -1.818814 | 1.200248 |
| 4 | 7 | 0 | -0.724755 | 1.051999 | 1.122915 |
| 5 | 7 | 0 | -1.327656 | 0.075205 | -1.287614 |
| 6 | 7 | 0 | 1.581781 | -0.779334 | 1.708450 |
| 7 | 7 | 0 | 1.605041 | 0.704247 | -0.537091 |
| 8 | 6 | 0 | 1.404272 | -2.288560 | -1.546185 |
| 9 | 1 | 0 | 2.063204 | -1.443908 | -1.683968 |
| 10 | 6 | 0 | 1.570414 | -3.466309 | -2.284812 |
| 11 | 1 | 0 | 2.384672 | -3.528408 | -2.997862 |
| 12 | 6 | 0 | 0.699045 | -4.515027 | -2.096088 |
| 13 | 1 | 0 | 0.798663 | -5.435853 | -2.662531 |
| 14 | 6 | 0 | -0.338272 | -4.386845 | -1.152146 |
| 15 | 6 | 0 | -0.417702 | -3.176512 | -0.442094 |
| 16 | 6 | 0 | -1.435654 | -2.992450 | 0.538138 |
| 17 | 6 | 0 | -1.302441 | -5.410476 | -0.888135 |
| 18 | 1 | 0 | -1.234042 | -6.337379 | -1.449417 |
| 19 | 6 | 0 | -2.280719 | -5.231343 | 0.040431 |
| 20 | 1 | 0 | -3.009561 | -6.012103 | 0.235224 |
| 21 | 6 | 0 | -2.368395 | -4.014830 | 0.786531 |
| 22 | 6 | 0 | -3.337203 | -3.764861 | 1.777495 |
| 23 | 1 | 0 | -4.082210 | -4.522577 | 2.000459 |
| 24 | 6 | 0 | -3.326954 | -2.564508 | 2.451533 |
| 25 | 1 | 0 | -4.060458 | -2.343585 | 3.218053 |
| 26 | 6 | 0 | -2.358116 | -1.604649 | 2.125840 |
| 27 | 1 | 0 | -2.324528 | -0.646175 | 2.629852 |
| 28 | 6 | 0 | -0.440325 | 1.495786 | 2.337489 |
| 29 | 1 | 0 | 0.305086 | 0.942249 | 2.892810 |
| 30 | 6 | 0 | -1.064142 | 2.617096 | 2.893277 |
| 31 | 1 | 0 | -0.787607 | 2.934114 | 3.892240 |
| 32 | 6 | 0 | -2.010210 | 3.297093 | 2.160871 |
| 33 | 1 | 0 | -2.507838 | 4.174387 | 2.562179 |
| 34 | 6 | 0 | -2.338735 | 2.839639 | 0.872887 |
| 35 | 6 | 0 | -1.665541 | 1.701540 | 0.397580 |
| 36 | 6 | 0 | -1.979757 | 1.183188 | -0.893175 |
| 37 | 6 | 0 | -3.321751 | 3.465329 | 0.043753 |
| 38 | 1 | 0 | -3.831589 | 4.343412 | 0.427656 |
| 39 | 6 | 0 | -3.613200 | 2.976526 | -1.189975 |
| 40 | 1 | 0 | -4.361512 | 3.454000 | -1.815026 |
| 41 | 6 | 0 | -2.944291 | 1.818463 | -1.692751 |
| 42 | 6 | 0 | -3.199259 | 1.253482 | -2.954834 |
| 43 | 1 | 0 | -3.938149 | 1.711374 | -3.605352 |
| 44 | 6 | 0 | -2.515158 | 0.123774 | -3.347011 |
| 45 | 1 | 0 | -2.693313 | -0.335602 | -4.312647 |
| 46 | 6 | 0 | -1.580490 | -0.444639 | -2.472553 |
| 47 | 1 | 0 | -1.028858 | -1.339256 | -2.741429 |
| 48 | 6 | 0 | 1.567890 | -1.570285 | 2.763753 |
| 49 | 1 | 0 | 0.709592 | -2.226829 | 2.862813 |
| 50 | 6 | 0 | 2.594185 | -1.560020 | 3.717590 |
| 51 | 1 | 0 | 2.542994 | -2.229980 | 4.568470 |
| 52 | 6 | 0 | 3.647150 | -0.686654 | 3.555122 |
| 53 | 1 | 0 | 4.454983 | -0.646190 | 4.279773 |
| 54 | 6 | 0 | 3.682243 | 0.159637 | 2.431504 |
| 55 | 6 | 0 | 2.612889 | 0.063608 | 1.520493 |
| 56 | 6 | 0 | 2.620670 | 0.859896 | 0.329999 |
| 57 | 6 | 0 | 4.745363 | 1.079578 | 2.174106 |
| 58 | 1 | 0 | 5.557519 | 1.143924 | 2.891925 |
| 59 | 6 | 0 | 4.748573 | 1.841947 | 1.049132 |
| 60 | 1 | 0 | 5.564442 | 2.529053 | 0.846543 |
| 61 | 6 | 0 | 3.693884 | 1.739151 | 0.090160 |
| 62 | 6 | 0 | 3.677513 | 2.458522 | -1.118447 |
| 63 | 1 | 0 | 4.486077 | 3.147822 | -1.341865 |
| 64 | 6 | 0 | 2.644069 | 2.266686 | -2.006269 |

| | | | | | |
|---|---|---|---|---|---|
| 65 | 1 | 0 | 2.605719 | 2.795926 | -2.951516 |
| 66 | 6 | 0 | 1.616126 | 1.375037 | -1.670852 |
| 67 | 1 | 0 | 0.781554 | 1.206358 | -2.341906 |
| 68 | 16 | 0 | 0.411614 | 4.447372 | -0.469323 |
| 69 | 8 | 0 | 0.983152 | 3.649128 | 0.579483 |
| 70 | 8 | 0 | -0.303601 | 3.862385 | -1.572398 |
| 71 | 8 | 0 | 1.614904 | 5.336839 | -1.008685 |
| 72 | 1 | 0 | 1.382219 | 5.853984 | -1.797960 |
| 73 | 16 | 0 | 4.930470 | -1.605181 | -0.947073 |
| 74 | 8 | 0 | 5.450663 | -2.947160 | -1.742751 |
| 75 | 1 | 0 | 6.006001 | -2.696975 | -2.494591 |
| 76 | 8 | 0 | 4.060876 | -2.193261 | 0.074384 |
| 77 | 8 | 0 | 6.138683 | -0.954285 | -0.416703 |
| 78 | 8 | 0 | 4.239162 | -0.797899 | -1.966072 |
| 79 | 16 | 0 | -5.053736 | -0.599658 | 0.080800 |
| 80 | 8 | 0 | -5.772844 | 0.332147 | -1.069953 |
| 81 | 1 | 0 | -5.980836 | 1.203340 | -0.705664 |
| 82 | 8 | 0 | -4.147478 | -1.433972 | -0.713007 |
| 83 | 8 | 0 | -6.143137 | -1.357780 | 0.719074 |
| 84 | 8 | 0 | -4.405472 | 0.360503 | 0.986516 |
| 85 | 8 | 0 | -0.592484 | 5.520241 | 0.139828 |
| 86 | 1 | 0 | -0.287316 | 5.892792 | 0.984043 |

Rotational constants (GHZ): 0.0616043 0.0474304

**Structures of DC-3-012**

DC1-3-012a, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.038116 | 0.628776 | -0.023795 |
| 2 | 7 | 0 | -1.219439 | 1.879913 | -0.925657 |
| 3 | 7 | 0 | 0.933809 | 2.228884 | 0.478111 |
| 4 | 7 | 0 | 1.227722 | -0.569584 | 0.849295 |
| 5 | 7 | 0 | 1.064595 | 0.337563 | -1.577824 |
| 6 | 7 | 0 | -1.203634 | 0.730548 | 1.668720 |
| 7 | 7 | 0 | -1.184728 | -0.898250 | -0.410892 |
| 8 | 6 | 0 | -2.288140 | 1.645022 | -1.666960 |
| 9 | 1 | 0 | -2.541234 | 0.609862 | -1.841970 |
| 10 | 6 | 0 | -3.061634 | 2.677853 | -2.212812 |
| 11 | 1 | 0 | -3.932453 | 2.424763 | -2.807068 |
| 12 | 6 | 0 | -2.707166 | 3.990379 | -1.990929 |
| 13 | 1 | 0 | -3.292538 | 4.806768 | -2.402437 |
| 14 | 6 | 0 | -1.559193 | 4.267363 | -1.225296 |
| 15 | 6 | 0 | -0.852843 | 3.164731 | -0.720667 |
| 16 | 6 | 0 | 0.326888 | 3.355306 | 0.040460 |
| 17 | 6 | 0 | -1.069020 | 5.581434 | -0.940767 |
| 18 | 1 | 0 | -1.619378 | 6.432451 | -1.330091 |
| 19 | 6 | 0 | 0.061198 | 5.764575 | -0.203514 |
| 20 | 1 | 0 | 0.427228 | 6.764693 | 0.007613 |
| 21 | 6 | 0 | 0.795504 | 4.649470 | 0.311932 |
| 22 | 6 | 0 | 1.966022 | 4.751604 | 1.087400 |
| 23 | 1 | 0 | 2.373823 | 5.729451 | 1.324362 |
| 24 | 6 | 0 | 2.571736 | 3.599554 | 1.536871 |
| 25 | 1 | 0 | 3.473079 | 3.636644 | 2.138032 |
| 26 | 6 | 0 | 2.023421 | 2.350046 | 1.215958 |
| 27 | 1 | 0 | 2.485234 | 1.438385 | 1.564146 |
| 28 | 6 | 0 | 1.303139 | -0.961636 | 2.109957 |
| 29 | 1 | 0 | 0.587517 | -0.534228 | 2.800263 |
| 30 | 6 | 0 | 2.262567 | -1.881719 | 2.551137 |
| 31 | 1 | 0 | 2.275685 | -2.164836 | 3.597396 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 6 | 0 | 3.164224 | -2.413012 | 1.657259 |
| 33 | 1 | 0 | 3.912572 | -3.132161 | 1.974539 |
| 34 | 6 | 0 | 3.112923 | -2.003100 | 0.313780 |
| 35 | 6 | 0 | 2.121439 | -1.072962 | -0.028815 |
| 36 | 6 | 0 | 2.024385 | -0.587555 | -1.356287 |
| 37 | 6 | 0 | 3.997672 | -2.469050 | -0.707929 |
| 38 | 1 | 0 | 4.757676 | -3.195343 | -0.438119 |
| 39 | 6 | 0 | 3.897259 | -2.011899 | -1.984901 |
| 40 | 1 | 0 | 4.575988 | -2.365950 | -2.754562 |
| 41 | 6 | 0 | 2.908364 | -1.043586 | -2.344991 |
| 42 | 6 | 0 | 2.766994 | -0.489534 | -3.628938 |
| 43 | 1 | 0 | 3.423940 | -0.809740 | -4.431661 |
| 44 | 6 | 0 | 1.797038 | 0.466329 | -3.842538 |
| 45 | 1 | 0 | 1.664697 | 0.923007 | -4.816837 |
| 46 | 6 | 0 | 0.960016 | 0.857887 | -2.790846 |
| 47 | 1 | 0 | 0.185851 | 1.599276 | -2.940329 |
| 48 | 6 | 0 | -1.188948 | 1.592655 | 2.668352 |
| 49 | 1 | 0 | -0.500770 | 2.425584 | 2.589915 |
| 50 | 6 | 0 | -2.013229 | 1.439459 | 3.790708 |
| 51 | 1 | 0 | -1.966350 | 2.173434 | 4.587173 |
| 52 | 6 | 0 | -2.864150 | 0.358205 | 3.864251 |
| 53 | 1 | 0 | -3.512631 | 0.215564 | 4.723244 |
| 54 | 6 | 0 | -2.896412 | -0.567835 | 2.806305 |
| 55 | 6 | 0 | -2.033411 | -0.328934 | 1.723476 |
| 56 | 6 | 0 | -2.029906 | -1.202362 | 0.601016 |
| 57 | 6 | 0 | -3.762595 | -1.704008 | 2.763474 |
| 58 | 1 | 0 | -4.424138 | -1.882796 | 3.605438 |
| 59 | 6 | 0 | -3.767513 | -2.533960 | 1.686536 |
| 60 | 1 | 0 | -4.437605 | -3.386889 | 1.647560 |
| 61 | 6 | 0 | -2.908880 | -2.297354 | 0.567402 |
| 62 | 6 | 0 | -2.912419 | -3.085084 | -0.596791 |
| 63 | 1 | 0 | -3.580549 | -3.937385 | -0.668795 |
| 64 | 6 | 0 | -2.072756 | -2.748066 | -1.632452 |
| 65 | 1 | 0 | -2.052484 | -3.321889 | -2.551557 |
| 66 | 6 | 0 | -1.216611 | -1.648140 | -1.499793 |
| 67 | 1 | 0 | -0.544881 | -1.374489 | -2.302170 |
| 68 | 16 | 0 | 0.676023 | -4.335613 | -0.294764 |
| 69 | 8 | 0 | 0.136937 | -3.515872 | 0.754257 |
| 70 | 8 | 0 | 1.036798 | -3.797392 | -1.579776 |
| 71 | 8 | 0 | -0.379769 | -5.511431 | -0.475847 |
| 72 | 1 | 0 | -0.191708 | -6.079394 | -1.241273 |
| 73 | 16 | 0 | -5.306178 | 0.051781 | -0.549535 |
| 74 | 8 | 0 | -6.463849 | 1.064074 | -0.952337 |
| 75 | 1 | 0 | -7.002124 | 0.753979 | -1.700488 |
| 76 | 8 | 0 | -4.539106 | 0.746014 | 0.449055 |
| 77 | 8 | 0 | -6.085294 | -1.169770 | 0.098150 |
| 78 | 8 | 0 | -4.694760 | -0.486877 | -1.736562 |
| 79 | 16 | 0 | 5.270675 | 1.116802 | 0.584215 |
| 80 | 8 | 0 | 6.272603 | -0.080298 | 0.077603 |
| 81 | 1 | 0 | 6.889254 | -0.325501 | 0.781538 |
| 82 | 8 | 0 | 4.381641 | 1.267355 | -0.570435 |
| 83 | 8 | 0 | 6.129893 | 2.285118 | 0.841917 |
| 84 | 8 | 0 | 4.626845 | 0.598697 | 1.802971 |
| 85 | 8 | 0 | 1.982648 | -5.086190 | 0.214089 |
| 86 | 1 | 0 | 1.940560 | -5.321109 | 1.156252 |
| 87 | 1 | 0 | -6.332312 | -1.021242 | 1.026682 |

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Rotational constants (GHZ): 0.0630740 0.0462165

DC1-3-012b, ferroin singlet

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| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.012281 | -0.474294 | 0.266391 |
| 2 | 7 | 0 | 0.593458 | -2.025334 | -0.720384 |
| 3 | 7 | 0 | -1.337059 | -1.703999 | 0.986920 |
| 4 | 7 | 0 | -0.790278 | 1.039630 | 1.214459 |
| 5 | 7 | 0 | -1.244197 | 0.042147 | -1.148355 |
| 6 | 7 | 0 | 1.251528 | -0.823056 | 1.696919 |
| 7 | 7 | 0 | 1.393902 | 0.691890 | -0.410657 |
| 8 | 6 | 0 | 1.591119 | -2.132428 | -1.580573 |
| 9 | 1 | 0 | 2.171670 | -1.240191 | -1.762263 |
| 10 | 6 | 0 | 1.876650 | -3.331005 | -2.246810 |
| 11 | 1 | 0 | 2.713132 | -3.361861 | -2.936120 |
| 12 | 6 | 0 | 1.092225 | -4.441745 | -2.024154 |
| 13 | 1 | 0 | 1.291247 | -5.379477 | -2.533733 |
| 14 | 6 | 0 | 0.014034 | -4.348550 | -1.124273 |
| 15 | 6 | 0 | -0.183124 | -3.108719 | -0.497198 |
| 16 | 6 | 0 | -1.244218 | -2.929960 | 0.425731 |
| 17 | 6 | 0 | -0.882062 | -5.420698 | -0.815331 |
| 18 | 1 | 0 | -0.730316 | -6.377205 | -1.306048 |
| 19 | 6 | 0 | -1.898780 | -5.250689 | 0.074291 |
| 20 | 1 | 0 | -2.571269 | -6.070364 | 0.307763 |
| 21 | 6 | 0 | -2.103467 | -3.996046 | 0.731530 |
| 22 | 6 | 0 | -3.105352 | -3.750179 | 1.688189 |
| 23 | 1 | 0 | -3.800973 | -4.538320 | 1.958737 |
| 24 | 6 | 0 | -3.176603 | -2.506554 | 2.274867 |
| 25 | 1 | 0 | -3.927014 | -2.281393 | 3.023721 |
| 26 | 6 | 0 | -2.272958 | -1.503801 | 1.898461 |
| 27 | 1 | 0 | -2.318249 | -0.521647 | 2.347965 |
| 28 | 6 | 0 | -0.537409 | 1.499402 | 2.428858 |
| 29 | 1 | 0 | 0.221545 | 0.983505 | 3.002686 |
| 30 | 6 | 0 | -1.218663 | 2.596327 | 2.969744 |
| 31 | 1 | 0 | -0.967280 | 2.929557 | 3.970192 |
| 32 | 6 | 0 | -2.185893 | 3.235046 | 2.226650 |
| 33 | 1 | 0 | -2.722944 | 4.091512 | 2.621777 |
| 34 | 6 | 0 | -2.476708 | 2.762097 | 0.935789 |
| 35 | 6 | 0 | -1.741964 | 1.657100 | 0.482509 |
| 36 | 6 | 0 | -1.987147 | 1.115623 | -0.804847 |
| 37 | 6 | 0 | -3.461721 | 3.334123 | 0.071585 |
| 38 | 1 | 0 | -4.022167 | 4.192593 | 0.428199 |
| 39 | 6 | 0 | -3.691385 | 2.820203 | -1.166248 |
| 40 | 1 | 0 | -4.439337 | 3.259369 | -1.819065 |
| 41 | 6 | 0 | -2.952977 | 1.692444 | -1.643284 |
| 42 | 6 | 0 | -3.127190 | 1.110650 | -2.910787 |
| 43 | 1 | 0 | -3.860807 | 1.521284 | -3.597316 |
| 44 | 6 | 0 | -2.359299 | 0.021565 | -3.256763 |
| 45 | 1 | 0 | -2.464476 | -0.455741 | -4.224321 |
| 46 | 6 | 0 | -1.428628 | -0.490377 | -2.345066 |
| 47 | 1 | 0 | -0.818017 | -1.345737 | -2.602421 |
| 48 | 6 | 0 | 1.159368 | -1.657586 | 2.719913 |
| 49 | 1 | 0 | 0.284344 | -2.293440 | 2.756917 |
| 50 | 6 | 0 | 2.134957 | -1.717737 | 3.722643 |
| 51 | 1 | 0 | 2.007375 | -2.419655 | 4.538935 |
| 52 | 6 | 0 | 3.232231 | -0.886114 | 3.662457 |

| | | | | | |
|---|---|---|---|---|---|
| 53 | 1 | 0 | 3.997715 | -0.911949 | 4.431988 |
| 54 | 6 | 0 | 3.359767 | -0.001173 | 2.577631 |
| 55 | 6 | 0 | 2.334522 | -0.018811 | 1.619959 |
| 56 | 6 | 0 | 2.409972 | 0.810675 | 0.472649 |
| 57 | 6 | 0 | 4.464727 | 0.885776 | 2.382175 |
| 58 | 1 | 0 | 5.251968 | 0.902314 | 3.129652 |
| 59 | 6 | 0 | 4.535872 | 1.682527 | 1.281561 |
| 60 | 1 | 0 | 5.383967 | 2.343095 | 1.131416 |
| 61 | 6 | 0 | 3.513135 | 1.654370 | 0.281443 |
| 62 | 6 | 0 | 3.551948 | 2.391276 | -0.915941 |
| 63 | 1 | 0 | 4.387463 | 3.054716 | -1.115379 |
| 64 | 6 | 0 | 2.524655 | 2.248488 | -1.819267 |
| 65 | 1 | 0 | 2.518633 | 2.796172 | -2.754148 |
| 66 | 6 | 0 | 1.454951 | 1.391354 | -1.530087 |
| 67 | 1 | 0 | 0.636142 | 1.272670 | -2.226238 |
| 68 | 16 | 0 | 0.134864 | 4.616631 | -0.420877 |
| 69 | 8 | 0 | 0.826775 | 3.821009 | 0.595018 |
| 70 | 8 | 0 | -0.421406 | 3.852943 | -1.547924 |
| 71 | 8 | 0 | 1.379448 | 5.485212 | -1.056753 |
| 72 | 1 | 0 | 1.066763 | 6.026057 | -1.795368 |
| 73 | 16 | 0 | 5.104731 | -1.222417 | -1.050931 |
| 74 | 8 | 0 | 6.004989 | -2.468552 | -1.452883 |
| 75 | 1 | 0 | 6.527551 | -2.323642 | -2.259429 |
| 76 | 8 | 0 | 4.341454 | -1.672082 | 0.081680 |
| 77 | 8 | 0 | 6.163273 | -0.125199 | -0.612806 |
| 78 | 8 | 0 | 4.466142 | -0.673658 | -2.219145 |
| 79 | 16 | 0 | -4.932694 | -0.767066 | -0.176146 |
| 80 | 8 | 0 | -5.763751 | -0.073558 | -1.340693 |
| 81 | 1 | 0 | -6.348235 | 0.635023 | -1.023198 |
| 82 | 8 | 0 | -3.945491 | -1.564795 | -0.850629 |
| 83 | 8 | 0 | -6.000017 | -1.706785 | 0.535940 |
| 84 | 8 | 0 | -4.580460 | 0.206106 | 0.822978 |
| 85 | 8 | 0 | -0.808195 | 5.608422 | 0.124461 |
| 86 | 1 | 0 | -6.233140 | -2.488619 | 0.008005 |
| 87 | 1 | 0 | 6.512534 | -0.264034 | 0.283913 |

Rotational constants (GHZ): 0.0627814 0.0477746

DC3-3-012, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.049442 | -0.290097 | 0.074141 |
| 2 | 7 | 0 | 1.211642 | -1.400365 | -0.985164 |
| 3 | 7 | 0 | -0.297967 | -2.140063 | 1.086454 |
| 4 | 7 | 0 | -1.258388 | 0.679838 | 1.101779 |
| 5 | 7 | 0 | -1.545114 | -0.341961 | -1.343643 |
| 6 | 7 | 0 | 1.710613 | 0.189653 | 1.384093 |
| 7 | 7 | 0 | 0.783819 | 1.585833 | -0.739753 |
| 8 | 6 | 0 | 1.931907 | -1.012696 | -2.024678 |
| 9 | 1 | 0 | 1.874648 | 0.033936 | -2.288083 |
| 10 | 6 | 0 | 2.737189 | -1.896564 | -2.751804 |
| 11 | 1 | 0 | 3.311920 | -1.518573 | -3.589428 |
| 12 | 6 | 0 | 2.785659 | -3.223037 | -2.389157 |
| 13 | 1 | 0 | 3.403427 | -3.931190 | -2.932567 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | 2.010372 | -3.666257 | -1.301521 |
| 15 | 6 | 0 | 1.235163 | -2.706896 | -0.626447 |
| 16 | 6 | 0 | 0.413585 | -3.102901 | 0.469838 |
| 17 | 6 | 0 | 1.960316 | -5.029734 | -0.870968 |
| 18 | 1 | 0 | 2.566621 | -5.757928 | -1.400953 |
| 19 | 6 | 0 | 1.167093 | -5.409333 | 0.166694 |
| 20 | 1 | 0 | 1.126251 | -6.447040 | 0.483316 |
| 21 | 6 | 0 | 0.368299 | -4.451387 | 0.865353 |
| 22 | 6 | 0 | -0.477038 | -4.769565 | 1.945853 |
| 23 | 1 | 0 | -0.550940 | -5.799906 | 2.280569 |
| 24 | 6 | 0 | -1.194756 | -3.771495 | 2.566333 |
| 25 | 1 | 0 | -1.851961 | -3.986496 | 3.401008 |
| 26 | 6 | 0 | -1.071988 | -2.453213 | 2.104879 |
| 27 | 1 | 0 | -1.612777 | -1.640702 | 2.573191 |
| 28 | 6 | 0 | -1.105018 | 1.139733 | 2.333493 |
| 29 | 1 | 0 | -0.138940 | 0.977407 | 2.792866 |
| 30 | 6 | 0 | -2.127322 | 1.803271 | 3.019268 |
| 31 | 1 | 0 | -1.943271 | 2.158929 | 4.026536 |
| 32 | 6 | 0 | -3.341820 | 1.996958 | 2.401570 |
| 33 | 1 | 0 | -4.152569 | 2.513368 | 2.905709 |
| 34 | 6 | 0 | -3.531492 | 1.511643 | 1.095632 |
| 35 | 6 | 0 | -2.450661 | 0.853316 | 0.486160 |
| 36 | 6 | 0 | -2.598075 | 0.315742 | -0.826038 |
| 37 | 6 | 0 | -4.759758 | 1.646983 | 0.375427 |
| 38 | 1 | 0 | -5.584232 | 2.160131 | 0.860556 |
| 39 | 6 | 0 | -4.894917 | 1.148527 | -0.881816 |
| 40 | 1 | 0 | -5.829312 | 1.254461 | -1.424360 |
| 41 | 6 | 0 | -3.810905 | 0.468676 | -1.518365 |
| 42 | 6 | 0 | -3.883275 | -0.086862 | -2.808237 |
| 43 | 1 | 0 | -4.802202 | 0.005999 | -3.379024 |
| 44 | 6 | 0 | -2.793241 | -0.751843 | -3.326341 |
| 45 | 1 | 0 | -2.822004 | -1.194673 | -4.315312 |
| 46 | 6 | 0 | -1.632005 | -0.863923 | -2.551578 |
| 47 | 1 | 0 | -0.756798 | -1.388595 | -2.919244 |
| 48 | 6 | 0 | 2.164401 | -0.530407 | 2.390748 |
| 49 | 1 | 0 | 1.638318 | -1.454930 | 2.601004 |
| 50 | 6 | 0 | 3.264467 | -0.134206 | 3.162648 |
| 51 | 1 | 0 | 3.600471 | -0.762713 | 3.979564 |
| 52 | 6 | 0 | 3.898160 | 1.048832 | 2.859652 |
| 53 | 1 | 0 | 4.756600 | 1.387562 | 3.431744 |
| 54 | 6 | 0 | 3.429428 | 1.831937 | 1.788007 |
| 55 | 6 | 0 | 2.318461 | 1.347573 | 1.069714 |
| 56 | 6 | 0 | 1.814807 | 2.097214 | -0.044577 |
| 57 | 6 | 0 | 4.034520 | 3.068218 | 1.403551 |
| 58 | 1 | 0 | 4.893672 | 3.418625 | 1.967276 |
| 59 | 6 | 0 | 3.546888 | 3.786802 | 0.358903 |
| 60 | 1 | 0 | 4.005904 | 4.726892 | 0.068105 |
| 61 | 6 | 0 | 2.424864 | 3.318359 | -0.392805 |
| 62 | 6 | 0 | 1.899294 | 4.010495 | -1.499420 |
| 63 | 1 | 0 | 2.339040 | 4.958634 | -1.793828 |
| 64 | 6 | 0 | 0.843004 | 3.470867 | -2.197558 |
| 65 | 1 | 0 | 0.416962 | 3.973979 | -3.058015 |
| 66 | 6 | 0 | 0.314284 | 2.241842 | -1.782671 |
| 67 | 1 | 0 | -0.508493 | 1.780596 | -2.315298 |
| 68 | 16 | 0 | -1.900170 | 4.334226 | -0.143840 |
| 69 | 8 | 0 | -0.911952 | 3.779084 | 0.739035 |
| 70 | 8 | 0 | -2.429038 | 3.600059 | -1.262810 |
| 71 | 8 | 0 | -1.271277 | 5.707613 | -0.642564 |
| 72 | 1 | 0 | -1.789519 | 6.134459 | -1.344929 |
| 73 | 16 | 0 | 4.997375 | -0.343001 | -0.509371 |
| 74 | 8 | 0 | 5.921420 | -1.265994 | -1.416580 |
| 75 | 1 | 0 | 6.467603 | -0.765345 | -2.045045 |
| 76 | 8 | 0 | 4.180030 | -1.262641 | 0.232637 |

| | | | | | |
|---|---|---|---|---|---|
| 77 | 8 | 0 | 6.028146 | 0.381903 | 0.459631 |
| 78 | 8 | 0 | 4.432154 | 0.717592 | -1.301342 |
| 79 | 16 | 0 | -3.945429 | -2.965675 | 0.190378 |
| 80 | 8 | 0 | -5.037451 | -2.532928 | -0.961794 |
| 81 | 1 | 0 | -5.623922 | -1.844693 | -0.618281 |
| 82 | 8 | 0 | -2.764008 | -3.303588 | -0.608912 |
| 83 | 8 | 0 | -4.531995 | -4.123164 | 0.886834 |
| 84 | 8 | 0 | -3.819928 | -1.775600 | 1.044940 |
| 85 | 8 | 0 | -3.180050 | 4.788943 | 0.683306 |
| 86 | 1 | 0 | -2.961349 | 5.136738 | 1.564208 |
| 87 | 1 | 0 | 6.312940 | -0.176032 | 1.202534 |

Rotational constants (GHZ): 0.0598483 0.0502309

**Structures of DC-3-003**

DC1-3-003, ferroin singlet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | -0.050933 | -0.465033 | 0.234104 |
| 2 | 7 | 0 | 0.557674 | -2.035439 | -0.723043 |
| 3 | 7 | 0 | -1.362975 | -1.683200 | 0.989152 |
| 4 | 7 | 0 | -0.808985 | 1.059613 | 1.175113 |
| 5 | 7 | 0 | -1.269020 | 0.044559 | -1.174800 |
| 6 | 7 | 0 | 1.289260 | -0.824069 | 1.751012 |
| 7 | 7 | 0 | 1.385259 | 0.668226 | -0.423740 |
| 8 | 6 | 0 | 1.549865 | -2.159219 | -1.587440 |
| 9 | 1 | 0 | 2.121077 | -1.268175 | -1.801570 |
| 10 | 6 | 0 | 1.844003 | -3.374829 | -2.218100 |
| 11 | 1 | 0 | 2.675883 | -3.417970 | -2.912279 |
| 12 | 6 | 0 | 1.073687 | -4.486454 | -1.955153 |
| 13 | 1 | 0 | 1.279556 | -5.437421 | -2.436697 |
| 14 | 6 | 0 | 0.001233 | -4.376640 | -1.050332 |
| 15 | 6 | 0 | -0.205163 | -3.120013 | -0.460943 |
| 16 | 6 | 0 | -1.259770 | -2.925047 | 0.466058 |
| 17 | 6 | 0 | -0.879713 | -5.448802 | -0.700594 |
| 18 | 1 | 0 | -0.720854 | -6.418360 | -1.162637 |
| 19 | 6 | 0 | -1.890920 | -5.262820 | 0.191986 |
| 20 | 1 | 0 | -2.551860 | -6.082369 | 0.456740 |
| 21 | 6 | 0 | -2.104290 | -3.990717 | 0.811851 |
| 22 | 6 | 0 | -3.101329 | -3.726636 | 1.768730 |
| 23 | 1 | 0 | -3.786404 | -4.513505 | 2.068362 |
| 24 | 6 | 0 | -3.180551 | -2.467093 | 2.319162 |
| 25 | 1 | 0 | -3.926852 | -2.227385 | 3.067618 |
| 26 | 6 | 0 | -2.290972 | -1.466753 | 1.904897 |
| 27 | 1 | 0 | -2.345145 | -0.471892 | 2.323958 |
| 28 | 6 | 0 | -0.548942 | 1.529347 | 2.383656 |
| 29 | 1 | 0 | 0.207288 | 1.012644 | 2.959876 |
| 30 | 6 | 0 | -1.220518 | 2.637106 | 2.915556 |
| 31 | 1 | 0 | -0.964801 | 2.977341 | 3.912510 |
| 32 | 6 | 0 | -2.185807 | 3.275550 | 2.169805 |
| 33 | 1 | 0 | -2.716625 | 4.138712 | 2.558871 |
| 34 | 6 | 0 | -2.482109 | 2.793829 | 0.882452 |
| 35 | 6 | 0 | -1.756971 | 1.678106 | 0.439135 |
| 36 | 6 | 0 | -2.003094 | 1.129127 | -0.844335 |
| 37 | 6 | 0 | -3.462143 | 3.365515 | 0.011877 |
| 38 | 1 | 0 | -4.018541 | 4.229861 | 0.360622 |
| 39 | 6 | 0 | -3.691799 | 2.843919 | -1.223166 |
| 40 | 1 | 0 | -4.435884 | 3.283019 | -1.880371 |
| 41 | 6 | 0 | -2.961688 | 1.706234 | -1.689898 |
| 42 | 6 | 0 | -3.140585 | 1.111707 | -2.951151 |

| | | | | | |
|---|---|---|---|---|---|
| 43 | 1 | 0 | -3.869396 | 1.521323 | -3.643286 |
| 44 | 6 | 0 | -2.384678 | 0.009741 | -3.282297 |
| 45 | 1 | 0 | -2.495251 | -0.478987 | -4.243493 |
| 46 | 6 | 0 | -1.459461 | -0.501635 | -2.364640 |
| 47 | 1 | 0 | -0.859128 | -1.367694 | -2.609775 |
| 48 | 6 | 0 | 1.205154 | -1.625395 | 2.796310 |
| 49 | 1 | 0 | 0.328821 | -2.259581 | 2.858206 |
| 50 | 6 | 0 | 2.194389 | -1.651455 | 3.788128 |
| 51 | 1 | 0 | 2.084803 | -2.326331 | 4.629369 |
| 52 | 6 | 0 | 3.285224 | -0.815839 | 3.680589 |
| 53 | 1 | 0 | 4.063318 | -0.813598 | 4.437964 |
| 54 | 6 | 0 | 3.393805 | 0.038889 | 2.568863 |
| 55 | 6 | 0 | 2.355160 | -0.010860 | 1.624679 |
| 56 | 6 | 0 | 2.407253 | 0.795352 | 0.453823 |
| 57 | 6 | 0 | 4.492378 | 0.925241 | 2.341208 |
| 58 | 1 | 0 | 5.288310 | 0.963623 | 3.078544 |
| 59 | 6 | 0 | 4.544224 | 1.695408 | 1.221804 |
| 60 | 1 | 0 | 5.386170 | 2.356721 | 1.043365 |
| 61 | 6 | 0 | 3.508954 | 1.638222 | 0.235699 |
| 62 | 6 | 0 | 3.542450 | 2.353016 | -0.974405 |
| 63 | 1 | 0 | 4.378288 | 3.011279 | -1.188877 |
| 64 | 6 | 0 | 2.514591 | 2.190594 | -1.874412 |
| 65 | 1 | 0 | 2.508627 | 2.713747 | -2.823500 |
| 66 | 6 | 0 | 1.446686 | 1.341644 | -1.560370 |
| 67 | 1 | 0 | 0.624061 | 1.209639 | -2.250157 |
| 68 | 16 | 0 | 0.287664 | 4.430708 | -0.422945 |
| 69 | 8 | 0 | 0.853552 | 3.638120 | 0.633147 |
| 70 | 8 | 0 | -0.420179 | 3.838767 | -1.527066 |
| 71 | 8 | 0 | 1.494180 | 5.317117 | -0.959843 |
| 72 | 1 | 0 | 1.265280 | 5.833829 | -1.750595 |
| 73 | 16 | 0 | 5.069127 | -1.260180 | -1.079743 |
| 74 | 8 | 0 | 5.964137 | -2.514272 | -1.467080 |
| 75 | 1 | 0 | 6.483381 | -2.383170 | -2.278178 |
| 76 | 8 | 0 | 4.308217 | -1.690933 | 0.061876 |
| 77 | 8 | 0 | 6.131988 | -0.159874 | -0.659744 |
| 78 | 8 | 0 | 4.428268 | -0.725619 | -2.253272 |
| 79 | 16 | 0 | -4.939910 | -0.745834 | -0.179966 |
| 80 | 8 | 0 | -5.771413 | -0.064590 | -1.351388 |
| 81 | 1 | 0 | -6.361102 | 0.642254 | -1.039666 |
| 82 | 8 | 0 | -3.953024 | -1.550726 | -0.846344 |
| 83 | 8 | 0 | -6.006815 | -1.677566 | 0.542637 |
| 84 | 8 | 0 | -4.586198 | 0.238485 | 0.807731 |
| 85 | 8 | 0 | -0.722159 | 5.504707 | 0.174060 |
| 86 | 1 | 0 | -0.419990 | 5.888639 | 1.014339 |
| 87 | 1 | 0 | 6.481404 | -0.285616 | 0.238913 |
| 88 | 1 | 0 | -6.244518 | -2.461613 | 0.019827 |

Rotational constants (GHZ): 0.0631972 0.0477014

DC3-3-003, ferroin triplet

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 26 | 0 | 0.177831 | -0.504987 | 0.166878 |
| 2 | 7 | 0 | 0.705742 | -2.181114 | -1.063492 |
| 3 | 7 | 0 | -0.986798 | -1.820906 | 0.965450 |
| 4 | 7 | 0 | -0.790156 | 1.198087 | 1.140468 |
| 5 | 7 | 0 | -1.410388 | 0.019512 | -1.223868 |
| 6 | 7 | 0 | 1.631436 | -0.573963 | 1.735496 |
| 7 | 7 | 0 | 1.456986 | 0.730159 | -0.580298 |
| 8 | 6 | 0 | 1.546447 | -2.302442 | -2.071764 |
| 9 | 1 | 0 | 2.116830 | -1.419246 | -2.333013 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 6 | 0 | 1.703307 | -3.507893 | -2.769684 |
| 11 | 1 | 0 | 2.409098 | -3.565376 | -3.590870 |
| 12 | 6 | 0 | 0.954502 | -4.602630 | -2.395831 |
| 13 | 1 | 0 | 1.058430 | -5.549501 | -2.917923 |
| 14 | 6 | 0 | 0.042638 | -4.491595 | -1.328525 |
| 15 | 6 | 0 | -0.041350 | -3.238801 | -0.691552 |
| 16 | 6 | 0 | -0.949327 | -3.048083 | 0.391767 |
| 17 | 6 | 0 | -0.786192 | -5.562646 | -0.870423 |
| 18 | 1 | 0 | -0.714793 | -6.526839 | -1.364499 |
| 19 | 6 | 0 | -1.644860 | -5.382150 | 0.167682 |
| 20 | 1 | 0 | -2.265921 | -6.202364 | 0.514858 |
| 21 | 6 | 0 | -1.747707 | -4.119064 | 0.831349 |
| 22 | 6 | 0 | -2.602032 | -3.880641 | 1.923907 |
| 23 | 1 | 0 | -3.234145 | -4.679704 | 2.300246 |
| 24 | 6 | 0 | -2.618460 | -2.634634 | 2.507316 |
| 25 | 1 | 0 | -3.267577 | -2.412196 | 3.346298 |
| 26 | 6 | 0 | -1.793746 | -1.626013 | 1.995898 |
| 27 | 1 | 0 | -1.806067 | -0.629588 | 2.414074 |
| 28 | 6 | 0 | -0.466027 | 1.764864 | 2.287226 |
| 29 | 1 | 0 | 0.374608 | 1.332983 | 2.818496 |
| 30 | 6 | 0 | -1.160534 | 2.858428 | 2.815076 |
| 31 | 1 | 0 | -0.859065 | 3.280353 | 3.767395 |
| 32 | 6 | 0 | -2.223523 | 3.369045 | 2.106218 |
| 33 | 1 | 0 | -2.794290 | 4.211291 | 2.487106 |
| 34 | 6 | 0 | -2.578642 | 2.792387 | 0.874990 |
| 35 | 6 | 0 | -1.818109 | 1.693091 | 0.428976 |
| 36 | 6 | 0 | -2.146868 | 1.069126 | -0.820303 |
| 37 | 6 | 0 | -3.661978 | 3.274138 | 0.079149 |
| 38 | 1 | 0 | -4.225099 | 4.132022 | 0.433762 |
| 39 | 6 | 0 | -3.974208 | 2.681365 | -1.099856 |
| 40 | 1 | 0 | -4.792425 | 3.056016 | -1.707969 |
| 41 | 6 | 0 | -3.229076 | 1.559806 | -1.576575 |
| 42 | 6 | 0 | -3.528765 | 0.904420 | -2.782982 |
| 43 | 1 | 0 | -4.358177 | 1.252310 | -3.391367 |
| 44 | 6 | 0 | -2.774639 | -0.177542 | -3.172399 |
| 45 | 1 | 0 | -2.986555 | -0.713468 | -4.090664 |
| 46 | 6 | 0 | -1.718340 | -0.589194 | -2.353391 |
| 47 | 1 | 0 | -1.102277 | -1.438738 | -2.625303 |
| 48 | 6 | 0 | 1.704640 | -1.285007 | 2.841395 |
| 49 | 1 | 0 | 0.950212 | -2.053918 | 2.972004 |
| 50 | 6 | 0 | 2.695589 | -1.060747 | 3.808336 |
| 51 | 1 | 0 | 2.719700 | -1.667689 | 4.706569 |
| 52 | 6 | 0 | 3.618848 | -0.059214 | 3.598874 |
| 53 | 1 | 0 | 4.387080 | 0.146438 | 4.339425 |
| 54 | 6 | 0 | 3.572094 | 0.699884 | 2.413043 |
| 55 | 6 | 0 | 2.545322 | 0.388505 | 1.501417 |
| 56 | 6 | 0 | 2.463402 | 1.076917 | 0.256599 |
| 57 | 6 | 0 | 4.501432 | 1.735310 | 2.086887 |
| 58 | 1 | 0 | 5.274088 | 1.991291 | 2.805872 |
| 59 | 6 | 0 | 4.435603 | 2.372406 | 0.888301 |
| 60 | 1 | 0 | 5.160268 | 3.139652 | 0.634036 |
| 61 | 6 | 0 | 3.429769 | 2.041593 | -0.071032 |
| 62 | 6 | 0 | 3.357419 | 2.616976 | -1.351312 |
| 63 | 1 | 0 | 4.087557 | 3.361777 | -1.651736 |
| 64 | 6 | 0 | 2.359549 | 2.220395 | -2.209258 |
| 65 | 1 | 0 | 2.278810 | 2.632977 | -3.208319 |
| 66 | 6 | 0 | 1.413375 | 1.283824 | -1.779329 |
| 67 | 1 | 0 | 0.583997 | 0.993322 | -2.410847 |
| 68 | 16 | 0 | 0.045587 | 4.340066 | -0.786589 |
| 69 | 8 | 0 | 0.767904 | 3.721572 | 0.285817 |
| 70 | 8 | 0 | -0.719733 | 3.592446 | -1.741543 |
| 71 | 8 | 0 | 1.120991 | 5.251656 | -1.546374 |
| 72 | 1 | 0 | 0.749048 | 5.656592 | -2.343775 |

| | | | | | |
|---|---|---|---|---|---|
| 73 | 16 | 0 | 4.646030 | -1.446548 | -0.681122 |
| 74 | 8 | 0 | 5.552110 | -2.628038 | -1.256713 |
| 75 | 1 | 0 | 6.148714 | -2.323889 | -1.956806 |
| 76 | 8 | 0 | 3.716183 | -2.077356 | 0.208773 |
| 77 | 8 | 0 | 5.694245 | -0.576881 | 0.157092 |
| 78 | 8 | 0 | 4.226145 | -0.585376 | -1.750850 |
| 79 | 16 | 0 | -4.715127 | -0.895298 | 0.382953 |
| 80 | 8 | 0 | -5.790256 | -0.165864 | -0.551357 |
| 81 | 1 | 0 | -6.315548 | 0.476599 | -0.052169 |
| 82 | 8 | 0 | -3.882490 | -1.647004 | -0.509252 |
| 83 | 8 | 0 | -5.628905 | -1.889203 | 1.241706 |
| 84 | 8 | 0 | -4.188193 | 0.040876 | 1.334177 |
| 85 | 8 | 0 | -0.966019 | 5.434595 | -0.200403 |
| 86 | 1 | 0 | -0.561107 | 5.943594 | 0.516935 |
| 87 | 1 | 0 | 5.981669 | -1.036703 | 0.958941 |
| 88 | 1 | 0 | -5.985413 | -2.608744 | 0.700523 |

Rotational constants (GHZ): 0.0608431 0.0499648