

## Development of new dinuclear Fe(III) coordination complexes with *in vitro* nanomolar antitrypanosomal activity

Felipe Figueirôa Moreira<sup>a, b</sup>, Juliana de Araujo Portes<sup>c</sup>, Nathália Florência Barros Azeredo<sup>d</sup>, Christiane Fernandes<sup>d, #, \*</sup>, Adolfo Horn Júnior<sup>d, #</sup>, Cristina Pinheiro Santiago<sup>d</sup>, Bruna Barriquel Segat<sup>e</sup>, Giovanni Finoto Caramori<sup>e</sup>, Letícia Maria Pequeno Madureira<sup>e</sup>, Dalber Ruben Sanchez Candela<sup>f</sup>, Marcelo Monteiro Marques<sup>g</sup>, Jackson Antônio Lamounier Camargos Resende<sup>h</sup>, Wanderley de Souza<sup>c</sup>, Renato Augusto DaMatta<sup>b</sup>, Sergio Henrique Seabra<sup>a, b, \*</sup>.

<sup>a</sup>Laboratório de Tecnologia em Bioquímica e Microscopia, Centro Universitário Estadual da Zona Oeste (UEZO), Rio de Janeiro, RJ, Brazil.

<sup>b</sup>Laboratório de Biologia Celular e Tecidual, Centro de Biociências e Biotecnologia, Universidade Estadual do Norte Fluminense Darcy Ribeiro (UENF), Campos dos Goytacazes, RJ, Brazil.

<sup>c</sup>Laboratório de Ultraestrutura Celular Hertha Meyer, Instituto de Biofísica Carlos Chagas Filho, Universidade Federal do Rio de Janeiro (UFRJ), RJ, Brazil.

<sup>d</sup>Laboratório de Ciências Químicas, Centro de Ciência e Tecnologia, Universidade Estadual do Norte Fluminense Darcy Ribeiro (UENF), Campos dos Goytacazes, RJ, Brazil.

<sup>e</sup>Departamento de Química, Universidade Federal de Santa Catarina (UFSC), Florianópolis, SC, Brazil.

<sup>f</sup>Departamento de Física, Universidade Federal Fluminense (UFF), Niterói, RJ, Brazil.

<sup>g</sup>Colégio Universitário Geraldo Reis, Universidade Federal Fluminense (UFF), Niterói, RJ, Brazil

<sup>h</sup>Instituto de Ciências Exatas e da Terra, Campus Universitário do Araguaia, Universidade Federal de Mato Grosso (UFMT), Barra do Garças, MT, Brazil.

\* Corresponding authors: Sergio Henrique Seabra: E-mail - [seabrash@gmail.com](mailto:seabrash@gmail.com);  
Christiane Fernandes: E-mail - [christiane.horn@ufsc.br](mailto:christiane.horn@ufsc.br)

# Current address: Departamento de Química, Universidade Federal de Santa Catarina (UFSC), Florianópolis, SC, Brazil.

## Supplementary Material

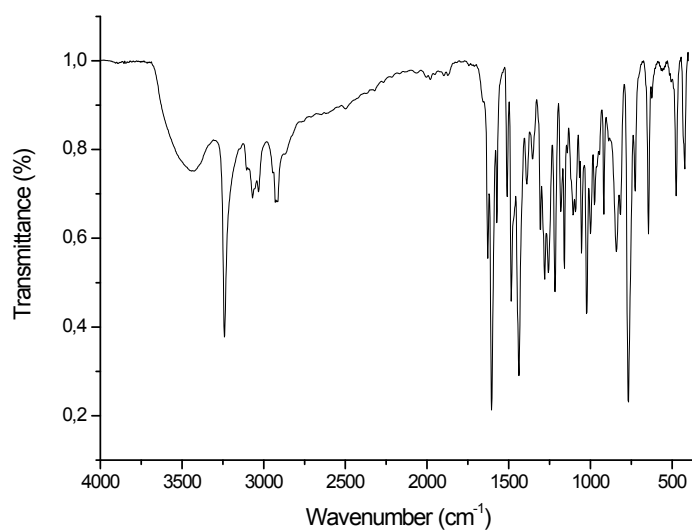
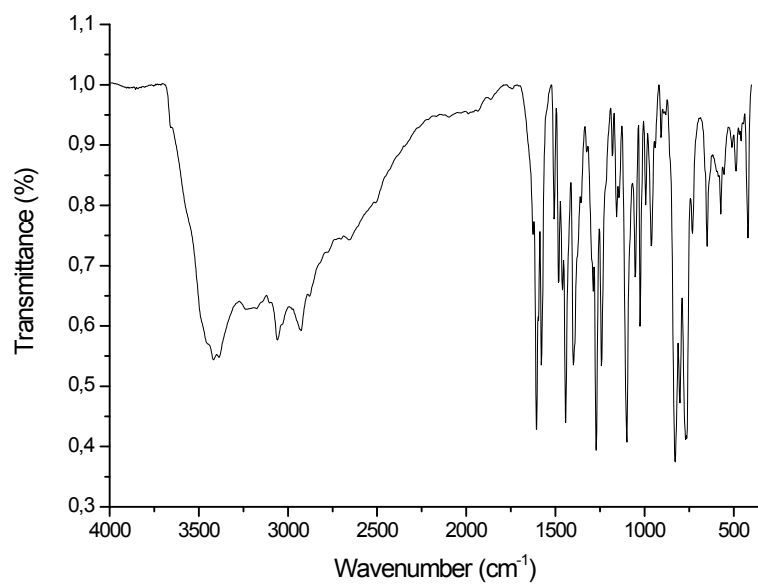


Figure S1. IR spectra of complexes **(1)** (top) and **(2)** (bottom).

Table S1. Calculated and measured bands in the IR region for complex **(1)**.

| Complex <b>1</b>            |                               |                          |
|-----------------------------|-------------------------------|--------------------------|
| Measured(cm <sup>-1</sup> ) | Calculated(cm <sup>-1</sup> ) | Shift(cm <sup>-1</sup> ) |
| 3449                        | 3444.9                        | 5.90                     |
| 3422                        | 3444.7                        | 22.7                     |
| 3382                        | 3124.0                        | 258                      |
| 3229                        | 3095.7                        | 133                      |
| 3176                        | 3092.3                        | 83.7                     |
| 3056                        | 3069.0                        | 13.0                     |

|      |        |      |
|------|--------|------|
| 2923 | 2934.5 | 11.5 |
| 1625 | 1609.2 | 15.8 |
| 1606 | 1607.3 | 1.30 |
| 1577 | 1572.3 | 5.30 |
| 1506 | 1504.3 | 1.70 |
| 1480 | 1477.8 | 2.20 |
| 1459 | 1449.7 | 9.30 |
| 1441 | 1436.9 | 4.10 |
| 1399 | 1396.3 | 2.70 |
| 1289 | 1289.9 | 0.90 |
| 1271 | 1257.4 | 13.6 |
| 1243 | 1246.0 | 3.00 |
| 1155 | 1150.5 | 4.50 |
| 1141 | 1132.4 | 8.60 |
| 1098 | 1097.1 | 0.90 |
| 1050 | 1049.9 | 0.10 |
| 1022 | 1026.6 | 4.60 |
| 990  | 986.31 | 3.69 |
| 963  | 964.25 | 1.25 |
| 828  | 829.00 | 1.00 |
| 798  | 786.23 | 11.8 |
| 769  | 768.70 | 0.30 |
| 763  | 763.23 | 0.23 |
| 730  | 716.90 | 14.1 |
| 648  | 637.30 | 10.3 |
| 571  | 563.09 | 7.91 |
| 489  | 484.06 | 4.94 |
| 418  | 426.16 | 8,16 |

Table S2. Calculated and measured bands in the IR region for complex (2).

| Complex 2                   |                               |                          |
|-----------------------------|-------------------------------|--------------------------|
| Measured(cm <sup>-1</sup> ) | Calculated(cm <sup>-1</sup> ) | Shift(cm <sup>-1</sup> ) |
| 3442                        | 3412.3                        | 29.7                     |
| 3240                        | 3134.4                        | 106                      |
| 3105                        | 3105.5                        | 0.50                     |
| 3065                        | 3073.9                        | 8.90                     |
| 3030                        | 2993.9                        | 36.1                     |
| 2925                        | 2930.9                        | 5.90                     |
| 2913                        | 2918.6                        | 5.60                     |
| 1627                        | 1615.3                        | 11.7                     |
| 1604                        | 1606.3                        | 2.30                     |
| 1571                        | 1571.0                        | 0.00                     |
| 1509                        | 1503.5                        | 5.50                     |
| 1482                        | 1460.6                        | 21.4                     |
| 1435                        | 1435.9                        | 0.90                     |
| 1390                        | 1395.3                        | 5.30                     |
| 1351                        | 1345.6                        | 5.40                     |
| 1305                        | 1307.5                        | 2.50                     |
| 1279                        | 1278.9                        | 0.10                     |
| 1255                        | 1255.6                        | 0.60                     |
| 1214                        | 1216.6                        | 2.60                     |
| 1180                        | 1178.8                        | 1.20                     |
| 1157                        | 1158.9                        | 1.90                     |
| 1105                        | 1103.3                        | 1.70                     |
| 1090                        | 1094.4                        | 4.40                     |
| 1052                        | 1059.8                        | 7.80                     |
| 1021                        | 1029.1                        | 8.10                     |
| 999                         | 985.50                        | 13.5                     |
| 974                         | 972.40                        | 2.60                     |
| 918                         | 918.90                        | 0.90                     |
| 839                         | 833.71                        | 5.29                     |
| 814                         | 806.45                        | 7.15                     |
| 767                         | 768.26                        | 1.26                     |
| 725                         | 717.15                        | 7.75                     |
| 643                         | 648.50                        | 5.50                     |
| 474                         | 472.37                        | 1.63                     |
| 421                         | 423.42                        | 2.42                     |

Table S3. Weight loss (%) data obtained by TGA for compounds (1) and (2).

| Compound | $\Delta T/^{\circ}\text{C}$ | Weight Loss/%     | Theoretical Weight Loss/% | Proposed Residue loss                              |
|----------|-----------------------------|-------------------|---------------------------|--|
| (1)      | 30-94                       | 7.1               | 8.0                       | 2 $\text{CH}_3\text{CH}_2\text{OH}$                |
|          | 151-211                     | 1.7               | 1.6                       | 1 $\text{H}_2\text{O}$                             |
|          | 211-505                     | 35.7              | 35.7                      | 2x $\text{C}_{12}\text{H}_{10}\text{OCl}$          |
|          | 505-670                     | 13.0%             | 13.5                      | 2x $\text{C}_5\text{H}_5\text{N}$                  |
|          | 670-999                     | 25.8              | 26.2                      | 2x $\text{C}_8\text{H}_{10}\text{N}_2$             |
|          | -                           | 16.5(residue)     | 17.2                      | $\text{Fe}_2\text{Cl}_2\text{O}$                   |
| (2)      | 30-130                      | 1.2               | 1.7                       | 1 $\text{H}_2\text{O}$                             |
|          | 160-502                     | 43,4              | 44.3                      | 2x $\text{C}_{13}\text{H}_{13}\text{O}_2\text{Cl}$ |
|          | 379-502                     | 11.6              | 11.2                      | 2 x $\text{C}_2\text{H}_4\text{O}_2$               |
|          | 502-686                     | 10.3              | 10.5                      | 2 x $\text{C}_3\text{H}_6\text{N}$                 |
|          | 686-999                     | 24.86             | 29,2                      | 4x $\text{C}_5\text{H}_4\text{N}$                  |
|          |                             | 19.9<br>(residue) | 20.1                      | $\text{Fe}_2\text{Cl}_2\text{O}_2$                 |

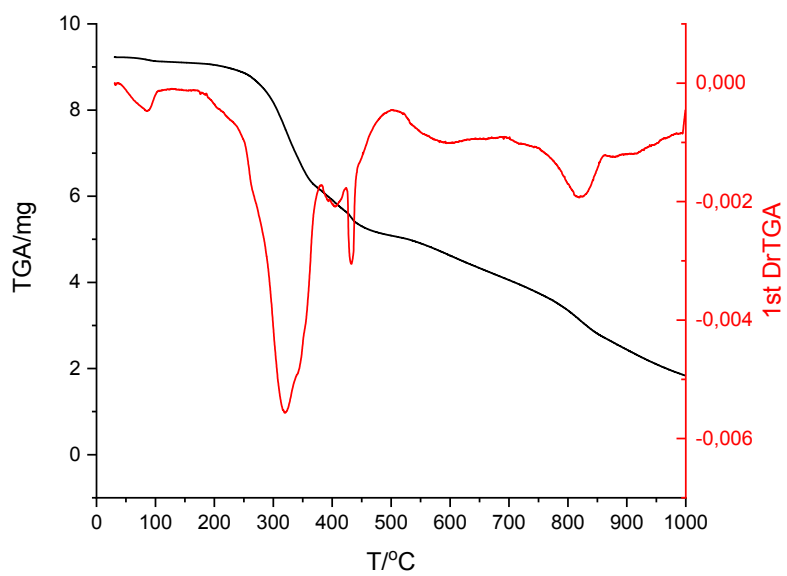
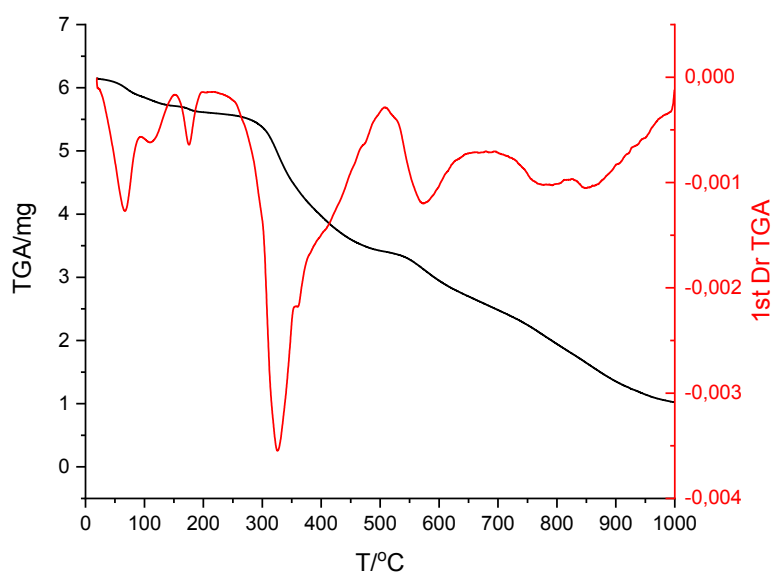


Figure S2. TGA analysis for complexes (1) (top) and (2) (bottom).

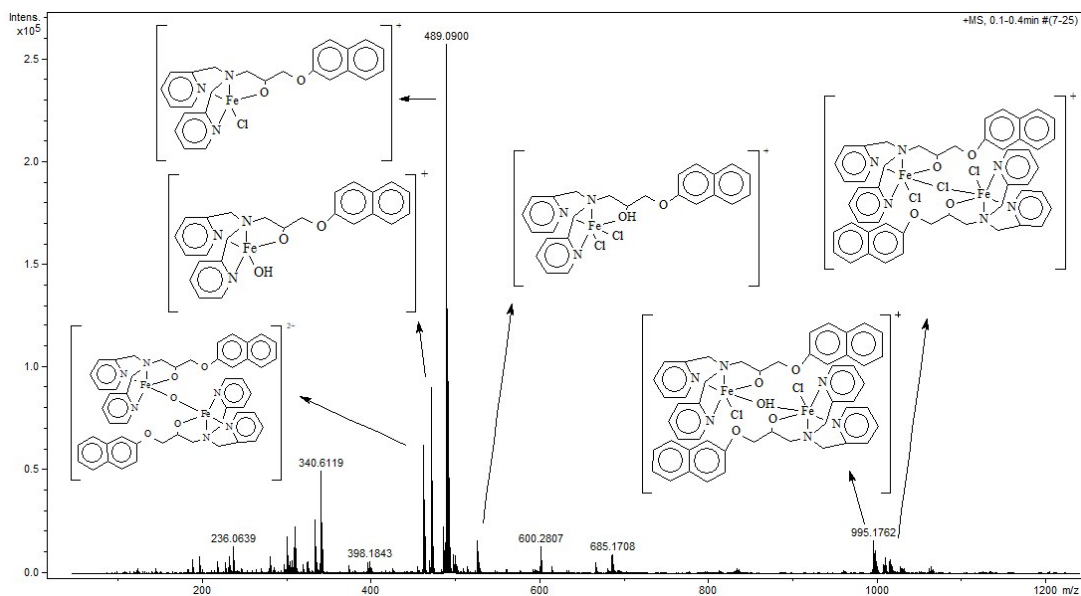


Figure S3. ESI(+)-MS in water/methanol (1:1) for complex **(2)**.

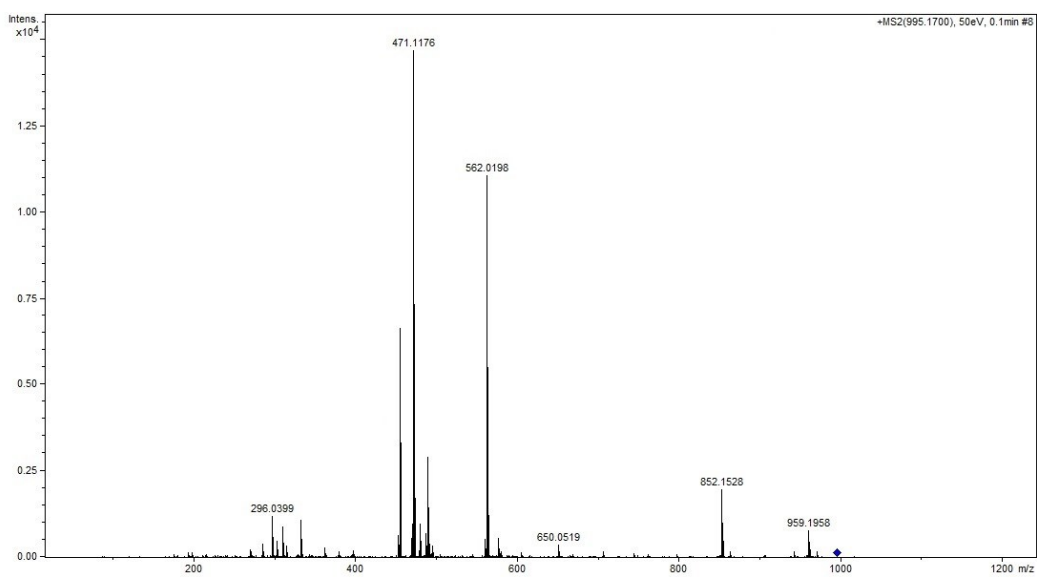


Figure S4. ESI(+)-MS/MS in water/methanol (1:1) for complex **(1)** of the species of  $m/z$  995.

Coordinates of optimized structures with DFT:

Complex 1A

|    |              |              |              |
|----|--------------|--------------|--------------|
| Cl | 5.658866579  | 7.355752025  | 16.324640056 |
| C  | 4.529531341  | 7.316976691  | 19.278632372 |
| H  | 4.351315186  | 6.730056362  | 18.390179216 |
| C  | 3.760920290  | 7.158713739  | 20.416286076 |
| H  | 2.963896345  | 6.434329578  | 20.431027238 |
| Fe | 4.799603266  | 11.386597000 | 17.008126497 |
| O  | 3.692579712  | 13.050703564 | 16.502693592 |
| H  | 3.818664739  | 13.987536262 | 16.707910958 |
| O  | 1.036482552  | 13.503351250 | 16.227427164 |
| N  | 3.437249778  | 10.847654634 | 18.261304051 |
| N  | 5.964332985  | 11.789685050 | 15.518141749 |
| N  | 3.668634719  | 10.487492047 | 15.686180043 |
| C  | 2.676584775  | 9.856790930  | 17.777343087 |
| C  | -0.910975991 | 13.797452073 | 17.528983949 |
| C  | -0.171969025 | 14.161145437 | 16.370165521 |
| C  | 3.046841164  | 9.377125079  | 16.411470651 |
| H  | 2.186250885  | 8.964898939  | 15.875501975 |
| H  | 3.799456429  | 8.587276287  | 16.521261950 |
| C  | 4.565780796  | 10.056888576 | 14.615312668 |
| H  | 5.018267988  | 9.105935985  | 14.927174920 |
| H  | 4.035374397  | 9.889870808  | 13.672062186 |
| C  | -0.658967281 | 15.090766484 | 15.491331643 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.106357152 | 15.380175207 | 14.611325975 |
| C | -0.431952887 | 12.855798573 | 18.461431261 |
| H | 0.535046614  | 12.404029305 | 18.292186475 |
| C | 5.680266489  | 11.037837747 | 14.447630525 |
| C | 1.846985676  | 13.795682489 | 15.120929752 |
| H | 1.325872505  | 13.604150908 | 14.173562823 |
| H | 2.170580204  | 14.846734510 | 15.134816231 |
| C | 3.067216772  | 12.871700789 | 15.237557655 |
| H | 3.777645773  | 13.090770842 | 14.427716874 |
| C | 6.411763624  | 11.140785899 | 13.272159822 |
| H | 6.157027479  | 10.518787183 | 12.429295083 |
| C | 2.621779596  | 11.407772009 | 15.223169345 |
| H | 2.270825126  | 11.132441862 | 14.224131726 |
| H | 1.782580404  | 11.349409066 | 15.919886805 |
| C | -2.170685913 | 14.410631056 | 17.749044900 |
| C | 1.636631056  | 9.310400541  | 18.514830210 |
| H | 1.041146234  | 8.517536000  | 18.091900295 |
| C | 3.172738314  | 11.331705360 | 19.470682234 |
| H | 3.802020396  | 12.143150421 | 19.801988062 |
| C | -2.648848043 | 15.361854081 | 16.822483244 |
| H | -3.607752071 | 15.823729282 | 16.997601768 |
| C | -1.907083302 | 15.691599606 | 15.725859320 |
| H | -2.268857378 | 16.420759208 | 15.018185222 |
| C | 7.459332482  | 12.044424835 | 13.200659753 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 8.037743456  | 12.142692902 | 12.295964912 |
| C  | -1.172518124 | 12.530539741 | 19.564116333 |
| H  | -0.797804193 | 11.810617102 | 20.277032041 |
| C  | 2.156788779  | 10.838072765 | 20.268274529 |
| H  | 1.981002540  | 11.268601930 | 21.239949507 |
| C  | 1.374745314  | 9.799774257  | 19.784544393 |
| H  | 0.570786207  | 9.387602272  | 20.373315801 |
| C  | -2.421312272 | 13.129310680 | 19.782422888 |
| H  | -2.992890816 | 12.860529898 | 20.657347774 |
| C  | -2.907901506 | 14.049216480 | 18.895585697 |
| H  | -3.866703748 | 14.516466423 | 19.060677041 |
| Fe | 6.690267514  | 8.588566323  | 17.706600671 |
| O  | 5.502863277  | 9.899082640  | 17.439959229 |
| O  | 7.797873422  | 6.924739609  | 18.211569607 |
| H  | 7.670902474  | 5.987586430  | 18.008372855 |
| O  | 10.454504546 | 6.470486863  | 18.478417464 |
| N  | 8.048400106  | 9.123171101  | 16.446972831 |
| N  | 5.530788147  | 8.190256816  | 19.201977399 |
| N  | 7.827036214  | 9.489851921  | 19.022085485 |
| C  | 8.811866750  | 10.114436960 | 16.925658915 |
| C  | 12.397113098 | 6.171947606  | 17.170641607 |
| C  | 11.661947195 | 5.811435478  | 18.332891439 |
| C  | 8.447198842  | 10.597799038 | 18.291709310 |
| H  | 9.310181530  | 11.010534960 | 18.823422077 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 7.694937270  | 11.388099297 | 18.182743959 |
| C | 6.934259276  | 9.924071666  | 20.095137512 |
| H | 6.481504523  | 10.874620728 | 19.782477871 |
| H | 7.468314019  | 10.093031119 | 21.035982304 |
| C | 12.151348524 | 4.883420605  | 19.212081053 |
| H | 11.601651168 | 4.596396197  | 20.094686106 |
| C | 11.915487339 | 7.111862104  | 16.237775407 |
| H | 10.949438196 | 7.564744857  | 16.409449407 |
| C | 5.819486748  | 8.944592061  | 20.269489732 |
| C | 9.647713780  | 6.181315727  | 19.588450703 |
| H | 10.172354351 | 6.374536467  | 20.533523612 |
| H | 9.323186673  | 5.130508853  | 19.578068062 |
| C | 8.427852383  | 7.106056897  | 19.474081108 |
| H | 7.720116347  | 6.889454808  | 20.286939614 |
| C | 5.092277009  | 8.845314139  | 21.447929493 |
| H | 5.350635225  | 9.469307715  | 22.288213104 |
| C | 8.874651074  | 8.569642149  | 19.483508296 |
| H | 9.229413576  | 8.846940933  | 20.480655048 |
| H | 9.711426793  | 8.625623459  | 18.783686619 |
| C | 13.655566844 | 5.557312189  | 16.947494259 |
| C | 9.849557878  | 10.658025711 | 16.182931361 |
| H | 10.447414828 | 11.451314963 | 16.601696846 |
| C | 8.307841856  | 8.635970115  | 15.237763123 |
| H | 7.676469097  | 7.824401108  | 14.910766549 |

|            |              |              |              |
|------------|--------------|--------------|--------------|
| C          | 14.136297031 | 4.607811909  | 17.874500973 |
| H          | 15.094224421 | 4.144815023  | 17.697021957 |
| C          | 13.398176339 | 4.281104381  | 18.974482551 |
| H          | 13.761898214 | 3.553261984  | 19.682512705 |
| C          | 4.044255733  | 7.942710222  | 21.525676771 |
| H          | 3.469170762  | 7.847218011  | 22.432785336 |
| C          | 12.652366110 | 7.434061082  | 15.131732814 |
| H          | 12.275667408 | 8.152653939  | 14.418522834 |
| C          | 9.321248441  | 9.126675102  | 14.435145259 |
| H          | 9.492916497  | 8.693655030  | 13.463841266 |
| C          | 10.106128850 | 10.165368597 | 14.913405072 |
| H          | 10.908252821 | 10.575336227 | 14.320605275 |
| C          | 13.899928045 | 6.833844683  | 14.910345827 |
| H          | 14.468592473 | 7.100214093  | 14.032789578 |
| C          | 14.388974875 | 5.915576496  | 15.797524715 |
| H          | 15.346830624 | 5.447223074  | 15.630087170 |
| Cl         | 5.824610043  | 12.616956130 | 18.397040020 |
| C          | 6.965153643  | 12.663966256 | 15.447479214 |
| H          | 7.139597097  | 13.248701077 | 16.338118164 |
| C          | 7.737884648  | 12.825781745 | 14.313120100 |
| H          | 8.534404485  | 13.550802824 | 14.303247340 |
| Complex 1B |              |              |              |
| Cl         | 5.658866579  | 7.355752025  | 16.324640056 |
| C          | 4.529531341  | 7.316976691  | 19.278632372 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 4.351315186  | 6.730056362  | 18.390179216 |
| C  | 3.760920290  | 7.158713739  | 20.416286076 |
| H  | 2.963896345  | 6.434329578  | 20.431027238 |
| Fe | 4.799603266  | 11.386597000 | 17.008126497 |
| O  | 3.692579712  | 13.050703564 | 16.502693592 |
| H  | 3.818664739  | 13.987536262 | 16.707910958 |
| O  | 1.036482552  | 13.503351250 | 16.227427164 |
| N  | 3.437249778  | 10.847654634 | 18.261304051 |
| N  | 5.964332985  | 11.789685050 | 15.518141749 |
| N  | 3.668634719  | 10.487492047 | 15.686180043 |
| C  | 2.676584775  | 9.856790930  | 17.777343087 |
| C  | -0.910975991 | 13.797452073 | 17.528983949 |
| C  | -0.171969025 | 14.161145437 | 16.370165521 |
| C  | 3.046841164  | 9.377125079  | 16.411470651 |
| H  | 2.186250885  | 8.964898939  | 15.875501975 |
| H  | 3.799456429  | 8.587276287  | 16.521261950 |
| C  | 4.565780796  | 10.056888576 | 14.615312668 |
| H  | 5.018267988  | 9.105935985  | 14.927174920 |
| H  | 4.035374397  | 9.889870808  | 13.672062186 |
| C  | -0.658967281 | 15.090766484 | 15.491331643 |
| H  | -0.106357152 | 15.380175207 | 14.611325975 |
| C  | -0.431952887 | 12.855798573 | 18.461431261 |
| H  | 0.535046614  | 12.404029305 | 18.292186475 |
| C  | 5.680266489  | 11.037837747 | 14.447630525 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.846985676  | 13.795682489 | 15.120929752 |
| H | 1.325872505  | 13.604150908 | 14.173562823 |
| H | 2.170580204  | 14.846734510 | 15.134816231 |
| C | 3.067216772  | 12.871700789 | 15.237557655 |
| H | 3.777645773  | 13.090770842 | 14.427716874 |
| C | 6.411763624  | 11.140785899 | 13.272159822 |
| H | 6.157027479  | 10.518787183 | 12.429295083 |
| C | 2.621779596  | 11.407772009 | 15.223169345 |
| H | 2.270825126  | 11.132441862 | 14.224131726 |
| H | 1.782580404  | 11.349409066 | 15.919886805 |
| C | -2.170685913 | 14.410631056 | 17.749044900 |
| C | 1.636631056  | 9.310400541  | 18.514830210 |
| H | 1.041146234  | 8.517536000  | 18.091900295 |
| C | 3.172738314  | 11.331705360 | 19.470682234 |
| H | 3.802020396  | 12.143150421 | 19.801988062 |
| C | -2.648848043 | 15.361854081 | 16.822483244 |
| H | -3.607752071 | 15.823729282 | 16.997601768 |
| C | -1.907083302 | 15.691599606 | 15.725859320 |
| H | -2.268857378 | 16.420759208 | 15.018185222 |
| C | 7.459332482  | 12.044424835 | 13.200659753 |
| H | 8.037743456  | 12.142692902 | 12.295964912 |
| C | -1.172518124 | 12.530539741 | 19.564116333 |
| H | -0.797804193 | 11.810617102 | 20.277032041 |
| C | 2.156788779  | 10.838072765 | 20.268274529 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 1.981002540  | 11.268601930 | 21.239949507 |
| C  | 1.374745314  | 9.799774257  | 19.784544393 |
| H  | 0.570786207  | 9.387602272  | 20.373315801 |
| C  | -2.421312272 | 13.129310680 | 19.782422888 |
| H  | -2.992890816 | 12.860529898 | 20.657347774 |
| C  | -2.907901506 | 14.049216480 | 18.895585697 |
| H  | -3.866703748 | 14.516466423 | 19.060677041 |
| Fe | 6.690267514  | 8.588566323  | 17.706600671 |
| O  | 5.488749957  | 10.067127337 | 17.621235249 |
| O  | 7.797873422  | 6.924739609  | 18.211569607 |
| H  | 7.670902474  | 5.987586430  | 18.008372855 |
| O  | 10.454504546 | 6.470486863  | 18.478417464 |
| N  | 8.048400106  | 9.123171101  | 16.446972831 |
| N  | 5.530788147  | 8.190256816  | 19.201977399 |
| N  | 7.827036214  | 9.489851921  | 19.022085485 |
| C  | 8.811866750  | 10.114436960 | 16.925658915 |
| C  | 12.397113098 | 6.171947606  | 17.170641607 |
| C  | 11.661947195 | 5.811435478  | 18.332891439 |
| C  | 8.447198842  | 10.597799038 | 18.291709310 |
| H  | 9.310181530  | 11.010534960 | 18.823422077 |
| H  | 7.694937270  | 11.388099297 | 18.182743959 |
| C  | 6.934259276  | 9.924071666  | 20.095137512 |
| H  | 6.481504523  | 10.874620728 | 19.782477871 |
| H  | 7.468314018  | 10.093031119 | 21.035982304 |

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| C | 12.151348524 | 4.883420605  | 19.212081053 |
| H | 11.601651168 | 4.596396197  | 20.094686106 |
| C | 11.915487339 | 7.111862104  | 16.237775407 |
| H | 10.949438196 | 7.564744857  | 16.409449407 |
| C | 5.819486748  | 8.944592061  | 20.269489732 |
| C | 9.647713780  | 6.181315727  | 19.588450703 |
| H | 10.172354351 | 6.374536467  | 20.533523612 |
| H | 9.323186673  | 5.130508853  | 19.578068062 |
| C | 8.427852383  | 7.106056897  | 19.474081108 |
| H | 7.720116347  | 6.889454808  | 20.286939614 |
| C | 5.092277009  | 8.845314139  | 21.447929493 |
| H | 5.350635225  | 9.469307715  | 22.288213104 |
| C | 8.874651074  | 8.569642149  | 19.483508296 |
| H | 9.229413576  | 8.846940933  | 20.480655048 |
| H | 9.711426793  | 8.625623459  | 18.783686619 |
| C | 13.655566844 | 5.557312189  | 16.947494259 |
| C | 9.849557878  | 10.658025711 | 16.182931361 |
| H | 10.447414828 | 11.451314963 | 16.601696846 |
| C | 8.307841856  | 8.635970115  | 15.237763123 |
| H | 7.676469097  | 7.824401108  | 14.910766549 |
| C | 14.136297031 | 4.607811909  | 17.874500973 |
| H | 15.094224421 | 4.144815023  | 17.697021957 |
| C | 13.398176339 | 4.281104381  | 18.974482551 |
| H | 13.761898214 | 3.553261984  | 19.682512705 |



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| C  | 4.044255733  | 7.942710222  | 21.525676771 |
| H  | 3.469170762  | 7.847218011  | 22.432785336 |
| C  | 12.652366110 | 7.434061082  | 15.131732814 |
| H  | 12.275667408 | 8.152653939  | 14.418522834 |
| C  | 9.321248441  | 9.126675102  | 14.435145259 |
| H  | 9.492916497  | 8.693655030  | 13.463841266 |
| C  | 10.106128850 | 10.165368597 | 14.913405072 |
| H  | 10.908252821 | 10.575336227 | 14.320605275 |
| C  | 13.899928045 | 6.833844683  | 14.910345827 |
| H  | 14.468592473 | 7.100214093  | 14.032789578 |
| C  | 14.388974875 | 5.915576496  | 15.797524715 |
| H  | 15.346830624 | 5.447223074  | 15.630087170 |
| Cl | 5.824610043  | 12.616956130 | 18.397040020 |
| C  | 6.965153643  | 12.663966256 | 15.447479214 |
| H  | 7.139597097  | 13.248701077 | 16.338118164 |
| C  | 7.737884648  | 12.825781745 | 14.313120100 |
| H  | 8.534404485  | 13.550802824 | 14.303247340 |

Complex 1C

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| Cl | 5.658866579 | 7.355752025 | 16.324640056 |
| C  | 4.529531341 | 7.316976691 | 19.278632372 |
| H  | 4.351315186 | 6.730056362 | 18.390179216 |
| C  | 3.760920290 | 7.158713739 | 20.416286076 |
| H  | 2.963896345 | 6.434329578 | 20.431027238 |

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| Fe | 4.799603266  | 11.386597000 | 17.008126497 |
| O  | 3.692579712  | 13.050703564 | 16.502693592 |
| H  | 3.818664739  | 13.987536262 | 16.707910958 |
| O  | 1.036482552  | 13.503351250 | 16.227427164 |
| N  | 3.437249778  | 10.847654634 | 18.261304051 |
| N  | 5.964332985  | 11.789685050 | 15.518141749 |
| N  | 3.668634719  | 10.487492047 | 15.686180043 |
| C  | 2.676584775  | 9.856790930  | 17.777343087 |
| C  | -0.910975991 | 13.797452073 | 17.528983949 |
| C  | -0.171969025 | 14.161145437 | 16.370165521 |
| C  | 3.046841164  | 9.377125079  | 16.411470651 |
| H  | 2.186250885  | 8.964898939  | 15.875501975 |
| H  | 3.799456429  | 8.587276287  | 16.521261950 |
| C  | 4.565780796  | 10.056888576 | 14.615312668 |
| H  | 5.018267988  | 9.105935985  | 14.927174920 |
| H  | 4.035374397  | 9.889870808  | 13.672062186 |
| C  | -0.658967281 | 15.090766484 | 15.491331643 |
| H  | -0.106357152 | 15.380175207 | 14.611325975 |
| C  | -0.431952887 | 12.855798573 | 18.461431261 |
| H  | 0.535046614  | 12.404029305 | 18.292186475 |
| C  | 5.680266489  | 11.037837747 | 14.447630525 |
| C  | 1.846985676  | 13.795682489 | 15.120929752 |
| H  | 1.325872505  | 13.604150908 | 14.173562823 |
| H  | 2.170580204  | 14.846734510 | 15.134816231 |

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| C | 3.067216772  | 12.871700789 | 15.237557655 |
| H | 3.777645773  | 13.090770842 | 14.427716874 |
| C | 6.411763624  | 11.140785899 | 13.272159822 |
| H | 6.157027479  | 10.518787183 | 12.429295083 |
| C | 2.621779596  | 11.407772009 | 15.223169345 |
| H | 2.270825126  | 11.132441862 | 14.224131726 |
| H | 1.782580404  | 11.349409066 | 15.919886805 |
| C | -2.170685913 | 14.410631056 | 17.749044900 |
| C | 1.636631056  | 9.310400541  | 18.514830210 |
| H | 1.041146234  | 8.517536000  | 18.091900295 |
| C | 3.172738314  | 11.331705360 | 19.470682234 |
| H | 3.802020396  | 12.143150421 | 19.801988062 |
| C | -2.648848043 | 15.361854081 | 16.822483244 |
| H | -3.607752071 | 15.823729282 | 16.997601768 |
| C | -1.907083302 | 15.691599606 | 15.725859320 |
| H | -2.268857378 | 16.420759208 | 15.018185222 |
| C | 7.459332482  | 12.044424835 | 13.200659753 |
| H | 8.037743456  | 12.142692902 | 12.295964912 |
| C | -1.172518124 | 12.530539741 | 19.564116333 |
| H | -0.797804193 | 11.810617102 | 20.277032041 |
| C | 2.156788779  | 10.838072765 | 20.268274529 |
| H | 1.981002540  | 11.268601930 | 21.239949507 |
| C | 1.374745314  | 9.799774257  | 19.784544393 |
| H | 0.570786207  | 9.387602272  | 20.373315801 |

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| C  | -2.421312272 | 13.129310680 | 19.782422888 |
| H  | -2.992890816 | 12.860529898 | 20.657347774 |
| C  | -2.907901506 | 14.049216480 | 18.895585697 |
| H  | -3.866703748 | 14.516466423 | 19.060677041 |
| Fe | 6.690267514  | 8.588566323  | 17.706600671 |
| O  | 5.471072792  | 9.958429900  | 17.406889346 |
| O  | 7.797873422  | 6.924739609  | 18.211569607 |
| H  | 7.670902474  | 5.987586430  | 18.008372855 |
| O  | 10.454504546 | 6.470486863  | 18.478417464 |
| N  | 8.048400106  | 9.123171101  | 16.446972831 |
| N  | 5.530788147  | 8.190256816  | 19.201977399 |
| N  | 7.827036214  | 9.489851921  | 19.022085485 |
| C  | 8.811866750  | 10.114436960 | 16.925658915 |
| C  | 12.397113098 | 6.171947606  | 17.170641607 |
| C  | 11.661947195 | 5.811435478  | 18.332891439 |
| C  | 8.447198842  | 10.597799038 | 18.291709310 |
| H  | 9.310181530  | 11.010534960 | 18.823422077 |
| H  | 7.694937270  | 11.388099297 | 18.182743959 |
| C  | 6.934259276  | 9.924071666  | 20.095137512 |
| H  | 6.481504523  | 10.874620728 | 19.782477871 |
| H  | 7.468314018  | 10.093031119 | 21.035982304 |
| C  | 12.151348524 | 4.883420605  | 19.212081053 |
| H  | 11.601651168 | 4.596396197  | 20.094686106 |
| C  | 11.915487339 | 7.111862104  | 16.237775407 |

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| H | 10.949438196 | 7.564744857  | 16.409449407 |
| C | 5.819486748  | 8.944592061  | 20.269489732 |
| C | 9.647713780  | 6.181315727  | 19.588450703 |
| H | 10.172354351 | 6.374536467  | 20.533523612 |
| H | 9.323186673  | 5.130508853  | 19.578068062 |
| C | 8.427852383  | 7.106056897  | 19.474081108 |
| H | 7.720116347  | 6.889454808  | 20.286939614 |
| C | 5.092277009  | 8.845314139  | 21.447929493 |
| H | 5.350635225  | 9.469307715  | 22.288213104 |
| C | 8.874651074  | 8.569642149  | 19.483508296 |
| H | 9.229413576  | 8.846940933  | 20.480655048 |
| H | 9.711426793  | 8.625623459  | 18.783686619 |
| C | 13.655566844 | 5.557312189  | 16.947494259 |
| C | 9.849557878  | 10.658025711 | 16.182931361 |
| H | 10.447414828 | 11.451314963 | 16.601696846 |
| C | 8.307841856  | 8.635970115  | 15.237763123 |
| H | 7.676469097  | 7.824401108  | 14.910766549 |
| C | 14.136297031 | 4.607811909  | 17.874500973 |
| H | 15.094224421 | 4.144815023  | 17.697021957 |
| C | 13.398176339 | 4.281104381  | 18.974482551 |
| H | 13.761898214 | 3.553261984  | 19.682512705 |
| C | 4.044255733  | 7.942710222  | 21.525676771 |
| H | 3.469170762  | 7.847218011  | 22.432785336 |
| C | 12.652366110 | 7.434061082  | 15.131732814 |

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| H  | 12.275667408 | 8.152653939  | 14.418522834 |
| C  | 9.321248441  | 9.126675102  | 14.435145259 |
| H  | 9.492916497  | 8.693655030  | 13.463841266 |
| C  | 10.106128850 | 10.165368597 | 14.913405072 |
| H  | 10.908252821 | 10.575336227 | 14.320605275 |
| C  | 13.899928045 | 6.833844683  | 14.910345827 |
| H  | 14.468592473 | 7.100214093  | 14.032789578 |
| C  | 14.388974875 | 5.915576496  | 15.797524715 |
| H  | 15.346830624 | 5.447223074  | 15.630087170 |
| Cl | 5.824610043  | 12.616956130 | 18.397040020 |
| C  | 6.965153643  | 12.663966256 | 15.447479214 |
| H  | 7.139597097  | 13.248701077 | 16.338118164 |
| C  | 7.737884648  | 12.825781745 | 14.313120100 |
| H  | 8.534404485  | 13.550802824 | 14.303247340 |

Complex 2A

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| Cl | 5.866344360 | 7.525870266  | 16.737984603 |
| C  | 4.460642834 | 7.700457689  | 19.568798179 |
| H  | 4.373021637 | 7.035515888  | 18.722487346 |
| C  | 3.556885000 | 7.664103408  | 20.613570557 |
| H  | 2.745027410 | 6.956444915  | 20.599124189 |
| Fe | 5.106516821 | 11.617976642 | 16.997395753 |
| O  | 4.311588634 | 13.306485160 | 16.104508841 |
| H  | 3.755490234 | 13.975011125 | 16.564538948 |

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| N | 3.563445719  | 11.313603395 | 18.142209370 |
| N | 6.442171493  | 11.764226704 | 15.622728106 |
| N | 4.044443858  | 10.634341532 | 15.677801300 |
| C | 2.826760223  | 10.279285681 | 17.710011222 |
| C | -0.740022850 | 12.256413055 | 17.088330820 |
| C | 0.214548690  | 12.849599655 | 16.231064335 |
| C | 3.321565179  | 9.627627011  | 16.458482538 |
| H | 2.508691814  | 9.166813019  | 15.887974963 |
| H | 4.038062958  | 8.847812180  | 16.739805406 |
| C | 4.992243047  | 10.071520913 | 14.717331138 |
| H | 5.345637697  | 9.114370526  | 15.122546918 |
| H | 4.529104239  | 9.880186583  | 13.743836580 |
| C | 1.061694361  | 13.812764588 | 16.706781431 |
| C | -1.609595512 | 11.244175509 | 16.634599836 |
| H | -1.550161903 | 10.926180986 | 15.603653412 |
| C | 6.187294101  | 10.961306293 | 14.583517712 |
| C | 2.478566708  | 14.010488207 | 14.725694918 |
| C | 3.612376562  | 12.966541107 | 14.914400913 |
| H | 4.322649731  | 13.020085987 | 14.081520580 |
| C | 7.012127158  | 10.935016625 | 13.467328560 |
| H | 6.780694901  | 10.274731605 | 12.647117509 |
| C | 3.063476726  | 11.544798583 | 15.070510737 |
| H | 2.723570357  | 11.163261043 | 14.101523707 |
| H | 2.207328743  | 11.594887934 | 15.747469208 |

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| C  | -0.830286486 | 12.685453511 | 18.437305736 |
| C  | 1.699092793  | 9.851763491  | 18.393770248 |
| H  | 1.121591268  | 9.026791562  | 18.009444354 |
| C  | 3.202612290  | 11.938756803 | 19.259126013 |
| H  | 3.831323431  | 12.763280532 | 19.559372142 |
| C  | 0.036166114  | 13.707170862 | 18.881251202 |
| H  | -0.053088099 | 14.062720380 | 19.896274461 |
| C  | 0.968020494  | 14.247302305 | 18.046775586 |
| H  | 1.631056679  | 15.033028483 | 18.372379391 |
| C  | 8.121034027  | 11.764268780 | 13.423165918 |
| H  | 8.772013048  | 11.762933846 | 12.563572750 |
| C  | -2.528249942 | 10.684594781 | 17.479732564 |
| H  | -3.197851290 | 9.917884527  | 17.121891958 |
| C  | 2.099998673  | 11.562201455 | 20.003135198 |
| H  | 1.852103034  | 12.098384969 | 20.903228260 |
| C  | 1.328908488  | 10.497262913 | 19.562739079 |
| H  | 0.453846143  | 10.182261834 | 20.107647724 |
| C  | -2.618535158 | 11.109626244 | 18.814022397 |
| H  | -3.357068900 | 10.664229273 | 19.462282611 |
| C  | -1.787301459 | 12.089359793 | 19.283255031 |
| H  | -1.860419799 | 12.431485508 | 20.304921762 |
| Fe | 6.789403021  | 8.841248544  | 18.126881086 |
| O  | 5.643959721  | 10.070264854 | 17.567154982 |
| O  | 7.824350719  | 7.207017265  | 18.792511820 |



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| H | 7.488743463  | 6.304212423  | 18.688121771 |
| O | 10.740040882 | 6.988540492  | 19.897717297 |
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| N | 5.485830273  | 8.548506395  | 19.533229193 |
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| C | 9.054644183  | 10.218692159 | 17.493968882 |
| C | 10.818132738 | 6.116576060  | 16.279397100 |
| C | 10.377131750 | 6.141023485  | 17.621109760 |
| C | 8.551358412  | 10.824572139 | 18.763223095 |
| H | 9.359206853  | 11.254861410 | 19.362532608 |
| H | 7.846802797  | 11.624272256 | 18.504524687 |
| C | 6.811482879  | 10.344095698 | 20.416498536 |
| H | 6.418978045  | 11.265857625 | 19.964214498 |
| H | 7.240800921  | 10.596392059 | 21.391472780 |
| C | 11.054891249 | 6.870915640  | 18.558491326 |
| C | 10.133120479 | 5.380048393  | 15.291711803 |
| H | 9.251446417  | 4.821786040  | 15.571464881 |
| C | 5.663119095  | 9.399345191  | 20.551172252 |
| C | 9.537599114  | 6.497866381  | 20.411796372 |
| H | 9.689165256  | 6.461964478  | 21.493655060 |
| H | 9.321481222  | 5.481559449  | 20.061100091 |
| C | 8.326457119  | 7.420393766  | 20.111284193 |
| H | 7.533787846  | 7.212998337  | 20.842662148 |
| C | 4.797672311  | 9.423870085  | 21.636676047 |

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| H | 4.969483173  | 10.122457099 | 22.439459028 |
| C | 8.757882579  | 8.887913350  | 20.150276723 |
| H | 8.942663532  | 9.185877463  | 21.186207961 |
| H | 9.703461452  | 8.944588271  | 19.607476290 |
| C | 11.977599950 | 6.844752769  | 15.910107530 |
| C | 10.227528585 | 10.617225728 | 16.870971187 |
| H | 10.836106865 | 11.385462966 | 17.319872536 |
| C | 8.641547961  | 8.673477365  | 15.841546461 |
| H | 7.989912078  | 7.894714482  | 15.478031515 |
| C | 12.656774234 | 7.582168259  | 16.904135498 |
| H | 13.549712061 | 8.124878802  | 16.633369804 |
| C | 12.205880298 | 7.603333131  | 18.188970738 |
| H | 12.722519848 | 8.149137948  | 18.962281889 |
| C | 3.725559060  | 8.547718202  | 21.670498655 |
| H | 3.043084001  | 8.548074941  | 22.505278885 |
| C | 10.583902027 | 5.358111907  | 14.000327564 |
| H | 10.060439795 | 4.782070208  | 13.252742146 |
| C | 9.788434546  | 9.023634821  | 15.154472191 |
| H | 10.041300014 | 8.516332322  | 14.238954689 |
| C | 10.601925026 | 10.015084731 | 15.680578970 |
| H | 11.512316190 | 10.305234856 | 15.181719723 |
| C | 11.737045416 | 6.070760661  | 13.637154925 |
| H | 12.085996809 | 6.029732607  | 12.616861121 |
| C | 12.418626408 | 6.800782502  | 14.572150945 |

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| H  | 13.312478481 | 7.343402597  | 14.302428500 |
| Cl | 6.044568447  | 12.921467694 | 18.377658896 |
| C  | 7.496610889  | 12.571965870 | 15.575596061 |
| H  | 7.632339200  | 13.216157001 | 16.430504897 |
| C  | 8.363394263  | 12.605480935 | 14.499286890 |
| H  | 9.201852594  | 13.281485721 | 14.504007936 |
| O  | 2.059140654  | 14.456985007 | 15.990699252 |
| H  | 0.216518073  | 12.537879108 | 15.196590558 |
| H  | 1.665341374  | 13.610975753 | 14.117999994 |
| H  | 2.879808258  | 14.898488656 | 14.230496523 |
| H  | 9.517454062  | 5.537988385  | 17.868669309 |

Complex 2B

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| Cl | 5.866342834 | 7.525869742  | 16.737985075 |
| C  | 4.460641985 | 7.700459087  | 19.568798880 |
| H  | 4.373020081 | 7.035517183  | 18.722488202 |
| C  | 3.556884416 | 7.664105649  | 20.613571510 |
| H  | 2.745026323 | 6.956447725  | 20.599125505 |
| Fe | 5.106517029 | 11.617976710 | 16.997395925 |
| O  | 4.311588872 | 13.306485416 | 16.104509393 |
| H  | 3.755490653 | 13.975011413 | 16.564539755 |
| N  | 3.563446325 | 11.313603948 | 18.142210120 |
| N  | 6.442171170 | 11.764226523 | 15.622727712 |
| N  | 4.044443369 | 10.634341903 | 15.677801855 |
| C  | 2.826760107 | 10.279286693 | 17.710012089 |

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| C | -0.740023050 | 12.256412257 | 17.088330349 |
| C | 0.214548575  | 12.849599295 | 16.231064220 |
| C | 3.321564491  | 9.627627725  | 16.458483338 |
| H | 2.508690873  | 9.166813909  | 15.887976005 |
| H | 4.038062087  | 8.847812702  | 16.739806206 |
| C | 4.992242152  | 10.071520823 | 14.717331557 |
| H | 5.345636768  | 9.114370494  | 15.122547498 |
| H | 4.529103004  | 9.880186295  | 13.743837198 |
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| C | -1.609594835 | 11.244174053 | 16.634599175 |
| H | -1.550160341 | 10.926179166 | 15.603652916 |
| C | 6.187293269  | 10.961306028 | 14.583517508 |
| C | 2.478566845  | 14.010489057 | 14.725695775 |
| C | 3.612376460  | 12.966541546 | 14.914401586 |
| H | 4.322649370  | 13.020086258 | 14.081521020 |
| C | 7.012125899  | 10.935016137 | 13.467328045 |
| H | 6.780693168  | 10.274731167 | 12.647117088 |
| C | 3.063476361  | 11.544799177 | 15.070511407 |
| H | 2.723569746  | 11.163261740 | 14.101524423 |
| H | 2.207328466  | 11.594888690 | 15.747469998 |
| C | -0.830287633 | 12.685452920 | 18.437305153 |
| C | 1.699092339  | 9.851765376  | 18.393771089 |
| H | 1.121590198  | 9.026793875  | 18.009445199 |
| C | 3.202613308  | 11.938757679 | 19.259126733 |

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| H  | 3.831324858  | 12.763281141 | 19.559372727 |
| C  | 0.036164209  | 13.707170773 | 18.881250906 |
| H  | -0.053090471 | 14.062720223 | 19.896274148 |
| C  | 0.968018878  | 14.247302388 | 18.046775752 |
| H  | 1.631054479  | 15.033028943 | 18.372379849 |
| C  | 8.121032867  | 11.764268136 | 13.423164908 |
| H  | 8.772011501  | 11.762933100 | 12.563571446 |
| C  | -2.528249132 | 10.684592741 | 17.479731679 |
| H  | -3.197849530 | 9.917881684  | 17.121891054 |
| C  | 2.099999384  | 11.562203168 | 20.003135906 |
| H  | 1.852104045  | 12.098387034 | 20.903228838 |
| C  | 1.328908376  | 10.497265212 | 19.562739773 |
| H  | 0.453845898  | 10.182264639 | 20.107648499 |
| C  | -2.618535118 | 11.109624256 | 18.814021427 |
| H  | -3.357068629 | 10.664226660 | 19.462281478 |
| C  | -1.787302278 | 12.089358427 | 19.283254257 |
| H  | -1.860421423 | 12.431484418 | 20.304920838 |
| Fe | 6.789402569  | 8.841247998  | 18.126880889 |
| O  | 5.595150580  | 10.024957642 | 17.597808076 |
| O  | 7.824349540  | 7.207016287  | 18.792511798 |
| H  | 7.488741315  | 6.304211721  | 18.688122462 |
| O  | 10.740040302 | 6.988538424  | 19.897718312 |
| N  | 8.276599996  | 9.257575494  | 16.977970333 |
| N  | 5.485830062  | 8.548507016  | 19.533229471 |

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| N | 7.806389780  | 9.797556027  | 19.495969224 |
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| C | 10.818133707 | 6.116577624  | 16.279397261 |
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| C | 8.551359127  | 10.824570964 | 18.763221783 |
| H | 9.359208099  | 11.254859870 | 19.362530846 |
| H | 7.846803817  | 11.624271423 | 18.504523585 |
| C | 6.811484220  | 10.344095535 | 20.416498225 |
| H | 6.418979824  | 11.265857842 | 19.964214551 |
| H | 7.240802875  | 10.596391426 | 21.391472321 |
| C | 11.054891176 | 6.870914947  | 18.558492343 |
| C | 10.133121897 | 5.380050949  | 15.291710916 |
| H | 9.251447508  | 4.821788598  | 15.571462963 |
| C | 5.663119777  | 9.399345876  | 20.551172316 |
| C | 9.537597897  | 6.497864867  | 20.411796369 |
| H | 9.689163422  | 6.461962347  | 21.493655073 |
| H | 9.321479599  | 5.481558218  | 20.061099492 |
| C | 8.326456595  | 7.420393035  | 20.111283900 |
| H | 7.533787349  | 7.212998595  | 20.842662189 |
| C | 4.797673222  | 9.423871684  | 21.636676282 |
| H | 4.969484756  | 10.122458792 | 22.439459038 |
| C | 8.757883125  | 8.887912297  | 20.150275494 |
| H | 8.942665213  | 9.185876705  | 21.186206445 |
| H | 9.703461532  | 8.944586405  | 19.607474169 |

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| C  | 11.977601736 | 6.844753772  | 15.910109165 |
| C  | 10.227528160 | 10.617223700 | 16.870968942 |
| H  | 10.836106849 | 11.385460932 | 17.319869747 |
| C  | 8.641546536  | 8.673475436  | 15.841545580 |
| H  | 7.989910330  | 7.894712541  | 15.478031245 |
| C  | 12.656775897 | 7.582167817  | 16.904138277 |
| H  | 13.549714281 | 8.124877995  | 16.633373696 |
| C  | 12.205881110 | 7.603331800  | 18.188973228 |
| H  | 12.722520788 | 8.149135182  | 18.962285305 |
| C  | 3.725559361  | 8.547720574  | 21.670499362 |
| H  | 3.043084477  | 8.548078024  | 22.505279734 |
| C  | 10.583904351 | 5.358115284  | 14.000326975 |
| H  | 10.060442537 | 4.782074188  | 13.252740811 |
| C  | 9.788432896  | 9.023632352  | 15.154470671 |
| H  | 10.041297900 | 8.516329354  | 14.238953316 |
| C  | 10.601923963 | 10.015082095 | 15.680576821 |
| H  | 11.512314802 | 10.305232065 | 15.181716897 |
| C  | 11.737048419 | 6.070763661  | 13.637155755 |
| H  | 12.086000655 | 6.029736066  | 12.616862220 |
| C  | 12.418629191 | 6.800784275  | 14.572152889 |
| H  | 13.312481737 | 7.343404131  | 14.302431532 |
| Cl | 6.044569622  | 12.921467407 | 18.377658752 |
| C  | 7.496610582  | 12.571965630 | 15.575595144 |
| H  | 7.632339299  | 13.216156818 | 16.430503875 |

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| C | 8.363393517 | 12.605480514 | 14.499285612 |
| H | 9.201851960 | 13.281485163 | 14.504006280 |
| O | 2.059140278 | 14.456985152 | 15.990700147 |
| H | 0.216518669 | 12.537878560 | 15.196590500 |
| H | 1.665341809 | 13.610977166 | 14.118000060 |
| H | 2.879808938 | 14.898489756 | 14.230498190 |
| H | 9.517454155 | 5.537988598  | 17.868668257 |

Complex 2C

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| Cl | 5.866348613  | 7.525869786  | 16.737984542 |
| C  | 4.460643608  | 7.700456398  | 19.568796387 |
| H  | 4.373023478  | 7.035515065  | 18.722485078 |
| C  | 3.556884857  | 7.664101079  | 20.613567935 |
| H  | 2.745027828  | 6.956441960  | 20.599120580 |
| Fe | 5.106516347  | 11.617976240 | 16.997395327 |
| O  | 4.311585866  | 13.306484272 | 16.104509144 |
| H  | 3.755485681  | 13.975008945 | 16.564538828 |
| N  | 3.563443963  | 11.313599260 | 18.142205454 |
| N  | 6.442173317  | 11.764230206 | 15.622730604 |
| N  | 4.044447648  | 10.634340467 | 15.677797565 |
| C  | 2.826760580  | 10.279281107 | 17.710004744 |
| C  | -0.740017996 | 12.256412147 | 17.088335485 |
| C  | 0.214552458  | 12.849597567 | 16.231066940 |
| C  | 3.321569127  | 9.627624126  | 16.458476669 |
| H  | 2.508697590  | 9.166809343  | 15.887967076 |



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| H | 4.038067393  | 8.847810022  | 16.739800205 |
| C | 4.992250275  | 10.071521778 | 14.717329715 |
| H | 5.345645405  | 9.114371852  | 15.122546052 |
| H | 4.529114320  | 9.880187077  | 13.743833856 |
| C | 1.061696490  | 13.812765565 | 16.706780632 |
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| H | -1.550155371 | 10.926174303 | 15.603662326 |
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| C | 2.478565938  | 14.010485605 | 14.725691948 |
| C | 3.612377348  | 12.966540527 | 14.914399282 |
| H | 4.322652738  | 13.020088316 | 14.081520942 |
| C | 7.012136215  | 10.935020796 | 13.467332650 |
| H | 6.780707752  | 10.274734583 | 12.647121489 |
| C | 3.063480434  | 11.544796304 | 15.070505449 |
| H | 2.723578172  | 11.163259551 | 14.101516678 |
| H | 2.207330295  | 11.594882698 | 15.747461322 |
| C | -0.830282098 | 12.685456848 | 18.437308951 |
| C | 1.699092358  | 9.851756587  | 18.393761056 |
| H | 1.121593168  | 9.026783846  | 18.009433399 |
| C | 3.202606910  | 11.938751216 | 19.259121787 |
| H | 3.831316573  | 12.763275143 | 19.559370498 |
| C | 0.036168942  | 13.707177117 | 18.881250955 |
| H | -0.053085637 | 14.062729615 | 19.896273127 |
| C | 0.968022372  | 14.247307355 | 18.046773476 |

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| H  | 1.631056997  | 15.033036000 | 18.372374443 |
| C  | 8.121041505  | 11.764275203 | 13.423172559 |
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| C  | -2.528242765 | 10.684592449 | 17.479742361 |
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| H  | 1.852093570  | 12.098376551 | 20.903220817 |
| C  | 1.328904293  | 10.497254498 | 19.562729584 |
| H  | 0.453841048  | 10.182252024 | 20.107635909 |
| C  | -2.618528174 | 11.109627813 | 18.814030952 |
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| C  | -1.787295781 | 12.089364053 | 19.283260360 |
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| Fe | 6.789404345  | 8.841249381  | 18.126881788 |
| O  | 5.751608261  | 10.120776267 | 17.291762725 |
| O  | 7.824352837  | 7.207019164  | 18.792513851 |
| H  | 7.488746759  | 6.304213955  | 18.688123212 |
| O  | 10.740042149 | 6.988544530  | 19.897715532 |
| N  | 8.276602883  | 9.257579225  | 16.977973540 |
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| N  | 7.806388171  | 9.797558626  | 19.495971670 |
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| C  | 10.377129364 | 6.141020291  | 17.621111468 |

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| H | 9.359204001  | 11.254865401 | 19.362535687 |
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| H | 9.251439313  | 4.821777896  | 15.571472349 |
| C | 5.663117664  | 9.399344468  | 20.551172135 |
| C | 9.537601791  | 6.497870360  | 20.411798120 |
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| H | 10.836105613 | 11.385469024 | 17.319876873 |
| C | 8.641551918  | 8.673480079  | 15.841549121 |

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| C  | 12.656765404 | 7.582170096  | 16.904126855 |
| H  | 13.549700865 | 8.124882537  | 16.633357151 |
| C  | 12.205875150 | 7.603336953  | 18.188963387 |
| H  | 12.722514753 | 8.149146083  | 18.962271461 |
| C  | 3.725557506  | 8.547715346  | 21.670496694 |
| H  | 3.043081931  | 8.548070992  | 22.505276502 |
| C  | 10.583889500 | 5.358102550  | 14.000330014 |
| H  | 10.060425448 | 4.782059239  | 13.252747085 |
| C  | 9.788438211  | 9.023639702  | 15.154475415 |
| H  | 10.041304233 | 8.516338823  | 14.238957163 |
| C  | 10.601926010 | 10.015091921 | 15.680582058 |
| H  | 11.512318234 | 10.305241952 | 15.181724667 |
| C  | 11.737030340 | 6.070752914  | 13.637152409 |
| H  | 12.085978396 | 6.029723926  | 12.616857500 |
| C  | 12.418612666 | 6.800778155  | 14.572144820 |
| H  | 13.312462634 | 7.343399754  | 14.302418434 |
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| C  | 7.496611406  | 12.571971268 | 15.575601082 |
| H  | 7.632336404  | 13.216162862 | 16.430510098 |
| C  | 8.363397596  | 12.605487654 | 14.499294220 |
| H  | 9.201854294  | 13.281494456 | 14.504017074 |
| O  | 2.059140885  | 14.456985567 | 15.990695638 |
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**H 2.879805708 14.898485126 14.230490831**

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