

ELECTRONIC SUPPLEMENTARY INFORMATION

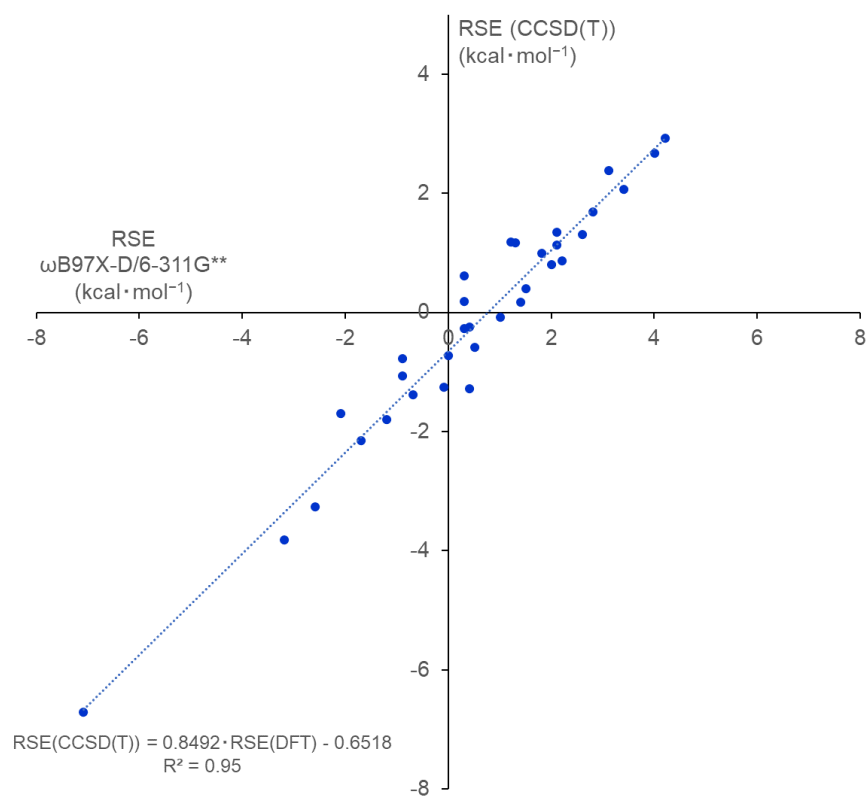


Figure S1: Correlation of the RSE values calculated at the (U)DF-CCSD(T)/aug-ccpVTZ//ωB97X-D/6-311G** level and at the ωB97X-D/6-311G** level

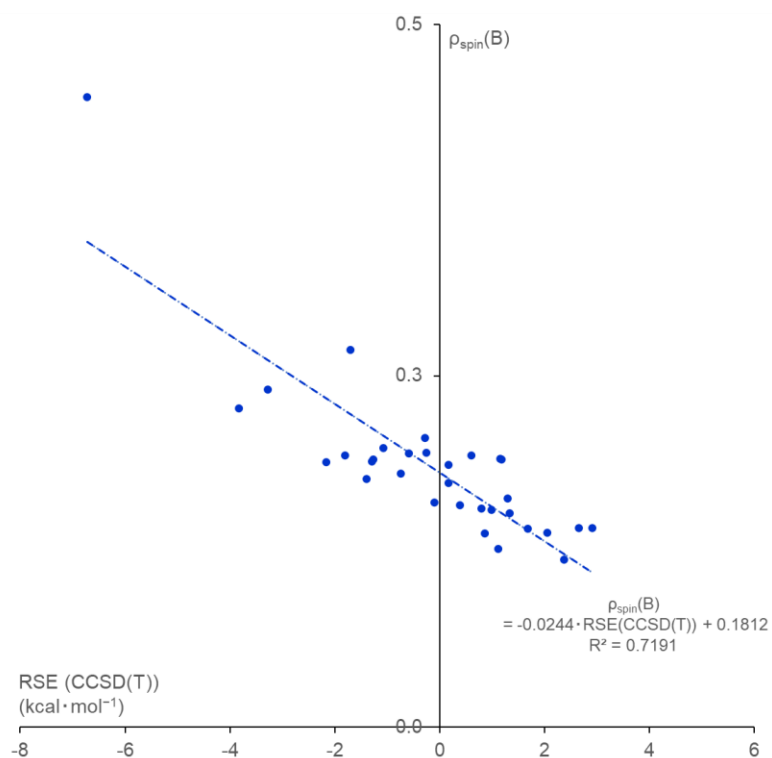


Figure S2: Plot of $\rho_{spin}(B)$ versus $RSE(CCSD(T))$

Table S1: Mulliken partial charges at the P- and O- atoms ($q(P)$ and $q(O)$, respectively), calculated at the (U) ω B97X-D/6-311G** level

| Radical | $q(P)$ | $q(O)$ | Radical | $q(P)$ | $q(O)$ |
|-----------|--------|--------|-----------|--------|--------|
| 1 | 0.717 | -0.498 | 17 | 0.758 | -0.526 |
| 2 | 0.770 | -0.505 | 18 | 0.800 | -0.530 |
| 3 | 0.750 | -0.517 | 19 | 0.801 | -0.531 |
| 4 | 0.786 | -0.510 | 20 | 0.786 | -0.521 |
| 5 | 0.756 | -0.525 | 21 | 0.780 | -0.522 |
| 6 | 0.785 | -0.526 | 22 | 0.822 | -0.540 |
| 7 | 0.768 | -0.525 | 23 | 0.794 | -0.494 |
| 8 | 0.962 | -0.499 | 24 | 0.840 | -0.511 |
| 9 | 0.741 | -0.523 | 25 | 0.879 | -0.524 |
| 10 | 0.785 | -0.527 | 26 | 0.892 | -0.522 |
| 11 | 0.728 | -0.537 | 27 | 0.870 | -0.543 |
| 12 | 0.844 | -0.533 | 28 | 0.888 | -0.543 |
| 13 | 0.823 | -0.537 | 29 | 0.822 | -0.522 |
| 14 | 0.742 | -0.540 | 30 | 0.877 | -0.553 |
| 15 | 0.745 | -0.528 | 31 | 0.822 | -0.520 |
| 16 | 0.773 | -0.527 | 32 | 0.904 | -0.553 |

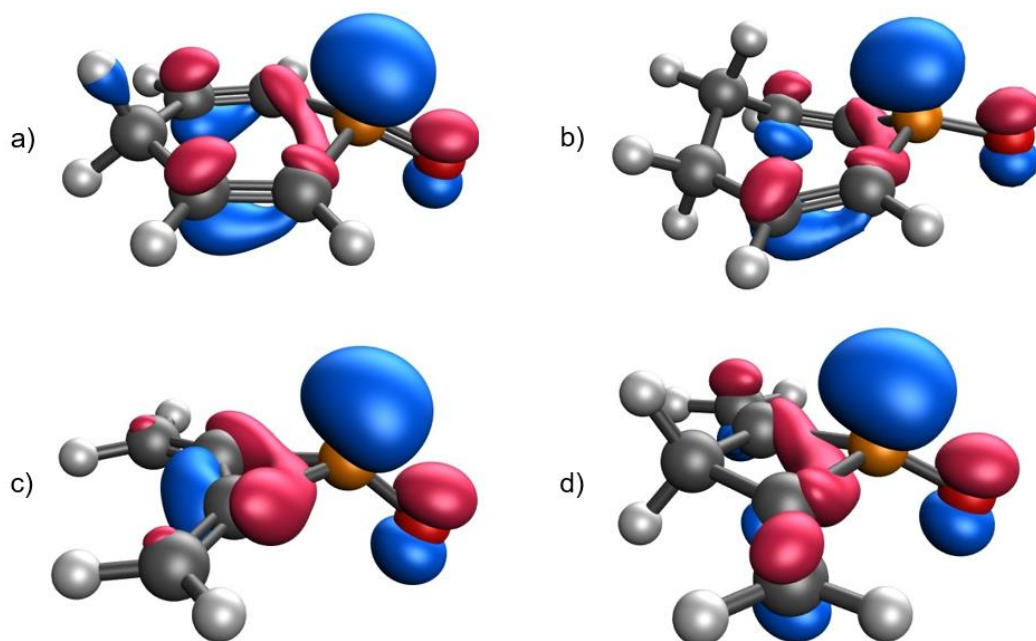


Figure S3: SOMO of radical a) 12, b) 18, c) 23, d) 24

Table S2: Dimerization energy of parent $H_2P^{\bullet}(O)$, and unsubstituted radical 8 and radical 33

| | ΔE_{dim} (kcal/mol) | ΔG_{dim} (kcal/mol) |
|-----------------------------------|---------------------------------------|---------------------------------------|
| $H_2P^{\bullet}(O)$, heterodimer | -79.1 | -63.1 |
| $H_2P^{\bullet}(O)$, homodimer | -58.0 | -42.0 |
| 8 , heterodimer | -57.2 | -42.1 |
| 8 , homodimer | -47.3 | -31.1 |
| 33 , heterodimer | -62.0 | -46.5 |
| 33 , homodimer | -58.8 | -41.4 |

Table S3: SBA in degree at the $U\omega B97X-D/6-311G^{}$ level, $\rho_{spin}(P)$, $\rho_{spin}(O)$ and $\rho_{spin}(B)$ values, and RSE values at the $(U)\omega B97X-D/6-311G^{**}$ level in kcal/mol**

| Radical | SBA | $\rho_{spin}(P)$ | $\rho_{spin}(O)$ | $\rho_{spin}(B)$ | RSE (DFT) |
|----------------|------------|------------------------------------|------------------------------------|------------------------------------|------------------|
| 8A | 360 | 0.376 | 0.221 | 0.403 | -3.9 |
| 8B | 360 | 0.323 | 0.215 | 0.462 | -7.7 |
| 8C | 360 | 0.277 | 0.224 | 0.499 | -4.5 |
| 8D | 360 | 0.243 | 0.208 | 0.549 | -9.7 |
| 8E | 360 | 0.361 | 0.205 | 0.434 | -6.4 |
| 8F | 347 | 0.445 | 0.264 | 0.291 | -3.0 |
| 8G | 360 | 0.327 | 0.206 | 0.467 | -6.0 |
| 8H | 359 | 0.351 | 0.199 | 0.450 | -4.5 |
| 8I | 355 | 0.399 | 0.241 | 0.360 | -5.1 |
| 8J | 360 | 0.369 | 0.192 | 0.439 | -10.9 |
| 8K | 360 | 0.300 | 0.197 | 0.503 | -8.0 |
| 8L | 360 | 0.293 | 0.182 | 0.524 | -15.9 |
| 8M | 360 | 0.361 | 0.215 | 0.424 | -9.2 |
| 8N | 354 | 0.384 | 0.224 | 0.392 | -2.5 |
| 8O | 360 | 0.360 | 0.197 | 0.444 | -2.8 |
| 8P | 360 | 0.329 | 0.197 | 0.474 | -4.9 |
| 33A | 360 | 0.309 | 0.177 | 0.514 | -5.9 |
| 33B | 345 | 0.494 | 0.249 | 0.257 | -1.9 |
| 33C | 360 | 0.223 | 0.158 | 0.618 | -9.6 |
| 33D | 360 | 0.273 | 0.184 | 0.543 | -5.1 |
| 33F | 360 | 0.288 | 0.160 | 0.552 | -2.2 |
| 33G | 350 | 0.452 | 0.217 | 0.331 | 0.4 |

Total Energies and optimized geometries in cartesian coordinates

1

8

E= -495.117297

| | | | |
|---|-----------|-----------|-----------|
| P | -0.020386 | -0.134429 | 0.175112 |
| C | 0.108364 | 0.021222 | 1.968277 |
| C | 1.471259 | -0.024865 | 1.184851 |
| H | 2.055959 | 0.889235 | 1.180400 |
| H | 2.062328 | -0.926790 | 1.309717 |
| H | -0.126482 | -0.855191 | 2.564359 |
| H | -0.142069 | 0.961740 | 2.447911 |
| O | -0.433670 | -1.432580 | -0.464252 |

1H

9

E= -495.756762

| | | | |
|---|-----------|-----------|-----------|
| P | -0.012376 | -0.212967 | 0.229807 |
| C | 0.125436 | -0.000762 | 1.998108 |
| C | 1.474946 | -0.032917 | 1.202574 |
| H | 2.048325 | 0.885898 | 1.141768 |
| H | 2.079247 | -0.920152 | 1.358797 |
| H | -0.061266 | -0.869444 | 2.620474 |
| H | -0.172409 | 0.938604 | 2.451474 |
| O | -0.485689 | -1.397247 | -0.525929 |
| H | -0.296145 | 1.057680 | -0.303421 |

2

6

E= -493.864503

| | | | |
|---|----------|----------|----------|
| C | 0.078989 | 0.033980 | 0.117280 |
| C | 0.079313 | 0.033775 | 1.454940 |

| | | | |
|---|-----------|-----------|-----------|
| P | 1.714629 | -0.072899 | 0.785702 |
| O | 2.633058 | -1.255408 | 0.785300 |
| H | -0.640850 | 0.013899 | 2.262306 |
| H | -0.641584 | 0.014334 | -0.689726 |

2H

7

E= -494.504268

| | | | |
|---|-----------|-----------|-----------|
| C | 0.084664 | 0.055580 | 0.159123 |
| C | 0.012328 | -0.056558 | 1.485676 |
| P | 1.659475 | -0.185946 | 0.894394 |
| O | 2.563157 | -1.354953 | 0.844355 |
| H | -0.740389 | -0.120569 | 2.259634 |
| H | -0.578947 | 0.128857 | -0.691736 |
| H | 2.324599 | 1.045403 | 1.035022 |

3

11

E= -534.459393

| | | | |
|---|-----------|-----------|-----------|
| P | 0.096163 | 0.025005 | 0.206654 |
| C | 0.125407 | -0.092956 | 2.060206 |
| C | 1.921419 | -0.120870 | 0.519425 |
| H | 2.595686 | 0.530112 | -0.034181 |
| H | 2.228801 | -1.162241 | 0.395651 |
| H | -0.062377 | -1.126455 | 2.361616 |
| H | -0.512333 | 0.578726 | 2.632092 |
| O | -0.633623 | -0.982495 | -0.625844 |
| C | 1.637203 | 0.244611 | 1.998868 |
| H | 1.804445 | 1.308500 | 2.174621 |
| H | 2.239250 | -0.321056 | 2.710873 |

3H

12
E= -535.100550
P 0.068007 -0.136944 0.209015
C 0.115607 -0.183294 2.041176
C 1.876663 -0.195361 0.502994
H 2.529826 0.406145 -0.126764
H 2.216985 -1.233158 0.505725
H 0.064289 -1.218333 2.385987
H -0.591613 0.427711 2.599336
O -0.707485 -1.042074 -0.671871
C 1.587217 0.307497 1.944949
H 1.641375 1.396431 1.998424
H 2.249663 -0.103075 2.706570
H -0.132823 1.249274 -0.031560

4

9
E= -533.217327
C -0.018987 -0.010904 -0.067003
C 0.181183 -0.452304 1.365419
C 1.486021 -0.304241 1.629292
P 1.781350 0.507894 0.036163
O 2.798298 0.056984 -0.962580
H 2.059796 -0.506988 2.522247
H -0.167918 -0.833398 -0.768672
H -0.761455 0.770114 -0.237883
H -0.603171 -0.795786 2.034387

4H

10
E= -533.856104
C 0.035451 0.030207 -0.035544

C 0.176297 -0.490487 1.381103
C 1.486683 -0.447891 1.651389
P 1.852296 0.379402 0.087446
O 2.858527 -0.043414 -0.912946
H 2.038113 -0.743071 2.533043
H -0.184862 -0.747500 -0.768973
H -0.638407 0.877459 -0.180291
H -0.636753 -0.802471 2.029897
H 1.914710 1.755857 0.427618

5

14
E= -573.793795
P -0.251598 0.158931 -0.079168
C 0.041939 -0.102516 1.736373
C 1.553048 0.088766 1.924972
C 2.005353 1.197992 0.961610
C 1.426453 0.874557 -0.420804
H -0.523353 0.642293 2.302743
H -0.321200 -1.092959 2.013121
H 2.071830 -0.841469 1.672022
H 1.801657 0.332339 2.960458
H 3.093896 1.279605 0.926970
H 1.619186 2.162089 1.310065
H 1.997873 0.088979 -0.924521
H 1.371673 1.738302 -1.083096
O -0.601782 -1.071504 -0.870665

5H

15
E= -574.436234
P -0.177839 -0.004785 -0.107362

C 0.085241 -0.216312 1.703976
C 1.565509 0.122315 1.947985
C 1.959600 1.217289 0.944442
C 1.456033 0.761546 -0.431629
H -0.571207 0.475138 2.239281
H -0.182933 -1.232716 1.994653
H 2.178770 -0.766522 1.768203
H 1.743231 0.434267 2.979116
H 3.037002 1.394999 0.939585
H 1.479053 2.161416 1.224843
H 2.096135 -0.024020 -0.844498
H 1.386782 1.564446 -1.166544
O -0.584656 -1.187700 -0.912977
H -1.073568 1.095063 -0.185009

6

12

E= -572.557714

C -0.257265 -0.116093 0.115670
C 0.100898 0.319270 1.546358
C 1.339449 -0.428236 1.980938
C 2.020901 -1.097618 1.050996
P 1.282165 -0.875238 -0.579964
O 1.121228 -2.058061 -1.488899
H -0.622522 0.701614 -0.503885
H -1.008125 -0.910936 0.112233
H -0.722937 0.138332 2.242584
H 0.304376 1.395136 1.583586
H 1.651958 -0.380231 3.019927
H 2.942070 -1.637267 1.226713

6H

13

E= -573.198239

C -0.228698 -0.066447 0.074511
C 0.031465 0.185072 1.572029
C 1.408799 -0.325103 1.911336
C 2.070513 -1.012105 0.982828
P 1.074342 -1.229190 -0.504490
O 0.676593 -2.604173 -0.906811
H -0.149809 0.859105 -0.499636
H -1.208107 -0.503466 -0.122250
H -0.705169 -0.325858 2.200351
H -0.046639 1.248964 1.812876
H 1.813226 -0.136307 2.901798
H 3.047122 -1.455493 1.129050
H 1.764827 -0.518207 -1.519450

7

12

E= -572.556709

C -0.018985 -0.004559 -0.021973
C 0.176807 0.275297 1.442167
C 1.222030 -0.281901 2.049869
C 2.133222 -1.151861 1.229328
P 1.541984 -0.884907 -0.511481
O 1.378256 -2.114676 -1.357449
H -0.173378 0.903962 -0.608107
H -0.862845 -0.675060 -0.215545
H -0.522530 0.915591 1.969083
H 1.428039 -0.124228 3.103144
H 2.027814 -2.216020 1.465108
H 3.186418 -0.887066 1.345339

7H

13
 E= -573.200113
 C -0.058339 -0.113172 -0.007476
 C 0.231039 0.337184 1.400899
 C 1.279806 -0.219126 2.007125
 C 2.060825 -1.237245 1.217472
 P 1.535436 -0.878777 -0.505970
 O 1.561863 -1.949559 -1.534377
 H -0.344167 0.701786 -0.675018
 H -0.845624 -0.873101 -0.048651
 H -0.394929 1.078760 1.884193
 H 1.569939 0.036508 3.019954
 H 1.778630 -2.265088 1.468275
 H 3.141724 -1.147207 1.339990
 H 2.316248 0.269318 -0.803216

8

10
 E= -571.326600
 C 0.190710 -0.353080 0.009545
 P 0.206270 -0.394636 1.740617
 O 1.124973 0.227216 2.720590
 C -0.886212 -1.106087 -0.376487
 C -1.652277 -1.683362 0.707804
 C -1.190377 -1.393616 1.964154
 H 0.890211 0.162921 -0.627711
 H -1.155080 -1.265378 -1.412576
 H -2.524604 -2.297472 0.525954
 H -1.605910 -1.716941 2.904616

8H

11

E= -571.954267
 C 0.108664 -0.269379 0.018738
 P 0.070782 -0.131748 1.828773
 O 1.312284 -0.244606 2.633234
 C -0.841489 -1.123200 -0.370925
 C -1.612810 -1.749440 0.732188
 C -1.249472 -1.371229 1.960350
 H 0.773084 0.281791 -0.631415
 H -1.057397 -1.362361 -1.406117
 H -2.407143 -2.457180 0.523391
 H -1.688265 -1.713912 2.886605
 H -0.656099 1.076826 2.006099

9

17
 E= -613.112090
 P 0.348191 0.049673 -0.190381
 C 0.202226 0.125821 1.641142
 O 1.111397 -1.137573 -0.708309
 C -0.728736 1.259430 2.093182
 H -0.182501 -0.848230 1.966503
 H 1.204108 0.237930 2.060954
 C -2.139932 1.150147 1.508694
 H -0.781802 1.255567 3.185627
 H -0.294244 2.224901 1.807855
 C -2.173625 1.252482 -0.018861
 H -2.586597 0.196534 1.817408
 H -2.765689 1.939816 1.934157
 C -1.411834 0.117876 -0.717901
 H -3.211027 1.244254 -0.365254
 H -1.752905 2.217774 -0.324715

H -1.851675 -0.856352 -0.472821
H -1.440842 0.225230 -1.804279

9H

18

E= -613.757420

P 0.281270 0.000776 -0.174343
C 0.160456 0.114038 1.638799
O 1.099068 -1.114237 -0.724054
C -0.762782 1.255221 2.090886
H -0.215646 -0.853283 1.988846
H 1.170292 0.230807 2.039756
C -2.181353 1.140400 1.525329
H -0.799953 1.268255 3.183676
H -0.331724 2.217005 1.787328
C -2.228585 1.212625 -0.003697
H -2.628573 0.195203 1.857541
H -2.799150 1.941204 1.941352
C -1.465076 0.067408 -0.685255
H -3.267974 1.195829 -0.343015
H -1.814785 2.174226 -0.330909
H -1.904239 -0.902101 -0.426580
H -1.497132 0.154660 -1.774083
H 0.730399 1.307598 -0.514578

10

15

E= -611.873798

P 0.072187 0.063920 -0.012522
C -0.006635 0.135338 1.818951
C 1.406458 0.006787 2.399817
C 2.315513 1.180676 2.029932

C 2.367573 1.509540 0.563736
C 1.490790 1.115073 -0.365145
O -1.188488 0.419156 -0.748489
H -0.467409 1.090700 2.092433
H -0.659475 -0.664098 2.174098
H 1.345737 -0.074021 3.488331
H 1.861595 -0.924312 2.043823
H 1.993959 2.084258 2.565968
H 3.332269 0.979094 2.381836
H 3.187765 2.155376 0.255840
H 1.617428 1.412364 -1.401408

10H

16

E= -612.515553

P -0.073100 0.189485 0.022553
C -0.062126 0.213311 1.840880
C 1.358607 -0.006876 2.371210
C 2.307210 1.134526 2.000867
C 2.325569 1.487521 0.539205
C 1.425272 1.116404 -0.371629
O -1.306413 0.655192 -0.665837
H -0.455671 1.186104 2.151774
H -0.752735 -0.552409 2.201241
H 1.332097 -0.121001 3.457904
H 1.757657 -0.946789 1.971716
H 2.044510 2.038659 2.566477
H 3.325914 0.880688 2.310934
H 3.156366 2.114453 0.220607
H 1.529657 1.432747 -1.405028
H 0.282817 -1.157861 -0.257273

11
15
E= -611.871883
C 0.064025 -0.086280 0.281449
P 0.077384 -0.060479 2.123183
O 1.440882 -0.291407 2.719885
C -0.070904 -1.474172 -0.299168
C -0.364391 -2.590679 0.361137
C -0.639742 -2.715063 1.836479
C -1.107834 -1.408648 2.492705
H -0.742567 0.561172 -0.081293
H 1.003416 0.371636 -0.041617
H 0.103410 -1.539075 -1.370431
H -0.395475 -3.518328 -0.203358
H -1.398496 -3.487466 1.997519
H 0.267461 -3.066566 2.341514
H -2.083081 -1.106909 2.096831
H -1.195982 -1.517661 3.575086

11H
16
E= -612.515409
C 0.019016 -0.114419 0.277519
P 0.085946 -0.121070 2.102212
O 1.435519 -0.263140 2.712792
C -0.055812 -1.504364 -0.306591
C -0.340452 -2.625076 0.351549
C -0.648997 -2.751806 1.820688
C -1.104214 -1.442098 2.475028
H -0.838280 0.488479 -0.046620
H 0.917276 0.398756 -0.078104
H 0.154383 -1.571750 -1.370267

H -0.332443 -3.556534 -0.207351
H -1.421911 -3.513087 1.961476
H 0.242528 -3.125678 2.337845
H -2.078270 -1.131513 2.080059
H -1.193019 -1.550595 3.557954
H -0.611176 1.064843 2.452792

12
13
E= -610.636539
C 0.345769 -0.328031 0.070211
P 0.000622 -0.017762 1.801494
O 1.167870 0.281866 2.695604
C -0.377990 -1.178114 -0.662197
C -1.502729 -2.036776 -0.162730
C -1.645965 -2.167482 1.325294
C -1.039863 -1.409221 2.242021
H 1.142249 0.254307 -0.380638
H -0.149429 -1.282254 -1.720222
H -2.448190 -1.654012 -0.575363
H -1.402198 -3.038768 -0.597323
H -2.305542 -2.964850 1.659469
H -1.206142 -1.578497 3.300528

12H
14
E= -611.275382
C 0.259201 -0.228529 0.101080
P 0.157776 -0.150237 1.895155
O 1.441184 -0.285374 2.634029
C -0.428685 -1.096884 -0.637345
C -1.429213 -2.092047 -0.138070

C -1.677120 -2.144104 1.337253
C -1.107205 -1.374993 2.262608
H 0.971837 0.441826 -0.369385
H -0.271368 -1.108935 -1.713853
H -2.385875 -1.910046 -0.646328
H -1.128429 -3.092084 -0.478294
H -2.400008 -2.893792 1.652122
H -1.355053 -1.510063 3.310886
H -0.505055 1.081668 2.130162

13

13

E= -610.638814

C -0.033709 -0.217172 0.053437
C 0.025374 0.237227 1.487037
C 1.112070 0.166179 2.263671
C 2.412307 -0.335530 1.823484
C 2.725087 -0.611867 0.542748
P 1.603259 -0.191694 -0.781099
O 1.684569 -0.978868 -2.054510
H -0.729212 0.392840 -0.526176
H -0.405426 -1.250765 -0.000209
H -0.905430 0.592408 1.918450
H 1.032620 0.476995 3.299670
H 3.160247 -0.498176 2.594323
H 3.715177 -0.962256 0.271987

13H

14

E= -611.279609

C -0.077741 0.020153 0.040917
P 0.119009 -0.120563 1.854573

O 1.479015 -0.419935 2.374372
C -0.391275 -1.283112 -0.631536
C -1.096423 -2.257460 -0.048932
C -1.576856 -2.202212 1.332267
C -1.174501 -1.307704 2.246938
H -0.908664 0.720305 -0.123085
H 0.821678 0.482840 -0.370966
H -0.048884 -1.409888 -1.653130
H -1.329370 -3.153120 -0.613837
H -2.290005 -2.968029 1.626040
H -1.528532 -1.364911 3.270419
H -0.424593 1.107627 2.306562

14

20

E= -652.420593

P 0.221816 0.104520 0.053921
C -0.059700 -0.275550 1.833230
O 1.054986 1.348905 -0.124437
C -0.365297 0.982521 2.661943
H -0.857277 -1.022974 1.910301
H 0.858977 -0.743878 2.195655
C -1.781988 1.540349 2.516561
H -0.198240 0.744152 3.717386
H 0.364060 1.752769 2.394013
C -2.234922 1.925261 1.100632
H -2.499299 0.816945 2.926012
H -1.850737 2.427691 3.153956
C -2.571686 0.733623 0.186151
H -3.131526 2.543460 1.199985
H -1.476589 2.558505 0.625421
H -2.922435 -0.102652 0.800907

H -3.413386 0.998984 -0.461082
C -1.439029 0.252577 -0.733824
H -1.275411 0.961666 -1.550695
H -1.701154 -0.707559 -1.187172

14H

21

E= -653.062829

P 0.150788 -0.092220 0.099916
C -0.139287 -0.262287 1.890297
O 1.302633 0.783702 -0.260276
C -0.378516 1.068920 2.614773
H -0.962691 -0.966816 2.056741
H 0.770830 -0.737620 2.268702
C -1.815920 1.586377 2.549154
H -0.111391 0.938687 3.667507
H 0.310016 1.821317 2.215161
C -2.357438 1.940883 1.160129
H -2.484044 0.846196 3.008806
H -1.877361 2.481440 3.176485
C -2.608012 0.752280 0.216068
H -3.306229 2.466206 1.304458
H -1.684859 2.658553 0.674550
H -2.925387 -0.119792 0.799290
H -3.451246 0.993826 -0.437697
C -1.432930 0.382088 -0.696072
H -1.172064 1.235184 -1.330183
H -1.718875 -0.433939 -1.366673
H 0.296362 -1.454020 -0.280271

15

18

E= -651.182964

C -0.051171 -0.022122 0.043548
C -0.012046 -0.043291 1.573679
C 1.377669 0.017779 2.213329
C 2.242130 -1.246862 2.047499
C 2.978150 -1.379543 0.737253
C 2.427165 -1.477590 -0.474747
P 0.655294 -1.499055 -0.796622
O 0.314699 -1.575369 -2.258800
H -1.084443 0.034322 -0.308462
H 0.479471 0.851675 -0.350159
H -0.589051 0.816062 1.928784
H -0.535525 -0.934288 1.940383
H 1.924495 0.886940 1.831293
H 1.238180 0.185400 3.285467
H 2.975995 -1.272567 2.855776
H 1.604052 -2.129686 2.189661
H 4.063646 -1.405036 0.799148
H 3.048686 -1.620169 -1.354381

15H

19

E= -651.823629

C -0.023770 0.002319 0.015688
C -0.003623 -0.042558 1.547937
C 1.374979 -0.000715 2.213934
C 2.243567 -1.261164 2.037763
C 2.983589 -1.362277 0.725670
C 2.435346 -1.448409 -0.484246
P 0.658906 -1.466333 -0.820657
O 0.318988 -1.603497 -2.262258
H -1.053964 0.085990 -0.343263

H 0.521460 0.871916 -0.363702
H -0.584080 0.810182 1.912141
H -0.537783 -0.937101 1.892057
H 1.930838 0.875105 1.861715
H 1.215352 0.143999 3.286584
H 2.975671 -1.292391 2.847390
H 1.610525 -2.148763 2.169373
H 4.069535 -1.365493 0.790540
H 3.058823 -1.517209 -1.370687
H 0.183909 -2.511356 0.022537

16

18
E= -651.181340

C 0.043059 0.000410 0.030597
C -0.009700 -0.009670 1.564862
C 1.377583 -0.030742 2.218838
C 2.379659 -1.051274 1.745343
C 2.196085 -2.170920 1.048251
C 0.889931 -2.743536 0.567471
P 0.065828 -1.688950 -0.712234
O 0.712547 -1.741648 -2.067321
H -0.818710 0.519431 -0.394730
H 0.939762 0.512140 -0.333229
H -0.522038 0.893360 1.908014
H -0.622008 -0.842736 1.923849
H 1.833578 0.955229 2.065969
H 1.263076 -0.126279 3.306101
H 3.405993 -0.815086 2.016529
H 3.079818 -2.738904 0.773841
H 0.182060 -2.889888 1.386931
H 1.039793 -3.716361 0.096787

16H

19
E= -651.825272
C 0.103532 0.007366 -0.007126
C -0.007992 -0.015378 1.523990
C 1.357140 -0.041683 2.223421
C 2.377325 -1.057887 1.778589
C 2.227688 -2.165955 1.055690
C 0.943064 -2.720616 0.499780
P 0.165154 -1.650024 -0.766895
O 0.742231 -1.712473 -2.136192
H -0.743662 0.522700 -0.466715
H 1.007711 0.533111 -0.327394
H -0.534142 0.882417 1.858983
H -0.629920 -0.854364 1.853039
H 1.816985 0.945812 2.093266
H 1.207083 -0.146088 3.305352
H 3.388596 -0.830876 2.108226
H 3.121799 -2.739185 0.832970
H 0.203903 -2.891980 1.288429
H 1.114907 -3.683343 0.014027
H -1.191467 -2.069854 -0.672456

17

18
E= -651.180817
P 0.091487 -0.569841 0.040216
C 0.037103 0.224646 1.699797
C 1.307613 0.015349 2.534857
C 2.449473 0.948986 2.200536
C 2.902255 1.334211 1.008830

C 2.473971 0.906297 -0.371121
C 1.852125 -0.493834 -0.478843
O -0.840805 0.075201 -0.949646
H 1.852436 -0.829361 -1.518882
H 2.433751 -1.217993 0.098462
H 3.362201 0.929022 -1.011164
H 1.789634 1.648450 -0.800500
H 3.712113 2.059965 1.012915
H 2.948410 1.377326 3.065885
H 1.635244 -1.030703 2.474807
H 1.048996 0.171219 3.585150
H -0.145139 1.290542 1.531413
H -0.837790 -0.176194 2.217231

17H

19
E= -651.825173
P 0.055639 -0.424495 -0.026935
C 0.026269 0.361793 1.613837
C 1.238507 0.033630 2.496492
C 2.474941 0.856809 2.215193
C 2.957990 1.276741 1.047303
C 2.466369 0.993559 -0.351169
C 1.801918 -0.376391 -0.546124
O -0.922992 0.119094 -1.008685
H 1.796967 -0.651926 -1.604202
H 2.359851 -1.149348 -0.008242
H 3.327749 1.054615 -1.021746
H 1.788646 1.790512 -0.683385
H 3.844300 1.905003 1.089578
H 3.025929 1.157326 3.102584
H 1.473686 -1.038219 2.438194

H 0.957190 0.203444 3.538693
H -0.051554 1.440473 1.451342
H -0.904199 0.042769 2.091020
H -0.115995 -1.798185 0.298096

18

16
E= -649.944805
C 0.113434 0.192672 0.017238
C 0.058868 0.104499 1.346731
C 1.274526 -0.005020 2.228515
C 1.956061 -1.380010 2.185474
C 2.701535 -1.732812 0.929299
C 2.658859 -1.168724 -0.281668
P 1.678530 0.222763 -0.867686
O 1.568095 0.295651 -2.362650
H -0.779818 0.305799 -0.589150
H -0.913262 0.098789 1.833221
H 2.006826 0.759351 1.939041
H 0.994226 0.208993 3.261981
H 2.670573 -1.439034 3.014405
H 1.217563 -2.167997 2.382454
H 3.372603 -2.582672 1.043096
H 3.315663 -1.548585 -1.060146
18H
17
E= -650.581020
C -0.044998 -0.050164 0.040185
C 0.028105 0.058102 1.364219
C 1.330273 0.114255 2.119900
C 2.027552 -1.248406 2.212834

C 2.603725 -1.821639 0.950027
C 2.454779 -1.432173 -0.316938
P 1.448939 -0.081198 -0.978541
O 2.141738 1.220269 -1.192286
H -1.003487 -0.086244 -0.468306
H -0.889903 0.090475 1.946652
H 2.005288 0.832379 1.641985
H 1.149379 0.478975 3.133120
H 2.851960 -1.165053 2.929920
H 1.345506 -1.995096 2.642163
H 3.240976 -2.687892 1.123580
H 3.003615 -1.974489 -1.083097
H 0.966311 -0.693698 -2.162529

19

16

E= -649.948474

C 0.287851 -0.033296 0.001586
C 0.037779 0.332281 1.461511
C 0.972628 -0.200853 2.507033
C 1.881902 -1.187220 2.496055
C 2.272137 -2.169041 1.484853
C 1.686474 -2.520447 0.326479
P 0.184090 -1.834209 -0.347702
O -0.074862 -2.183466 -1.785724
H -0.458378 0.443484 -0.637477
H 1.275860 0.305526 -0.323526
H 0.061944 1.425299 1.539658
H -0.983522 0.050814 1.747592
H 0.888644 0.334178 3.450542
H 2.436683 -1.304456 3.423224
H 3.167549 -2.725261 1.752338

H 2.112392 -3.329894 -0.259293

19H

17

E= -650.587840

C 0.340170 0.079231 -0.039964
C -0.061778 0.024304 1.441057
C 1.122242 -0.059062 2.363262
C 2.033572 -1.035027 2.394505
C 2.069624 -2.269570 1.606714
C 1.512689 -2.574292 0.427545
P 0.597855 -1.569281 -0.762486
O 1.161846 -1.599262 -2.138522
H -0.438609 0.545391 -0.649210
H 1.254911 0.658877 -0.183870
H -0.649992 0.909283 1.689315
H -0.720902 -0.837983 1.616311
H 1.247556 0.761063 3.064174
H 2.827749 -0.950934 3.130544
H 2.656437 -3.059320 2.072307
H 1.684400 -3.575052 0.037392
H -0.706168 -2.124719 -0.648284

20

16

E= -649.943116

C 0.018563 -0.011130 -0.062378
C -0.016862 0.081251 1.435736
C 1.058034 0.013540 2.213784
C 2.484874 -0.095083 1.728894
C 2.867416 -1.288022 0.887683
C 2.147019 -1.973187 -0.005198

P 0.443359 -1.737306 -0.547127
O 0.250173 -2.063856 -2.001761
H -0.943269 0.231551 -0.514464
H 0.776992 0.647353 -0.500949
H -0.994667 0.156699 1.900469
H 0.920095 0.067689 3.288909
H 2.736272 0.807376 1.150859
H 3.152372 -0.071153 2.592743
H 3.904209 -1.596919 1.009553
H 2.620140 -2.804836 -0.521185

20H

17
E= -650.585148
C 0.049331 0.018375 -0.097640
C -0.020201 0.054758 1.400869
C 1.043660 -0.023749 2.193103
C 2.474572 -0.097784 1.715129
C 2.869789 -1.284669 0.870241
C 2.153266 -1.965296 -0.024592
P 0.490833 -1.660132 -0.666617
O 0.382307 -1.914637 -2.127921
H -0.902246 0.279836 -0.562903
H 0.810646 0.697748 -0.495402
H -1.006883 0.102234 1.850160
H 0.893297 -0.009604 3.267797
H 2.709954 0.811098 1.141201
H 3.139713 -0.067790 2.580374
H 3.901827 -1.601401 1.010778
H 2.634776 -2.789087 -0.546241
H -0.346293 -2.469432 0.143746

21

16
E= -649.953472
C -0.091733 -0.137067 0.012343
C -0.039540 -0.041719 1.504000
C 1.096519 0.029719 2.210627
C 2.429348 -0.105019 1.622347
C 2.768792 -1.071064 0.758791
C 1.878736 -2.215148 0.387001
P 0.429465 -1.774120 -0.694689
O 0.725531 -1.691332 -2.164071
H -1.084923 0.088592 -0.376609
H 0.619353 0.562160 -0.443269
H -0.987036 0.034555 2.028240
H 1.036805 0.231286 3.276999
H 3.186891 0.611005 1.929839
H 3.764796 -1.065715 0.327381
H 1.427246 -2.647366 1.285819
H 2.421981 -3.003819 -0.134984

21H

17
E= -650.596569
C -0.034899 -0.048254 -0.013394
C -0.022330 0.026053 1.484161
C 1.097348 0.049867 2.218127
C 2.442632 -0.100884 1.659792
C 2.786290 -1.045105 0.775048
C 1.878602 -2.154651 0.336804
P 0.440203 -1.672243 -0.705591
O 0.621768 -1.711266 -2.179969
H -1.010773 0.210222 -0.427631

H 0.702763 0.641903 -0.438897
H -0.980237 0.124145 1.984830
H 1.017647 0.226491 3.287572
H 3.207756 0.584476 2.014690
H 3.801196 -1.059170 0.391977
H 1.428677 -2.628182 1.217358
H 2.420596 -2.923456 -0.216574
H -0.564859 -2.545037 -0.204933

22_planar

14

E= -648.719481

P 0.043675 -0.035944 0.106264
C 0.336426 0.302428 1.739278
O 1.046695 -0.732157 -0.719232
C -0.516736 0.955005 2.657048
H 1.304326 -0.039073 2.086212
C -1.774399 1.489401 2.526717
H -0.088778 1.047202 3.652044
C -2.650009 1.563128 1.401213
H -2.175495 1.932775 3.432293
C -2.497944 1.122317 0.110279
H -3.597186 2.051594 1.605657
H -3.348079 1.321614 -0.537170
C -1.439767 0.453874 -0.545550
H -1.557032 0.204027 -1.593238

22_nonplanar

14

E= -648.718340

C -0.002736 -0.041173 0.004161
P 0.054501 0.041729 1.799453

O 1.428873 0.197770 2.378990
C -1.133326 -0.157664 -0.711432
C -2.504174 -0.127613 -0.230729
C -3.021798 0.553087 0.813539
C -2.351062 1.443715 1.745256
C -1.083325 1.379850 2.184166
H 0.963453 -0.070649 -0.491947
H -1.033326 -0.302682 -1.784758
H -3.216369 -0.651608 -0.862280
H -4.101966 0.512993 0.924345
H -2.973502 2.248738 2.129397
H -0.707138 2.126254 2.878341

22H

15

E= -649.357821

C -0.032422 0.113327 -0.016597
C -0.002639 0.044172 1.323032
C 1.164868 -0.133051 2.167236
C 2.417291 0.343594 1.977878
C 2.915319 1.154683 0.881855
C 2.544559 1.094069 -0.406220
P 1.432559 -0.181084 -1.019513
H 1.968894 -1.352778 -0.421509
H -0.958878 0.317267 -0.544173
H -0.944735 0.123908 1.861392
H 0.970136 -0.604539 3.126610
H 3.111866 0.210558 2.802794
H 3.674255 1.881794 1.163029
H 2.935351 1.799324 -1.132957
O 1.227376 -0.225860 -2.489314

23

10

E= -571.248424

| | | | |
|---|-----------|-----------|-----------|
| C | 0.075297 | 0.018310 | 0.043853 |
| C | 0.075443 | 0.017987 | 1.528533 |
| P | 1.706922 | -0.044113 | 0.786003 |
| O | 2.652220 | -1.205581 | 0.785474 |
| C | -0.763984 | 0.002420 | 2.552487 |
| C | -0.764425 | 0.002519 | -0.979865 |
| H | -1.837978 | 0.064432 | 2.404130 |
| H | -0.399581 | -0.076388 | 3.570431 |
| H | -1.838404 | 0.063996 | -0.831179 |
| H | -0.400286 | -0.075903 | -1.997934 |

23H

11

E= -571.883213

| | | | |
|---|-----------|-----------|-----------|
| C | 0.064798 | -0.000126 | 0.096134 |
| C | 0.030428 | -0.034466 | 1.565420 |
| P | 1.664815 | -0.195079 | 0.864385 |
| O | 2.620438 | -1.325420 | 0.860180 |
| C | -0.811248 | -0.046617 | 2.589727 |
| C | -0.727871 | 0.035201 | -0.966032 |
| H | -1.879908 | 0.080458 | 2.444286 |
| H | -0.455992 | -0.191768 | 3.603511 |
| H | -1.802445 | 0.155576 | -0.865434 |
| H | -0.325109 | -0.063207 | -1.967622 |
| H | 2.228650 | 1.097262 | 0.908042 |

24

13

E= -610.604929

| | | | |
|---|-----------|-----------|-----------|
| C | 0.163408 | 0.249188 | -0.088850 |
| C | 0.135610 | 0.142164 | 1.435391 |
| C | 1.643475 | 0.249133 | 1.659979 |
| P | 1.915732 | 0.719782 | -0.071141 |
| O | 2.996919 | 0.248404 | -0.986185 |
| C | 2.412596 | 0.041159 | 2.719321 |
| C | -0.754206 | 0.041277 | -1.022533 |
| H | -0.438102 | 0.936441 | 1.920960 |
| H | -0.248471 | -0.827991 | 1.760416 |
| H | -1.770469 | -0.241946 | -0.766227 |
| H | -0.512683 | 0.136589 | -2.075071 |
| H | 1.991792 | -0.242083 | 3.679215 |
| H | 3.490583 | 0.136441 | 2.655139 |

24H

14

E= -611.238820

| | | | |
|---|-----------|-----------|-----------|
| C | 0.150140 | 0.272036 | -0.045208 |
| C | 0.097397 | 0.189252 | 1.480468 |
| C | 1.610398 | 0.256733 | 1.689251 |
| P | 1.905970 | 0.775591 | -0.037013 |
| O | 2.970835 | 0.276329 | -0.937933 |
| C | 2.393139 | -0.096278 | 2.694629 |
| C | -0.710138 | -0.063810 | -0.991361 |
| H | -0.420846 | 1.045585 | 1.924363 |
| H | -0.361655 | -0.727474 | 1.858836 |
| H | -1.706799 | -0.424673 | -0.754429 |
| H | -0.440735 | 0.000401 | -2.039939 |
| H | 1.986691 | -0.463201 | 3.632639 |
| H | 3.472810 | -0.040691 | 2.608394 |
| H | 1.826783 | 2.193299 | 0.042024 |

25

16

E= -649.941567

| | | | |
|---|-----------|-----------|-----------|
| C | -0.120681 | -0.392808 | 0.117214 |
| C | 0.023136 | -0.025243 | 1.581657 |
| C | 1.514929 | 0.230673 | 1.896630 |
| C | 2.329473 | -0.718792 | 1.049251 |
| P | 1.508074 | -0.810152 | -0.556231 |
| O | 1.702447 | -1.985915 | -1.463685 |
| C | -1.247504 | -0.419991 | -0.590662 |
| H | -0.320147 | -0.879291 | 2.175096 |
| H | -0.598632 | 0.833388 | 1.844503 |
| H | 1.731018 | 0.097848 | 2.958208 |
| H | 1.775243 | 1.262595 | 1.635544 |
| C | 3.428089 | -1.386636 | 1.386656 |
| H | 3.861165 | -1.298214 | 2.378656 |
| H | 3.918500 | -2.050345 | 0.682791 |
| H | -2.202825 | -0.160787 | -0.143399 |
| H | -1.252698 | -0.718606 | -1.633331 |

25H

17

E= -650.578559

| | | | |
|---|-----------|-----------|-----------|
| C | -0.087504 | -0.424907 | 0.122394 |
| C | 0.051629 | -0.048696 | 1.585442 |
| C | 1.539878 | 0.251625 | 1.874446 |
| C | 2.345760 | -0.735237 | 1.066607 |
| P | 1.536188 | -0.921798 | -0.548320 |
| O | 1.686570 | -2.180947 | -1.322507 |
| C | -1.205791 | -0.442556 | -0.591693 |
| H | -0.260308 | -0.903727 | 2.194947 |
| H | -0.592663 | 0.794102 | 1.845067 |

| | | | |
|---|----------|----------|----------|
| H | 1.771860 | 0.186744 | 2.939357 |
|---|----------|----------|----------|

| | | | |
|---|----------|----------|----------|
| H | 1.776083 | 1.272071 | 1.549199 |
|---|----------|----------|----------|

| | | | |
|---|----------|-----------|----------|
| C | 3.379898 | -1.467921 | 1.455778 |
|---|----------|-----------|----------|

| | | | |
|---|----------|-----------|----------|
| H | 3.796300 | -1.380348 | 2.455414 |
|---|----------|-----------|----------|

| | | | |
|---|----------|-----------|----------|
| H | 3.834787 | -2.189956 | 0.785368 |
|---|----------|-----------|----------|

| | | | |
|---|-----------|-----------|-----------|
| H | -2.160250 | -0.149129 | -0.162941 |
|---|-----------|-----------|-----------|

| | | | |
|---|-----------|-----------|-----------|
| H | -1.210802 | -0.765922 | -1.627555 |
|---|-----------|-----------|-----------|

| | | | |
|---|----------|----------|-----------|
| H | 1.954782 | 0.242054 | -1.246481 |
|---|----------|----------|-----------|

26

14

E= -648.714570

| | | | |
|---|-----------|-----------|-----------|
| C | -0.015062 | -0.007552 | -0.025238 |
|---|-----------|-----------|-----------|

| | | | |
|---|----------|----------|----------|
| C | 0.022873 | 0.032017 | 1.307696 |
|---|----------|----------|----------|

| | | | |
|---|----------|-----------|----------|
| P | 1.526865 | -0.037515 | 2.331761 |
|---|----------|-----------|----------|

| | | | |
|---|----------|-----------|----------|
| O | 2.658030 | -0.949256 | 1.965254 |
|---|----------|-----------|----------|

| | | | |
|---|-----------|----------|----------|
| C | -1.109591 | 0.154228 | 2.229456 |
|---|-----------|----------|----------|

| | | | |
|---|-----------|-----------|----------|
| C | -0.830618 | -0.023312 | 3.532070 |
|---|-----------|-----------|----------|

| | | | |
|---|----------|-----------|----------|
| C | 0.568454 | -0.315136 | 3.854977 |
|---|----------|-----------|----------|

| | | | |
|---|----------|-----------|----------|
| C | 1.068961 | -0.696665 | 5.031264 |
|---|----------|-----------|----------|

| | | | |
|---|-----------|----------|----------|
| H | -2.103298 | 0.382437 | 1.860048 |
|---|-----------|----------|----------|

| | | | |
|---|-----------|----------|----------|
| H | -1.577574 | 0.047771 | 4.315000 |
|---|-----------|----------|----------|

| | | | |
|---|----------|-----------|----------|
| H | 0.426306 | -0.848009 | 5.893081 |
|---|----------|-----------|----------|

| | | | |
|---|----------|-----------|----------|
| H | 2.128452 | -0.887887 | 5.158189 |
|---|----------|-----------|----------|

| | | | |
|---|-----------|----------|-----------|
| H | -0.957935 | 0.031925 | -0.561962 |
|---|-----------|----------|-----------|

| | | | |
|---|----------|-----------|-----------|
| H | 0.891027 | -0.101311 | -0.612946 |
|---|----------|-----------|-----------|

26H

15

E= -649.352337

| | | | |
|---|-----------|-----------|-----------|
| C | -0.024006 | -0.025092 | -0.022880 |
|---|-----------|-----------|-----------|

| | | | |
|---|----------|----------|----------|
| C | 0.013698 | 0.030437 | 1.306670 |
|---|----------|----------|----------|

P 1.528063 -0.089379 2.320542
O 2.614848 -1.033002 1.958759
C -1.117361 0.153812 2.229079
C -0.836823 -0.022569 3.532284
C 0.562032 -0.314295 3.854094
C 1.061611 -0.707852 5.023597
H -2.117832 0.351315 1.860213
H -1.590233 0.019598 4.311144
H 0.427052 -0.834740 5.895661
H 2.116228 -0.932404 5.138788
H -0.962585 0.039288 -0.565268
H 0.880295 -0.155056 -0.607060
H 1.933888 1.266574 2.416764

27

19

E= -689.264151

C -0.234518 -0.396928 0.189284
C -0.086335 -0.044548 1.651838
C 1.376561 -0.019208 2.115289
C 2.066792 -1.384530 1.993159
C 2.145895 -1.878758 0.566774
P 0.588572 -1.913680 -0.353348
O 0.681821 -2.140839 -1.831577
C -0.924182 0.317777 -0.699186
H -0.552900 0.929068 1.826632
H -0.638244 -0.773066 2.259293
H 1.930021 0.720336 1.527068
H 1.412980 0.305140 3.159084
H 3.079688 -1.331514 2.402294
H 1.518151 -2.114963 2.601308
C 3.261722 -2.287937 -0.035909

H 4.214955 -2.280236 0.485105
H 3.250942 -2.628324 -1.065613
H -1.432210 1.233027 -0.408618
H -0.989254 0.010986 -1.737388

27H

20

E= -689.903652

C -0.198467 -0.386119 0.151111
C -0.103183 -0.078415 1.625993
C 1.348076 -0.064142 2.132056
C 2.061666 -1.414817 1.961954
C 2.157375 -1.840546 0.516748
P 0.586183 -1.931408 -0.386421
O 0.655998 -2.185982 -1.849073
C -0.746190 0.401249 -0.767675
H -0.579019 0.886355 1.823479
H -0.667093 -0.830754 2.193560
H 1.908226 0.708258 1.595020
H 1.352433 0.209133 3.191041
H 3.067170 -1.364496 2.389313
H 1.514000 -2.177163 2.532073
C 3.283934 -2.086888 -0.142240
H 4.252047 -2.013767 0.345924
H 3.264324 -2.363883 -1.191267
H -1.199447 1.351931 -0.500033
H -0.749610 0.114254 -1.814192
H -0.128567 -2.898273 0.372813

28

17

E= -688.028830

| | | | | | | | |
|----------------|-----------|-----------|-----------|----------------|-----------|-----------|-----------|
| C | 0.038407 | 0.105220 | -0.030874 | H | -2.148135 | 0.835361 | 3.960181 |
| C | 0.001994 | -0.028772 | 1.294222 | H | -0.256934 | 1.869635 | 4.930797 |
| C | 1.221697 | -0.031568 | 2.186735 | H | 2.097872 | 2.750353 | 4.689025 |
| C | 1.178776 | -0.998164 | 3.341370 | H | 3.241162 | 1.913638 | 3.484615 |
| C | 0.103055 | -1.614754 | 3.835109 | H | -0.909120 | 0.212150 | -0.546825 |
| C | -1.272329 | -1.477602 | 3.337786 | H | 0.950597 | 0.218921 | -0.524016 |
| C | -2.289006 | -2.237120 | 3.759837 | H | 1.490007 | -1.234979 | 2.964185 |
| P | -1.588167 | -0.168394 | 2.130253 | | | | |
| O | -2.804688 | -0.320955 | 1.269804 | 29 | | | |
| H | 2.106048 | -0.238549 | 1.575652 | 22 | | | |
| H | 1.371633 | 0.978342 | 2.593467 | E= -728.570293 | | | |
| H | 2.136026 | -1.185907 | 3.818534 | C | -0.232694 | -0.300759 | 0.171648 |
| H | 0.230957 | -2.291002 | 4.676685 | C | -0.006465 | -0.399417 | 1.664534 |
| H | -2.134123 | -3.017136 | 4.499326 | C | 1.347961 | 0.162155 | 2.132934 |
| H | -3.289341 | -2.108231 | 3.362642 | C | 2.572649 | -0.722020 | 1.891550 |
| H | 0.981888 | 0.191493 | -0.562410 | C | 2.875995 | -1.072901 | 0.425004 |
| H | -0.874591 | 0.122685 | -0.615658 | C | 1.964840 | -2.139527 | -0.137552 |
| | | | | P | 0.418676 | -1.615741 | -0.918360 |
| 28H | | | | O | -0.533032 | -2.740656 | -1.218537 |
| 18 | | | | C | -0.915125 | 0.695305 | -0.389319 |
| E= -688.668260 | | | | H | -0.803725 | 0.165656 | 2.157278 |
| C | 0.015013 | 0.149436 | 0.021161 | H | -0.107445 | -1.439736 | 1.992648 |
| C | 0.010614 | -0.001745 | 1.340054 | H | 1.501441 | 1.138609 | 1.658849 |
| P | 1.586695 | -0.025339 | 2.226200 | H | 1.278901 | 0.348192 | 3.209450 |
| O | 2.830903 | 0.141749 | 1.431633 | H | 3.444465 | -0.204241 | 2.304276 |
| C | -1.224507 | -0.108874 | 2.201023 | H | 2.468252 | -1.655083 | 2.456725 |
| C | -1.189092 | 0.713334 | 3.465401 | H | 2.822872 | -0.163328 | -0.185398 |
| C | -0.119918 | 1.288846 | 4.022022 | H | 3.906023 | -1.434037 | 0.355056 |
| C | 1.253050 | 1.218203 | 3.505752 | C | 2.249314 | -3.441773 | -0.115961 |
| C | 2.251448 | 1.998706 | 3.919905 | H | 3.185002 | -3.804670 | 0.301271 |
| H | -2.101969 | 0.175429 | 1.611253 | H | 1.553106 | -4.173847 | -0.510586 |
| H | -1.382486 | -1.160238 | 2.480976 | H | -1.377611 | 1.470402 | 0.216613 |

H -1.049738 0.767995 -1.463343

29H

23

E= -729.212075

C -0.263799 -0.370624 0.215329

C -0.034284 -0.452860 1.706682

C 1.320115 0.143043 2.134611

C 2.564676 -0.693510 1.826739

C 2.800390 -1.058867 0.348315

C 1.905883 -2.177177 -0.132561

P 0.273565 -1.769599 -0.809772

O -0.655490 -2.926068 -0.932653

C -0.831349 0.676844 -0.377164

H -0.833412 0.097866 2.210477

H -0.106018 -1.492318 2.045515

H 1.421504 1.131295 1.671236

H 1.290772 0.309041 3.216245

H 3.436050 -0.133778 2.181713

H 2.533731 -1.622243 2.407207

H 2.670745 -0.165443 -0.274842

H 3.840454 -1.374924 0.227539

C 2.216065 -3.467147 -0.043070

H 3.175976 -3.791206 0.351149

H 1.511155 -4.231170 -0.354397

H -1.202383 1.520508 0.199421

H -0.956803 0.731861 -1.454191

H 0.577313 -1.112599 -2.031880

30

20

E= -727.335829

C -0.153446 -0.999890 0.558220

C -0.117806 0.108487 1.307385

P 1.512022 0.563264 1.968825

O 2.562632 -0.487544 1.766332

C -1.282696 1.010088 1.421769

C -1.720240 1.647734 2.507568

C -1.152727 1.592228 3.903761

C 0.283880 2.128776 4.055316

C 1.348008 1.127759 3.682591

C 2.247689 0.658944 4.548704

H -1.850461 1.132366 0.502627

H -2.611284 2.257263 2.384299

H -1.804196 2.173915 4.559417

H -1.181618 0.561114 4.273993

H 0.394189 3.039272 3.456784

H 0.449292 2.412880 5.098572

H 2.243375 0.983688 5.585542

H 3.002335 -0.057264 4.243682

H -1.064337 -1.295779 0.046012

H 0.720469 -1.633032 0.454360

30H

21

E= -727.973374

C 0.085310 0.206464 -0.036264

C -0.022509 0.154354 1.292210

P 1.503816 -0.130347 2.249179

O 1.878587 -1.538702 2.543377

C -1.336213 0.179575 1.973403

C -1.717175 0.911333 3.022033

C -0.983664 1.949123 3.824359

C 0.497474 2.196283 3.511769

C 1.313572 0.942942 3.694134
C 1.845694 0.544786 4.844743
H -2.083842 -0.474268 1.531521
H -2.746381 0.773167 3.346342
H -1.532190 2.893678 3.719436
H -1.071043 1.674678 4.882664
H 0.601942 2.578894 2.490388
H 0.868858 2.977717 4.180445
H 1.767512 1.150883 5.743745
H 2.363591 -0.405640 4.919554
H -0.790474 0.298820 -0.672188
H 1.047939 0.156674 -0.535474
H 2.438451 0.574458 1.443573

31

20

E= -727.328367

C 0.054422 0.252504 0.057867
C -0.001751 0.001789 1.362685
P 1.553278 -0.206573 2.298448
O 1.884857 -1.614943 2.705471
C -1.299516 -0.143323 2.123172
C -1.694921 1.020805 3.001680
C -0.947594 1.994644 3.513754
C 0.549070 2.202535 3.385392
C 1.350769 0.952793 3.674880
C 1.901132 0.667599 4.853388
H -2.104345 -0.309241 1.398758
H -1.258746 -1.051701 2.738203
H -2.754417 1.037512 3.245129
H -1.460588 2.735848 4.119959
H 0.786227 2.578041 2.382498

H 0.856976 2.984276 4.083831
H 1.813964 1.349405 5.694549
H 2.439037 -0.261117 5.010164
H -0.850954 0.361228 -0.533575
H 0.998498 0.351289 -0.467360

31H

21

E= -727.970551

C -0.024490 0.253290 0.082762
C -0.002711 -0.000716 1.387442
P 1.585316 -0.137684 2.253184
O 2.073100 -1.501609 2.592560
C -1.247042 -0.181376 2.225399
C -1.692875 1.058330 2.971211
C -0.960727 2.058577 3.453870
C 0.544959 2.235440 3.423118
C 1.323659 0.963693 3.667883
C 1.781298 0.574560 4.852720
H -2.064077 -0.502735 1.573430
H -1.094339 -0.998741 2.942072
H -2.766804 1.118655 3.127206
H -1.498240 2.864882 3.945329
H 0.838116 2.677288 2.461010
H 0.823717 2.966906 4.186003
H 1.644441 1.184633 5.741367
H 2.296199 -0.374478 4.961993
H -0.960289 0.324937 -0.464867
H 0.887218 0.394427 -0.489611
H 2.433143 0.615696 1.398001

32

18
E= -726.107527
C -0.027770 -0.885529 0.409168
C -0.110802 0.109380 1.304210
P 1.453561 0.650801 2.036898
O 2.614804 -0.240997 1.714469
C -1.365721 0.820729 1.542374
C -1.729514 1.640197 2.542343
C -1.071077 2.049856 3.779482
C 0.116726 1.743559 4.326478
C 1.223776 0.940977 3.808969
C 2.209984 0.508999 4.608145
H -2.118771 0.636097 0.779836
H -2.734466 2.042714 2.453432
H -1.701475 2.684944 4.395207
H 0.299381 2.140761 5.322220
H 2.191415 0.714833 5.674308
H 3.041709 -0.062223 4.212689
H -0.905935 -1.214918 -0.138326
H 0.912268 -1.389653 0.217756

32H

19
E= -726.748487
C -0.046915 -1.051794 0.565485
C -0.089985 0.039977 1.335367
P 1.498019 0.591336 2.018238
O 2.648488 -0.291913 1.686698
C -1.311204 0.820984 1.521356
C -1.631316 1.705043 2.481587
C -0.961958 2.113825 3.715097

C 0.192743 1.739399 4.292147
C 1.245827 0.856150 3.795428
C 2.146329 0.288346 4.603690
H -2.066707 0.648446 0.758465
H -2.608028 2.166277 2.366462
H -1.558361 2.807125 4.301271
H 0.387858 2.147140 5.281200
H 2.106338 0.433915 5.679390
H 2.934589 -0.337511 4.199657
H -0.939012 -1.426735 0.072028
H 0.883153 -1.591253 0.423144
H 1.572410 1.922373 1.536138

33

20
E= -802.323468
C -0.069633 -0.066425 0.113225
C -0.082851 -0.009856 1.499752
C 1.227667 -0.016007 2.102994
C 1.781150 0.025455 3.442779
C 3.125456 -0.009455 3.358296
C 3.577646 -0.078366 1.920731
C 2.271891 -0.077307 1.191025
P 1.576733 -0.125770 -0.381685
O 2.195448 -0.192983 -1.726455
C -1.473107 -0.054979 -0.404115
C -2.270513 0.015488 0.874566
C -1.460201 0.040558 1.950800
H -1.722662 -0.953327 -0.980045
H -3.351902 0.041382 0.893035
H -1.775262 0.089977 2.984561
H 4.170543 -0.980634 1.732640

H 3.814888 0.008328 4.191830
H 1.201140 0.076145 4.354582
H 4.211698 0.777063 1.661504
H -1.681966 0.804429 -1.051236

33H

21

E= -802.952786

C -0.066305 0.041980 0.109835
C -0.079700 0.024321 1.462074
C 1.257221 0.018324 2.078310
C 1.788003 -0.015270 3.438231
C 3.130274 -0.025901 3.361494
C 3.576013 0.002318 1.923522
C 2.276738 0.032458 1.189781
P 1.635466 0.102583 -0.499949
O 2.112043 -0.844404 -1.540943
C -1.468281 0.026534 -0.401472
C -2.272309 0.001819 0.871434
C -1.458730 0.001843 1.941827
H -1.670638 -0.853463 -1.023770
H -3.353758 -0.018351 0.891011
H -1.762744 -0.016264 2.979768
H 4.173014 -0.881412 1.668229
H 3.817730 -0.055552 4.196253
H 1.196114 -0.032909 4.343464
H 1.796229 1.472397 -0.837843
H 4.205108 0.875344 1.712883
H -1.708516 0.903665 -1.013992

34

20

E= -802.315422

C -0.078453 0.021962 0.187163
C -0.141781 0.071956 1.664669
C 1.181760 0.075197 2.280333
C 1.715617 0.056134 3.512141
C 3.212864 -0.003214 3.389903
C 3.458155 -0.010973 1.905985
C 2.271166 0.027701 1.280144
P 1.624929 0.149664 -0.403257
O 2.141727 -0.719568 -1.509395
C -1.321576 -0.022433 -0.317335
C -2.298493 -0.017335 0.826241
C -1.427714 0.048379 2.050017
H -1.605611 -0.058951 -1.359639
H -2.927127 -0.917387 0.822939
H -1.806867 0.050620 3.062586
H 4.438454 -0.043391 1.451703
H 3.624934 -0.899541 3.871509
H 1.185492 0.057726 4.454493
H -2.987419 0.835138 0.759940
H 3.703099 0.853399 3.871264

34H

21

E= -802.953455

C -0.072540 0.067615 0.187060
C -0.140540 0.056878 1.663472
C 1.182770 0.060186 2.279322
C 1.718788 0.029076 3.510512
C 3.216277 0.011802 3.381832
C 3.455424 0.041858 1.897341
C 2.268479 0.073479 1.276544

| | | | | | | | |
|----------------|-----------|-----------|-----------|----------------|-----------|-----------|-----------|
| P | 1.637463 | 0.097991 | -0.427566 | H | -1.649607 | 0.897284 | 2.618473 |
| O | 2.100275 | -0.908156 | -1.416550 | H | 4.558093 | -0.058487 | 1.525109 |
| C | -1.311610 | 0.029915 | -0.321177 | H | 4.037479 | 0.021613 | 4.093896 |
| C | -2.293248 | -0.001802 | 0.817760 | H | 1.499285 | -0.859072 | 4.132277 |
| C | -1.427498 | 0.021300 | 2.046275 | H | 1.490191 | 0.899299 | 4.071358 |
| H | -1.593285 | 0.012778 | -1.365044 | H | -1.699456 | -0.861240 | 2.654062 |
| H | -2.920101 | -0.902298 | 0.777336 | | | | |
| H | -1.810909 | 0.000218 | 3.056897 | 35H | | | |
| H | 4.435511 | 0.027999 | 1.440688 | 21 | | | |
| H | 3.654482 | -0.886146 | 3.836960 | E= -802.951729 | | | |
| H | 1.192580 | 0.007564 | 4.454675 | C | -0.032477 | 0.013808 | 0.157492 |
| H | 1.823588 | 1.442277 | -0.834771 | C | -0.033895 | 0.006881 | 1.513000 |
| H | -2.983135 | 0.851257 | 0.778390 | C | 1.287160 | 0.007958 | 2.123402 |
| H | 3.687194 | 0.867638 | 3.882809 | C | 1.824223 | -0.007826 | 3.518694 |
| | | | | C | 3.313524 | -0.004298 | 3.289460 |
| 35 | | | | C | 3.581213 | 0.011098 | 1.970832 |
| 20 | | | | C | 2.318502 | 0.015424 | 1.243739 |
| E= -802.317754 | | | | P | 1.676290 | 0.098166 | -0.453824 |
| C | -0.034941 | -0.095126 | 0.165320 | O | 2.165964 | -0.818845 | -1.513027 |
| C | -0.034914 | -0.055852 | 1.537003 | C | -1.404526 | 0.005850 | -0.332932 |
| C | 1.270585 | -0.054838 | 2.140685 | C | -2.235174 | -0.011337 | 0.725431 |
| C | 1.818439 | 0.001952 | 3.532763 | C | -1.444497 | -0.012273 | 2.008369 |
| C | 3.308394 | 0.000626 | 3.295653 | H | -1.693977 | 0.000980 | -1.374539 |
| C | 3.577510 | -0.043004 | 1.979637 | H | -3.315692 | -0.031651 | 0.690739 |
| C | 2.315729 | -0.093484 | 1.252244 | H | -1.675900 | 0.856551 | 2.636011 |
| P | 1.642722 | 0.060338 | -0.377829 | H | 4.562068 | 0.007330 | 1.516200 |
| O | 2.231417 | -0.445555 | -1.650787 | H | 4.040311 | -0.021972 | 4.089832 |
| C | -1.406535 | -0.047623 | -0.324863 | H | 1.498157 | -0.897885 | 4.070342 |
| C | -2.234841 | -0.004747 | 0.732589 | H | 1.810548 | 1.480756 | -0.745701 |
| C | -1.450422 | -0.000939 | 2.021301 | H | 1.494198 | 0.861312 | 4.100131 |
| H | -1.695475 | -0.064289 | -1.366294 | H | -1.650864 | -0.902765 | 2.614360 |
| H | -3.315303 | 0.014061 | 0.694054 | | | | |

36

22

E= -878.597681

| | | | |
|---|-----------|-----------|-----------|
| C | 0.042927 | -0.016692 | -0.087968 |
| C | 0.012157 | -0.018964 | 1.315938 |
| C | 1.352808 | -0.018426 | 1.940901 |
| C | 2.408262 | -0.015757 | 1.014665 |
| P | 1.746428 | 0.165281 | -0.654080 |
| O | 2.283983 | -0.627221 | -1.806547 |
| C | -1.126543 | -0.052896 | -0.835465 |
| C | 3.732720 | -0.050975 | 1.429747 |
| C | -2.346123 | -0.105639 | -0.171955 |
| H | -1.086174 | -0.050053 | -1.918727 |
| H | -3.268280 | -0.149193 | -0.739376 |
| C | -2.386713 | -0.098667 | 1.220252 |
| C | -1.215700 | -0.054071 | 1.967655 |
| H | -3.343317 | -0.131929 | 1.728975 |
| H | -1.265995 | -0.056728 | 3.050648 |
| C | 4.008729 | -0.103128 | 2.790446 |
| H | 4.536424 | -0.047832 | 0.702323 |
| H | 5.036259 | -0.145916 | 3.131897 |
| C | 2.968544 | -0.096545 | 3.716678 |
| C | 1.643159 | -0.052926 | 3.300353 |
| H | 3.194005 | -0.129332 | 4.776437 |
| H | 0.846044 | -0.055869 | 4.035206 |

36H

23

E= -879.235427

| | | | |
|---|----------|-----------|-----------|
| C | 0.043507 | 0.018514 | -0.081936 |
| C | 0.009040 | -0.022569 | 1.318244 |
| C | 1.353056 | -0.022044 | 1.944777 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.403258 | 0.019436 | 1.018097 |
| P | 1.756010 | 0.120238 | -0.674579 |
| O | 2.247452 | -0.803776 | -1.728034 |
| C | -1.122864 | -0.014278 | -0.829776 |
| C | 3.725984 | -0.012379 | 1.430588 |
| H | 1.905200 | 1.493908 | -0.995762 |
| C | -2.345964 | -0.077690 | -0.169864 |
| H | -1.082525 | 0.000699 | -1.913228 |
| H | -3.267443 | -0.109453 | -0.739128 |
| C | -2.387560 | -0.104695 | 1.220489 |
| C | -1.216747 | -0.078369 | 1.970514 |
| H | -3.344835 | -0.153039 | 1.727020 |
| H | -1.267908 | -0.107679 | 3.052983 |
| C | 4.007013 | -0.075184 | 2.791673 |
| H | 4.529846 | 0.002896 | 0.703064 |
| H | 5.035509 | -0.106180 | 3.131421 |
| C | 2.968912 | -0.102569 | 3.717490 |
| C | 1.641662 | -0.077238 | 3.303003 |
| H | 3.196489 | -0.150435 | 4.776359 |
| H | 0.845518 | -0.106839 | 4.038185 |

37

23

E= -841.651529

| | | | |
|---|-----------|-----------|-----------|
| P | -0.017480 | -0.418811 | 0.149283 |
| O | -0.009732 | 0.261357 | 1.489088 |
| C | 1.347314 | -0.131445 | -0.954365 |
| C | 2.794448 | -0.009232 | -0.575649 |
| C | 3.475500 | 0.132527 | -1.902455 |
| C | 2.563346 | 0.084808 | -2.885509 |
| C | 1.229819 | -0.083421 | -2.304560 |
| C | -1.393080 | -0.128136 | -0.939930 |

C -2.835773 -0.001762 -0.545959
C -3.530357 0.142272 -1.865485
C -2.628769 0.092030 -2.858114
C -0.034273 -0.161914 -3.103850
H 3.147995 -0.889651 -0.026188
H 4.542518 0.263989 -2.019651
H 2.758460 0.168211 -3.947673
H -3.186072 -0.881369 0.006890
H -4.598172 0.276796 -1.971411
H -3.002659 0.861376 0.109049
H 2.970757 0.853665 0.077221
H -0.037229 0.637183 -3.855814
H -0.038520 -1.097612 -3.681115
C -1.289680 -0.080146 -2.291279
H -2.834857 0.176146 -3.918149

37H

24

E= -842.289856

P -0.071487 -0.191562 0.166401
O -0.062632 0.795521 1.282392
C 1.306180 -0.146403 -0.971149
C 2.757516 -0.128753 -0.586521
C 3.453241 -0.008496 -1.907072
C 2.545111 0.046652 -2.891674
C 1.199124 -0.030879 -2.312534
C -1.440352 -0.111929 -0.979836
C -2.893265 -0.058069 -0.604633
C -3.577220 0.079556 -1.929628
C -2.661652 0.111756 -2.908337
C -0.058253 0.023926 -3.120090
H 3.055892 -1.035925 -0.046386

H 4.528302 0.028915 -2.019344
H 2.748571 0.139385 -3.951416
H -3.217491 -0.957950 -0.067147
H -4.650262 0.143885 -2.048820
H -3.102635 0.791066 0.056921
H 2.983507 0.715482 0.075884
H -0.045025 0.927366 -3.743264
H -0.066494 -0.813650 -3.830259
C -1.321787 0.000715 -2.320499
H -2.855836 0.209292 -3.969386
H -0.089754 -1.533925 0.629612

38

23

E= -841.642753

P -0.051043 0.969316 -0.012138
O -0.055155 0.712802 1.463776
C 1.304992 0.329692 -0.988577
C 2.528922 -0.061418 -0.585892
C 3.296324 -0.554484 -1.774781
C 2.329408 -0.377907 -2.908145
C 1.182038 0.144604 -2.452860
C -1.431573 0.382052 -0.987135
C -2.669201 0.038234 -0.583152
C -3.456017 -0.425365 -1.771192
C -2.484297 -0.286040 -2.905483
C -0.061268 0.524471 -3.209759
H 3.598716 -1.601659 -1.648194
H 2.545191 -0.644608 -3.934473
H -3.039092 0.061014 0.432577
H -4.358722 0.180982 -1.920894
H 2.900611 -0.052841 0.429398

H -0.040705 1.610467 -3.377865
H -0.070784 0.052495 -4.194083
C -1.317269 0.192163 -2.451479
H 4.221298 0.017127 -1.925209
H -2.711249 -0.544087 -3.931618
H -3.797983 -1.460226 -1.643943

38H

24

E= -842.280400

P -0.138808 -0.760410 0.134367
O -0.133690 -0.221765 1.518732
C 1.243938 -0.343969 -0.942176
C 2.454289 0.115803 -0.589714
C 3.241917 0.414523 -1.829188
C 2.290804 0.067868 -2.935953
C 1.134611 -0.372087 -2.418340
C -1.481535 -0.269669 -0.961392
C -2.669893 0.255916 -0.626406
C -3.421764 0.597059 -1.877017
C -2.475172 0.198626 -2.969956
C -0.117453 -0.827826 -3.118148
H 4.166550 -0.174968 -1.871699
H 2.520638 0.174925 -3.987909
H -3.028397 0.433623 0.378407
H -3.668197 1.665722 -1.913567
H 2.807261 0.274344 0.420252
H -0.101934 -0.529236 -4.168040
H -0.147759 -1.926278 -3.100053
C -1.352360 -0.303914 -2.435883
H -0.176872 -2.177570 0.051485
H 3.546618 1.468185 -1.861732

H -2.683322 0.318059 -4.025095
H -4.376537 0.058936 -1.933259

39

23

E= -841.644989

P -0.061638 -0.439498 0.127354
O -0.068480 0.244810 1.463783
C 1.319001 -0.134632 -0.969104
C 2.734310 -0.002855 -0.594604
C 3.467806 0.139301 -1.705527
C 2.571000 0.103275 -2.908394
C 1.202488 -0.080175 -2.315964
C -1.436139 -0.143892 -0.979355
C -2.855262 -0.023624 -0.615669
C -3.581539 0.112016 -1.732361
C -2.675320 0.083515 -2.928374
C -0.050379 -0.166109 -3.128042
H 4.539769 0.270138 -1.757296
H 2.828742 -0.715875 -3.592316
H -3.221588 -0.029404 0.401919
H -4.654043 0.234776 -1.792098
H 3.092799 -0.006472 0.425775
H -0.049956 0.630003 -3.884458
H -0.045576 -1.102810 -3.706218
C -1.309808 -0.088119 -2.325281
H -2.739727 1.008513 -3.515277
H 2.631826 1.028947 -3.494624
H -2.920140 -0.738327 -3.613728

39H

24

E= -842.283483
P -0.054554 -0.174011 0.190625
O -0.061957 0.805372 1.310311
C 1.328743 -0.101288 -0.952668
C 2.753677 -0.059999 -0.588001
C 3.489354 0.027564 -1.703157
C 2.582582 0.060678 -2.897970
C 1.208873 -0.025706 -2.293833
C -1.432831 -0.114784 -0.959501
C -2.859930 -0.088109 -0.601974
C -3.590856 -0.008084 -1.720789
C -2.678541 0.034130 -2.911068
C -0.047172 -0.021661 -3.103096
H 4.567572 0.078660 -1.762911
H 2.772137 -0.771659 -3.587453
H -3.232520 -0.118115 0.413178
H -4.669227 0.032131 -1.785881
H 3.121445 -0.086530 0.429005
H -0.049891 0.856960 -3.762153
H -0.041276 -0.884717 -3.783695
C -1.307042 -0.038196 -2.300061
H -2.807809 0.954676 -3.494152
H 2.705342 0.982659 -3.480208
H -2.856061 -0.800311 -3.601203
H -0.049196 -1.523942 0.628928

40

25

E= -917.914457
C 0.026230 0.320493 0.107070
C 0.019317 0.237745 1.506186
C 1.272859 0.541499 2.298471

C 2.536160 -0.070759 1.732294
C 2.795100 -0.018905 0.355820
P 1.569617 0.750291 -0.719911
O 1.662030 0.432232 -2.182547
C -1.128860 0.073405 -0.633162
C -1.167388 -0.110794 2.141662
H 1.403743 1.632187 2.329735
H 1.140296 0.217955 3.332604
C 3.474170 -0.679738 2.558649
C 3.968831 -0.551451 -0.175195
C 4.895618 -1.147930 0.666826
H 4.136282 -0.505756 -1.245514
H 5.806880 -1.568753 0.258393
C 4.646202 -1.211103 2.033033
H 5.365532 -1.681180 2.693917
H 3.285272 -0.741097 3.625561
C -2.304606 -0.265354 0.019972
H -1.089832 0.134842 -1.715017
H -3.203833 -0.464254 -0.551112
C -2.321522 -0.357027 1.407066
H -3.237079 -0.626706 1.921075
H -1.189093 -0.192647 3.223594

40H

26

E= -918.553053

C 0.027284 0.272033 0.063451
C 0.027080 0.254715 1.462793
C 1.284815 0.601201 2.232206
C 2.538033 -0.052150 1.687665
C 2.786991 -0.065237 0.310601
P 1.564458 0.663816 -0.804861

O 1.645321 0.275510 -2.237687
C -1.117323 -0.049889 -0.658745
C -1.151912 -0.077759 2.121659
H 1.420291 1.691432 2.207213
H 1.157980 0.333247 3.282816
C 3.469310 -0.642520 2.535521
C 3.929760 -0.666703 -0.206743
C 4.851559 -1.248543 0.653300
H 4.079384 -0.683663 -1.280807
H 5.743551 -1.718745 0.256469
C 4.618968 -1.232504 2.022901
H 5.332213 -1.691168 2.698465
H 3.291262 -0.648212 3.606009
C -2.287364 -0.376083 0.013958
H -1.076220 -0.053588 -1.742528
H -3.182186 -0.627917 -0.542897
C -2.301190 -0.386786 1.403149
H -3.210301 -0.647185 1.933420
H -1.170653 -0.102926 3.206414
H 1.712194 2.054883 -0.556208

41

24

E= -879.735887

C -0.034658 -0.007560 0.087311
C -0.043143 -0.042291 1.453197
C 1.369654 -0.009736 1.960815
C 2.180732 0.064579 0.706686
C 1.364903 0.055670 -0.355970
P -1.428074 -0.282315 2.546315
O -1.146147 -0.017366 3.998366
C -1.136344 -0.025030 -0.856005

C -2.421665 0.334893 -0.672183
C -3.070696 0.842595 0.521490
C -2.725895 0.709072 1.836883
C -3.735887 1.419948 2.690901
C -4.689666 1.988165 1.689116
C -4.301707 1.642207 0.454326
H 3.260160 0.126783 0.690267
H -5.547525 2.592723 1.949680
H 1.602620 -0.898813 2.558844
H 1.661592 0.106618 -1.396310
H -4.789828 1.912833 -0.473802
H -3.058726 0.308254 -1.552379
H -0.856595 -0.308394 -1.867314
H -4.224225 0.732951 3.392283
H -3.259888 2.189390 3.310793
H 1.532683 0.847155 2.625656

41H

25

E= -880.371499

C 0.013891 -0.080775 0.039998
C 0.024143 0.061960 1.505159
C 1.319354 0.072907 1.919729
C 2.226560 -0.093635 0.736491
C 1.270862 -0.183942 -0.410535
C -1.196945 0.158542 2.284904
C -1.414039 -0.250415 3.550846
C -0.482730 -0.892901 4.460936
C 0.869628 -0.774274 4.542240
C 1.388131 -1.673127 5.625768
C 0.143863 -2.307094 6.161556

C -0.921701 -1.843349 5.495890
P 1.899767 0.336146 3.590949
O 3.366510 0.176168 3.790786
H 0.136358 -3.036451 6.960079
H 1.576570 -0.323231 -1.438542
H 1.936387 -1.110312 6.390871
H -1.955223 -2.124645 5.655307
H -0.890308 -0.118421 -0.554743
H -2.059884 0.530240 1.738534
H -2.433818 -0.174174 3.919056
H 2.922828 0.747997 0.638543
H 2.853039 -0.988939 0.830860
H 2.098168 -2.411021 5.232947
H 1.391289 1.622618 3.919350

42

24

E= -879.727597

C 0.030264 -0.038188 0.004463
C 0.044784 -0.073942 1.486211
C 1.315340 0.027925 1.925067
C 2.240795 0.124045 0.754281
C 1.307644 0.086475 -0.412322
P -1.363622 -0.030895 2.578885
C -2.613574 -1.089355 1.874129
C -3.477065 -1.802628 2.624400
C -4.493037 -2.448094 1.736920
C -4.094337 -1.976945 0.375965
C -2.997112 -1.194571 0.446231
C -2.347321 -0.615904 -0.725736
C -1.105155 -0.141422 -0.906998
O -1.069105 -0.246687 4.032341

H -5.513171 -2.142155 2.003207
H 2.835003 1.046625 0.785005
H -3.450462 -1.886175 3.702209
H -4.608283 -2.252736 -0.535764
H 1.626880 0.128945 -1.445634
H -0.865190 0.173775 -1.919095
H -2.977903 -0.633240 -1.610800
H 1.620545 0.050789 2.962220
H -4.470271 -3.542387 1.817701
H 2.960985 -0.703847 0.733279

42H

25

E= -880.365878

C 0.016481 0.197284 0.164173
C 0.004938 0.252182 1.644126
C 1.181268 -0.184517 2.120712
C 2.072136 -0.558532 0.978267
C 1.229055 -0.255529 -0.218360
P -1.288174 0.915870 2.696437
C -2.814540 0.272811 2.005982
C -3.838672 -0.147932 2.764733
C -4.994292 -0.506961 1.884752
C -4.476138 -0.213953 0.513567
C -3.199971 0.220971 0.576920
C -2.390095 0.540333 -0.597394
C -1.058886 0.530446 -0.768227
O -1.102249 0.702503 4.156224
H -5.884862 0.084534 2.132713
H 3.004957 0.019473 0.992338
H -3.837465 -0.200976 3.845077
H -5.044921 -0.362875 -0.395095

H 1.547977 -0.410918 -1.240857
H -0.707911 0.731572 -1.776969
H -2.981427 0.748323 -1.485234
H 1.451899 -0.239547 3.166507
H -5.283253 -1.559428 1.999346
H 2.365331 -1.615308 1.018211
H -1.331671 2.272440 2.280710

43

24

E= -879.734811

C -0.091513 -0.021738 0.044991
C -0.074528 -0.046551 1.412185
C 1.309822 -0.004086 1.884970
C 2.136636 0.042119 0.830571
C 1.339394 0.021399 -0.433730
P -1.458391 -0.295431 2.521883
O -1.164502 -0.029820 3.970967
C -1.186623 -0.020817 -0.887280
C -2.476332 0.342831 -0.692081
C -3.112428 0.829860 0.502275
C -2.762583 0.710881 1.818956
C -3.737911 1.418543 2.649621
C -4.677691 1.962540 1.862892
C -4.386263 1.635482 0.433829
H -5.524208 2.551794 2.187562
H 1.579063 -0.007442 2.932394
H 1.529712 0.900427 -1.061497
H -4.264490 2.534227 -0.183150
H -3.109474 0.347766 -1.575989
H -0.911239 -0.272179 -1.908637
H -3.670876 1.472159 3.727685

H 3.216416 0.088875 0.863252
H -5.192910 1.047769 -0.023845
H 1.569503 -0.859494 -1.047268

43H

25

E= -880.371493

C 0.072834 -0.014339 0.069004
C 0.086829 -0.103300 1.427982
C 1.375580 -0.631264 1.875900
C 2.160070 -0.840452 0.808001
C 1.424440 -0.456257 -0.436506
P -1.213649 0.443710 2.538129
C -2.688263 -0.264919 1.799067
C -3.745784 -0.929581 2.560715
C -4.753386 -1.243140 1.732454
C -4.418151 -0.796521 0.344765
C -3.040852 -0.195701 0.485355
C -2.316808 0.312990 -0.652178
C -0.976975 0.391010 -0.831371
O -1.003000 0.131349 3.977332
H -3.689567 -1.108498 3.625765
H -5.130508 -0.047948 -0.026019
H 1.339513 -1.286888 -1.147473
H -0.640700 0.706945 -1.815882
H -2.932909 0.573481 -1.509342
H 1.621012 -0.799177 2.915646
H -5.679011 -1.732732 2.002047
H 3.173618 -1.216986 0.818311
H -4.428512 -1.622608 -0.376397
H 1.924705 0.362682 -0.969731
H -1.334899 1.825774 2.232814

44

26
 E= -955.982548

| | | | |
|---|-----------|-----------|-----------|
| C | -0.006510 | -0.013502 | -0.016506 |
| C | -0.010513 | -0.020147 | 1.384268 |
| C | 1.229523 | -0.005357 | 2.047358 |
| C | 2.417198 | -0.024553 | 1.314437 |
| C | 2.396928 | -0.048872 | -0.071124 |
| C | 1.176254 | -0.037001 | -0.736212 |
| P | 1.333048 | 0.128638 | 3.856095 |
| C | -1.317380 | -0.034427 | 2.053451 |
| C | -1.709195 | -0.641248 | 3.183101 |
| C | -0.958782 | -1.488774 | 4.118243 |
| C | 0.392062 | -1.302373 | 4.461862 |
| C | 1.021111 | -2.186741 | 5.339530 |
| C | 0.328516 | -3.252324 | 5.892367 |
| C | -1.014307 | -3.429630 | 5.579451 |
| C | -1.646929 | -2.554097 | 4.713027 |
| H | -2.101126 | 0.465036 | 1.490318 |
| H | -2.768473 | -0.568512 | 3.414359 |
| H | 2.061691 | -2.026415 | 5.600940 |
| H | 0.827087 | -3.930323 | 6.574891 |
| H | -1.571082 | -4.251163 | 6.015423 |
| H | -2.695125 | -2.699226 | 4.473453 |
| H | 3.366376 | -0.005786 | 1.839372 |
| H | 3.325739 | -0.060536 | -0.629038 |
| H | 1.146517 | -0.042284 | -1.819759 |
| H | -0.955271 | -0.004633 | -0.542763 |
| O | 0.876573 | 1.452862 | 4.409110 |

44H

E= -956.634561

| | | | |
|---|-----------|-----------|-----------|
| C | -0.003142 | -0.006620 | 0.012454 |
| C | 0.012121 | -0.013245 | 1.412454 |
| C | 1.258283 | 0.008272 | 2.056651 |
| C | 2.440115 | 0.075214 | 1.321744 |
| C | 2.399644 | 0.115212 | -0.063579 |
| C | 1.172607 | 0.067685 | -0.716706 |
| C | -1.281633 | -0.054901 | 2.109770 |
| C | -1.673442 | 0.539352 | 3.248264 |
| C | -0.934332 | 1.422236 | 4.162604 |
| C | -1.638089 | 2.473096 | 4.763187 |
| C | -1.004213 | 3.369258 | 5.608573 |
| C | 0.349337 | 3.224903 | 5.894085 |
| C | 1.058124 | 2.171273 | 5.337452 |
| C | 0.423948 | 1.273705 | 4.481014 |
| P | 1.400259 | -0.112589 | 3.854600 |
| H | 0.587688 | -1.233458 | 4.160011 |
| O | 2.799885 | -0.156840 | 4.359373 |
| H | -2.725537 | 0.430202 | 3.499271 |
| H | -2.058533 | -0.581440 | 1.561128 |
| H | 3.384022 | 0.079002 | 1.855847 |
| H | 3.320464 | 0.165580 | -0.632630 |
| H | 1.132362 | 0.084150 | -1.799876 |
| H | -0.956444 | -0.043629 | -0.504350 |
| H | 2.106565 | 2.016516 | 5.567808 |
| H | 0.844747 | 3.920488 | 6.561164 |
| H | -1.569368 | 4.181852 | 6.050656 |
| H | -2.694345 | 2.592236 | 4.545539 |

8A

| | | | | | | | |
|----|-------------|-----------|-----------|------------|-------------|-----------|-----------|
| E= | -885.844765 | | | H | -3.334893 | -6.050290 | 4.291193 |
| C | 0.084153 | 0.152720 | -0.194453 | H | -3.808024 | -5.070178 | 2.898094 |
| C | 0.038050 | 0.069034 | 1.334676 | H | -2.253464 | -5.927093 | 2.898165 |
| C | 1.473736 | 0.073882 | 1.888757 | | | | |
| C | -0.661730 | -1.200576 | 1.770116 | 8AH | | | |
| P | -0.938685 | -1.702867 | 3.420091 | 35 | | | |
| O | -0.574233 | -1.041501 | 4.702156 | E: | -886.477383 | | |
| C | -1.214221 | -2.203147 | 1.021082 | C | -0.027003 | -0.024222 | 0.013261 |
| C | -1.817648 | -3.297936 | 1.757375 | C | 0.007989 | 0.015323 | 1.543735 |
| C | -1.769433 | -3.210265 | 3.121720 | C | 1.469953 | 0.083400 | 2.026156 |
| C | -2.292572 | -4.159379 | 4.178468 | C | -0.649198 | -1.259060 | 2.102880 |
| C | -3.320926 | -3.425261 | 5.056977 | C | -0.721671 | 1.228633 | 2.071556 |
| C | -2.960510 | -5.371170 | 3.520604 | C | -1.231289 | 2.274191 | 1.408895 |
| C | -1.122746 | -4.636877 | 5.056948 | C | -1.850228 | 3.335632 | 2.235512 |
| C | -0.724445 | 1.285497 | 1.888787 | C | -1.835760 | 3.139571 | 3.559668 |
| H | -1.210590 | -2.196698 | -0.061520 | C | -2.334663 | 4.032331 | 4.671973 |
| H | -2.276369 | -4.130324 | 1.238927 | C | -3.265190 | 3.226114 | 5.595427 |
| H | -0.232487 | 2.213080 | 1.580817 | P | -1.102996 | 1.492989 | 3.834644 |
| H | -1.752403 | 1.300794 | 1.516415 | O | -0.065950 | 1.279863 | 4.884401 |
| H | -0.754398 | 1.266391 | 2.981694 | C | -1.117910 | 4.520454 | 5.481889 |
| H | 0.590930 | 1.072273 | -0.499041 | C | -3.095091 | 5.237081 | 4.110358 |
| H | 0.632759 | -0.690661 | -0.623564 | H | -1.206930 | 2.370501 | 0.328701 |
| H | -0.921877 | 0.166119 | -0.623544 | H | -2.280867 | 4.211811 | 1.762709 |
| H | 1.995344 | 0.985102 | 1.580728 | H | 2.015422 | -0.804232 | 1.690895 |
| H | 1.473591 | 0.038414 | 2.981666 | H | 1.967695 | 0.967784 | 1.619369 |
| H | 2.035532 | -0.787132 | 1.516424 | H | 1.523490 | 0.135268 | 3.116141 |
| H | -3.711468 | -4.098785 | 5.825821 | H | 0.506795 | -0.907604 | -0.347529 |
| H | -2.867125 | -2.566699 | 5.559614 | H | -1.053724 | -0.072365 | -0.361541 |
| H | -4.160027 | -3.067323 | 4.454164 | H | 0.458403 | 0.855284 | -0.419410 |
| H | -1.483650 | -5.326785 | 5.825748 | H | -0.140017 | -2.144861 | 1.712728 |
| H | -0.372033 | -5.155143 | 4.454102 | H | -0.582018 | -1.295103 | 3.194243 |
| H | -0.639178 | -3.794752 | 5.559638 | H | -1.703607 | -1.317329 | 1.817609 |

| | | | | | | | |
|--------------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -1.451615 | 5.139695 | 6.320342 | C | -2.044138 | -2.827508 | 0.389828 |
| H | -0.543313 | 3.679014 | 5.876133 | C | -3.737965 | -0.125806 | -0.308917 |
| H | -0.453947 | 5.120137 | 4.853485 | C | -3.366767 | 1.077042 | -1.070694 |
| H | -3.647085 | 3.867713 | 6.394576 | C | -0.564685 | 1.726468 | -2.560122 |
| H | -4.118944 | 2.824103 | 5.042217 | C | -2.294054 | 3.236608 | -2.369043 |
| H | -2.733973 | 2.394164 | 6.067176 | C | 0.867430 | -1.805915 | -2.428838 |
| H | -3.445652 | 5.869822 | 4.930247 | C | 3.071547 | -1.509993 | -3.055998 |
| H | -2.454038 | 5.849980 | 3.470233 | C | -2.196340 | -1.731236 | 2.385528 |
| H | -3.966670 | 4.923166 | 3.528328 | C | -4.121566 | -2.296563 | 1.228745 |
| H | -2.266551 | 0.691347 | 3.993114 | H | -4.083594 | 1.565164 | -1.726025 |
| {8A} ₂ | | | | H | -4.743198 | -0.534765 | -0.371201 |
| 68 | | | | H | 3.796747 | 1.891801 | 0.393023 |
| E= -1771.794547 | | | | H | 3.965238 | 0.406334 | -1.699198 |
| C | 1.155806 | 2.575326 | 2.238378 | H | -4.192410 | -3.253794 | 1.753952 |
| C | 1.892531 | 1.391894 | 2.367707 | H | -4.716688 | -1.565048 | 1.782891 |
| C | 1.203447 | 0.486104 | 3.183004 | H | -4.576947 | -2.428333 | 0.242579 |
| C | 3.156399 | 1.685250 | 2.893614 | H | -2.312399 | -2.640476 | 2.983511 |
| C | 2.101674 | 0.797355 | 1.117594 | H | -1.123578 | -1.549268 | 2.267489 |
| C | 3.086709 | 1.081821 | 0.248847 | H | -2.637592 | -0.900467 | 2.943280 |
| C | 3.207782 | 0.201617 | -0.948070 | H | -2.124871 | -3.824762 | 0.833788 |
| C | 2.347143 | -0.823650 | -1.020946 | H | -2.387330 | -2.887240 | -0.646936 |
| C | 2.200780 | -1.811584 | -2.002050 | H | -0.987870 | -2.542710 | 0.399083 |
| C | 2.513231 | -3.040088 | -1.407784 | H | -1.767823 | 3.965357 | -2.992778 |
| P | 1.294429 | -0.683493 | 0.442426 | H | -2.928456 | 2.636103 | -3.027692 |
| O | 1.132523 | -1.844739 | 1.351518 | H | -2.943743 | 3.787774 | -1.683401 |
| O | -0.084689 | -0.218120 | -0.265819 | H | -0.015867 | 3.948923 | -1.410078 |
| P | -1.405310 | 0.530410 | 0.454015 | H | -1.141149 | 3.722091 | -0.061198 |
| C | -2.087349 | 1.483422 | -0.922648 | H | 0.165431 | 2.562130 | -0.329086 |
| C | -1.383382 | 2.433877 | -1.671691 | H | 0.057531 | 2.403971 | -3.153173 |
| C | -0.567234 | 3.200999 | -0.831795 | H | 0.091853 | 1.051525 | -2.002774 |
| C | -2.748987 | -0.682442 | 0.425882 | H | -1.162080 | 1.121139 | -3.247835 |
| C | -2.784510 | -1.894515 | 1.125609 | H | 0.692147 | -2.603249 | -3.157597 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 0.189106 | -1.956957 | -1.584897 | C | -1.347368 | 1.387816 | -2.283464 |
| H | 0.605515 | -0.851410 | -2.891885 | C | -1.456608 | -1.668928 | -2.060396 |
| H | 2.333975 | -3.870343 | -2.097498 | C | 4.323308 | 0.071676 | 3.550136 |
| H | 3.561012 | -3.074347 | -1.096844 | C | 4.914344 | -1.669052 | 1.066774 |
| H | 1.897562 | -3.194040 | -0.516790 | C | 5.024087 | 1.387692 | 0.843949 |
| H | 2.994154 | -2.261966 | -3.846790 | H | -2.170472 | 1.392558 | -3.004444 |
| H | 2.833964 | -0.537394 | -3.496931 | H | -1.360964 | 2.340508 | -1.746735 |
| H | 4.112743 | -1.488423 | -2.720961 | H | -0.410060 | 1.330544 | -2.844810 |
| H | 3.062781 | 2.152247 | 3.878766 | H | -3.942931 | 0.056731 | -0.718950 |
| H | 3.755718 | 0.777599 | 3.004527 | H | -3.147147 | -0.762690 | 0.628067 |
| H | 3.708139 | 2.378717 | 2.251703 | H | -3.083611 | 1.003041 | 0.499721 |
| H | 1.007464 | 3.027465 | 3.224309 | H | -2.281946 | -1.719591 | -2.777067 |
| H | 1.664417 | 3.306745 | 1.604592 | H | -0.520714 | -1.760233 | -2.619578 |
| H | 0.172064 | 2.375715 | 1.806272 | H | -1.534863 | -2.530422 | -1.391388 |
| H | 1.174849 | 0.845236 | 4.216225 | H | 6.097938 | 1.392397 | 1.054085 |
| H | 0.171732 | 0.370346 | 2.839804 | H | 4.894819 | 1.330438 | -0.240924 |
| H | 1.666964 | -0.503168 | 3.166721 | H | 4.607829 | 2.340392 | 1.183031 |

8B

34

E= -1388.711869

| | | | |
|----|-----------|-----------|-----------|
| C | -0.040647 | -0.025133 | 0.076419 |
| C | -0.033639 | 0.074714 | 1.452959 |
| C | 1.264580 | 0.074692 | 2.090186 |
| C | 2.357838 | -0.025180 | 1.253710 |
| Si | 4.178528 | -0.059179 | 1.683951 |
| Si | -1.494712 | -0.059069 | -1.100746 |
| P | 1.645192 | -0.114650 | -0.326277 |
| O | 2.297091 | -0.234642 | -1.654390 |
| H | -0.944503 | 0.149795 | 2.036350 |
| H | 1.360233 | 0.149754 | 3.167624 |
| C | -3.059600 | 0.071817 | -0.073748 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.347368 | 1.387816 | -2.283464 |
| C | -1.456608 | -1.668928 | -2.060396 |
| C | 4.323308 | 0.071676 | 3.550136 |
| C | 4.914344 | -1.669052 | 1.066774 |
| C | 5.024087 | 1.387692 | 0.843949 |
| H | -2.170472 | 1.392558 | -3.004444 |
| H | -1.360964 | 2.340508 | -1.746735 |
| H | -0.410060 | 1.330544 | -2.844810 |
| H | -3.942931 | 0.056731 | -0.718950 |
| H | -3.147147 | -0.762690 | 0.628067 |
| H | -3.083611 | 1.003041 | 0.499721 |
| H | -2.281946 | -1.719591 | -2.777067 |
| H | -0.520714 | -1.760233 | -2.619578 |
| H | -1.534863 | -2.530422 | -1.391388 |
| H | 6.097938 | 1.392397 | 1.054085 |
| H | 4.894819 | 1.330438 | -0.240924 |
| H | 4.607829 | 2.340392 | 1.183031 |
| H | 5.986151 | -1.719752 | 1.281312 |
| H | 4.432936 | -2.530537 | 1.537896 |
| H | 4.784229 | -1.760338 | -0.015657 |
| H | 5.374051 | 0.056553 | 3.854270 |
| H | 3.884356 | 1.002908 | 3.919931 |
| H | 3.821632 | -0.762822 | 4.048677 |

8BH

35

E: -1389.338413

| | | | |
|----|-----------|-----------|----------|
| C | 0.018815 | 0.023044 | 0.005599 |
| Si | -0.022863 | 0.002852 | 1.881283 |
| C | 1.714661 | 0.042203 | 2.589620 |
| C | -0.839432 | -1.588841 | 2.442349 |
| P | -0.970035 | -2.130807 | 4.171678 |

| | | | | | | | | |
|--------------------------|-----------|-----------|-----------|----|--------------|-----------|-----------|--|
| O | -1.410028 | -1.179740 | 5.231106 | E= | -2777.525419 | | | |
| C | -1.432051 | -2.544087 | 1.706554 | C | 1.618359 | -3.453089 | -1.714057 | |
| C | -2.049587 | -3.666286 | 2.457615 | Si | 1.995512 | -1.791301 | -2.505641 | |
| C | -1.952817 | -3.612298 | 3.796571 | C | 3.639139 | -1.879648 | -3.420164 | |
| Si | -2.655510 | -4.781195 | 5.083036 | C | 2.161939 | -0.447301 | -1.203421 | |
| C | -3.920481 | -3.827549 | 6.080113 | P | 0.930574 | 0.819544 | -0.806788 | |
| C | -3.430021 | -6.244309 | 4.199981 | O | -0.118992 | 0.156105 | 0.227052 | |
| C | -1.245951 | -5.337574 | 6.190213 | P | -1.142623 | -1.151333 | -0.021405 | |
| C | -1.030000 | 1.424722 | 2.565171 | C | -2.817207 | -0.457035 | -0.063774 | |
| H | -1.478682 | -2.524079 | 0.620913 | C | -3.500538 | -1.002673 | 0.974950 | |
| H | -2.549460 | -4.469812 | 1.923142 | C | -2.669320 | -1.738262 | 1.956971 | |
| H | -0.546473 | 2.386336 | 2.368670 | C | -1.345231 | -1.775311 | 1.666411 | |
| H | -2.029071 | 1.448385 | 2.121210 | Si | 0.074212 | -2.226236 | 2.788617 | |
| H | -1.149963 | 1.310778 | 3.646523 | C | 0.750528 | -0.607458 | 3.469232 | |
| H | 0.483725 | 0.944181 | -0.358047 | C | 3.262553 | -0.133911 | -0.485020 | |
| H | 0.593786 | -0.818902 | -0.390712 | C | 3.155659 | 1.079215 | 0.395841 | |
| H | -0.990005 | -0.025223 | -0.414777 | C | 1.977241 | 1.729068 | 0.345142 | |
| H | 2.238244 | 0.953970 | 2.286889 | Si | 1.370152 | 3.272877 | 1.209497 | |
| H | 1.688790 | 0.024503 | 3.683381 | C | -0.190081 | 2.818754 | 2.155170 | |
| H | 2.304745 | -0.813822 | 2.250373 | C | 2.722974 | 3.899141 | 2.355529 | |
| H | -4.291523 | -4.418514 | 6.922843 | C | 0.962203 | 4.487552 | -0.165320 | |
| H | -3.472401 | -2.909094 | 6.470449 | C | 0.596305 | -1.300178 | -3.653100 | |
| H | -4.775508 | -3.542396 | 5.460900 | O | 0.263440 | 1.539925 | -1.933627 | |
| H | -1.604176 | -6.027977 | 6.959707 | C | -0.550665 | -3.330138 | 4.178925 | |
| H | -0.464545 | -5.846049 | 5.618440 | C | 1.434903 | -3.068195 | 1.803307 | |
| H | -0.791602 | -4.482574 | 6.699954 | Si | -3.461200 | 0.754405 | -1.338260 | |
| H | -3.858242 | -6.945661 | 4.922205 | C | -2.732979 | 0.351409 | -3.019724 | |
| H | -4.236189 | -5.924610 | 3.533159 | C | -5.343538 | 0.666836 | -1.332051 | |
| H | -2.691325 | -6.788992 | 3.604855 | C | -2.865116 | 2.465593 | -0.834624 | |
| H | 0.318975 | -2.694299 | 4.389403 | H | -3.107158 | -2.157514 | 2.856128 | |
| {8B} ₂ | | | | H | -4.568453 | -0.887792 | 1.124184 | |
| 68 | | | | H | 4.193588 | -0.687156 | -0.531767 | |

| | | | | | | | |
|---|-----------|-----------|-----------|-----------|--------------|-----------|-----------|
| H | 3.992431 | 1.381179 | 1.014089 | H | 2.413871 | -3.769877 | -1.029407 |
| H | -5.763264 | 1.371563 | -2.060917 | H | 0.680316 | -3.401119 | -1.148977 |
| H | -5.693656 | -0.339630 | -1.591957 | H | 0.619577 | -1.887541 | -4.579338 |
| H | -5.748162 | 0.927795 | -0.345760 | H | -0.371446 | -1.474047 | -3.166199 |
| H | -3.203517 | 0.958771 | -3.803601 | H | 0.645402 | -0.234968 | -3.905136 |
| H | -1.663957 | 0.600433 | -3.001287 | 8C | | | |
| H | -2.850594 | -0.705130 | -3.288489 | 34 | | | |
| H | -3.371118 | 3.245184 | -1.418839 | E= | -2672.195820 | | |
| H | -3.037905 | 2.662544 | 0.230007 | P | 0.010953 | 0.063215 | 0.177195 |
| H | -1.789550 | 2.534399 | -1.038401 | C | 0.048822 | 0.097548 | 1.924187 |
| H | 0.260877 | -3.576198 | 4.875257 | C | 1.734857 | -0.003132 | -0.102327 |
| H | -1.341294 | -2.829633 | 4.752320 | O | -1.119982 | -0.029964 | -0.758689 |
| H | -0.956973 | -4.269306 | 3.784262 | C | 2.452955 | -0.094518 | -1.436128 |
| H | 2.277102 | -3.328531 | 2.457488 | C | 2.114772 | 1.148211 | -2.324560 |
| H | 1.082378 | -3.985283 | 1.317229 | F | 0.809366 | 1.405220 | -2.313383 |
| H | 1.812578 | -2.395550 | 1.022044 | C | 2.295745 | -0.028133 | 1.150891 |
| H | 1.641984 | -0.773247 | 4.087456 | C | 1.380733 | 0.026567 | 2.250676 |
| H | 1.017542 | 0.054904 | 2.636886 | C | -1.133996 | 0.119891 | 2.874680 |
| H | -0.004244 | -0.092984 | 4.076580 | C | -0.655107 | 0.129703 | 4.363111 |
| H | -0.806395 | 3.704604 | 2.351109 | F | -0.078255 | -1.034736 | 4.673701 |
| H | -0.781521 | 2.098622 | 1.578406 | C | 4.002656 | -0.146867 | -1.234488 |
| H | 0.053945 | 2.346542 | 3.114375 | F | 4.434545 | 0.844703 | -0.451941 |
| H | 0.333535 | 5.311614 | 0.193169 | F | 4.357594 | -1.297192 | -0.654871 |
| H | 1.874210 | 4.913250 | -0.601849 | F | 4.653886 | -0.048976 | -2.387483 |
| H | 0.426418 | 3.960036 | -0.965102 | C | 2.005537 | -1.408483 | -2.166713 |
| H | 2.404172 | 4.811743 | 2.874421 | F | 1.990958 | -2.429686 | -1.309839 |
| H | 2.964649 | 3.146875 | 3.117122 | F | 0.776005 | -1.270902 | -2.656004 |
| H | 3.638221 | 4.132124 | 1.797110 | F | 2.814090 | -1.732083 | -3.171474 |
| H | 3.603174 | -2.643779 | -4.206969 | F | 2.736948 | 2.232322 | -1.860169 |
| H | 3.875723 | -0.916963 | -3.888816 | F | 2.482983 | 0.966556 | -3.589481 |
| H | 4.460765 | -2.139413 | -2.740274 | C | -2.006341 | 1.395631 | 2.630763 |
| H | 1.507679 | -4.220567 | -2.491370 | F | -1.383024 | 2.478640 | 3.096192 |

C -1.998683 -1.168235 2.642871
F -2.698003 -1.060331 1.516227
F -2.220739 1.589314 1.331986
F -3.190271 1.306811 3.229971
F -1.210858 -2.238034 2.532390
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F 0.241553 1.092538 4.589127
F -1.663208 0.326968 5.204526
H 3.356716 -0.083507 1.336417
H 1.754382 0.012282 3.262271

8CH

35

E: -2672.827458

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F 0.009200 -0.023453 1.360026
C 1.454635 -0.015476 -0.556484
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F 2.750009 0.466943 1.411153
C 1.449194 0.372804 -2.025550
C 2.139469 -0.230145 -2.998308
C 2.025411 0.362832 -4.338451
C 1.243750 1.442025 -4.441757
C 1.017160 2.260822 -5.701628
C 1.905207 3.555333 -5.632261
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O 0.801606 3.156844 -2.191909
C 1.978296 -1.477946 -0.366440
F 1.756882 -1.934989 0.860099
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F -0.741740 -0.919415 -0.455860
C 1.414722 1.446247 -6.977333

F 0.993715 2.026510 -8.094623
C -0.485309 2.662614 -5.830112
F -0.681876 3.575448 -6.772783
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F -1.224249 1.589185 -6.120984
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F 1.366730 4.455955 -4.823064
F 3.118577 3.255393 -5.174969
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H -0.749242 1.348646 -2.860470

{8C}2

68

E= -5344.498772

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C -3.201109 -1.830948 0.946677
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C 2.771984 -0.572934 0.186202
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| | | | | | | | |
|---|-----------|-----------|-----------|-----------|--------------|-----------|-----------|
| C | -4.532952 | -1.608402 | 1.740126 | F | -0.179487 | -2.631997 | -3.095055 |
| C | -3.319840 | 0.463809 | -0.079386 | F | -1.229536 | -1.083443 | -2.026952 |
| C | -2.719267 | 1.804524 | -0.167700 | F | -0.437117 | 1.071378 | -4.902192 |
| C | -1.547459 | 1.971387 | 0.447227 | F | -0.848716 | 1.371339 | -2.806416 |
| C | -0.824372 | 3.299890 | 0.616136 | F | 1.058397 | 1.933900 | -3.627505 |
| C | -1.323615 | 4.347319 | -0.436778 | F | 1.375500 | 4.247730 | 0.770334 |
| C | -1.135759 | 3.853983 | 2.055199 | F | 1.186132 | 2.163174 | 1.219020 |
| C | 0.717794 | 3.137443 | 0.447810 | F | 1.014903 | 2.832766 | -0.818045 |
| O | -0.803575 | 0.260888 | 2.602195 | F | -0.850620 | 5.153442 | 2.149403 |
| C | -0.584645 | -1.365572 | -3.163546 | F | -2.427026 | 3.699440 | 2.340155 |
| C | 0.093977 | 1.019815 | -3.681333 | F | -0.430714 | 3.212671 | 2.975751 |
| C | 3.454383 | -0.972633 | 1.493094 | F | -0.556222 | 5.430184 | -0.474376 |
| C | 4.839517 | -1.633403 | 1.173768 | F | -1.343921 | 3.832102 | -1.664761 |
| C | 3.681197 | 0.285188 | 2.397635 | F | -2.569607 | 4.745129 | -0.147906 |
| C | 2.603140 | -2.009212 | 2.286875 | F | -4.931186 | -2.711033 | 2.366391 |
| H | 3.171252 | 0.692932 | -2.896086 | F | -4.392412 | -0.648206 | 2.646262 |
| H | 4.437560 | 0.438729 | -0.707536 | F | -5.515150 | -1.237928 | 0.905620 |
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| H | -3.264101 | 2.585197 | -0.678791 | F | -4.041721 | -1.935503 | -1.307146 |
| F | 5.329142 | -2.304003 | 2.211120 | F | -2.382490 | -3.213190 | -0.819671 |
| F | 4.739438 | -2.482476 | 0.152409 | F | -2.561297 | -3.947796 | 1.873524 |
| F | 5.742203 | -0.702518 | 0.834721 | F | -0.986172 | -2.574586 | 1.368138 |
| F | 3.035039 | -2.169889 | 3.531821 | F | -2.229699 | -2.211283 | 3.093736 |
| F | 1.332562 | -1.621605 | 2.345235 | | | | |
| F | 2.635975 | -3.199859 | 1.680201 | 8D | | | |
| F | 4.577266 | 0.040810 | 3.354477 | 34 | | | |
| F | 4.133486 | 1.317538 | 1.683669 | E= | -3175.000232 | | |
| F | 2.547429 | 0.654027 | 2.977857 | C | 0.061182 | 0.147495 | 0.134156 |
| F | 0.748367 | -1.310150 | -5.569237 | F | 0.179847 | 0.396438 | 1.449072 |
| F | 2.343308 | 0.000418 | -4.965571 | Si | 1.798460 | -0.020918 | -0.691914 |
| F | 2.220344 | -1.992942 | -4.158867 | C | 2.832096 | 1.545003 | -0.228848 |
| F | -1.467841 | -1.265040 | -4.149578 | F | 3.815309 | 1.763577 | -1.111932 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|--------------|-----------|-----------|
| F | -0.668017 | 1.129011 | -0.405431 | E: | -3175.623591 | | |
| F | -0.649663 | -0.994687 | 0.010993 | C | -0.292911 | -0.000689 | 0.271524 |
| C | 1.549711 | -0.028098 | -2.605169 | F | -0.542410 | -0.149283 | 1.588789 |
| F | 0.570156 | -0.883481 | -2.950465 | F | 1.039165 | 0.146402 | 0.140710 |
| C | 2.606133 | -1.559208 | -0.112447 | Si | -0.905520 | -1.535689 | -0.727498 |
| C | 2.005883 | -2.646940 | 0.505241 | C | -0.319219 | -3.079003 | 0.084375 |
| C | 2.882436 | -3.727583 | 0.852184 | P | -0.716451 | -4.782347 | -0.438384 |
| C | 4.218212 | -3.549096 | 0.522294 | O | -0.567326 | -5.156547 | -1.860704 |
| Si | 5.604282 | -4.708956 | 0.819012 | F | -0.871485 | 1.137703 | -0.120271 |
| C | 6.767745 | -4.837926 | -0.718752 | C | -0.244349 | -1.376758 | -2.535471 |
| F | 7.654003 | -3.833972 | -0.750015 | F | 1.029908 | -1.787548 | -2.613927 |
| F | 1.221730 | 1.179018 | -3.083982 | C | -2.833781 | -1.503686 | -0.777814 |
| F | 2.668823 | -0.426850 | -3.231357 | F | -3.314535 | -2.696981 | -1.176498 |
| P | 4.281050 | -1.985872 | -0.220300 | F | -0.968300 | -2.105996 | -3.390666 |
| O | 5.420114 | -1.240960 | -0.777670 | F | -0.283897 | -0.099374 | -2.952677 |
| C | 6.671512 | -4.166115 | 2.331901 | F | -3.335801 | -1.262569 | 0.446374 |
| F | 6.007353 | -4.386282 | 3.481183 | F | -3.317202 | -0.572893 | -1.606995 |
| C | 4.905054 | -6.471348 | 1.185058 | C | 0.503599 | -3.150279 | 1.144565 |
| F | 4.352924 | -7.004570 | 0.082400 | C | 0.881313 | -4.515078 | 1.570577 |
| F | 7.834467 | -4.826809 | 2.402319 | C | 0.369369 | -5.518817 | 0.836758 |
| F | 6.949074 | -2.853384 | 2.274851 | Si | 0.634212 | -7.314621 | 1.143262 |
| F | 5.846466 | -7.313782 | 1.621408 | C | 1.406588 | -7.581885 | 2.893769 |
| F | 3.938857 | -6.425980 | 2.128154 | F | 2.506928 | -6.816431 | 3.059401 |
| F | 7.455491 | -5.989593 | -0.723865 | C | -1.067848 | -8.224476 | 1.100811 |
| F | 6.055712 | -4.787355 | -1.858335 | F | -1.975172 | -7.550548 | 1.835086 |
| F | 2.068868 | 2.647328 | -0.186941 | C | 1.811282 | -8.126304 | -0.151832 |
| F | 3.398204 | 1.399186 | 0.982137 | F | 1.441537 | -7.850809 | -1.404253 |
| H | 0.946611 | -2.692293 | 0.721158 | F | -1.543657 | -8.290011 | -0.153458 |
| H | 2.508716 | -4.619434 | 1.337639 | F | -1.003960 | -9.470452 | 1.582428 |
| | | | | F | 3.066255 | -7.669952 | 0.016755 |
| | | | | F | 1.844478 | -9.461168 | -0.015208 |
| | | | | F | 0.536178 | -7.230175 | 3.856651 |

8DH

| | | | | | | | |
|-------------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| F | 1.765836 | -8.850043 | 3.111186 | C | -1.252045 | 4.639097 | -2.128035 |
| H | 0.887742 | -2.290638 | 1.682658 | C | -1.953677 | -3.699187 | 0.040058 |
| H | 1.530809 | -4.653198 | 2.427878 | C | -3.713766 | -3.313998 | 2.566435 |
| H | -1.995011 | -4.981611 | 0.138149 | H | -0.004166 | 0.086009 | 4.766420 |
| {8D}₂ | | | | H | -1.926966 | -1.526378 | 4.147251 |
| 68 | | | | H | 3.040593 | 1.201958 | -2.728974 |
| E= -6350.104781 | | | | H | 1.324145 | 3.115528 | -2.662234 |
| C | 3.764583 | -1.935843 | -0.474578 | F | -4.537998 | -3.875005 | 2.115807 |
| Si | 2.605480 | -1.796375 | -1.942028 | F | -3.107111 | -4.016174 | 3.145468 |
| C | 1.391469 | -3.218009 | -1.934503 | F | -4.150217 | -2.589262 | 3.260356 |
| C | 3.608303 | -1.769125 | -3.529924 | F | -2.733434 | -4.342177 | -0.379839 |
| C | 1.637238 | -0.178329 | -1.879567 | F | -1.483137 | -3.165846 | -0.791809 |
| C | 2.043114 | 1.017524 | -2.339064 | F | -1.207296 | -4.339943 | 0.517879 |
| C | 1.040071 | 2.120199 | -2.332895 | F | -4.625796 | -1.730171 | -0.146145 |
| C | -0.191484 | 1.800579 | -1.910638 | F | -4.090959 | -0.419537 | 0.919952 |
| Si | -1.727134 | 2.866253 | -1.739885 | F | -3.161770 | -0.822888 | -0.544720 |
| C | -2.999965 | 2.210077 | -2.947283 | F | 3.157412 | 2.726778 | 4.452420 |
| P | -0.113169 | 0.053344 | -1.452006 | F | 1.557961 | 2.240209 | 5.018291 |
| O | -1.087101 | -0.906981 | -2.026797 | F | 2.873482 | 1.057004 | 4.962353 |
| O | -0.216746 | 0.195992 | 0.157054 | F | 4.206732 | 1.692571 | 1.672149 |
| P | 0.218342 | -0.938591 | 1.317191 | F | 3.898881 | 0.003451 | 2.107222 |
| C | 0.660727 | 0.114681 | 2.718449 | F | 3.154955 | 0.695012 | 0.660591 |
| Si | 1.953076 | 1.466357 | 2.683444 | F | 1.893991 | 3.761160 | 1.708669 |
| C | 3.444312 | 0.907695 | 1.694373 | F | 0.842836 | 2.644623 | 0.813056 |
| C | -1.325602 | -1.496149 | 2.080495 | F | 0.309688 | 3.309199 | 2.362722 |
| Si | -2.695605 | -2.463835 | 1.235482 | F | -3.286749 | 3.263250 | 0.147902 |
| C | -3.746542 | -1.238039 | 0.281469 | F | -2.549963 | 1.654571 | 0.263778 |
| C | -1.231613 | -1.173298 | 3.389994 | F | -1.623310 | 3.076775 | 0.735475 |
| C | -0.129652 | -0.265419 | 3.745483 | F | -3.955260 | 2.732212 | -2.837968 |
| C | 1.179005 | 2.938956 | 1.811849 | F | -2.662710 | 2.327519 | -3.980806 |
| C | 2.428630 | 1.910790 | 4.443565 | F | -3.168967 | 1.143516 | -2.772628 |
| C | -2.356504 | 2.701910 | 0.017147 | F | -2.121585 | 5.297799 | -2.045482 |

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|-----------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| F | -0.490648 | 5.003966 | -1.432361 | C | 3.828223 | -3.152190 | 1.424320 |
| F | -0.860124 | 4.734728 | -3.144920 | C | 3.855927 | -2.516241 | -2.574547 |
| F | 4.194388 | -2.687846 | -3.629070 | C | 4.491638 | 0.389957 | -3.317115 |
| F | 2.956955 | -1.686791 | -4.404156 | P | 0.011546 | 0.696434 | 0.003225 |
| F | 4.308401 | -0.928378 | -3.549177 | Si | -3.548769 | -0.784622 | 2.092440 |
| F | 4.320501 | -2.877237 | -0.531392 | C | -5.174775 | -0.039398 | 2.693193 |
| F | 4.488794 | -1.117281 | -0.445947 | Si | -3.582816 | 2.141122 | -0.363107 |
| F | 3.205620 | -1.929195 | 0.464477 | C | -5.454627 | 2.365198 | -0.460055 |
| F | 1.904540 | -4.161465 | -2.144240 | C | -3.640784 | -2.665786 | 2.205945 |
| F | 0.912653 | -3.307385 | -0.955540 | C | -2.136625 | -0.173636 | 3.181436 |
| F | 0.600190 | -3.075405 | -2.674309 | C | -2.940450 | 3.111292 | 1.121147 |
| | | | | C | -2.792539 | 2.814635 | -1.935707 |
| 8E | | | | C | -4.592619 | -0.509441 | -3.268293 |
| 88 | | | | C | -3.907502 | -3.135184 | -1.840525 |
| E= -3604.866416 | | | | H | 1.336389 | -2.504833 | -1.098991 |
| C | 5.440734 | 2.429765 | 0.195244 | H | -1.250215 | -2.539861 | -1.088591 |
| Si | 3.572083 | 2.167451 | 0.235786 | H | 3.013187 | 4.282831 | -0.952280 |
| Si | 3.156499 | -0.116412 | -0.125593 | H | 3.141663 | 2.940526 | -2.100195 |
| C | 1.324405 | -0.450466 | -0.409451 | H | 1.691297 | 3.117878 | -1.104470 |
| C | 0.762325 | -1.628937 | -0.808845 | H | 3.103693 | 3.772771 | 2.084054 |
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| C | -1.285533 | -0.487673 | -0.400252 | H | 3.404150 | 2.154331 | 2.730268 |
| Si | -3.117732 | -0.151136 | -0.125754 | H | 5.685823 | 3.469021 | 0.436787 |
| Si | -4.500153 | -1.361618 | -1.588310 | H | 5.954878 | 1.787571 | 0.915942 |
| C | -6.227899 | -1.414540 | -0.830691 | H | 5.850126 | 2.215204 | -0.796294 |
| C | 2.779641 | 3.224482 | -1.108091 | H | 2.461328 | -1.598884 | 3.988700 |
| C | 2.917696 | 2.706278 | 1.920375 | H | 2.112603 | -0.014718 | 3.276543 |
| Si | 3.680601 | -1.312967 | 1.822539 | H | 1.335799 | -1.461382 | 2.627780 |
| C | 5.300942 | -0.708654 | 2.576326 | H | 5.567238 | -1.300449 | 3.457916 |
| Si | 4.482883 | -0.866113 | -1.910374 | H | 6.124065 | -0.783996 | 1.859612 |
| C | 6.245002 | -1.097151 | -1.275203 | H | 5.224485 | 0.337230 | 2.888343 |
| C | 2.268542 | -1.073003 | 3.048264 | H | 4.011764 | -3.734587 | 2.332988 |

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| H | 2.906017 | -3.527109 | 0.969710 | H | -4.662949 | -3.709340 | -2.386975 |
| H | 4.649081 | -3.349049 | 0.728459 | H | -2.983663 | -3.167535 | -2.424647 |
| H | 6.915637 | -1.393308 | -2.088224 | H | -3.727177 | -3.639947 | -0.887123 |
| H | 6.637135 | -0.175356 | -0.836224 | H | -3.140758 | 4.180590 | 0.997401 |
| H | 6.288061 | -1.875883 | -0.507780 | H | -3.424001 | 2.785136 | 2.046793 |
| H | 4.530101 | -2.896522 | -3.348941 | H | -1.861281 | 2.983002 | 1.242671 |
| H | 3.796315 | -3.269240 | -1.783105 | O | -0.645555 | 2.307396 | -0.021715 |
| H | 2.862587 | -2.410471 | -3.019760 | | | | |
| H | 5.062699 | 0.012725 | -4.171647 | SEH | | | |
| H | 3.475130 | 0.603396 | -3.660164 | 89 | | | |
| H | 4.944443 | 1.335407 | -3.004582 | E: -3605.495049 | | | |
| H | -3.750462 | -2.993708 | 3.244609 | C | -5.504215 | 2.390716 | 0.119786 |
| H | -4.490606 | -3.058726 | 1.639893 | Si | -3.624816 | 2.201693 | 0.067650 |
| H | -2.730745 | -3.122017 | 1.804357 | C | -2.861306 | 3.065962 | 1.548355 |
| H | -2.318709 | -0.414857 | 4.233696 | C | -2.973826 | 2.964717 | -1.525074 |
| H | -1.190555 | -0.639255 | 2.889272 | Si | -3.185029 | -0.112536 | 0.111617 |
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| | | | | C | 4.447334 | -1.339498 | 3.379440 |
| 8FH | | | | C | 5.223513 | -0.259372 | 3.788223 |
| 77 | | | | C | 5.226648 | 0.897903 | 3.026594 |
| E: -2036.718486 | | | | C | 4.446985 | 0.988888 | 1.875938 |
| C | -4.449727 | 0.988559 | 1.873783 | C | 2.776476 | 1.306285 | -0.531232 |
| C | -3.650336 | -0.075502 | 1.468015 | C | 2.300754 | 2.416245 | 0.176989 |
| C | -3.681084 | -1.249014 | 2.229334 | C | 2.105433 | 3.635776 | -0.448971 |
| C | -4.449136 | -1.339028 | 3.378481 | C | 2.367336 | 3.771657 | -1.809240 |
| C | -5.226804 | -0.259503 | 3.785969 | C | 2.826996 | 2.677553 | -2.523945 |
| C | -5.230393 | 0.897374 | 3.023725 | C | 3.029947 | 1.453439 | -1.891046 |
| C | -2.814228 | -0.070498 | 0.171907 | C | -3.443894 | -1.153982 | -0.721318 |
| C | -2.776331 | 1.306778 | -0.531465 | C | -2.749456 | -2.272970 | -1.161395 |
| C | -3.027064 | 1.453565 | -1.891839 | C | -3.384785 | -3.243214 | -1.932795 |
| C | -2.822908 | 2.677531 | -2.524620 | C | -4.721265 | -3.108346 | -2.270325 |
| C | -2.364708 | 3.771817 | -1.809246 | C | -5.428274 | -1.993589 | -1.827548 |
| C | -2.105510 | 3.636277 | -0.448430 | C | -4.796188 | -1.032674 | -1.057207 |
| C | -2.302038 | 2.416890 | 0.177450 | H | 1.278393 | -0.471603 | 2.603305 |
| C | -1.336081 | -0.323578 | 0.472793 | H | -1.278713 | -0.471303 | 2.603508 |
| C | -0.738781 | -0.434686 | 1.664471 | H | 4.481264 | 1.898821 | 1.291155 |
| C | 0.738344 | -0.434992 | 1.664332 | H | 5.842360 | 1.740986 | 3.319569 |
| C | 1.335636 | -0.324364 | 0.472572 | H | 5.829489 | -0.328313 | 4.684367 |
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| O | -0.000880 | -1.012034 | -1.988906 | H | 3.107964 | -2.110204 | 1.900635 |
| C | 2.813892 | -0.071033 | 0.172198 | H | 3.360513 | 0.604941 | -2.475476 |

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|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 3.020484 | 2.763499 | -3.587023 | C | -3.691908 | -0.931609 | -5.862920 |
| H | 2.202940 | 4.721094 | -2.305699 | C | -4.249358 | 0.336483 | -5.982050 |
| H | 1.733238 | 4.479032 | 0.121847 | C | -4.343101 | 1.140376 | -4.856922 |
| H | 2.054487 | 2.311690 | 1.227936 | C | -2.849041 | -1.151756 | -2.125389 |
| H | 1.699532 | -2.393130 | -0.938328 | C | -3.955884 | -2.039958 | -1.516655 |
| H | 2.820711 | -4.100329 | -2.278913 | C | -5.104418 | -2.405058 | -2.211158 |
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| H | 5.359775 | -0.176693 | -0.697947 | C | -4.734520 | -3.356431 | 0.367474 |
| H | -4.484398 | 1.898173 | 1.288538 | C | -3.795030 | -2.520020 | -0.211894 |
| H | -5.847260 | 1.739972 | 3.315666 | C | -2.586306 | -0.007167 | -1.134803 |
| H | -5.833577 | -0.328616 | 4.681560 | C | -3.560690 | 0.572901 | -0.408247 |
| H | -4.452120 | -2.259749 | 3.951024 | C | -3.174264 | 1.756491 | 0.340247 |
| H | -3.107746 | -2.109245 | 1.901314 | C | -1.884548 | 2.138934 | 0.251105 |
| H | -3.356263 | 0.604854 | -2.476730 | C | -1.368375 | 3.413418 | 0.946037 |
| H | -3.014226 | 2.763204 | -3.588111 | C | -1.760700 | 3.220238 | 2.428705 |
| H | -2.199296 | 4.721131 | -2.305601 | C | -2.893649 | 3.823260 | 2.973474 |
| H | -1.734443 | 4.479685 | 0.122896 | C | -3.288340 | 3.555102 | 4.281087 |
| H | -2.057790 | 2.312551 | 1.228891 | C | -2.551319 | 2.685273 | 5.071535 |
| H | -5.358235 | -0.174314 | -0.704542 | C | -1.424777 | 2.073399 | 4.535455 |
| H | -6.476766 | -1.877617 | -2.078103 | C | -1.040588 | 2.326998 | 3.227326 |
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| H | -2.819723 | -4.103401 | -2.273011 | O | 0.131060 | 0.288846 | -0.587018 |
| H | -1.700034 | -2.395315 | -0.932001 | P | 1.132870 | -0.212144 | 0.561843 |
| H | 0.000155 | 1.246341 | -1.039862 | C | 2.590157 | -0.706248 | -0.488690 |
| | | | | C | 2.370309 | -2.010964 | -0.699756 |
| {8F}2 | | | | C | 1.352908 | -2.690491 | 0.116579 |
| 152 | | | | C | 0.636870 | -1.935995 | 0.954858 |
| E= -4072.288732 | | | | C | 0.008836 | -2.472461 | 2.257179 |
| C | -3.885051 | 0.684625 | -3.624408 | C | 0.017001 | -4.011343 | 2.174130 |
| C | -3.318912 | -0.579783 | -3.490337 | C | 0.745388 | -4.824148 | 3.033096 |
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| C | -0.089881 | -6.804877 | 1.935122 | C | -3.107997 | -0.293194 | 2.781561 |
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| C | -0.777717 | -4.621536 | 1.197810 | C | 3.770883 | 0.066721 | -1.141631 |
| C | 0.143966 | 3.660050 | 0.748970 | C | 4.586926 | -0.997841 | -1.922222 |
| C | 1.006350 | 3.980376 | 1.795316 | C | 4.522946 | -1.125612 | -3.305865 |
| C | 2.340240 | 4.284216 | 1.555963 | C | 5.204425 | -2.148112 | -3.963385 |
| C | 2.839515 | 4.292609 | 0.262919 | C | 5.963915 | -3.059400 | -3.247883 |
| C | 1.978786 | 4.025068 | -0.791583 | C | 6.039853 | -2.941017 | -1.862840 |
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| C | -2.028567 | 4.685757 | 0.355045 | C | 3.305077 | 1.139198 | -2.147760 |
| C | -1.745927 | 5.916046 | 0.958762 | C | 4.180132 | 2.132913 | -2.591575 |
| C | -2.266749 | 7.096799 | 0.458891 | C | 3.826025 | 2.984129 | -3.628964 |
| C | -3.073182 | 7.082342 | -0.676004 | C | 2.576645 | 2.881504 | -4.231329 |
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| C | -2.826845 | 4.686091 | -0.782821 | C | 2.062427 | 1.045196 | -2.763182 |
| O | 1.244443 | 0.719534 | 1.705202 | C | 4.690858 | 0.725756 | -0.081542 |
| C | -1.576856 | -1.991734 | -2.402829 | C | 6.062485 | 0.861531 | -0.333325 |
| C | -1.479488 | -3.348745 | -2.111341 | C | 6.903872 | 1.501682 | 0.564709 |
| C | -0.349992 | -4.082858 | -2.465839 | C | 6.397069 | 2.019806 | 1.750323 |
| C | 0.700543 | -3.475883 | -3.133683 | C | 5.040970 | 1.899465 | 2.007657 |
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| C | -0.512732 | -1.398918 | -3.089570 | H | 1.335560 | -3.772270 | 0.119416 |
| C | 0.947654 | -1.956933 | 3.384675 | H | 2.962776 | -2.611899 | -1.374064 |
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| C | 1.316914 | -0.908075 | 5.535114 | H | -3.911282 | 2.310889 | 0.912322 |
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| C | 3.196846 | -1.553610 | 4.202020 | H | 0.904880 | -0.466672 | 6.436127 |
| C | 2.334780 | -2.037387 | 3.230279 | H | 3.361231 | -0.588539 | 6.117751 |
| C | -1.430398 | -2.023566 | 2.570215 | H | 4.267562 | -1.612862 | 4.043593 |
| C | -2.286222 | -2.879296 | 3.274997 | H | 2.754347 | -2.473503 | 2.331877 |
| C | -3.532453 | -2.453923 | 3.710320 | H | 1.355595 | -4.382463 | 3.810350 |
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|---|-----------|-----------|-----------|-----------|--------------|-----------|-----------|
| H | -0.129953 | -7.884448 | 1.844664 | H | -0.006080 | 3.565011 | -1.399143 |
| H | -1.456638 | -6.445210 | 0.308883 | H | -1.104643 | 5.943234 | 1.832610 |
| H | -1.361710 | -4.001130 | 0.528610 | H | -2.036306 | 8.034846 | 0.951433 |
| H | -1.971829 | -3.888258 | 3.506291 | H | -3.477198 | 8.006600 | -1.073118 |
| H | -4.170638 | -3.141611 | 4.254555 | H | -3.959588 | 5.845225 | -2.188042 |
| H | -4.915963 | -0.807443 | 3.818240 | H | -3.051501 | 3.757628 | -1.291343 |
| H | -3.397277 | 0.737214 | 2.620927 | H | -5.273538 | -2.040783 | -3.215891 |
| H | -1.232653 | -0.013640 | 1.822288 | H | -6.944385 | -3.505614 | -2.189668 |
| H | 3.939282 | -0.425559 | -3.889606 | H | -6.615261 | -4.373088 | 0.109185 |
| H | 5.138770 | -2.221906 | -5.043188 | H | -4.572213 | -3.711587 | 1.378219 |
| H | 6.496373 | -3.852840 | -3.759911 | H | -2.924983 | -2.227523 | 0.363423 |
| H | 6.630854 | -3.644461 | -1.287078 | H | -2.298778 | -3.858357 | -1.622595 |
| H | 5.418690 | -1.848697 | -0.133148 | H | -0.303754 | -5.137655 | -2.217993 |
| H | 6.488034 | 0.458706 | -1.244132 | H | 1.579670 | -4.044629 | -3.415842 |
| H | 7.960359 | 1.588562 | 0.336090 | H | 1.422776 | -1.631914 | -3.972606 |
| H | 7.052972 | 2.511792 | 2.459935 | H | -0.586114 | -0.358290 | -3.388200 |
| H | 4.616644 | 2.300893 | 2.921123 | H | -2.796609 | -2.369995 | -4.562629 |
| H | 3.143997 | 1.234221 | 1.344448 | H | -3.611575 | -1.575946 | -6.731235 |
| H | 5.153250 | 2.245173 | -2.132681 | H | -4.603594 | 0.692290 | -6.942789 |
| H | 4.528642 | 3.740566 | -3.960607 | H | -4.772562 | 2.133262 | -4.930777 |
| H | 2.297226 | 3.554371 | -5.033975 | H | -3.976024 | 1.332691 | -2.763062 |
| H | 0.705906 | 1.819997 | -4.230085 | | | | |
| H | 1.379322 | 0.273861 | -2.447480 | 8G | | | |
| H | -3.481446 | 4.510923 | 2.377576 | 76 | | | |
| H | -4.174795 | 4.036668 | 4.679205 | E= | -2538.960308 | | |
| H | -2.855616 | 2.480079 | 6.091778 | O | 0.000138 | 2.046813 | 0.249328 |
| H | -0.843009 | 1.374836 | 5.126628 | P | 0.000032 | 0.604506 | -0.116913 |
| H | -0.177620 | 1.810762 | 2.821074 | C | 1.341341 | -0.455293 | -0.422045 |
| H | 0.648016 | 3.991119 | 2.815053 | Si | 3.172543 | -0.109908 | -0.148776 |
| H | 2.992349 | 4.509481 | 2.392590 | C | 3.551641 | -0.933806 | 1.532170 |
| H | 3.885964 | 4.506230 | 0.077252 | C | -1.341327 | -0.455170 | -0.422138 |
| H | 2.336525 | 4.058187 | -1.811432 | Si | -3.172529 | -0.109822 | -0.148876 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.562176 | 1.757628 | -0.054515 | C | 2.816857 | 4.064149 | -0.119964 |
| C | -0.723261 | -1.649388 | -0.735083 | C | 2.531161 | 2.695299 | -0.187988 |
| C | 0.723246 | -1.649448 | -0.734995 | H | 5.681258 | 1.459338 | 0.246762 |
| H | 1.280064 | -2.552200 | -0.957949 | H | 6.189186 | 3.892957 | 0.367700 |
| H | -1.280174 | -2.552090 | -0.958033 | H | 4.355940 | 5.560063 | 0.132992 |
| C | 4.216009 | -0.911353 | -1.533321 | H | 2.014766 | 4.793550 | -0.222654 |
| C | 3.562315 | 1.757594 | -0.055971 | H | 1.506838 | 2.359931 | -0.343592 |
| C | -4.215961 | -0.910210 | -1.534058 | C | -5.609591 | -0.777031 | -1.526431 |
| C | -3.551832 | -0.935031 | 1.531380 | C | -6.374411 | -1.363703 | -2.541748 |
| C | 5.609653 | -0.778322 | -1.525664 | C | -5.745600 | -2.083553 | -3.564691 |
| C | 6.374496 | -1.365768 | -2.540514 | C | -4.351970 | -2.216732 | -3.572317 |
| C | 5.745696 | -2.086245 | -3.563022 | C | -3.587150 | -1.630060 | -2.557001 |
| C | 4.352052 | -2.219276 | -3.570680 | H | -6.098716 | -0.217090 | -0.730727 |
| C | 3.587208 | -1.631830 | -2.555829 | H | -7.458456 | -1.260108 | -2.535815 |
| H | 6.098770 | -0.217894 | -0.730298 | H | -6.340521 | -2.539900 | -4.354462 |
| H | 7.458553 | -1.262290 | -2.534557 | H | -3.862845 | -2.776673 | -4.368021 |
| H | 6.340635 | -2.543195 | -4.352430 | H | -2.503105 | -1.733654 | -2.562933 |
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| H | 2.503152 | -1.735309 | -2.561786 | C | -5.123728 | -1.482869 | 3.294620 |
| C | 4.845470 | -0.876440 | 2.063880 | C | -4.107878 | -2.144760 | 3.994583 |
| C | 5.123342 | -1.480345 | 3.295987 | C | -2.814004 | -2.201787 | 3.462944 |
| C | 4.107386 | -2.141615 | 3.996383 | C | -2.535981 | -1.596922 | 2.231343 |
| C | 2.813557 | -2.198981 | 3.464672 | H | -5.635892 | -0.363147 | 1.518547 |
| C | 2.535685 | -1.595076 | 2.232566 | H | -6.130177 | -1.438511 | 3.708159 |
| H | 5.635739 | -0.362067 | 1.519072 | H | -4.324140 | -2.615259 | 4.952592 |
| H | 6.129756 | -1.435722 | 3.709582 | H | -2.023818 | -2.716644 | 4.007415 |
| H | 4.323531 | -2.611366 | 4.954786 | H | -1.529533 | -1.641281 | 1.817804 |
| H | 2.023288 | -2.713354 | 4.009480 | C | -4.879029 | 2.188698 | 0.145681 |
| H | 1.529271 | -1.639699 | 1.818971 | C | -5.164634 | 3.557509 | 0.214846 |
| C | 4.879167 | 2.188739 | 0.144072 | C | -4.133387 | 4.495252 | 0.083815 |
| C | 5.164864 | 3.557588 | 0.212096 | C | -2.816535 | 4.064182 | -0.116381 |
| C | 4.133709 | 4.495294 | 0.080079 | C | -2.530929 | 2.695370 | -0.185546 |

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|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -5.681192 | 1.459268 | 0.247605 | C | 3.008470 | 2.539208 | -1.211543 |
| H | -6.188957 | 3.892820 | 0.370571 | P | 0.000013 | 0.654675 | 0.343437 |
| H | -4.355548 | 5.559992 | 0.137616 | O | 0.000056 | 2.129399 | 0.109413 |
| H | -2.014372 | 4.793612 | -0.218305 | C | 3.459695 | 0.162924 | 1.723141 |
| H | -1.506606 | 2.360060 | -0.341271 | C | 4.282577 | 1.190155 | 2.193646 |
| | | | | C | 4.490973 | 1.370769 | 3.556387 |
| 8GH | | | | C | 3.878226 | 0.525442 | 4.472289 |
| 77 | | | | C | 3.054017 | -0.501154 | 4.024355 |
| E: -2539.589636 | | | | C | 2.847399 | -0.676827 | 2.662575 |
| C | -3.008305 | 2.539297 | -1.211380 | C | 4.049394 | -1.657310 | -0.709368 |
| C | -3.783434 | 1.378041 | -1.089624 | C | 4.665583 | -2.549374 | 0.172905 |
| C | -5.062413 | 1.366989 | -1.659832 | C | 5.271317 | -3.712122 | -0.291220 |
| C | -5.556089 | 2.478851 | -2.331541 | C | 5.269873 | -4.003009 | -1.649178 |
| C | -4.774686 | 3.622046 | -2.445156 | C | 4.666009 | -3.126255 | -2.544093 |
| C | -3.502820 | 3.649570 | -1.885276 | C | 4.064503 | -1.965124 | -2.076715 |
| Si | -3.179911 | -0.101968 | -0.114214 | C | -4.049456 | -1.657182 | -0.709529 |
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| C | -4.282444 | 1.189965 | 2.193777 | C | -5.271685 | -3.711846 | -0.291548 |
| C | -4.490839 | 1.370425 | 3.556540 | C | -5.270216 | -4.002660 | -1.649522 |
| C | -3.878151 | 0.524950 | 4.472342 | C | -4.666190 | -3.125941 | -2.544361 |
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| C | -2.847397 | -0.677172 | 2.662489 | H | 1.290936 | -2.254028 | -1.359015 |
| C | -1.337745 | -0.371516 | -0.337094 | H | -1.290906 | -2.254000 | -1.359090 |
| C | -0.741442 | -1.427557 | -0.916826 | H | 4.679138 | -2.331654 | 1.236276 |
| C | 0.741454 | -1.427585 | -0.916772 | H | 5.747348 | -4.389830 | 0.408769 |
| C | 1.337764 | -0.371586 | -0.336965 | H | 5.742672 | -4.908991 | -2.011921 |
| Si | 3.179945 | -0.101992 | -0.114189 | H | 4.668864 | -3.345514 | -3.606088 |
| C | 3.783500 | 1.377885 | -1.089781 | H | 3.609139 | -1.281314 | -2.787832 |
| C | 5.062424 | 1.366676 | -1.660109 | H | 4.757888 | 1.863271 | 1.486977 |
| C | 5.556140 | 2.478445 | -2.331942 | H | 5.128454 | 2.176326 | 3.903226 |
| C | 4.774839 | 3.621708 | -2.445555 | H | 4.037794 | 0.668518 | 5.535254 |
| C | 3.503029 | 3.649391 | -1.885552 | H | 2.570205 | -1.160277 | 4.736684 |

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|--------------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 2.196307 | -1.479385 | 2.325134 | O | -1.328889 | -1.382632 | 1.544488 |
| H | 5.681025 | 0.477449 | -1.583975 | C | 1.925323 | 1.495472 | -0.680976 |
| H | 6.548697 | 2.450808 | -2.767973 | Si | 1.844733 | 2.746542 | -2.101172 |
| H | 5.156501 | 4.490172 | -2.971452 | C | 2.808774 | 1.849642 | -3.484753 |
| H | 2.889344 | 4.538993 | -1.973333 | C | -1.470824 | 1.404628 | 1.312062 |
| H | 2.011229 | 2.586369 | -0.781238 | Si | -1.121169 | 1.961953 | 3.096587 |
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| H | -5.743122 | -4.908558 | -2.012337 | Si | -3.693075 | -1.391169 | -1.526690 |
| H | -4.669029 | -3.345143 | -3.606368 | C | -2.817586 | -2.015238 | -3.105347 |
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| H | -4.757704 | 1.863200 | 1.487188 | H | -2.785491 | 3.022385 | 0.830872 |
| H | -5.128273 | 2.175980 | 3.903471 | C | -3.131386 | 1.235641 | -0.438327 |
| H | -4.037714 | 0.667908 | 5.535325 | H | -3.929372 | 1.696679 | -1.009059 |
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| H | -2.196366 | -1.479740 | 2.324955 | H | 3.555788 | 2.331212 | 0.451264 |
| H | -5.681085 | 0.477810 | -1.583707 | C | 3.194756 | 0.189467 | 0.873627 |
| H | -6.548691 | 2.451337 | -2.767478 | H | 4.029613 | 0.100201 | 1.560786 |
| H | -5.156315 | 4.490580 | -2.970962 | C | 4.931424 | -2.681296 | 0.786818 |
| H | -2.889056 | 4.539117 | -1.973062 | C | 2.429604 | -3.626393 | 2.261367 |
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| H | -0.000075 | 0.284659 | 1.712397 | C | 2.883458 | 4.301366 | -1.711721 |
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| {8G} ₂ | | | | C | -5.373182 | -0.671131 | -2.080663 |
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| E= -5078.052482 | | | | C | -0.111170 | 3.580559 | 3.186689 |
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| O | -0.189753 | -0.341529 | -0.538403 | C | -3.991767 | 2.108575 | 2.954218 |
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| H | -4.456386 | 3.331802 | 6.616481 | H | -7.223713 | 2.187392 | -1.870654 |
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| H | -3.861664 | 1.766046 | 1.928710 | C | -5.003557 | -4.965501 | 0.221704 |
| C | 0.229649 | 4.124654 | 4.430796 | C | -4.599531 | -4.835120 | 1.555781 |
| C | 0.969962 | 5.311067 | 4.496839 | C | -3.926070 | -3.681060 | 1.973626 |
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| H | -0.081101 | 3.625024 | 5.347161 | H | -4.809113 | -5.631397 | 2.268480 |
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| H | 0.023215 | 3.799647 | 1.040888 | C | -2.776136 | -3.461130 | -5.051543 |
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| C | 0.486700 | 0.024384 | 6.444822 | C | -0.933876 | -1.941644 | -4.630543 |
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| C | 0.469136 | -1.593675 | 4.638838 | H | -4.383947 | -3.416760 | -3.608110 |
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| H | 0.710665 | 0.280745 | 7.479250 | H | 0.032214 | -1.528581 | -4.916845 |
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| C | -6.256481 | -1.454341 | -2.833236 | C | 1.560004 | -5.020187 | 4.528774 |
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|---|-----------|-----------|-----------|-----------------|-----------|-----------|-----------|
| C | 2.889852 | -5.094162 | -0.839391 | C | -2.396521 | 3.772523 | -3.874087 |
| C | 2.552487 | -5.869444 | -1.955242 | C | -2.280386 | 2.854418 | -2.823565 |
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| C | 1.560480 | -3.923069 | -3.007642 | H | 0.898970 | 4.557640 | -4.277886 |
| C | 1.897846 | -3.147786 | -1.891792 | H | -1.342321 | 5.099820 | -5.214784 |
| H | 3.406883 | -5.549633 | 0.003903 | H | -3.377142 | 4.009741 | -4.284003 |
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| H | 1.043449 | -3.467597 | -3.850937 | C | 2.976904 | 2.463365 | -4.731780 |
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| C | 7.729413 | -2.689609 | 0.892582 | C | 3.347271 | 0.578507 | -3.251869 |
| C | 7.039082 | -1.484186 | 0.718226 | H | 2.558030 | 3.452127 | -4.912931 |
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| H | 5.070516 | -4.821132 | 1.055663 | H | 4.771682 | 0.023442 | -6.301898 |
| H | 7.557729 | -4.828521 | 1.149680 | H | 4.472771 | -1.067669 | -4.084862 |
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| H | 5.103108 | -0.542384 | 0.529721 | 8H | | | |
| C | 2.953082 | 5.347222 | -2.639804 | 214 | | | |
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| C | 3.575204 | 4.395171 | -0.498177 | C | -3.614138 | 1.871661 | -2.908562 |
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| C | -5.922223 | 1.791188 | 1.633102 | C | -0.701745 | -3.035619 | 3.719413 |
| P | -0.049286 | 0.306702 | -0.633165 | C | -0.978918 | -2.234352 | 4.820181 |
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| C | 0.674153 | -0.234557 | 1.638800 | C | -6.492584 | -2.665420 | 0.370339 |
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| C | 5.286667 | 1.441768 | -2.253124 | H | -9.318659 | -3.419349 | 2.082682 |
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| C | -6.790736 | 2.700764 | 1.022025 | C | -8.611345 | -0.107677 | -2.688841 |
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| C | 5.543266 | -2.576150 | -2.033532 | H | 4.898091 | 0.643006 | 6.518810 |
| H | 6.687104 | -2.861630 | 1.137596 | H | 2.503380 | 0.781119 | 7.159226 |
| H | 8.808093 | -3.109923 | -0.061729 | H | 0.807872 | 1.316191 | 5.431846 |
| H | 8.867082 | -3.007941 | -2.537200 | H | 1.479066 | 1.727586 | 3.122135 |
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| C | 4.581821 | -4.114653 | 2.330795 | C | 3.325422 | 5.943921 | 0.184029 |
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| C | 4.218218 | -3.857444 | 4.696582 | C | 4.577953 | 3.895122 | 0.054910 |
| C | 3.724541 | -2.580507 | 4.475745 | H | 2.276890 | 3.755170 | 2.538014 |
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| H | 8.367819 | -1.166471 | 1.952563 | C | 2.180199 | 2.586540 | -3.893947 |
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| C | 4.524904 | 1.069540 | 4.450950 | C | 0.942910 | 4.564360 | -3.300174 |
| C | 4.145118 | 0.873056 | 5.773108 | C | 1.105089 | 4.253510 | -1.957333 |
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| H | 5.573322 | 0.976709 | 4.192044 | H | 0.394997 | 5.454280 | -3.591850 |

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|-----------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 0.694079 | 4.895985 | -1.187776 | C | -4.113495 | 3.661227 | 2.778961 |
| H | 1.935111 | 2.908941 | -0.533227 | C | -3.628430 | 4.930612 | 3.074447 |
| C | 4.133732 | -0.622124 | -4.488651 | C | -2.265294 | 5.182678 | 3.036577 |
| C | 4.004443 | -1.635684 | -5.430698 | C | -1.389273 | 4.158682 | 2.695662 |
| C | 2.997223 | -2.585182 | -5.297118 | C | -1.876838 | 2.891979 | 2.404869 |
| C | 2.111659 | -2.503845 | -4.229104 | Si | -3.846044 | 1.366452 | -1.699171 |
| C | 2.237662 | -1.481481 | -3.296620 | C | -2.754099 | 1.486489 | -3.234333 |
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| H | 4.696148 | -1.690757 | -6.264419 | C | -2.202342 | 2.747434 | -5.240250 |
| H | 2.903632 | -3.385554 | -6.022943 | C | -1.484654 | 1.663053 | -5.736461 |
| H | 1.326540 | -3.242746 | -4.110344 | C | -1.396582 | 0.498933 | -4.986894 |
| H | 1.531210 | -1.438573 | -2.477036 | C | -2.039346 | 0.407042 | -3.756996 |
| | | | | C | -4.023592 | 3.139822 | -1.087065 |
| 8HH | | | | C | -2.889633 | 3.845992 | -0.668282 |
| 215 | | | | C | -2.969620 | 5.179959 | -0.301621 |
| E: -7056.320484 | | | | C | -4.194983 | 5.837096 | -0.337065 |
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| C | -2.570923 | -3.521250 | 0.549604 | C | -5.243029 | 3.819432 | -1.126133 |
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| C | -2.396494 | -5.382566 | 2.107068 | C | -5.881534 | 0.817279 | -3.644521 |
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| C | -0.404572 | -4.464664 | 1.128176 | C | -7.951199 | -0.340654 | -3.211212 |
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| C | -3.338768 | -2.605329 | -2.302877 | C | -6.425695 | 0.128481 | -1.416957 |
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| C | -2.861435 | -2.847557 | -5.063432 | O | 0.080869 | -0.824947 | -2.026357 |
| C | -4.081504 | -2.365089 | -4.605511 | C | -5.460013 | -2.818080 | -0.113045 |
| C | -4.316483 | -2.248785 | -3.242537 | C | -6.126180 | -3.745792 | -0.921751 |
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| C | -3.251691 | 2.612771 | 2.440483 | C | -7.479139 | -2.634010 | 1.232096 |

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| C | -6.160530 | -2.285133 | 0.972019 | C | 3.459836 | -2.572149 | 2.626312 |
| C | -0.662120 | -0.253805 | 1.543144 | C | 4.378450 | -2.803518 | 3.655052 |
| C | 0.807791 | -0.213743 | 1.522736 | C | 3.961339 | -3.258469 | 4.902159 |
| C | 1.393582 | -0.009398 | 0.327722 | C | 2.613244 | -3.489960 | 5.148357 |
| Si | 3.272988 | 0.045737 | 0.095752 | C | 1.683875 | -3.274171 | 4.137441 |
| Si | 3.799461 | 1.904901 | 1.511206 | C | 2.110366 | -2.831706 | 2.893571 |
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| C | 1.758030 | 2.224199 | 3.505326 | C | 3.575612 | 3.218348 | -2.569465 |
| C | 1.006900 | 1.834259 | 4.607572 | C | 2.959474 | 4.416323 | -2.897224 |
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| C | 3.523367 | -4.782999 | 0.062133 | C | 8.037218 | 0.501145 | -1.992516 |
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| C | 1.948112 | -5.565676 | -1.580732 | C | 7.369125 | 1.545574 | -4.048823 |
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| C | 4.496631 | -2.100279 | -3.270129 | C | 3.738035 | 4.688809 | 0.809656 |
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| C | -7.826248 | 0.287257 | 3.566403 | H | 5.940361 | -3.667564 | -0.801401 |
| C | -8.600148 | 1.030692 | 2.683600 | H | 8.393472 | -3.597590 | -1.003234 |
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| C | -6.604650 | 1.696885 | 1.517419 | H | 8.561426 | -0.571051 | 2.034414 |
| C | -3.252175 | -0.204816 | 3.585062 | H | 6.131801 | -0.628053 | 2.230833 |
| C | -2.682737 | 0.381775 | 4.721058 | H | 5.437971 | -2.645890 | 3.482470 |
| C | -2.105322 | -0.398296 | 5.716589 | H | 4.694490 | -3.440036 | 5.680799 |
| C | -2.077981 | -1.782157 | 5.592953 | H | 2.290571 | -3.846084 | 6.120766 |
| C | -2.654041 | -2.385863 | 4.480779 | H | 0.628165 | -3.458811 | 4.305486 |
| C | -3.241202 | -1.601420 | 3.497369 | H | 1.372451 | -2.704946 | 2.110856 |
| H | 1.347890 | -0.346967 | 2.451181 | H | 1.553428 | -0.623967 | -4.064099 |
| H | -1.161543 | -0.403714 | 2.491002 | H | 1.337544 | -2.644971 | -5.401066 |
| H | 4.771329 | 4.710763 | 1.140568 | H | 3.105932 | -4.383460 | -5.351040 |
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| H | 1.336227 | 6.796894 | -0.332353 | H | 5.401958 | -1.957545 | -2.687910 |
| H | 0.065274 | 4.666470 | -0.376579 | H | 6.468281 | -0.149099 | -0.707399 |
| H | 1.124311 | 2.588306 | 0.362900 | H | 8.806744 | 0.158964 | -1.310142 |
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| H | 4.259161 | -0.046315 | 3.738700 | H | 3.491150 | 5.350116 | -2.755402 |
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| H | 4.275082 | -5.007627 | 0.814171 | H | -1.883896 | 6.171664 | 3.265971 |
| H | 3.227292 | -6.852073 | -0.424115 | H | -0.323630 | 4.352910 | 2.645890 |
| H | 1.478309 | -6.381282 | -2.119159 | H | -1.167276 | 2.112720 | 2.153520 |
| H | 0.806435 | -4.029631 | -2.564787 | H | -5.856102 | -0.348931 | 4.109776 |
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|---|-----------|-----------|-----------|--------------------------|----------------|-----------|-----------|
| H | -9.678141 | 1.061830 | 2.797044 | H | -1.958199 | -0.520275 | -3.208351 |
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| H | -2.671804 | 1.462216 | 4.821141 | H | -4.260612 | 6.878416 | -0.041675 |
| H | -1.668500 | 0.078028 | 6.587590 | H | -2.082128 | 5.704071 | 0.034145 |
| H | -1.609033 | -2.387975 | 6.360567 | H | -1.925846 | 3.344299 | -0.629503 |
| H | -2.634147 | -3.463636 | 4.362309 | H | -0.054020 | 1.479560 | -1.218064 |
| H | -3.661348 | -2.098096 | 2.630749 | {8H} ₂ | | | |
| H | -5.614591 | -4.187879 | -1.770003 | 428 | | | |
| H | -7.941170 | -4.820395 | -1.313190 | E= | -14111.2680154 | | |
| H | -9.158178 | -3.819351 | 0.599405 | C | 3.504218 | 4.825818 | -4.285286 |
| H | -7.995663 | -2.182012 | 2.071486 | C | 2.696473 | 4.003783 | -3.482167 |
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| H | -0.410463 | -6.108010 | 2.509755 | C | 3.746570 | 4.531393 | -5.619217 |
| H | 0.669896 | -4.483702 | 0.987463 | Si | 2.271647 | 4.578062 | -1.730276 |
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| H | -4.852791 | -2.068358 | -5.307386 | C | 3.871285 | 8.471331 | -1.228698 |
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| H | -5.199864 | 1.268546 | -4.357815 | Si | 3.179186 | 3.348007 | 0.160263 |
| H | -7.333037 | 0.346689 | -5.152327 | Si | 5.626575 | 3.285539 | 0.087061 |
| H | -8.878225 | -0.773186 | -3.571342 | C | 6.352821 | 2.910677 | 1.803949 |
| H | -8.279221 | -0.914013 | -1.158883 | C | 7.729784 | 3.092390 | 1.989211 |
| H | -6.190568 | 0.038131 | -0.364377 | C | 8.330529 | 2.844854 | 3.216813 |
| H | -3.358681 | 3.524764 | -3.619577 | C | 7.572199 | 2.383072 | 4.289575 |
| H | -2.272375 | 3.663671 | -5.816553 | C | 6.212227 | 2.160138 | 4.120073 |
| H | -0.990380 | 1.732251 | -6.699216 | C | 5.621666 | 2.423392 | 2.888936 |
| H | -0.837307 | -0.354098 | -5.354924 | C | 2.594185 | 1.421577 | 0.267964 |

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|----|-----------|-----------|-----------|----|-----------|-----------|----------|
| C | 3.567205 | 0.665328 | 0.797407 | C | -6.643085 | -4.355771 | 0.349319 |
| C | 3.582675 | -0.785789 | 0.580670 | C | -6.576190 | -2.986509 | 0.565783 |
| C | 2.601298 | -1.391474 | -0.102084 | C | -5.670122 | -2.458408 | 1.476405 |
| Si | 3.281183 | -3.175225 | -0.718676 | Si | -4.333851 | 1.008258 | 4.407296 |
| Si | 1.868598 | -5.126533 | -1.031357 | C | -4.461658 | 1.001299 | 6.304334 |
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| C | 0.331762 | -8.221294 | 2.101104 | C | -3.894314 | 2.030348 | 8.438198 |
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| C | 2.034642 | -6.678470 | 1.398546 | C | -6.066426 | 0.685136 | 3.685736 |
| P | 1.480642 | 0.095391 | -0.533503 | C | -6.893552 | -0.372704 | 4.068027 |
| O | 1.340744 | 0.240627 | -2.001096 | C | -8.162837 | -0.541119 | 3.529441 |
| O | 0.022134 | 0.125192 | 0.223943 | C | -8.637291 | 0.346521 | 2.575839 |
| P | -1.528483 | -0.644080 | 0.088696 | C | -7.833843 | 1.403735 | 2.165957 |
| C | -2.860773 | 0.209085 | -1.072432 | C | -6.575970 | 1.570562 | 2.725392 |
| Si | -3.680435 | 0.357995 | -2.893498 | C | -4.019037 | 2.821616 | 3.946567 |
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| C | -3.941125 | -3.029692 | -8.020776 | C | -3.103220 | 3.306100 | 3.011444 |
| C | -2.919851 | -2.499182 | -7.245422 | Si | -0.935986 | -0.569461 | 5.260398 |
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| C | -3.874616 | 0.402148 | -0.199730 | C | -1.038805 | -3.023646 | 6.730000 |
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| C | 1.576922 | -0.779791 | 3.764477 | C | -5.426958 | 3.529469 | -5.089432 |
| C | -0.784078 | 1.188640 | 5.941675 | Si | 2.833197 | 4.884703 | 2.130514 |
| C | -0.445517 | 1.432250 | 7.279455 | C | 1.309623 | 6.026207 | 2.150600 |
| C | -0.340063 | 2.724519 | 7.771250 | C | 0.465566 | 5.967341 | 3.264599 |
| C | -0.578281 | 3.811245 | 6.936084 | C | -0.525276 | 6.916697 | 3.482859 |
| C | -0.877545 | 3.591192 | 5.601005 | C | -0.711648 | 7.952853 | 2.579231 |
| C | -0.945936 | 2.292770 | 5.109845 | C | 0.103567 | 8.026124 | 1.457334 |
| Si | -5.577935 | 2.013917 | -2.615508 | C | 1.094925 | 7.076737 | 1.252153 |
| C | -7.159114 | 1.389773 | -1.745126 | C | 0.438332 | 4.482713 | -1.334384 |
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| Si | -2.430161 | 1.243835 | -4.819068 | Si | 4.402517 | -3.058270 | -2.937395 |
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| C | -0.753931 | 3.453746 | -5.393160 | C | 4.104742 | -4.457566 | -5.448037 |
| C | -0.385351 | 4.792995 | -5.419823 | C | 3.422812 | -4.907763 | -6.569176 |
| C | -1.036262 | 5.704261 | -4.600447 | C | 2.059586 | -4.665779 | -6.704576 |
| C | -2.006271 | 5.257090 | -3.712692 | C | 1.400981 | -3.935519 | -5.728069 |
| C | -2.334464 | 3.910127 | -3.664743 | C | 2.096713 | -3.486243 | -4.611951 |
| C | -5.280208 | 3.552322 | -1.520420 | Si | 4.978958 | -3.818784 | 1.024437 |
| C | -5.092014 | 4.841409 | -2.027379 | C | 6.554968 | -2.746272 | 1.220582 |
| C | -5.109658 | 5.958643 | -1.199002 | C | 7.802178 | -3.141577 | 0.721226 |
| C | -5.336157 | 5.817456 | 0.162437 | C | 8.963519 | -2.436429 | 1.017636 |
| C | -5.549074 | 4.549488 | 0.689231 | C | 8.911829 | -1.302811 | 1.815930 |
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|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 5.804558 | -0.063933 | -5.387977 | C | 6.471853 | 6.364703 | -2.542339 |
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| C | 6.056391 | -5.416482 | -3.233513 | C | 1.514300 | -0.777433 | -6.309181 |
| C | 7.259320 | -6.093550 | -3.378732 | C | 1.306852 | -0.509994 | -4.962331 |
| C | 8.463875 | -5.425334 | -3.188937 | C | 0.088562 | -0.002976 | -4.536401 |
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| C | 2.733477 | 2.915421 | 6.394834 | C | -4.769841 | 0.715010 | -6.485324 |
| C | 2.378373 | 2.148325 | 5.298999 | C | -4.317044 | -3.303317 | -2.524717 |
| C | 2.392169 | 2.691644 | 4.018770 | C | -4.681036 | -4.555070 | -3.043712 |
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| C | 5.636096 | -5.605834 | 0.902969 | H | -4.507324 | 0.416396 | 1.855067 |
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| C | -1.347645 | -4.152200 | 3.224935 | H | 0.413736 | 5.115197 | -6.078991 |
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| C | -6.847442 | -3.782167 | 7.162849 | H | -2.251499 | 2.799372 | -7.322597 |
| C | -5.558997 | -3.364162 | 7.464459 | H | -3.567669 | 2.942533 | -9.374792 |
| C | -4.687353 | -3.008071 | 6.442734 | H | -5.683213 | 1.667611 | -9.602452 |
| H | 4.433022 | 1.075524 | 1.295723 | H | -6.456450 | 0.240869 | -7.715498 |
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| H | 5.164671 | -4.666205 | -5.376887 | H | 7.122447 | 8.633213 | 3.390616 |
| H | 3.959334 | -5.451445 | -7.339578 | H | 7.236516 | 6.259158 | 4.136002 |
| H | 1.522600 | -5.025303 | -7.575650 | H | 5.481709 | 4.703716 | 3.541305 |
| H | 0.350304 | -3.694514 | -5.830769 | H | 3.347268 | 5.833260 | 4.820512 |
| H | 1.562292 | -2.898658 | -3.884195 | H | 3.331393 | 4.872151 | 7.065513 |
| H | 5.769063 | -2.193604 | -5.299480 | H | 2.716059 | 2.477568 | 7.386323 |
| H | 6.307237 | -0.049062 | -6.349113 | H | 2.071218 | 1.127695 | 5.446565 |
| H | 5.678132 | 2.080268 | -5.223648 | H | 2.110039 | 2.061289 | 3.179766 |
| H | 4.545820 | 2.011263 | -3.038842 | H | 0.600871 | 5.181147 | 3.994681 |
| H | 4.029834 | -0.120027 | -1.970075 | H | -1.151352 | 6.841541 | 4.365363 |
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| H | 8.796814 | 1.806323 | -3.558366 | H | -1.401541 | -2.131568 | -3.399415 |
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| H | 6.117030 | 0.381067 | 0.316824 | H | -1.563486 | -8.011576 | 1.114497 |
| H | 8.342947 | 3.437638 | 1.162295 | H | 0.002796 | -9.038240 | 2.733816 |
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| H | 6.280943 | 6.541260 | -3.595266 | H | 4.752490 | -6.266698 | 2.763117 |
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|---|-----------|-----------|-----------|---|------------|-----------|-----------|
| H | 6.717519 | -5.344289 | -0.932588 | H | -9.320903 | -3.579480 | -2.355140 |
| H | 6.253074 | -3.934846 | 3.592121 | H | -10.583044 | -1.942658 | -3.727620 |
| H | 5.535104 | -4.403715 | 5.882787 | H | -9.346596 | -0.201132 | -4.992030 |
| H | 3.108120 | -4.543510 | 6.418975 | H | -6.919451 | -0.088990 | -4.880507 |
| H | 1.448306 | -4.146048 | 4.650162 | H | -5.253504 | -4.613584 | -3.964517 |
| H | 2.154209 | -3.717551 | 2.334903 | H | -4.584421 | -6.687429 | -2.846558 |
| H | 7.889522 | -4.019285 | 0.096944 | H | -3.167061 | -6.605020 | -0.812593 |
| H | 9.910302 | -2.775204 | 0.611450 | H | -2.535388 | -4.410576 | 0.151905 |
| H | 9.812863 | -0.740479 | 2.032576 | H | -3.293688 | -2.344478 | -0.899095 |
| H | 7.631273 | -0.013399 | 2.967737 | H | -8.151215 | 1.775342 | -4.145318 |
| H | 5.620509 | -1.307183 | 2.538274 | H | -9.009071 | 2.708134 | -6.226033 |
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| H | 3.497426 | -0.587687 | 2.844372 | H | -8.029530 | 3.339650 | -2.066633 |
| H | 1.047233 | -0.568313 | 2.838459 | H | -10.239616 | 2.759772 | -1.199291 |
| H | -0.494277 | -3.441967 | 5.889988 | H | -10.684687 | 0.461966 | -0.358024 |
| H | -1.001537 | -4.877338 | 7.800779 | H | -8.855596 | -1.186888 | -0.308053 |
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| H | -0.272685 | 0.602825 | 7.955954 | H | -5.354560 | 6.685317 | 0.812172 |
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| H | -0.520387 | 4.822618 | 7.322472 | H | -5.722385 | 2.468817 | 0.289578 |
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| H | -7.243435 | -2.327650 | 0.029292 | C | -1.289133 | -0.007853 | 2.139717 |
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| H | -8.246392 | -4.194076 | 5.582414 | C | -3.225710 | 0.783765 | 3.245702 |
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| 42 | | | | H | 2.236488 | 0.004479 | 4.007746 |
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8IH

43

E: -1191.278866

C 0.056386 0.017825 -0.009119
C 0.004576 -0.012283 1.393723
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C 2.407605 -0.074805 1.499183
C 2.470212 -0.036038 0.114637
C 1.301802 0.010901 -0.630905
C -1.313124 -0.006915 2.069061
C -1.903361 1.005709 2.715568
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P -2.395533 -1.466100 2.243508
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C 1.133778 -0.110565 3.664732
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C -7.315506 -2.224780 4.582641
C -7.184800 -1.886899 3.243997
C -6.002249 -1.336976 2.757283
C -3.925319 -1.243145 5.974712
C -5.866208 -0.976197 1.301065
H -1.457359 1.991150 2.803505
H -3.770999 1.473611 3.859826

H -8.010358 -2.054300 2.560403
H -8.241306 -2.657323 4.945111
H -6.361042 -2.284971 6.502435
H 1.351750 0.038978 -1.714227
H 3.432471 -0.046347 -0.384897
H 3.322168 -0.118414 2.081261
H -6.796795 -1.170214 0.765374
H -5.617586 0.082396 1.180988
H -5.067300 -1.554639 0.828264
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H -4.147088 -1.699201 6.940822
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H -1.816819 -0.828145 -0.655784
H -1.818482 0.931626 -0.554142
H 0.765363 0.829869 4.083569
H 0.468240 -0.901411 4.021321
H 2.127505 -0.294938 4.075891
H -1.756628 -2.183143 3.290912

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84

E= -2381.413614

C 3.231235 -2.876424 -1.196905
C 2.737343 -2.361997 0.012848
C 3.620888 -1.882656 0.994939
C 4.990306 -1.943183 0.758521
C 5.485664 -2.453599 -0.429792
C 4.608074 -2.908341 -1.401928
C 1.291407 -2.428150 0.338402
P -0.109335 -1.607570 -0.488217
P -0.100318 1.712236 0.620299

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 1.301493 | 2.526922 | -0.210315 | C | 0.809226 | 3.419278 | -1.099895 |
| C | 2.748181 | 2.454528 | 0.110570 | H | 1.433783 | -4.034272 | 1.740397 |
| C | 3.626446 | 1.971598 | -0.874493 | H | -1.135095 | -3.902273 | 2.157489 |
| C | 4.996887 | 2.026479 | -0.642642 | H | -1.124056 | 4.012048 | -2.021740 |
| C | 5.498298 | 2.534775 | 0.544032 | H | 1.446551 | 4.132914 | -1.612191 |
| C | 4.625827 | 2.993041 | 1.519130 | H | 5.675833 | 1.646021 | -1.398209 |
| C | 3.248226 | 2.966824 | 1.318711 | H | 6.569065 | 2.568061 | 0.712787 |
| C | 3.119238 | 1.418478 | -2.182245 | H | 5.017508 | 3.396290 | 2.447672 |
| C | 2.329007 | 3.516590 | 2.378476 | H | -4.870665 | 0.903205 | -3.038469 |
| C | 3.120353 | -1.327389 | 2.304337 | H | -6.506756 | 1.645707 | -1.341924 |
| C | 2.306239 | -3.422373 | -2.253618 | H | -5.720534 | 2.701873 | 0.746390 |
| C | 0.798013 | -3.318052 | 1.229785 | H | -4.866277 | -0.778535 | 3.183911 |
| C | -0.627918 | -3.257842 | 1.446971 | H | -6.509987 | -1.514859 | 1.492040 |
| C | -1.280726 | -2.331428 | 0.712335 | H | -5.733701 | -2.574531 | -0.598235 |
| C | -2.727007 | -2.045340 | 0.874823 | H | 5.673326 | -1.565480 | 1.511792 |
| C | -3.161827 | -1.438200 | 2.066037 | H | 6.555718 | -2.491272 | -0.602106 |
| C | -4.527312 | -1.251614 | 2.267769 | H | 4.994975 | -3.313248 | -2.331752 |
| C | -5.449668 | -1.665229 | 1.321601 | H | 1.588036 | -4.126806 | -1.825695 |
| C | -5.012604 | -2.259072 | 0.148222 | H | 1.725542 | -2.627949 | -2.731169 |
| C | -3.657227 | -2.451769 | -0.095648 | H | 2.871514 | -3.938276 | -3.031877 |
| C | -2.190864 | -1.001559 | 3.136440 | H | 3.854042 | -0.641317 | 2.730857 |
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| C | -1.272152 | 2.441384 | -0.576611 | H | 2.937162 | -2.126776 | 3.029085 |
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| C | -3.160530 | 1.555928 | -1.925210 | H | 1.745748 | 2.724749 | 2.857187 |
| C | -4.527296 | 1.374782 | -2.123193 | H | 2.899076 | 4.029168 | 3.155434 |
| C | -5.445384 | 1.791865 | -1.174402 | H | 3.848612 | 0.729320 | -2.611198 |
| C | -5.002750 | 2.383756 | -0.002126 | H | 2.175802 | 0.884946 | -2.054611 |
| C | -3.645955 | 2.571025 | 0.238032 | H | 2.936991 | 2.218637 | -2.906373 |
| C | -2.194240 | 1.115558 | -2.998313 | H | -2.664304 | 2.526299 | 2.156831 |
| C | -3.193383 | 3.232320 | 1.512395 | H | -2.507886 | 4.059537 | 1.308823 |
| C | -0.617586 | 3.365245 | -1.312879 | H | -4.047371 | 3.619658 | 2.070867 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -2.684699 | 0.432395 | -3.695142 | C | -4.846886 | 1.273452 | -0.102218 |
| H | -1.822019 | 1.967501 | -3.574287 | C | -5.564988 | 0.096238 | -0.134507 |
| H | -1.321153 | 0.611650 | -2.577093 | C | -4.906679 | -1.113794 | -0.069541 |
| H | -4.067757 | -3.500183 | -1.926593 | C | -3.518663 | -1.191253 | 0.054100 |
| H | -2.681840 | -2.410839 | -2.017706 | C | -2.751181 | 2.671082 | -0.062262 |
| H | -2.527020 | -3.944112 | -1.169470 | C | -2.071687 | 2.812586 | -1.437452 |
| H | -2.676435 | -0.315644 | 3.833992 | C | -2.889042 | -2.612776 | 0.125244 |
| H | -1.821215 | -1.854838 | 3.712106 | C | -1.749784 | -2.806099 | -0.896194 |
| H | -1.316472 | -0.502023 | 2.712747 | C | 2.070859 | -2.812727 | -1.436709 |
| O | -0.194470 | 0.128455 | -0.407151 | C | 3.765526 | -3.830571 | 0.034377 |
| O | -0.204743 | -2.146601 | -2.139866 | C | 3.928435 | 3.705679 | -0.198811 |

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E= -1662.362976

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.518476 | 1.191371 | 0.054255 | C | -1.736881 | 2.931134 | 1.071820 |
| C | 2.793313 | -0.030328 | 0.119824 | H | 1.291778 | -0.010468 | 2.525429 |
| C | 3.456499 | -1.285398 | 0.013024 | H | -1.291716 | 0.009778 | 2.525598 |
| C | 4.847044 | -1.273131 | -0.102675 | H | 5.396977 | -2.198609 | -0.169896 |
| C | 5.564969 | -0.095819 | -0.134815 | H | 6.645539 | -0.121493 | -0.221875 |
| C | 4.906492 | 1.114106 | -0.069462 | H | 5.501358 | 2.012703 | -0.116532 |
| C | 1.326896 | 0.001827 | 0.376701 | H | -5.501629 | -2.012325 | -0.116860 |
| P | -0.000033 | 0.000089 | -0.751888 | H | -6.645565 | 0.122096 | -0.221426 |
| C | -1.326978 | -0.002146 | 0.376866 | H | -5.396702 | 2.199022 | -0.169151 |
| C | -0.721034 | -0.006033 | 1.605604 | H | 1.544011 | -3.770467 | -1.497649 |
| C | 0.720967 | 0.005381 | 1.605513 | H | 1.350998 | -2.024366 | -1.649987 |
| C | 2.751610 | -2.671125 | -0.062156 | H | 2.818579 | -2.783116 | -2.233828 |
| C | 1.738591 | -2.931519 | 1.072989 | H | 1.492345 | -3.996816 | 1.095657 |
| C | 2.888665 | 2.612834 | 0.125384 | H | 2.161698 | -2.664143 | 2.045574 |
| C | 2.376400 | 2.917634 | 1.546050 | H | 0.805101 | -2.392006 | 0.953630 |
| C | -2.793343 | 0.030312 | 0.119889 | H | 3.218239 | -4.775298 | -0.007561 |
| C | -3.456327 | 1.285506 | 0.013255 | H | 4.474978 | -3.840340 | -0.795683 |

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|------------|-----------|-----------|-----------|----|--------------|-----------|-----------|
| H | 4.323208 | -3.810548 | 0.975195 | E: | -1662.984534 | | |
| H | 1.576137 | 3.873697 | -1.059450 | C | 3.617821 | 1.124627 | 0.147797 |
| H | 1.988896 | 2.351735 | -1.862415 | C | 2.786007 | -0.039901 | 0.134398 |
| H | 0.806228 | 2.396988 | -0.547748 | C | 3.291140 | -1.279047 | -0.335972 |
| H | 2.028867 | 3.954406 | 1.598236 | C | 4.569902 | -1.287320 | -0.904297 |
| H | 1.544157 | 2.276701 | 1.830545 | C | 5.348728 | -0.157955 | -0.971166 |
| H | 3.177398 | 2.790974 | 2.280027 | C | 4.885175 | 1.021892 | -0.418345 |
| H | 3.429694 | 4.677445 | -0.176500 | C | 1.336784 | 0.063584 | 0.462673 |
| H | 4.736772 | 3.746885 | 0.535167 | C | 0.675039 | 0.072720 | 1.622537 |
| H | 4.361708 | 3.577832 | -1.194582 | C | -0.794749 | 0.136158 | 1.523574 |
| H | -1.575533 | -3.873257 | -1.058931 | C | -1.342454 | 0.143735 | 0.297925 |
| H | -1.985243 | -2.349850 | -1.860593 | P | 0.078413 | 0.223447 | -0.867721 |
| H | -0.805168 | -2.398067 | -0.543614 | O | 0.135640 | -0.666953 | -2.061182 |
| H | -2.031215 | -3.954856 | 1.598834 | C | 2.620587 | -2.683550 | -0.299919 |
| H | -1.547534 | -2.277034 | 1.832763 | C | 1.315030 | -2.823635 | 0.490825 |
| H | -3.181316 | -2.792184 | 2.279313 | C | 3.257770 | 2.477916 | 0.824393 |
| H | -3.429763 | -4.677119 | -0.179123 | C | 4.330501 | 3.555269 | 0.565972 |
| H | -4.737673 | -3.747188 | 0.531742 | C | -2.833989 | 0.139104 | 0.116775 |
| H | -4.360484 | -3.576508 | -1.197374 | C | -3.551945 | -1.056667 | 0.410237 |
| H | -1.544508 | 3.770121 | -1.498800 | C | -4.935146 | -0.959345 | 0.576395 |
| H | -1.352348 | 2.023915 | -1.651425 | C | -5.612326 | 0.229712 | 0.408739 |
| H | -2.820156 | 2.783340 | -2.233882 | C | -4.922741 | 1.352209 | -0.001001 |
| H | -3.217224 | 4.775354 | -0.006353 | C | -3.539865 | 1.341264 | -0.173178 |
| H | -4.474649 | 3.841142 | -0.794222 | C | -2.931423 | -2.481774 | 0.478640 |
| H | -4.321874 | 3.810364 | 0.976550 | C | -2.154225 | -2.767849 | -0.817684 |
| H | -1.490702 | 3.996443 | 1.094576 | C | -2.879826 | 2.622364 | -0.736912 |
| H | -2.158735 | 2.663344 | 2.044827 | C | -3.890488 | 3.766758 | -0.948854 |
| H | -0.803464 | 2.391799 | 0.951067 | C | -1.818832 | 3.209938 | 0.212238 |
| O | -0.000251 | -0.000278 | -2.234653 | C | -2.319526 | 2.301746 | -2.140746 |
| | | | | C | -2.049165 | -2.712630 | 1.723110 |
| 8JH | | | | C | -4.022380 | -3.571003 | 0.551318 |
| 79 | | | | C | 2.333561 | -3.140065 | -1.743520 |

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|---|-----------|-----------|-----------|--------------------------|-----------|-----------|-----------|
| C | 3.604958 | -3.668510 | 0.374275 | H | 3.037482 | 3.238762 | 2.849071 |
| C | 1.935513 | 3.090832 | 0.333588 | H | 2.411654 | 1.602799 | 2.651193 |
| C | 3.209132 | 2.279045 | 2.351217 | H | 4.156040 | 1.870545 | 2.714220 |
| H | -1.403398 | 0.149302 | 2.421558 | H | 4.017512 | 4.481223 | 1.054558 |
| H | 1.151901 | -0.014833 | 2.591830 | H | 5.303569 | 3.287328 | 0.983757 |
| H | -5.483892 | 2.256778 | -0.179190 | H | 4.450691 | 3.768327 | -0.499770 |
| H | -6.684571 | 0.273510 | 0.563489 | H | 1.912246 | -4.150711 | -1.733419 |
| H | -5.509529 | -1.833394 | 0.841605 | H | 1.615011 | -2.467882 | -2.216900 |
| H | 5.540198 | 1.878222 | -0.446634 | H | 3.241670 | -3.164264 | -2.350842 |
| H | 6.328425 | -0.194060 | -1.434047 | H | 3.139370 | -4.655745 | 0.443433 |
| H | 4.962253 | -2.206887 | -1.316702 | H | 4.538698 | -3.791019 | -0.175341 |
| H | -1.646510 | 3.095421 | -2.480700 | H | 3.851749 | -3.337377 | 1.387357 |
| H | -1.790973 | 1.352485 | -2.205944 | H | 1.029498 | -3.879711 | 0.491640 |
| H | -3.144764 | 2.231140 | -2.854384 | H | 1.421300 | -2.507995 | 1.530549 |
| H | -1.414582 | 4.134487 | -0.210821 | H | 0.488787 | -2.285610 | 0.035870 |
| H | -2.274787 | 3.449448 | 1.177337 | H | 0.179647 | 1.593765 | -1.181062 |
| H | -0.986646 | 2.545625 | 0.406030 | {8J} ₂ | | | |
| H | -3.361542 | 4.617213 | -1.387519 | 156 | | | |
| H | -4.691617 | 3.494498 | -1.639640 | E= -3324.813303 | | | |
| H | -4.334726 | 4.104809 | -0.008480 | C | -3.551882 | -2.608571 | 1.377161 |
| H | -1.676628 | -3.750858 | -0.756564 | C | -3.380331 | -1.192828 | 1.466910 |
| H | -2.840013 | -2.778176 | -1.669707 | C | -4.424535 | -0.317373 | 1.032832 |
| H | -1.378940 | -2.042517 | -1.048417 | C | -5.512859 | -0.894193 | 0.372049 |
| H | -1.839705 | -3.781834 | 1.824364 | C | -5.651964 | -2.255815 | 0.221820 |
| H | -1.092584 | -2.203686 | 1.667561 | C | -4.699848 | -3.097119 | 0.754683 |
| H | -2.567327 | -2.385517 | 2.629727 | C | -2.105520 | -0.662350 | 2.056151 |
| H | -3.536361 | -4.547129 | 0.478834 | C | -1.908547 | -0.462460 | 3.379082 |
| H | -4.572008 | -3.553514 | 1.496785 | C | -0.659137 | 0.158810 | 3.783230 |
| H | -4.735012 | -3.498753 | -0.273924 | C | 0.165059 | 0.506123 | 2.775337 |
| H | 1.844457 | 4.113798 | 0.709644 | C | 1.495347 | 1.179540 | 2.772279 |
| H | 1.901872 | 3.132694 | -0.758669 | C | 1.585803 | 2.595837 | 2.671772 |
| H | 1.069358 | 2.545478 | 0.693358 | C | 2.814618 | 3.134292 | 2.293575 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.925991 | 2.343511 | 2.085219 | C | 2.033258 | -3.429267 | -3.143838 |
| C | 3.863064 | 0.990677 | 2.347837 | C | 4.854500 | 1.078486 | -1.752481 |
| C | 2.667640 | 0.378159 | 2.723127 | C | 6.086830 | 1.742505 | -1.102007 |
| C | 0.479921 | 3.593221 | 3.121277 | C | 1.849249 | -0.393421 | -3.218516 |
| C | 0.337644 | 3.458462 | 4.650553 | C | 0.546866 | 0.190657 | -3.579712 |
| C | 2.716275 | -1.105027 | 3.169631 | C | -3.906623 | -2.132744 | -2.977496 |
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| C | -4.531272 | 1.224726 | 1.273787 | C | -0.832126 | 4.004687 | -1.215856 |
| C | -4.242202 | 1.605107 | 2.737827 | C | 0.528270 | 3.365445 | -3.224096 |
| C | -2.561203 | -3.667503 | 1.938455 | C | 3.002587 | -5.038469 | -1.571767 |
| C | -3.053040 | -5.108230 | 1.689746 | C | 1.196245 | -3.578657 | -0.775482 |
| P | -0.822824 | 0.342875 | 1.252222 | C | 5.212018 | 0.828774 | -3.232978 |
| P | 0.776674 | 0.372386 | -1.043669 | C | 3.737278 | 2.121743 | -1.679580 |
| C | -0.256636 | 0.547420 | -2.576351 | C | 0.880848 | 5.054285 | 2.838687 |
| C | -1.645143 | 1.073927 | -2.782304 | C | -0.898294 | 3.415269 | 2.466022 |
| C | -2.697302 | 0.128327 | -2.994260 | C | 2.332547 | -1.198233 | 4.659179 |
| C | -3.980304 | 0.620010 | -3.235568 | C | 1.810905 | -2.010252 | 2.326973 |
| C | -4.247716 | 1.970613 | -3.293158 | C | -3.644576 | 2.029103 | 0.310321 |
| C | -3.220897 | 2.871016 | -3.125706 | C | -5.971269 | 1.729282 | 1.017994 |
| C | -1.903841 | 2.472337 | -2.883628 | C | -1.208078 | -3.566221 | 1.232925 |
| C | -2.543352 | -1.418628 | -3.090338 | C | -2.383028 | -3.553699 | 3.468447 |
| C | -1.678916 | -2.028479 | -1.985591 | H | -2.678709 | -0.684649 | 4.109466 |
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| C | -1.362122 | 4.901697 | -3.478240 | H | 0.271635 | 0.314898 | -4.620049 |
| C | 2.139637 | -0.533138 | -1.921889 | H | 2.527275 | -0.720061 | -3.997221 |
| C | 3.407643 | -1.134980 | -1.387903 | H | -4.800459 | -0.062552 | -3.389481 |
| C | 3.481977 | -2.547920 | -1.182230 | H | -5.257746 | 2.321006 | -3.474574 |
| C | 4.606012 | -3.054251 | -0.528700 | H | -3.460052 | 3.920864 | -3.184604 |
| C | 5.641882 | -2.243469 | -0.120567 | H | 4.687120 | -4.109707 | -0.326550 |
| C | 5.624092 | -0.907587 | -0.453285 | H | 6.483524 | -2.661625 | 0.420318 |
| C | 4.554922 | -0.321528 | -1.134599 | H | 6.485885 | -0.315619 | -0.190608 |
| C | 2.440262 | -3.602621 | -1.662334 | H | 2.920317 | 4.198040 | 2.148500 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 4.857589 | 2.795504 | 1.763189 | H | -0.185492 | 4.876065 | -1.065753 |
| H | 4.764886 | 0.405984 | 2.245741 | H | -1.828828 | 4.245879 | -0.834923 |
| H | -6.297445 | -0.268459 | -0.021436 | H | -0.414957 | 3.182197 | -0.637008 |
| H | -6.517180 | -2.662768 | -0.289958 | H | 1.089004 | 4.303996 | -3.233919 |
| H | -4.863591 | -4.159432 | 0.669255 | H | 1.072552 | 2.690779 | -2.576310 |
| H | -3.879574 | 3.095355 | 0.396881 | H | 0.519364 | 2.968776 | -4.243197 |
| H | -2.583560 | 1.910717 | 0.506225 | H | -0.565522 | 5.648252 | -3.441885 |
| H | -3.833220 | 1.725053 | -0.719615 | H | -1.571785 | 4.682674 | -4.529307 |
| H | -4.502051 | 2.655566 | 2.896074 | H | -2.243129 | 5.372056 | -3.037821 |
| H | -4.845245 | 1.000524 | 3.422439 | H | -0.386829 | 4.188267 | 5.026838 |
| H | -3.200239 | 1.490415 | 3.011356 | H | -0.008144 | 2.464822 | 4.935198 |
| H | -6.021173 | 2.780696 | 1.310530 | H | 1.296064 | 3.638207 | 5.145392 |
| H | -6.249351 | 1.685066 | -0.037749 | H | -1.533414 | 4.266866 | 2.728685 |
| H | -6.715313 | 1.184046 | 1.605284 | H | -0.818777 | 3.373443 | 1.381056 |
| H | -1.967852 | -4.488723 | 3.855817 | H | -1.412189 | 2.523488 | 2.809483 |
| H | -1.696982 | -2.758380 | 3.746040 | H | 0.077948 | 5.709965 | 3.184784 |
| H | -3.341697 | -3.380766 | 3.965898 | H | 1.788402 | 5.352145 | 3.368705 |
| H | -2.293400 | -5.798238 | 2.065549 | H | 1.019242 | 5.235422 | 1.768985 |
| H | -3.985395 | -5.328459 | 2.217484 | H | 2.453112 | -2.228945 | 5.008312 |
| H | -3.187613 | -5.325795 | 0.627136 | H | 2.979946 | -0.556053 | 5.263104 |
| H | -0.489335 | -4.248689 | 1.696717 | H | 1.299977 | -0.907529 | 4.838271 |
| H | -1.315585 | -3.847411 | 0.184879 | H | 1.995568 | -3.059394 | 2.580716 |
| H | -0.783625 | -2.567584 | 1.262806 | H | 0.755347 | -1.818496 | 2.496447 |
| H | -1.737255 | -3.119289 | -2.041923 | H | 2.019741 | -1.876969 | 1.265154 |
| H | -0.629619 | -1.773737 | -2.082554 | H | 4.115114 | -2.724960 | 3.401397 |
| H | -2.025124 | -1.728181 | -0.995686 | H | 4.490613 | -1.690222 | 2.026617 |
| H | -2.002316 | -2.885082 | -4.594608 | H | 4.853866 | -1.149864 | 3.681582 |
| H | -2.547128 | -1.341760 | -5.273559 | H | 0.438503 | -4.253540 | -1.184044 |
| H | -0.926219 | -1.491142 | -4.578179 | H | 1.440708 | -3.916161 | 0.233466 |
| H | -3.731550 | -3.210689 | -2.938150 | H | 0.752892 | -2.590845 | -0.686186 |
| H | -4.434327 | -1.850778 | -2.064738 | H | 1.626894 | -4.372945 | -3.517134 |
| H | -4.553478 | -1.950815 | -3.839064 | H | 1.258649 | -2.679872 | -3.279745 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 2.893159 | -3.168030 | -3.766959 | C | -1.103317 | 0.217952 | -0.876907 |
| H | 2.246768 | -5.727063 | -1.956995 | C | -4.929157 | -1.111983 | 3.638670 |
| H | 3.908721 | -5.167099 | -2.170670 | C | -5.018405 | -1.503958 | 4.981176 |
| H | 3.210747 | -5.347120 | -0.545276 | C | -6.181984 | -2.076064 | 5.481007 |
| H | 2.914366 | 1.884029 | -2.344291 | C | -7.274883 | -2.270111 | 4.653127 |
| H | 3.337507 | 2.232338 | -0.673166 | C | -7.209005 | -1.884706 | 3.324741 |
| H | 4.132307 | 3.088261 | -2.006425 | C | -6.048170 | -1.312167 | 2.819079 |
| H | 6.207688 | 2.741103 | -1.527460 | C | -3.855265 | -1.285654 | 5.923922 |
| H | 5.960014 | 1.854640 | -0.022473 | C | -6.024765 | -0.881626 | 1.368788 |
| H | 7.017219 | 1.204019 | -1.294908 | H | -1.684145 | 2.106271 | 2.379045 |
| H | 5.517560 | 1.768100 | -3.704928 | H | -3.991178 | 1.590833 | 3.431759 |
| H | 6.034025 | 0.113287 | -3.324487 | H | -8.060145 | -2.029406 | 2.673490 |
| H | 4.358488 | 0.439151 | -3.789846 | H | -8.178899 | -2.720151 | 5.043790 |
| O | 0.049682 | -0.552577 | 0.088173 | H | -6.227848 | -2.370830 | 6.520487 |
| O | 1.148533 | 1.667273 | -0.422902 | H | 1.450901 | 0.095577 | -1.666463 |

8K

42

E= -2381.574566

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.115391 | 0.064908 | 0.006600 | F | -7.165346 | -1.204054 | 0.740636 |
| C | -0.021037 | -0.015410 | 1.399055 | F | -5.878425 | 0.446746 | 1.246679 |
| C | 1.144617 | -0.127024 | 2.168942 | F | -5.029088 | -1.458351 | 0.680324 |
| C | 2.396485 | -0.159472 | 1.566591 | F | -2.733856 | -1.885776 | 5.499713 |
| C | 2.509322 | -0.084120 | 0.188529 | F | -3.577637 | 0.018292 | 6.077501 |
| C | 1.370024 | 0.032036 | -0.589929 | F | -4.114262 | -1.772155 | 7.146831 |
| C | -1.356305 | 0.003537 | 2.036270 | F | -0.771886 | 0.224418 | -2.176743 |
| C | -2.061824 | 1.096957 | 2.469289 | F | -1.984991 | -0.778212 | -0.708749 |
| C | -3.344546 | 0.810371 | 3.054603 | F | -1.749967 | 1.369151 | -0.637157 |
| C | -3.686318 | -0.517036 | 3.099474 | F | 0.549654 | 0.940388 | 4.194191 |
| P | -2.354129 | -1.369101 | 2.389616 | F | 0.309237 | -1.205904 | 4.111100 |
| O | -2.137694 | -2.810251 | 2.158307 | F | 2.277629 | -0.344113 | 4.230161 |
| C | 1.065064 | -0.186375 | 3.678733 | | | | |

8KH

43

| | | | | | |
|-----------------|-----------|-----------|--------------------------|-----------|-----------|
| E: -2382.200664 | | | F 0.185102 | -2.665344 | 3.192300 |
| P -0.082584 | 0.436566 | -0.085019 | F -1.978630 | 3.510697 | 3.425900 |
| C -0.018742 | 0.092115 | 1.712788 | F -0.069902 | 2.734786 | 2.805254 |
| C 1.706121 | 0.091403 | -0.274845 | H 3.276495 | -0.288224 | 1.119098 |
| O -1.089343 | -0.209760 | -0.958507 | H 1.582362 | -0.287509 | 3.071318 |
| C 2.442306 | 0.026293 | -1.558260 | H -3.421892 | 1.976524 | 4.292954 |
| C 2.819494 | 1.173444 | -2.273068 | H -4.268722 | -0.238977 | 4.989120 |
| C 3.501212 | 1.072268 | -3.480179 | H -3.138525 | -2.284590 | 4.180779 |
| C 3.822449 | -0.168299 | -4.001894 | H 3.782551 | 1.973278 | -4.008022 |
| C 3.463634 | -1.312818 | -3.311592 | H 4.351567 | -0.242873 | -4.943482 |
| C 2.780145 | -1.222058 | -2.105132 | H 3.709185 | -2.287693 | -3.710012 |
| C 2.477518 | 2.557467 | -1.773484 | H -0.086822 | 1.845208 | -0.089176 |
| F 2.781958 | 2.733462 | -0.480387 | | | |
| C 2.439609 | -2.509231 | -1.383658 | {8K} ₂ | | |
| F 2.671485 | -3.580175 | -2.158715 | 84 | | |
| C 2.223078 | -0.108847 | 0.941152 | E= -4763.245427 | | |
| C 1.257877 | -0.108444 | 2.053393 | C -3.481723 | -2.695852 | 0.290391 |
| C -1.185723 | 0.027896 | 2.622390 | C -2.769972 | -1.797347 | 1.100977 |
| C -1.679998 | -1.220073 | 3.034557 | C -3.435644 | -0.775869 | 1.795478 |
| C -2.778315 | -1.310004 | 3.881040 | C -4.822331 | -0.695172 | 1.697694 |
| C -3.410914 | -0.165030 | 4.332757 | C -5.536027 | -1.596451 | 0.925431 |
| C -2.939187 | 1.075164 | 3.940631 | C -4.867048 | -2.582757 | 0.216251 |
| C -1.839975 | 1.175525 | 3.095784 | C -1.307576 | -1.971140 | 1.283160 |
| C -1.013958 | -2.507710 | 2.596755 | C -0.733689 | -2.794214 | 2.174220 |
| F -1.749020 | -3.578232 | 2.936003 | C 0.733985 | -2.794067 | 2.174228 |
| C -1.393064 | 2.559226 | 2.686234 | C 1.307757 | -1.970872 | 1.283191 |
| F -1.712514 | 2.816339 | 1.404286 | C 2.770177 | -1.796896 | 1.101284 |
| F 3.197739 | -2.666909 | -0.280194 | C 3.435591 | -0.775403 | 1.796014 |
| F 1.163773 | -2.569814 | -1.004758 | C 4.822300 | -0.694604 | 1.698597 |
| F 3.127609 | 3.508400 | -2.457877 | C 5.536260 | -1.595791 | 0.926472 |
| F 1.163434 | 2.814967 | -1.909167 | C 4.867531 | -2.582088 | 0.217043 |
| F -0.818236 | -2.569220 | 1.280366 | C 3.482196 | -2.695279 | 0.290812 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 2.684355 | 0.195073 | 2.669813 | H | 5.342922 | 0.095560 | 2.228559 |
| C | 2.767191 | -3.774156 | -0.481072 | H | 6.615943 | -1.517567 | 0.860813 |
| C | -2.684727 | 0.194675 | 2.669475 | H | 5.425272 | -3.279258 | -0.400241 |
| C | -2.766476 | -3.774802 | -0.481169 | H | -5.343144 | 0.095012 | 2.227437 |
| P | 0.000066 | -1.304615 | 0.192494 | H | -6.615699 | -1.518298 | 0.859492 |
| O | -0.000208 | 0.315600 | 0.607711 | H | -5.424580 | -3.280021 | -0.401115 |
| P | 0.000008 | 1.762330 | -0.099721 | H | -5.444440 | -0.292786 | -1.862505 |
| O | 0.000324 | 2.800793 | 0.952330 | H | -6.646619 | 1.531803 | -0.713795 |
| C | 1.337973 | 1.777959 | -1.345316 | H | -5.388342 | 3.463422 | 0.177298 |
| C | 0.739250 | 1.852484 | -2.539518 | H | 5.444192 | -0.293311 | -1.861945 |
| C | -0.739680 | 1.852590 | -2.539366 | H | 6.646365 | 1.531627 | -0.713763 |
| C | -1.338204 | 1.778205 | -1.345045 | H | 5.388133 | 3.463728 | 0.176334 |
| C | -2.801057 | 1.695742 | -1.117250 | F | 2.140291 | 4.399671 | -0.759547 |
| C | -3.512717 | 0.594158 | -1.628536 | F | 2.078630 | 3.734299 | 0.858607 |
| C | -4.895668 | 0.560136 | -1.479750 | F | 3.468752 | 4.720843 | 0.363383 |
| C | -5.569308 | 1.579001 | -0.828855 | F | 3.489823 | -1.420497 | -2.359338 |
| C | -4.861718 | 2.656595 | -0.321671 | F | 1.896564 | -0.835919 | -1.874644 |
| C | -3.478755 | 2.739524 | -0.461478 | F | 2.606536 | -0.286818 | -3.386543 |
| C | -2.836749 | -0.546090 | -2.349138 | F | 2.267892 | -4.479516 | 0.188742 |
| C | -2.755218 | 3.963533 | 0.034992 | F | 1.995470 | -3.351713 | -1.131851 |
| C | 2.800839 | 1.695577 | -1.117551 | F | 3.466399 | -4.334069 | -1.104784 |
| C | 3.478549 | 2.739643 | -0.462236 | F | 3.302486 | 1.065725 | 2.895181 |
| C | 4.861499 | 2.656704 | -0.322306 | F | 1.763952 | 0.542742 | 2.200314 |
| C | 5.569069 | 1.578846 | -0.828955 | F | 2.402194 | -0.275653 | 3.617121 |
| C | 4.895436 | 0.559765 | -1.479517 | F | -1.994168 | -3.352502 | -1.131335 |
| C | 3.512498 | 0.593797 | -1.628410 | F | -2.267869 | -4.480418 | 0.188894 |
| C | 2.755065 | 3.963962 | 0.033565 | F | -3.465415 | -4.334412 | -1.105455 |
| C | 2.836551 | -0.546580 | -2.348808 | F | -3.302869 | 1.065444 | 2.894366 |
| H | 1.292480 | 1.903313 | -3.471018 | F | -2.403103 | -0.275922 | 3.617006 |
| H | -1.293080 | 1.903421 | -3.470762 | F | -1.764046 | 0.542141 | 2.200373 |
| H | -1.305882 | -3.417190 | 2.854644 | F | -3.468865 | 4.720312 | 0.365128 |
| H | 1.306310 | -3.416985 | 2.854597 | F | -2.078879 | 3.733415 | 0.859990 |

F -2.140305 4.399585 -0.757819
F -3.490320 -1.419762 -2.360447
F -2.606090 -0.285974 -3.386636
F -1.897124 -0.835958 -1.874573

8L

78

E= -5235.015639

C 3.714861 0.002336 0.045705
C 2.636707 -0.922810 0.111494
C 2.863058 -2.324175 0.004860
C 4.184321 -2.757837 -0.110613
C 5.241442 -1.872399 -0.142902
C 5.005064 -0.515316 -0.077936
C 1.257873 -0.422714 0.368471
C 0.685050 -0.225085 1.597209
C -0.684744 0.225649 1.597118
C -1.257660 0.422958 0.368306
P 0.000019 -0.000111 -0.760283
O 0.000343 0.000167 -2.243048
C 1.751521 -3.411161 -0.070657
C 0.707345 -3.332881 1.063425
C 3.573355 1.550601 0.116849
C 4.907758 2.252981 -0.209587
C -2.636640 0.922783 0.111429
C -3.714688 -0.002539 0.045860
C -5.004954 0.514929 -0.077856
C -5.241524 1.871964 -0.143209
C -4.184541 2.757551 -0.111069
C -2.863222 2.324096 0.004630
C -3.572983 -1.550809 0.116989
C -2.557263 -2.098362 -0.906270

C -1.751881 3.411307 -0.070550
C -2.341349 4.834285 0.025983
C -0.708809 3.333760 1.064595
C -1.061619 3.327569 -1.445103
C -3.185225 -2.003537 1.537655
C -4.907845 -2.253359 -0.207206
C 1.062482 -3.327732 -1.445847
C 2.340568 -4.834226 0.027025
C 2.555908 2.098401 -0.904589
C 3.187956 2.003177 1.538204
H -1.220454 0.423366 2.517034
H 1.220649 -0.422724 2.517203
H -4.409322 3.810362 -0.178290
H -6.257031 2.242150 -0.230269
H -5.856143 -0.145994 -0.124926
H 5.856312 0.145518 -0.125255
H 6.256896 -2.242761 -0.229821
H 4.408962 -3.810697 -0.177546
F -0.255940 4.066294 -1.506043
F -0.631962 2.350273 -1.658382
F -1.779481 3.538841 -2.242222
F -0.134544 4.264198 1.087263
F -1.195237 3.215876 2.037180
F 0.002888 2.523844 0.945236
F -1.520470 5.554140 -0.015955
F -3.010351 5.070618 -0.804077
F -2.876101 4.993815 0.966801
F -2.733074 -3.165447 -1.067846
F -2.636979 -1.591438 -1.870810
F -1.531011 -2.012852 -0.556144
F -3.187819 -3.097003 1.589840
F -2.191618 -1.662701 1.822150

| | | | | | | | |
|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| F | -3.903544 | -1.627163 | 2.271632 | C | 4.898133 | -0.757829 | -1.254284 |
| F | -4.746378 | -3.333637 | -0.184895 | C | 5.274297 | 0.408333 | -1.877221 |
| F | -5.686846 | -2.033670 | 0.526772 | C | 4.624560 | 1.575951 | -1.550546 |
| F | -5.277404 | -1.993558 | -1.202977 | C | 3.488465 | 1.580575 | -0.742126 |
| F | 2.732394 | 3.165192 | -1.067326 | C | 3.639733 | -2.173175 | 0.347714 |
| F | 2.632947 | 1.590790 | -1.868988 | C | 3.263127 | -3.291580 | -0.673170 |
| F | 1.530386 | 2.014182 | -0.552009 | F | 4.342766 | -3.694004 | -1.360702 |
| F | 3.190221 | 3.096646 | 1.590439 | C | 2.877289 | 2.980150 | -0.426140 |
| F | 2.194958 | 1.661904 | 1.824368 | C | 3.897822 | 4.156459 | -0.726989 |
| F | 3.907677 | 1.627022 | 2.270918 | F | 4.015779 | 4.371383 | -2.044887 |
| F | 4.746373 | 3.333274 | -0.187518 | C | 0.851267 | -0.058818 | -1.403497 |
| F | 5.687830 | 2.033636 | 0.523347 | C | -0.607138 | -0.161902 | -1.417893 |
| F | 5.275854 | 1.992664 | -1.205769 | C | -2.758387 | -0.266069 | -0.379060 |
| F | 0.256554 | -4.066157 | -1.507195 | C | -3.695541 | 0.809315 | -0.511240 |
| F | 0.633419 | -2.350309 | -1.659820 | C | -4.705611 | 0.692060 | -1.469156 |
| F | 1.780937 | -3.539590 | -2.242277 | C | -4.891797 | -0.450530 | -2.208093 |
| F | 1.519524 | -5.553900 | -0.014748 | C | -4.196108 | -1.578910 | -1.845778 |
| F | 3.009816 | -5.071304 | -0.802617 | C | -3.189169 | -1.542477 | -0.883537 |
| F | 2.874930 | -4.993246 | 0.968155 | C | -3.841186 | 2.124860 | 0.318591 |
| F | 0.133139 | -4.263351 | 1.086181 | C | -5.180955 | 2.025018 | 1.155104 |
| F | 1.192719 | -3.214203 | 2.036432 | F | -5.006814 | 1.178633 | 2.168326 |
| F | -0.004340 | -2.523156 | 0.942672 | C | -2.641420 | -2.946459 | -0.459970 |
| | | | | C | -2.334363 | -3.025921 | 1.075390 |
| 8LH | | | | F | -3.479338 | -3.097620 | 1.761065 |
| 79 | | | | C | 1.629391 | 3.286773 | -1.336662 |
| E: -5235.629154 | | | | F | 0.496360 | 2.776323 | -0.860750 |
| P | 0.059660 | 0.342748 | 1.021485 | C | 2.550047 | 3.140791 | 1.108852 |
| C | 1.444658 | 0.144569 | -0.219880 | F | 3.609536 | 3.592634 | 1.777394 |
| C | -1.256596 | -0.064118 | -0.246525 | F | 1.414900 | 4.591500 | -1.490124 |
| O | 0.084111 | -0.276240 | 2.362230 | F | 1.828023 | 2.764718 | -2.549142 |
| C | 2.947822 | 0.330002 | -0.306645 | C | 4.991880 | -2.572046 | 1.076966 |
| C | 3.800340 | -0.810912 | -0.394139 | F | 5.172393 | -1.790055 | 2.139323 |

| | | | | | | | |
|---|-----------|-----------|-----------|--------------------------|-----------|-----------|-----------|
| C | 2.577053 | -2.147077 | 1.497674 | H | -1.120210 | -0.338148 | -2.356653 |
| F | 1.355484 | -2.292764 | 0.993185 | H | 1.404370 | -0.121716 | -2.333985 |
| F | 4.948582 | -3.841189 | 1.480264 | H | -4.442302 | -2.496996 | -2.350165 |
| F | 6.092893 | -2.464755 | 0.331780 | H | -5.631860 | -0.484766 | -2.996513 |
| C | -2.724965 | 2.411273 | 1.359200 | H | -5.366507 | 1.519413 | -1.660239 |
| F | -1.663675 | 2.936715 | 0.737408 | H | 5.461987 | -1.649300 | -1.464630 |
| C | -3.905538 | 3.383886 | -0.622039 | H | 6.103557 | 0.417835 | -2.572286 |
| F | -5.120079 | 3.542353 | -1.167407 | H | 5.004042 | 2.483419 | -1.984320 |
| F | -3.091355 | 3.277390 | 2.296737 | H | -0.013818 | 1.727781 | 1.034219 |
| F | -2.354229 | 1.298085 | 1.985945 | | | | |
| C | -3.739364 | -4.069852 | -0.697599 | {8L} ₂ | | | |
| F | -3.800919 | -4.427269 | -1.991793 | 156 | | | |
| C | -1.388065 | -3.378078 | -1.286414 | E= -10470.0948458 | | | |
| F | -0.273955 | -2.860339 | -0.785470 | C | -4.690834 | -0.050704 | -0.408754 |
| F | -3.462593 | -5.173878 | -0.013148 | C | -3.669077 | 0.866958 | -0.803755 |
| F | -4.954369 | -3.672943 | -0.331295 | C | -3.820269 | 2.260140 | -0.520188 |
| F | -1.224097 | -4.699388 | -1.318695 | C | -4.857855 | 2.644480 | 0.329885 |
| F | -1.501598 | -2.959000 | -2.552834 | C | -5.744790 | 1.733636 | 0.859674 |
| F | -1.603248 | -4.101846 | 1.366106 | C | -5.676223 | 0.416769 | 0.463746 |
| F | -1.680004 | -1.973036 | 1.521406 | C | -2.462685 | 0.395725 | -1.563855 |
| F | -3.638988 | 4.512393 | 0.030087 | C | -2.379681 | 0.327180 | -2.895583 |
| F | -3.027377 | 3.264139 | -1.615103 | C | -1.112439 | -0.129474 | -3.490037 |
| F | -5.527164 | 3.214158 | 1.647500 | C | -0.128936 | -0.450714 | -2.647924 |
| F | -6.222707 | 1.588520 | 0.452114 | C | 1.243986 | -0.848081 | -3.100431 |
| F | 1.545753 | 3.997359 | 1.297734 | C | 2.168563 | 0.191508 | -3.432901 |
| F | 2.220473 | 1.992452 | 1.692726 | C | 3.429174 | -0.179033 | -3.901553 |
| F | 3.478473 | 5.295486 | -0.182061 | C | 3.789640 | -1.498717 | -4.067241 |
| F | 5.114979 | 3.914184 | -0.249283 | C | 2.879065 | -2.489558 | -3.780521 |
| F | 2.744129 | -3.132008 | 2.376360 | C | 1.592471 | -2.214578 | -3.310153 |
| F | 2.665521 | -1.002481 | 2.159905 | C | 1.878774 | 1.721866 | -3.427410 |
| F | 2.744063 | -4.365563 | -0.088337 | C | 1.053373 | 2.098485 | -4.673756 |
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| C | -0.783958 | -3.301381 | -3.297197 | C | 6.175112 | -1.261394 | -0.083759 |
| C | -2.958774 | 3.416877 | -1.109977 | C | 0.707848 | -3.654204 | 4.429711 |
| C | -1.587743 | 3.469036 | -0.437507 | C | 0.001848 | -5.226253 | 2.653535 |
| C | -4.976174 | -1.448749 | -1.037734 | C | -3.695687 | 1.198069 | 3.721939 |
| C | -3.783081 | -2.393792 | -1.196816 | C | -1.621103 | 0.810126 | 4.986720 |
| P | -0.906264 | -0.419302 | -0.962026 | C | 4.748604 | -1.347136 | 1.896301 |
| O | -1.066984 | -1.762415 | -0.353274 | C | 3.794822 | -1.735502 | -0.420850 |
| O | -0.078407 | 0.524520 | 0.081523 | C | 2.874766 | 5.271454 | 1.382018 |
| P | 1.042100 | -0.332774 | 1.044656 | C | 1.107860 | 3.593235 | 1.154009 |
| C | 0.334668 | -0.633927 | 2.697317 | C | 1.162527 | 2.215790 | -2.169371 |
| C | -0.920339 | -1.418921 | 2.875944 | C | 3.181064 | 2.546368 | -3.501155 |
| C | -0.913573 | -2.833337 | 2.722442 | C | 1.154486 | -4.659182 | -3.927317 |
| C | -2.141302 | -3.462035 | 2.521507 | C | 0.934958 | -3.891199 | -1.568099 |
| C | -3.330945 | -2.763110 | 2.533824 | C | -2.788903 | 3.331383 | -2.644380 |
| C | -3.333044 | -1.419949 | 2.848466 | C | -3.610509 | 4.794871 | -0.860086 |
| C | -2.144493 | -0.720284 | 3.055529 | C | -6.027976 | -2.238905 | -0.230243 |
| C | 0.326765 | -3.746913 | 2.938648 | C | -5.591311 | -1.178912 | -2.427281 |
| C | 1.559731 | -3.427980 | 2.079243 | H | 3.255891 | 0.749807 | 3.611972 |
| C | -2.236319 | 0.736594 | 3.575767 | H | 1.265524 | -0.499225 | 4.629777 |
| C | -1.556741 | 1.745493 | 2.643300 | H | -1.003349 | -0.192919 | -4.565939 |
| C | 1.283459 | -0.252521 | 3.574870 | H | -3.200432 | 0.621346 | -3.537945 |
| C | 2.396014 | 0.487889 | 3.005351 | H | 4.156062 | 0.576633 | -4.152225 |
| C | 2.355928 | 0.750355 | 1.679302 | H | 4.780545 | -1.754202 | -4.425966 |
| C | 3.470166 | 1.409059 | 0.918815 | H | 3.187698 | -3.512181 | -3.928288 |
| C | 3.511836 | 2.836594 | 0.871678 | H | -4.987954 | 3.681269 | 0.593652 |
| C | 4.499214 | 3.443788 | 0.096833 | H | -6.516307 | 2.058469 | 1.548889 |
| C | 5.414202 | 2.706879 | -0.622903 | H | -6.433314 | -0.256103 | 0.832756 |
| C | 5.410103 | 1.333902 | -0.518743 | H | -2.184805 | -4.525179 | 2.343711 |
| C | 4.494668 | 0.642610 | 0.279943 | H | -4.264065 | -3.282089 | 2.344551 |
| C | 2.546368 | 3.785866 | 1.636260 | H | -4.282831 | -0.911898 | 2.921701 |
| C | 2.632216 | 3.603458 | 3.167577 | H | 6.166255 | 0.792297 | -1.063580 |
| C | 4.761517 | -0.892070 | 0.425106 | H | 6.148293 | 3.204585 | -1.247022 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 4.561932 | 4.518601 | 0.037993 | F | -1.265847 | -2.699288 | -2.538045 |
| F | 4.124626 | -2.779924 | -0.425366 | F | -0.974496 | -2.869865 | -4.283849 |
| F | 2.774565 | -1.715919 | -0.050930 | F | 0.436464 | -5.472404 | -3.799439 |
| F | 3.786550 | -1.380337 | -1.451670 | F | 1.170138 | -4.386124 | -4.986499 |
| F | 5.113396 | -2.376212 | 1.959211 | F | 2.130471 | -5.067073 | -3.658135 |
| F | 5.406331 | -0.717272 | 2.503377 | F | 1.539936 | -4.331648 | 4.648268 |
| F | 3.760157 | -1.332317 | 2.339485 | F | 1.015941 | -2.645083 | 4.702964 |
| F | 6.355691 | -2.314225 | 0.145320 | F | -0.138675 | -3.933122 | 5.063230 |
| F | 6.271116 | -1.156325 | -1.167098 | F | 2.294909 | -4.230394 | 2.194271 |
| F | 6.960139 | -0.675054 | 0.401763 | F | 1.299536 | -3.355072 | 1.024631 |
| F | 2.213731 | 4.485050 | 3.661905 | F | 2.050859 | -2.507859 | 2.378407 |
| F | 2.066485 | 2.742733 | 3.513047 | F | 0.900194 | -5.822076 | 2.833303 |
| F | 3.670375 | 3.496390 | 3.494950 | F | -0.779511 | -5.619627 | 3.307774 |
| F | 2.135134 | 5.879822 | 1.908537 | F | -0.296047 | -5.380949 | 1.612596 |
| F | 3.860882 | 5.552512 | 1.762645 | F | -1.763823 | 1.813716 | 5.400527 |
| F | 2.814809 | 5.536997 | 0.323492 | F | -2.107226 | 0.093742 | 5.655094 |
| F | 0.423526 | 4.194529 | 1.760299 | F | -0.553390 | 0.603349 | 4.982628 |
| F | 1.018648 | 3.919285 | 0.117303 | F | -1.779651 | 2.765261 | 2.974310 |
| F | 0.774630 | 2.561313 | 1.203228 | F | -0.475854 | 1.639552 | 2.630844 |
| F | 1.124150 | 3.308874 | -2.181151 | F | -1.926385 | 1.632098 | 1.623820 |
| F | 0.135127 | 1.875161 | -2.108205 | F | -3.701809 | 2.220847 | 4.108663 |
| F | 1.689749 | 1.911846 | -1.264050 | F | -4.215410 | 1.206542 | 2.763634 |
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| F | 1.528983 | 1.722351 | -5.583801 | F | -0.963550 | 4.220624 | -0.929503 |
| F | 0.038078 | 1.707014 | -4.629768 | F | -1.688655 | 3.748572 | 0.612885 |
| F | 2.929987 | 3.603172 | -3.381622 | F | -1.058861 | 2.520567 | -0.469093 |
| F | 3.872565 | 2.279023 | -2.700245 | F | -2.525664 | 4.319090 | -3.031871 |
| F | 3.689533 | 2.451221 | -4.463562 | F | -1.990334 | 2.656746 | -2.939736 |
| F | 0.393004 | -4.819779 | -1.358356 | F | -3.716246 | 3.019087 | -3.132705 |
| F | 1.996727 | -4.058860 | -1.365038 | F | -2.985450 | 5.559125 | -1.328104 |
| F | 0.554970 | -3.128551 | -0.890190 | F | -4.610217 | 4.865917 | -1.298089 |
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|-----------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| F | -3.102357 | -2.062863 | -1.973111 | C | 4.698317 | -1.618312 | -0.401733 |
| F | -3.215514 | -2.504821 | -0.274613 | C | 3.317226 | -1.511173 | -0.200259 |
| F | -4.148685 | -3.378668 | -1.502406 | Si | 3.049313 | 2.684903 | 0.498613 |
| F | -6.137727 | -3.228637 | -0.678794 | C | 1.887467 | 3.255185 | -0.860871 |
| F | -5.716600 | -2.377551 | 0.807964 | Si | 2.327054 | -3.125368 | -0.378819 |
| F | -7.017142 | -1.776132 | -0.244162 | C | 3.526163 | -4.572604 | -0.260063 |
| F | -5.894991 | -2.123907 | -2.889004 | C | 1.079463 | -3.356266 | 1.005737 |
| F | -6.471249 | -0.534130 | -2.350104 | C | 1.533218 | -3.192471 | -2.078968 |
| F | -4.874762 | -0.697884 | -3.094807 | C | 2.322566 | 2.898794 | 2.219877 |
| | | | | C | 4.549481 | 3.820559 | 0.428997 |
| 8M | | | | C | -1.533074 | 3.190904 | -2.079166 |
| 78 | | | | C | -3.526817 | 4.572724 | -0.262556 |
| E= -2668.115761 | | | | C | -1.888084 | -3.256148 | -0.861268 |
| C | -3.623538 | -0.902977 | 0.171317 | C | -2.321270 | -2.897368 | 2.220034 |
| C | -2.789478 | 0.234319 | 0.090601 | H | 1.288168 | -0.110233 | 2.512265 |
| C | -3.317425 | 1.511261 | -0.199846 | H | -1.287848 | 0.113957 | 2.512131 |
| C | -4.698574 | 1.618205 | -0.401001 | H | 5.135637 | -2.586179 | -0.620002 |
| C | -5.535142 | 0.518566 | -0.321461 | H | 6.602253 | -0.630019 | -0.479701 |
| C | -4.996111 | -0.724528 | -0.037863 | H | 5.664222 | 1.576050 | 0.019811 |
| C | -1.328983 | 0.091120 | 0.363080 | H | -5.663770 | -1.576534 | 0.019424 |
| C | -0.721138 | 0.053207 | 1.591490 | H | -6.602322 | 0.629551 | -0.479182 |
| C | 0.721385 | -0.051015 | 1.591571 | H | -5.136141 | 2.586049 | -0.618865 |
| C | 1.329124 | -0.090830 | 0.363198 | H | 0.888242 | -4.071664 | -2.171755 |
| P | 0.000054 | -0.000319 | -0.767602 | H | 0.941165 | -2.309582 | -2.329328 |
| Si | -2.327510 | 3.125504 | -0.379173 | H | 2.320684 | -3.272606 | -2.835031 |
| C | -1.080792 | 3.358443 | 1.005870 | H | 0.673683 | -4.372236 | 0.970258 |
| Si | -3.048672 | -2.684761 | 0.498882 | H | 1.556863 | -3.218102 | 1.980531 |
| C | -4.548833 | -3.820569 | 0.431004 | H | 0.241995 | -2.664729 | 0.943930 |
| C | 2.789555 | -0.234218 | 0.090608 | H | 2.955710 | -5.506772 | -0.271155 |
| C | 3.623838 | 0.902910 | 0.171580 | H | 4.224471 | -4.611341 | -1.100582 |
| C | 4.996359 | 0.724215 | -0.037679 | H | 4.106906 | -4.550129 | 0.666646 |
| C | 5.535110 | -0.518893 | -0.321830 | H | 1.536570 | 4.272963 | -0.664240 |

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|-----------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 2.416320 | 3.258012 | -1.818433 | C | -1.339369 | 0.097175 | 0.337604 |
| H | 1.007346 | 2.624524 | -0.980701 | C | 1.325906 | -0.063995 | 0.349406 |
| H | 2.112971 | 3.957929 | 2.400679 | O | -0.048566 | -0.955444 | -2.022040 |
| H | 1.396387 | 2.347131 | 2.378432 | C | 2.774404 | -0.207404 | 0.032947 |
| H | 3.047632 | 2.569787 | 2.970907 | C | 3.610774 | 0.934986 | 0.030600 |
| H | 4.217406 | 4.850760 | 0.592759 | C | 4.946987 | 0.762582 | -0.350810 |
| H | 5.286265 | 3.588728 | 1.203520 | C | 5.450125 | -0.473694 | -0.718129 |
| H | 5.050884 | 3.789406 | -0.542417 | C | 4.622478 | -1.579985 | -0.671041 |
| H | -1.533938 | -4.272324 | -0.662236 | C | 3.277353 | -1.486783 | -0.292411 |
| H | -2.419537 | -3.263673 | -1.817380 | Si | 3.136864 | 2.714289 | 0.513666 |
| H | -1.010058 | -2.623489 | -0.985896 | C | 2.382949 | 2.831976 | 2.234027 |
| H | -2.109786 | -3.956129 | 2.400846 | Si | 2.378571 | -3.170615 | -0.243946 |
| H | -1.396109 | -2.344040 | 2.378605 | C | 3.642821 | -4.443931 | 0.338688 |
| H | -3.046974 | -2.569671 | 2.971023 | C | 0.730792 | 0.007997 | 1.546218 |
| H | -4.216524 | -4.850678 | 0.594898 | C | -0.745792 | 0.103865 | 1.538073 |
| H | -5.284922 | -3.588457 | 1.206108 | C | -2.793433 | 0.243263 | 0.039989 |
| H | -5.051134 | -3.789913 | -0.539958 | C | -3.628386 | -0.897055 | 0.081414 |
| H | -0.887974 | 4.069908 | -2.172795 | C | -4.981629 | -0.725989 | -0.232358 |
| H | -0.941082 | 2.307758 | -2.328691 | C | -5.503393 | 0.507673 | -0.581365 |
| H | -2.320410 | 3.270326 | -2.835445 | C | -4.672372 | 1.612910 | -0.594676 |
| H | -2.956408 | 5.506912 | -0.274206 | C | -3.309941 | 1.519436 | -0.282608 |
| H | -4.224671 | 4.610622 | -1.103490 | Si | -3.096289 | -2.674691 | 0.518167 |
| H | -4.108044 | 4.551106 | 0.663871 | C | -4.643478 | -3.747863 | 0.596910 |
| H | -0.673327 | 4.373639 | 0.967711 | Si | -2.391731 | 3.185594 | -0.323010 |
| H | -1.559523 | 3.224090 | 1.980551 | C | -1.720923 | 3.524529 | -2.047661 |
| H | -0.244397 | 2.665343 | 0.947114 | C | 0.974792 | -3.229277 | 0.998235 |
| O | -0.000045 | -0.002925 | -2.251492 | C | 1.785934 | -3.639675 | -1.954083 |
| | | | | C | 4.710558 | 3.747148 | 0.588000 |
| 8MH | | | | C | 2.059458 | 3.530445 | -0.794357 |
| 79 | | | | C | -2.004334 | -3.392208 | -0.825335 |
| E: -2668.740040 | | | | C | -2.344383 | -2.776092 | 2.242130 |
| P | -0.000379 | 0.029224 | -0.906296 | C | -3.631894 | 4.548505 | 0.064867 |

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| C | -1.043401 | 3.329720 | 0.975455 | H | 3.001955 | 2.285884 | 2.952633 |
| H | -1.299754 | 0.196610 | 2.466188 | H | 4.447461 | 4.756313 | 0.920738 |
| H | 1.279681 | -0.013402 | 2.481456 | H | 5.438594 | 3.346262 | 1.298932 |
| H | -5.101857 | 2.576784 | -0.845216 | H | 5.199258 | 3.844235 | -0.385382 |
| H | -6.554158 | 0.608566 | -0.829426 | H | 1.301260 | -4.621227 | -1.935955 |
| H | -5.649750 | -1.578795 | -0.205849 | H | 1.072993 | -2.901469 | -2.327767 |
| H | 5.617631 | 1.613439 | -0.362736 | H | 2.627623 | -3.691639 | -2.651697 |
| H | 6.486024 | -0.574909 | -1.022299 | H | 3.132211 | -5.394420 | 0.523965 |
| H | 5.039315 | -2.547408 | -0.930541 | H | 4.424210 | -4.638588 | -0.400694 |
| H | -1.158934 | 4.463809 | -2.061092 | H | 4.127445 | -4.137752 | 1.270347 |
| H | -1.068418 | 2.738449 | -2.432701 | H | 0.640586 | -4.266061 | 1.107432 |
| H | -2.553594 | 3.622993 | -2.750831 | H | 1.291523 | -2.871324 | 1.982070 |
| H | -0.668036 | 4.357762 | 0.994369 | H | 0.114155 | -2.644753 | 0.681483 |
| H | -1.438689 | 3.096475 | 1.968612 | H | 0.084621 | 1.373392 | -1.331695 |
| H | -0.193789 | 2.675568 | 0.794491 | | | | |
| H | -3.095712 | 5.495224 | 0.184540 | {8M} ₂ | | | |
| H | -4.368004 | 4.693251 | -0.730153 | 156 | | | |
| H | -4.171639 | 4.350553 | 0.995216 | E= -5336.332421 | | | |
| H | -1.543766 | -4.327172 | -0.491264 | C | -4.665638 | 0.840721 | -0.275907 |
| H | -2.628723 | -3.620069 | -1.695248 | C | -4.028621 | -0.232865 | -0.947453 |
| H | -1.216899 | -2.720640 | -1.172437 | C | -4.387943 | -0.569106 | -2.277900 |
| H | -2.244024 | -3.828198 | 2.527988 | C | -5.253219 | 0.303079 | -2.953502 |
| H | -1.359539 | -2.319081 | 2.326310 | C | -5.756766 | 1.447863 | -2.364017 |
| H | -3.010288 | -2.297731 | 2.967395 | C | -5.488611 | 1.685826 | -1.028744 |
| H | -4.344660 | -4.764653 | 0.871697 | C | -3.055272 | -1.092354 | -0.214277 |
| H | -5.358115 | -3.401428 | 1.349233 | C | -3.420587 | -2.299750 | 0.298703 |
| H | -5.159320 | -3.812160 | -0.365247 | C | -2.459174 | -2.986129 | 1.100967 |
| H | 1.886800 | 4.578072 | -0.527314 | C | -1.303152 | -2.311167 | 1.334050 |
| H | 2.576321 | 3.511701 | -1.758511 | C | -0.152574 | -2.956172 | 2.028179 |
| H | 1.084139 | 3.066563 | -0.933465 | C | 0.627196 | -3.854674 | 1.264555 |
| H | 2.363713 | 3.881638 | 2.544481 | C | 1.705276 | -4.484010 | 1.894182 |
| H | 1.364934 | 2.450906 | 2.302056 | C | 1.970902 | -4.292087 | 3.240103 |

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|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 1.133657 | -3.482141 | 3.988368 | Si | 3.884452 | -0.320183 | -4.006847 |
| C | 0.064002 | -2.787194 | 3.410409 | C | 3.624699 | 1.523716 | -4.252490 |
| Si | 0.189998 | -4.476382 | -0.481453 | Si | 5.018375 | 0.064654 | 1.784037 |
| C | -1.221779 | -5.724688 | -0.379174 | C | 6.531624 | -0.725078 | 2.588043 |
| Si | -1.026459 | -1.775080 | 4.593058 | C | 1.561205 | 6.287961 | 2.416733 |
| C | -2.852514 | -2.173277 | 4.380365 | C | -0.015411 | 4.324777 | 4.149950 |
| Si | -4.015268 | -2.136869 | -3.319494 | C | -1.742345 | 3.490618 | -4.151191 |
| C | -2.523020 | -1.908947 | -4.428896 | C | 1.098194 | 4.256924 | -3.738998 |
| Si | -4.948012 | 0.988176 | 1.607966 | C | 5.548948 | 1.803847 | 1.303028 |
| C | -3.498006 | 1.215010 | 2.767440 | C | 3.715243 | 0.112769 | 3.124877 |
| P | -1.535305 | -0.652770 | 0.694777 | C | 5.409337 | -0.713900 | -5.050481 |
| P | 1.553127 | 0.918027 | 0.200630 | C | 2.432087 | -1.239671 | -4.752918 |
| C | 1.296526 | 2.631250 | -0.292759 | C | -0.205930 | -3.120901 | -1.709896 |
| C | 0.112315 | 3.522009 | -0.121049 | C | 1.639178 | -5.473719 | -1.145912 |
| C | -0.146109 | 4.212382 | 1.077991 | C | -0.579251 | -2.257802 | 6.358664 |
| C | -1.309423 | 4.994797 | 1.140804 | C | -0.710850 | 0.070388 | 4.455670 |
| C | -2.170554 | 5.118898 | 0.067665 | C | -3.809824 | -3.767325 | -2.409337 |
| C | -1.845206 | 4.505740 | -1.132400 | C | -5.509869 | -2.402706 | -4.443915 |
| C | -0.702967 | 3.714196 | -1.264100 | C | -6.092521 | 2.455046 | 1.914899 |
| Si | 0.992904 | 4.499305 | 2.572649 | C | -5.885731 | -0.561643 | 2.124965 |
| C | 2.519116 | 3.428215 | 2.676789 | H | 4.371566 | 2.212975 | -1.578246 |
| Si | -0.266703 | 3.162272 | -3.033701 | H | 2.603577 | 4.062015 | -1.196886 |
| C | 0.167541 | 1.348033 | -3.169161 | H | -2.644262 | -3.966435 | 1.521428 |
| C | 2.431049 | 3.029162 | -0.920616 | H | -4.421474 | -2.685673 | 0.147667 |
| C | 3.385287 | 1.992818 | -1.187712 | H | 2.341426 | -5.153742 | 1.325745 |
| C | 3.032626 | 0.723110 | -0.856809 | H | 2.806542 | -4.798270 | 3.711729 |
| C | 3.978388 | -0.425709 | -0.964342 | H | 1.322259 | -3.386596 | 5.052024 |
| C | 4.266727 | -0.965651 | -2.242779 | H | -5.542927 | 0.088386 | -3.975459 |
| C | 5.064607 | -2.117391 | -2.295863 | H | -6.390374 | 2.122873 | -2.929162 |
| C | 5.580027 | -2.712200 | -1.160036 | H | -5.957217 | 2.539219 | -0.554243 |
| C | 5.396578 | -2.088529 | 0.060517 | H | -1.543917 | 5.532732 | 2.054917 |
| C | 4.639678 | -0.919064 | 0.190412 | H | -3.069455 | 5.720637 | 0.150359 |

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| H | -2.500319 | 4.649442 | -1.983983 | H | 0.282490 | 0.315269 | 4.839781 |
| H | 5.888690 | -2.506947 | 0.930176 | H | -0.780086 | 0.443419 | 3.432421 |
| H | 6.163494 | -3.623611 | -1.232789 | H | -3.429231 | -1.656192 | 5.154179 |
| H | 5.293930 | -2.567860 | -3.255078 | H | -3.251984 | -1.878799 | 3.410562 |
| H | 3.896527 | 0.970988 | 3.778986 | H | -3.021168 | -3.248070 | 4.498261 |
| H | 2.704691 | 0.184834 | 2.728805 | H | -1.251452 | -1.737392 | 7.048373 |
| H | 3.770453 | -0.795295 | 3.727017 | H | -0.686905 | -3.331408 | 6.537450 |
| H | 5.986841 | 2.299744 | 2.175281 | H | 0.442119 | -1.967237 | 6.621452 |
| H | 6.307617 | 1.772322 | 0.515261 | H | 2.199319 | 6.568067 | 3.260929 |
| H | 4.719121 | 2.416311 | 0.953774 | H | 2.136494 | 6.433121 | 1.497461 |
| H | 6.831932 | -0.098133 | 3.434276 | H | 0.714269 | 6.979285 | 2.390072 |
| H | 6.321947 | -1.722741 | 2.985213 | H | 3.046881 | 3.651085 | 3.610113 |
| H | 7.384051 | -0.796126 | 1.907162 | H | 2.291041 | 2.364296 | 2.664483 |
| H | 3.493913 | 1.686959 | -5.328124 | H | 3.198104 | 3.638056 | 1.848635 |
| H | 2.746296 | 1.918236 | -3.748510 | H | 0.622406 | 4.509768 | 5.020003 |
| H | 4.496861 | 2.104684 | -3.940708 | H | -0.842328 | 5.038973 | 4.191074 |
| H | 5.324586 | -0.187306 | -6.006506 | H | -0.432356 | 3.321105 | 4.245114 |
| H | 6.328925 | -0.374873 | -4.564790 | H | 1.145845 | 4.110081 | -4.823190 |
| H | 5.521420 | -1.776928 | -5.278030 | H | 0.863012 | 5.310285 | -3.557396 |
| H | 2.342674 | -0.996964 | -5.816577 | H | 2.091007 | 4.057007 | -3.337360 |
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| H | 1.498173 | -0.963816 | -4.265634 | H | 1.068328 | 1.068592 | -2.622356 |
| H | -0.373378 | -3.569699 | -2.693942 | H | -0.658876 | 0.741218 | -2.795762 |
| H | -1.096537 | -2.548263 | -1.447660 | H | -1.516002 | 3.106414 | -5.151274 |
| H | 0.633446 | -2.428922 | -1.798953 | H | -2.648063 | 2.995656 | -3.800751 |
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| H | 1.432609 | -5.741743 | -2.187263 | H | -1.601981 | -1.898509 | -3.848206 |
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|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -5.423558 | -3.392245 | -4.904043 | C | 0.895199 | -0.250641 | 1.486413 |
| H | -6.452423 | -2.374140 | -3.889917 | C | 0.937183 | -0.968175 | 0.327176 |
| H | -5.572510 | -1.675234 | -5.257508 | P | -0.330798 | -0.279174 | -0.682965 |
| H | -3.027707 | 0.266898 | 3.015568 | O | -0.500613 | -0.355705 | -2.158425 |
| H | -2.735552 | 1.873122 | 2.353363 | C | -3.680318 | 0.609539 | 0.836735 |
| H | -3.868704 | 1.662598 | 3.696201 | C | -3.363032 | 0.163082 | 2.120354 |
| H | -6.291042 | 2.508756 | 2.990122 | C | -3.964944 | -0.973410 | 2.642463 |
| H | -5.632372 | 3.402390 | 1.619939 | C | -4.890590 | -1.684120 | 1.886928 |
| H | -7.057031 | 2.363133 | 1.409052 | C | -5.195837 | -1.261876 | 0.599745 |
| H | -6.243076 | -0.455192 | 3.154318 | C | -4.594818 | -0.122947 | 0.078989 |
| H | -6.752710 | -0.732075 | 1.480198 | C | 1.824629 | -2.087044 | -0.038460 |
| H | -5.253357 | -1.451278 | 2.086707 | C | 1.290217 | -3.273793 | -0.574186 |
| O | 0.153780 | -0.024134 | -0.225702 | C | 2.144945 | -4.301149 | -0.967382 |
| O | 1.802065 | 0.840969 | 1.921005 | C | 3.516576 | -4.178345 | -0.816304 |
| | | | | C | 4.045022 | -3.019591 | -0.269584 |
| 8N | | | | C | 3.219757 | -1.963924 | 0.115086 |
| 70 | | | | C | -0.178689 | -3.468837 | -0.709836 |
| E= -1957.502965 | | | | C | -1.011045 | -3.404830 | 0.410570 |
| C | 0.827759 | 4.559492 | -0.096285 | C | -2.381519 | -3.571195 | 0.280727 |
| C | 0.112383 | 3.570449 | -0.769189 | C | -2.940220 | -3.800055 | -0.971154 |
| C | 0.738715 | 2.864034 | -1.798008 | C | -2.120051 | -3.875947 | -2.089071 |
| C | 2.052764 | 3.147310 | -2.145932 | C | -0.746625 | -3.714639 | -1.958691 |
| C | 2.756898 | 4.141258 | -1.474845 | C | 3.855734 | -0.741853 | 0.683306 |
| C | 2.142688 | 4.843610 | -0.445642 | C | 4.667155 | -0.852280 | 1.812458 |
| C | -1.321003 | 3.323473 | -0.441720 | C | 5.263508 | 0.271995 | 2.372104 |
| C | -1.763613 | 2.097464 | 0.082771 | C | 5.055529 | 1.522307 | 1.806160 |
| C | -3.134743 | 1.888911 | 0.301385 | C | 4.256206 | 1.641148 | 0.674022 |
| C | -4.037035 | 2.913076 | 0.012468 | C | 3.663582 | 0.519114 | 0.115342 |
| C | -3.596187 | 4.133467 | -0.472996 | H | -0.133557 | 1.497696 | 2.377724 |
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| C | -0.774462 | 1.037928 | 0.376513 | H | 5.117878 | -2.910868 | -0.156022 |
| C | -0.035419 | 0.856900 | 1.509799 | H | 4.173226 | -4.984932 | -1.121371 |

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|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 1.717286 | -5.210581 | -1.374332 | C | -1.390572 | 2.363425 | 0.127267 |
| H | -1.889799 | 5.278865 | -1.099356 | C | -0.762173 | 3.536064 | -0.326010 |
| H | -4.307408 | 4.923882 | -0.683613 | C | -1.528165 | 4.683239 | -0.536488 |
| H | -5.093295 | 2.745891 | 0.191287 | C | -2.898667 | 4.672957 | -0.337370 |
| H | 0.189091 | 2.103451 | -2.342477 | C | -3.522675 | 3.505911 | 0.072861 |
| H | 2.523201 | 2.597186 | -2.953224 | C | -2.783933 | 2.348104 | 0.311261 |
| H | 3.779636 | 4.367655 | -1.755579 | C | 0.691468 | 3.601784 | -0.648372 |
| H | 2.685917 | 5.617316 | 0.085436 | C | 1.500129 | 4.560883 | -0.038130 |
| H | 0.347379 | 5.109602 | 0.705940 | C | 2.831380 | 4.706123 | -0.409453 |
| H | -2.658672 | 0.726273 | 2.720788 | C | 3.368066 | 3.896183 | -1.402470 |
| H | -3.719246 | -1.298124 | 3.647372 | C | 2.572130 | 2.927480 | -2.004414 |
| H | -5.367969 | -2.566311 | 2.299147 | C | 1.243357 | 2.776234 | -1.630787 |
| H | -5.906618 | -1.817262 | -0.001746 | C | -3.516585 | 1.129901 | 0.758304 |
| H | -4.833973 | 0.206845 | -0.926066 | C | -3.266616 | 0.539345 | 1.997914 |
| H | 4.816265 | -1.827110 | 2.265027 | C | -4.008190 | -0.555106 | 2.421105 |
| H | 5.885290 | 0.168741 | 3.254459 | C | -5.010511 | -1.075808 | 1.611373 |
| H | 5.513122 | 2.402196 | 2.244237 | C | -5.259239 | -0.503482 | 0.371073 |
| H | 4.079766 | 2.611772 | 0.226804 | C | -4.517154 | 0.591519 | -0.052091 |
| H | 3.032979 | 0.626467 | -0.760414 | C | 0.174102 | 0.892804 | 1.458238 |
| H | -0.110211 | -3.738116 | -2.835888 | C | 0.883602 | -0.399645 | 1.446037 |
| H | -2.550023 | -4.043424 | -3.069845 | C | 1.442146 | -2.380584 | -0.024586 |
| H | -4.013730 | -3.911962 | -1.073000 | C | 0.771413 | -3.495241 | -0.558200 |
| H | -3.015503 | -3.505653 | 1.155724 | C | 1.487023 | -4.607786 | -0.989262 |
| H | -0.577341 | -3.214099 | 1.385859 | C | 2.868164 | -4.639304 | -0.884781 |
| | | | | C | 3.537553 | -3.550825 | -0.348735 |
| 8NH | | | | C | 2.849175 | -2.415455 | 0.076600 |
| 71 | | | | C | -0.713155 | -3.510547 | -0.645576 |
| E: -1958.137896 | | | | C | -1.483495 | -3.569469 | 0.516639 |
| P | -0.532605 | -0.317078 | -0.698583 | C | -2.867465 | -3.530729 | 0.443372 |
| C | 0.687664 | -1.171430 | 0.366447 | C | -3.496971 | -3.428635 | -0.792529 |
| C | -0.589600 | 1.147569 | 0.390984 | C | -2.737344 | -3.383870 | -1.954069 |
| O | -0.212677 | -0.127298 | -2.143582 | C | -1.349895 | -3.431175 | -1.882445 |

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|---|-----------|-----------|-----------|-------------------|--------------|-----------|-----------|
| C | 3.648861 | -1.283246 | 0.624269 | H | -3.456899 | -3.563539 | 1.351608 |
| C | 4.447872 | -1.490230 | 1.748366 | H | -0.987605 | -3.627371 | 1.479307 |
| C | 5.187038 | -0.447561 | 2.295972 | H | -1.776030 | -0.932123 | -0.430564 |
| C | 5.134624 | 0.815248 | 1.722265 | | | | |
| C | 4.351038 | 1.027361 | 0.592424 | {8N} ₂ | | | |
| C | 3.617778 | -0.013811 | 0.043480 | 140 | | | |
| H | 0.294228 | 1.586239 | 2.283973 | E= | -3915.124315 | | |
| H | 1.570530 | -0.655404 | 2.244475 | C | 3.716942 | -3.317017 | -0.812349 |
| H | 4.619309 | -3.559903 | -0.275328 | C | 2.641284 | -3.489054 | 0.078909 |
| H | 3.422402 | -5.507713 | -1.221635 | C | 2.800651 | -3.114805 | 1.421191 |
| H | 0.945223 | -5.454620 | -1.395235 | C | 3.998131 | -2.532674 | 1.862689 |
| H | -1.035276 | 5.581881 | -0.890063 | C | 5.056867 | -2.341214 | 0.964468 |
| H | -3.481521 | 5.569711 | -0.513253 | C | 4.916859 | -2.748792 | -0.372086 |
| H | -4.595210 | 3.484919 | 0.230729 | C | 1.347000 | -4.051057 | -0.414798 |
| H | 0.633354 | 2.021740 | -2.117673 | C | 0.551399 | -3.342968 | -1.353153 |
| H | 2.982657 | 2.288300 | -2.778209 | C | -0.602844 | -3.973025 | -1.899228 |
| H | 4.402676 | 4.016721 | -1.704760 | C | -0.931491 | -5.276907 | -1.481885 |
| H | 3.446406 | 5.457784 | 0.072809 | C | -0.159443 | -5.956789 | -0.536651 |
| H | 1.079517 | 5.199983 | 0.731365 | C | 0.975822 | -5.339769 | -0.004222 |
| H | -2.497699 | 0.953411 | 2.639003 | C | 0.954791 | -1.999059 | -1.828908 |
| H | -3.808944 | -0.996148 | 3.391361 | P | 1.676204 | -0.589762 | -0.808948 |
| H | -5.593873 | -1.926719 | 1.945448 | O | 0.513634 | -0.107286 | 0.406399 |
| H | -6.033232 | -0.908704 | -0.270930 | P | -1.100286 | 0.304048 | 0.727081 |
| H | -4.707502 | 1.035389 | -1.023186 | C | -1.159768 | 1.962045 | 1.663620 |
| H | 4.473278 | -2.473100 | 2.207428 | C | -1.162400 | 3.373425 | 1.177700 |
| H | 5.797344 | -0.623515 | 3.174851 | C | 0.022526 | 4.159930 | 1.168428 |
| H | 5.701980 | 1.633401 | 2.151521 | C | -0.045392 | 5.516522 | 0.797833 |
| H | 4.297189 | 2.010259 | 0.140780 | C | -1.262632 | 6.120845 | 0.480428 |
| H | 2.998468 | 0.164094 | -0.829380 | C | -2.437983 | 5.369915 | 0.561730 |
| H | -0.752762 | -3.357081 | -2.783854 | C | -2.406617 | 4.006669 | 0.908180 |
| H | -3.222357 | -3.295627 | -2.919292 | C | -1.490649 | -3.333473 | -2.923156 |
| H | -4.578224 | -3.376864 | -0.846747 | C | -1.806746 | -4.040587 | -4.099925 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -2.651585 | -3.478560 | -5.069327 | C | -1.392680 | 3.451467 | -2.279322 |
| C | -3.194849 | -2.199702 | -4.870013 | C | -2.716911 | 3.362301 | -2.721207 |
| C | -2.888699 | -1.494392 | -3.695150 | C | -3.028142 | 2.603644 | -3.857708 |
| C | -2.045821 | -2.055205 | -2.729242 | C | -1.997059 | 1.956397 | -4.553972 |
| C | 1.350375 | 3.650743 | 1.617751 | C | -0.672579 | 2.056910 | -4.110451 |
| C | 2.098208 | 4.378555 | 2.565003 | O | -2.002313 | 0.140218 | -0.565397 |
| C | 3.360198 | 3.927164 | 2.975556 | C | -1.403444 | -0.669739 | 2.308842 |
| C | 3.884896 | 2.731916 | 2.456977 | C | -1.269016 | -2.134864 | 2.468432 |
| C | 3.139383 | 1.997332 | 1.524229 | C | -2.156637 | -3.028460 | 1.818380 |
| C | 1.893705 | 2.470055 | 1.101517 | C | -1.965519 | -4.414364 | 1.953634 |
| C | -3.732673 | 3.323631 | 1.015312 | C | -0.946695 | -4.923606 | 2.759780 |
| C | -4.092555 | 2.256906 | 0.175004 | C | -0.115090 | -4.045066 | 3.456491 |
| C | -5.389145 | 1.729590 | 0.224833 | C | -0.253714 | -2.651539 | 3.319640 |
| C | -6.334537 | 2.241104 | 1.125306 | C | -3.387890 | -2.577718 | 1.105044 |
| C | -5.974744 | 3.291299 | 1.984325 | C | -3.718968 | -3.113979 | -0.149975 |
| C | -4.683756 | 3.833340 | 1.921701 | C | -4.931221 | -2.791870 | -0.770397 |
| C | 1.051574 | -1.653884 | -3.139226 | C | -5.849469 | -1.953954 | -0.122194 |
| C | 1.412613 | -0.260907 | -3.410979 | C | -5.534450 | -1.425360 | 1.138997 |
| C | 1.589226 | 0.537167 | -2.329169 | C | -4.307672 | -1.723114 | 1.742179 |
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| C | 3.700319 | 3.650855 | -1.775857 | C | 1.600998 | -1.251536 | 6.324145 |
| C | 2.741214 | 4.661331 | -1.867561 | C | 2.360407 | -0.219905 | 5.753705 |
| C | 1.442131 | 4.336764 | -2.257226 | C | 2.275751 | 0.019442 | 4.373314 |
| C | 1.059093 | 3.002296 | -2.498751 | C | 1.439653 | -0.759599 | 3.564241 |
| C | 4.489156 | 1.320877 | -1.983798 | C | -1.547390 | 0.222622 | 3.308068 |
| C | 4.703473 | 0.432323 | -3.056287 | C | -1.446961 | 1.654069 | 2.946600 |
| C | 5.844304 | -0.378662 | -3.102729 | H | -1.685037 | -0.077116 | 4.340544 |
| C | 6.798089 | -0.317728 | -2.075688 | H | -1.615298 | 2.423450 | 3.692077 |
| C | 6.593757 | 0.557131 | -0.999278 | H | 1.564741 | 0.079114 | -4.429346 |
| C | 5.453998 | 1.369642 | -0.958376 | H | 0.858314 | -2.351168 | -3.946326 |
| C | -0.350802 | 2.789737 | -2.953100 | H | -1.816901 | -5.749351 | -1.896856 |

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|---|-----------|-----------|-----------|-----------|--------------|-----------|-----------|
| H | -0.439135 | -6.956275 | -0.220592 | H | -5.148771 | -3.188918 | -1.756464 |
| H | 1.599779 | -5.859488 | 0.715429 | H | -6.798243 | -1.715253 | -0.592966 |
| H | 0.707366 | 5.122945 | -2.394328 | H | -6.238431 | -0.779342 | 1.652354 |
| H | 3.014093 | 5.693769 | -1.677672 | H | -4.078231 | -1.317900 | 2.721556 |
| H | 4.730103 | 3.902957 | -1.546423 | H | 0.154864 | -2.811953 | 5.962913 |
| H | 0.874863 | 6.089798 | 0.756804 | H | 1.655485 | -1.446107 | 7.390478 |
| H | -1.297275 | 7.164266 | 0.186816 | H | 3.006815 | 0.391883 | 6.374807 |
| H | -3.396305 | 5.829422 | 0.343817 | H | 2.851214 | 0.819633 | 3.922902 |
| H | 0.670773 | -4.433471 | 4.096624 | H | 1.389228 | -0.562593 | 2.496660 |
| H | -0.810856 | -5.995361 | 2.855446 | H | -1.375451 | -5.024034 | -4.266379 |
| H | -2.648494 | -5.088727 | 1.448796 | H | -2.878769 | -4.034004 | -5.973982 |
| H | 1.685769 | 5.288890 | 2.990332 | H | -3.847979 | -1.761577 | -5.618673 |
| H | 3.925533 | 4.498415 | 3.704930 | H | -3.299501 | -0.507090 | -3.513706 |
| H | 4.856811 | 2.374877 | 2.784211 | H | -1.841818 | -1.481369 | -1.831151 |
| H | 3.515948 | 1.059356 | 1.127027 | H | 1.974944 | -3.244834 | 2.109542 |
| H | 1.341400 | 1.927443 | 0.352361 | H | 4.088967 | -2.218776 | 2.897723 |
| H | -3.377632 | 1.833633 | -0.521124 | H | 5.981000 | -1.878428 | 1.295887 |
| H | -5.646799 | 0.913739 | -0.440078 | H | 5.733117 | -2.605892 | -1.070277 |
| H | -7.338505 | 1.828824 | 1.158393 | H | 3.600767 | -3.609437 | -1.851473 |
| H | -6.695269 | 3.690552 | 2.691125 | | | | |
| H | -4.408089 | 4.653933 | 2.578348 | 8P | | | |
| H | -1.161383 | 4.043962 | -1.403547 | 94 | | | |
| H | -3.499693 | 3.878182 | -2.174679 | E= | -4653.891627 | | |
| H | -4.055000 | 2.525957 | -4.200367 | C | 2.616198 | -2.594447 | 1.997278 |
| H | -2.218959 | 1.379774 | -5.446269 | C | 2.875940 | -2.304779 | 0.648469 |
| H | 0.113806 | 1.594497 | -4.691854 | C | 2.521739 | -3.262592 | -0.309556 |
| H | 3.996116 | 0.404772 | -3.876403 | C | 1.895382 | -4.444713 | 0.068261 |
| H | 5.995306 | -1.044076 | -3.946745 | C | 1.613326 | -4.695069 | 1.397698 |
| H | 7.687875 | -0.938051 | -2.116858 | C | 1.982572 | -3.775007 | 2.363624 |
| H | 7.323790 | 0.614784 | -0.198155 | C | 3.537067 | -1.028517 | 0.237744 |
| H | 5.311709 | 2.054311 | -0.128411 | C | 2.791111 | 0.145044 | 0.071307 |
| H | -3.015105 | -3.768478 | -0.650275 | C | 3.459449 | 1.304551 | -0.354699 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.827395 | 1.278032 | -0.600195 | F | -3.891963 | -2.861715 | -3.056099 |
| C | 5.553295 | 0.112344 | -0.422115 | C | 2.724858 | 2.593987 | -0.555913 |
| C | 4.906439 | -1.036504 | -0.002614 | C | 2.040214 | 2.867254 | -1.748960 |
| C | 1.336179 | 0.182149 | 0.336065 | C | 1.336637 | 4.053938 | -1.913431 |
| C | 0.687245 | 0.952026 | 1.269562 | C | 1.318099 | 5.001484 | -0.904599 |
| C | -0.743891 | 0.871564 | 1.268470 | C | 2.023965 | 4.773237 | 0.262193 |
| C | -1.312179 | 0.050640 | 0.323572 | C | 2.724082 | 3.584279 | 0.436530 |
| C | -2.754205 | -0.093394 | 0.040478 | C | 2.125379 | 1.927478 | -2.934463 |
| C | -3.577381 | 1.047730 | -0.022844 | F | 3.396657 | 1.775000 | -3.336804 |
| C | -4.937923 | 0.929699 | -0.286665 | C | 3.553034 | 3.441865 | 1.695613 |
| C | -5.517699 | -0.308607 | -0.487862 | F | 3.393175 | 2.265044 | 2.314092 |
| C | -4.722860 | -1.437765 | -0.432125 | C | 2.919056 | -3.139793 | -1.768288 |
| C | -3.358345 | -1.341939 | -0.179314 | F | 2.884379 | -1.908180 | -2.262459 |
| C | -3.067497 | 2.443128 | 0.174347 | C | 3.103260 | -1.681201 | 3.102074 |
| C | -2.445308 | 3.157269 | -0.859530 | F | 4.433523 | -1.513311 | 3.047581 |
| C | -2.030114 | 4.469945 | -0.668837 | P | 0.059316 | -0.644924 | -0.505419 |
| C | -2.216986 | 5.099954 | 0.548061 | O | 0.133979 | -1.668453 | -1.570138 |
| C | -2.848078 | 4.421368 | 1.574994 | F | -3.287547 | 1.934385 | -2.714351 |
| C | -3.277684 | 3.111791 | 1.390781 | F | -1.851721 | 3.483514 | -3.121473 |
| C | -2.603942 | -2.634013 | -0.188926 | F | -3.569292 | 1.211468 | 2.800286 |
| C | -2.319602 | -3.332627 | 0.994227 | F | -3.860362 | 3.151282 | 3.679300 |
| C | -1.721614 | -4.584966 | 0.952536 | F | -4.012093 | -2.508392 | 2.432409 |
| C | -1.389658 | -5.161262 | -0.261887 | F | -2.416479 | -3.638710 | 3.335066 |
| C | -1.652564 | -4.484492 | -1.437364 | F | -2.456909 | -1.277530 | -2.776905 |
| C | -2.260672 | -3.235386 | -1.404830 | F | -1.859026 | -3.111857 | -3.727376 |
| C | -2.208014 | 2.544045 | -2.223839 | F | 1.641051 | 0.708103 | -2.680419 |
| F | -1.208534 | 1.647224 | -2.207609 | F | 1.441499 | 2.403440 | -3.985546 |
| C | -4.007918 | 2.450164 | 2.542605 | F | 4.863022 | 3.575910 | 1.432739 |
| F | -5.327729 | 2.368390 | 2.312791 | F | 3.242407 | 4.390043 | 2.596032 |
| C | -2.701024 | -2.771748 | 2.346475 | F | 4.187759 | -3.587083 | -1.921743 |
| F | -2.046883 | -1.639254 | 2.636850 | F | 2.148549 | -3.910009 | -2.549531 |
| C | -2.603287 | -2.601682 | -2.739080 | F | 2.549641 | -0.463146 | 3.069318 |

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|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| F | 2.829390 | -2.190332 | 4.314964 | C | 5.616972 | 0.043817 | -0.200595 |
| H | 1.216728 | 1.559614 | 1.987582 | C | 4.905242 | 1.153928 | -0.626545 |
| H | -1.326824 | 1.405139 | 2.001880 | C | 3.523666 | 1.201792 | -0.478710 |
| H | -5.540703 | 1.827862 | -0.338598 | C | 2.825285 | -2.157282 | 1.102760 |
| H | -6.577973 | -0.392157 | -0.691416 | C | 2.513962 | -2.205705 | 2.470653 |
| H | -5.155526 | -2.417808 | -0.590371 | C | 1.655890 | -3.174333 | 2.973274 |
| H | 5.320013 | 2.181741 | -0.936612 | C | 1.115456 | -4.129773 | 2.128219 |
| H | 6.619171 | 0.099767 | -0.613666 | C | 1.492207 | -4.156300 | 0.799223 |
| H | 5.460099 | -1.956555 | 0.138789 | C | 2.342238 | -3.183517 | 0.285541 |
| H | -1.569983 | 5.002073 | -1.488844 | C | 3.200201 | -1.286975 | 3.454751 |
| H | -1.887088 | 6.121382 | 0.691189 | F | 2.728991 | -1.452388 | 4.701165 |
| H | -3.013420 | 4.908143 | 2.526397 | C | 2.843210 | -3.381557 | -1.130264 |
| H | -1.525196 | -5.110363 | 1.876760 | F | 2.056503 | -4.211193 | -1.827437 |
| H | -0.924882 | -6.139528 | -0.289976 | C | 2.753854 | 2.398758 | -0.947119 |
| H | -1.381108 | -4.917404 | -2.390352 | C | 2.211382 | 2.447076 | -2.239706 |
| H | 1.625162 | -5.164908 | -0.691585 | C | 1.399905 | 3.503088 | -2.638502 |
| H | 1.121176 | -5.615528 | 1.685963 | C | 1.134475 | 4.545294 | -1.768488 |
| H | 1.791570 | -3.976613 | 3.408510 | C | 1.714113 | 4.551385 | -0.512203 |
| H | 2.038763 | 5.519604 | 1.044597 | C | 2.519556 | 3.493988 | -0.104054 |
| H | 0.774753 | 5.928881 | -1.037221 | C | 0.726890 | 0.642547 | 1.368577 |
| H | 0.810225 | 4.232808 | -2.840815 | C | -0.737927 | 0.553555 | 1.333593 |
| | | | | C | -2.745308 | -0.061594 | -0.035064 |
| 8PH | | | | C | -3.568596 | 1.069937 | 0.150227 |
| 95 | | | | C | -4.933621 | 1.006137 | -0.103640 |
| E: -4654.522658 | | | | C | -5.520167 | -0.171531 | -0.528954 |
| P | 0.105064 | -0.439058 | -0.872160 | C | -4.729597 | -1.291037 | -0.702891 |
| C | 1.369870 | 0.175159 | 0.293297 | C | -3.357364 | -1.248610 | -0.471010 |
| C | -1.289930 | 0.022187 | 0.233752 | C | -3.038682 | 2.386363 | 0.635565 |
| O | 0.238723 | -1.836966 | -1.363034 | C | -2.465163 | 3.319499 | -0.239249 |
| C | 2.841281 | 0.126095 | 0.103780 | C | -1.941226 | 4.517180 | 0.233806 |
| C | 3.569558 | -0.997204 | 0.519849 | C | -1.993609 | 4.821776 | 1.582349 |
| C | 4.949853 | -1.028851 | 0.370231 | C | -2.617861 | 3.946332 | 2.453722 |

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|---|-----------|-----------|-----------|--------------------------|--------------|-----------|-----------|
| C | -3.144231 | 2.746499 | 1.987941 | F | 4.064209 | -3.970899 | -1.076144 |
| C | -2.622254 | -2.532540 | -0.713956 | F | 4.519465 | -1.541778 | 3.502414 |
| C | -2.346689 | -3.434321 | 0.321704 | F | 3.072003 | 0.018153 | 3.173374 |
| C | -1.761836 | -4.666313 | 0.052660 | H | 1.231874 | 1.059931 | 2.227505 |
| C | -1.434481 | -5.020824 | -1.243126 | H | -1.311419 | 0.891361 | 2.183499 |
| C | -1.691757 | -4.140944 | -2.277252 | H | -5.535417 | 1.895239 | 0.037295 |
| C | -2.286051 | -2.914933 | -2.018323 | H | -6.584784 | -0.215673 | -0.722152 |
| C | -2.463049 | 3.084018 | -1.733045 | H | -5.171947 | -2.224595 | -1.027649 |
| F | -1.970749 | 4.145975 | -2.399201 | H | 5.419002 | 1.993180 | -1.078642 |
| C | -3.879716 | 1.870680 | 2.983403 | H | 6.693275 | 0.013046 | -0.318237 |
| F | -3.685992 | 2.294896 | 4.242875 | H | 5.496754 | -1.904103 | 0.698456 |
| C | -2.680400 | -3.111633 | 1.759657 | H | -1.502224 | 5.217053 | -0.462973 |
| F | -2.464586 | -4.169420 | 2.565658 | H | -1.575289 | 5.750396 | 1.949728 |
| C | -2.554934 | -2.006047 | -3.195830 | H | -2.698860 | 4.191677 | 3.503841 |
| F | -1.914277 | -2.415150 | -4.297338 | H | -1.571692 | -5.352384 | 0.866582 |
| C | 2.581768 | 1.409688 | -3.279453 | H | -0.971813 | -5.978581 | -1.446918 |
| F | 1.892618 | 1.588151 | -4.416743 | H | -1.414319 | -4.395980 | -3.290150 |
| C | 3.216844 | 3.614782 | 1.233106 | H | 1.115780 | -4.924100 | 0.138885 |
| F | 2.785653 | 4.689043 | 1.917336 | H | 0.424437 | -4.866723 | 2.517701 |
| F | -1.713955 | 2.032669 | -2.094010 | H | 1.413166 | -3.180686 | 4.026823 |
| F | -3.695880 | 2.876091 | -2.207550 | H | 1.547594 | 5.382671 | 0.159217 |
| F | -5.204157 | 1.894197 | 2.769083 | H | 0.497835 | 5.362120 | -2.083089 |
| F | -3.493376 | 0.588901 | 2.949839 | H | 0.978806 | 3.506679 | -3.634154 |
| F | -1.929248 | -2.111842 | 2.246309 | H | 0.054679 | 0.547735 | -1.873608 |
| F | -3.962493 | -2.760965 | 1.926840 | | | | |
| F | -3.865763 | -1.971344 | -3.506011 | {8P} ₂ | | | |
| F | -2.176949 | -0.735313 | -2.979664 | 188 | | | |
| F | 3.884016 | 1.496996 | -3.594598 | E= | -9307.783504 | | |
| F | 2.353471 | 0.153171 | -2.885859 | C | -2.213733 | 0.905997 | 4.077369 |
| F | 3.036621 | 2.558739 | 2.033864 | C | -3.270003 | -0.011672 | 3.909656 |
| F | 4.540829 | 3.766083 | 1.071955 | C | -4.599999 | 0.358866 | 4.238088 |
| F | 2.994539 | -2.272228 | -1.843627 | C | -4.851961 | 1.650928 | 4.725410 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.804911 | 2.564444 | 4.901096 | C | -5.174030 | 0.673056 | -3.320206 |
| C | -2.498154 | 2.187742 | 4.580526 | C | -0.417531 | -0.788005 | -4.499188 |
| C | -3.034600 | -1.411428 | 3.415487 | C | -3.077325 | -3.557782 | 0.224027 |
| C | -2.821020 | -1.741237 | 2.044485 | C | -2.111175 | -4.407760 | -0.364191 |
| C | -2.916711 | -3.098255 | 1.645145 | C | -2.377563 | -4.992141 | -1.609435 |
| C | -3.059451 | -4.099236 | 2.626012 | C | -3.574643 | -4.734400 | -2.282652 |
| C | -3.157168 | -3.781955 | 3.980835 | C | -4.520538 | -3.886883 | -1.705480 |
| C | -3.176461 | -2.436776 | 4.362398 | C | -4.295780 | -3.298657 | -0.449213 |
| C | -2.695875 | -0.651301 | 1.044187 | C | -0.778421 | -4.661855 | 0.296998 |
| C | -3.632833 | 0.312805 | 0.935621 | C | -5.400432 | -2.440445 | 0.136499 |
| C | -3.528792 | 1.251498 | -0.187712 | C | -5.761140 | -0.600404 | 4.049370 |
| C | -2.508274 | 1.086869 | -1.054024 | C | -0.804243 | 0.538417 | 3.684569 |
| C | -2.347112 | 1.908511 | -2.276927 | P | -1.449180 | -0.351332 | -0.375221 |
| C | -2.332529 | 3.330984 | -2.167626 | O | -1.041971 | -1.568911 | -1.300195 |
| C | -2.093216 | 4.109315 | -3.309637 | O | -0.033122 | 0.396568 | 0.242375 |
| C | -1.931400 | 3.514709 | -4.566050 | P | 1.597357 | 0.050720 | 0.924290 |
| C | -2.106481 | 2.134781 | -4.691836 | C | 2.726202 | 1.298643 | 0.005519 |
| C | -2.338488 | 1.320050 | -3.567051 | C | 2.777966 | 2.784243 | 0.070809 |
| C | -2.723948 | 4.049586 | -0.905858 | C | 2.806822 | 3.506601 | 1.290985 |
| C | -1.806877 | 4.247946 | 0.144051 | C | 2.816021 | 4.916008 | 1.266614 |
| C | -2.236418 | 4.877245 | 1.324903 | C | 2.802541 | 5.625565 | 0.065706 |
| C | -3.555681 | 5.320994 | 1.459523 | C | 2.888661 | 4.916404 | -1.136470 |
| C | -4.454913 | 5.155430 | 0.397969 | C | 2.924196 | 3.514934 | -1.151657 |
| C | -4.053291 | 4.526471 | -0.792429 | C | 3.026765 | 2.899758 | 2.649768 |
| C | -2.785822 | -0.086468 | -3.863827 | C | 2.057204 | 3.048053 | 3.670034 |
| C | -4.177094 | -0.357321 | -3.809938 | C | 2.370256 | 2.664238 | 4.983874 |
| C | -4.657865 | -1.586705 | -4.287859 | C | 3.640310 | 2.175360 | 5.304151 |
| C | -3.785501 | -2.536535 | -4.825339 | C | 4.602431 | 2.047656 | 4.299262 |
| C | -2.416502 | -2.264352 | -4.877317 | C | 4.313948 | 2.398240 | 2.969889 |
| C | -1.902133 | -1.046336 | -4.406447 | C | 3.290797 | 2.859446 | -2.455282 |
| C | -0.381888 | 3.792859 | -0.007898 | C | 4.634800 | 2.959956 | -2.893696 |
| C | -5.053752 | 4.348059 | -1.918181 | C | 5.019171 | 2.302757 | -4.074941 |

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|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.093853 | 1.552676 | -4.812232 | H | -4.490401 | 0.364148 | 1.593113 |
| C | 2.766410 | 1.471369 | -4.378857 | H | -4.293929 | 2.004058 | -0.324536 |
| C | 2.351887 | 2.128466 | -3.208864 | H | 4.517086 | 1.072220 | -1.155890 |
| C | 0.696269 | 3.646254 | 3.387651 | H | 4.307112 | -1.434986 | -1.170262 |
| C | 5.412477 | 2.289477 | 1.932658 | H | 2.749391 | -5.868657 | -1.387947 |
| C | 5.678867 | 3.708839 | -2.086117 | H | 2.496660 | -6.737669 | 0.936915 |
| C | 0.921801 | 2.049752 | -2.755330 | H | 2.432669 | -5.107075 | 2.824856 |
| C | 2.498254 | -1.391625 | -0.018797 | H | 2.965849 | 5.446776 | -2.080448 |
| C | 3.539499 | -0.843583 | -0.696024 | H | 2.782835 | 6.709942 | 0.066762 |
| C | 3.668083 | 0.601870 | -0.677411 | H | 2.866727 | 5.450096 | 2.210568 |
| C | 2.461001 | -2.864854 | 0.233957 | H | -2.059534 | 5.189271 | -3.205232 |
| C | 2.440196 | -3.370636 | 1.562177 | H | -1.733837 | 4.124592 | -5.440925 |
| C | 2.438517 | -4.757380 | 1.797112 | H | -2.103339 | 1.671888 | -5.673808 |
| C | 2.500500 | -5.670179 | 0.745259 | H | -3.322661 | -2.165029 | 5.403159 |
| C | 2.626093 | -5.180930 | -0.556600 | H | -3.262621 | -4.565725 | 4.723105 |
| C | 2.632815 | -3.802874 | -0.830676 | H | -3.139678 | -5.131168 | 2.299332 |
| C | 2.591637 | -2.517266 | 2.787078 | H | -1.530918 | 5.018949 | 2.137559 |
| C | 3.859573 | -1.971248 | 3.101023 | H | -3.880688 | 5.797490 | 2.378895 |
| C | 4.016536 | -1.273032 | 4.308809 | H | -5.476426 | 5.512074 | 0.493242 |
| C | 2.950501 | -1.129463 | 5.202298 | H | -5.725058 | -1.787160 | -4.257149 |
| C | 1.711452 | -1.701189 | 4.900712 | H | -4.170343 | -3.477451 | -5.205407 |
| C | 1.523105 | -2.404426 | 3.701618 | H | -1.736600 | -2.999359 | -5.297593 |
| C | 5.058944 | -2.160253 | 2.194648 | H | 6.051069 | 2.367746 | -4.408102 |
| C | 0.185528 | -3.033057 | 3.397902 | H | 4.406847 | 1.032339 | -5.711658 |
| C | 2.972366 | -3.457794 | -2.255723 | H | 2.047445 | 0.885343 | -4.942073 |
| C | 4.338131 | -3.363384 | -2.617782 | H | 1.620313 | 2.772968 | 5.762358 |
| C | 4.679519 | -3.095002 | -3.953543 | H | 3.881589 | 1.909469 | 6.328378 |
| C | 3.686243 | -2.983318 | -4.933403 | H | 5.597301 | 1.688678 | 4.546582 |
| C | 2.344686 | -3.167505 | -4.581730 | H | -1.638604 | -5.649931 | -2.056061 |
| C | 1.969270 | -3.409458 | -3.248481 | H | -3.766754 | -5.190655 | -3.248157 |
| C | 5.447806 | -3.619544 | -1.612445 | H | -5.453326 | -3.683573 | -2.223388 |
| C | 0.530510 | -3.688201 | -2.891584 | H | -5.870512 | 1.940670 | 4.966838 |

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|---|-----------|-----------|-----------|-----------|--------------|-----------|-----------|
| H | -4.008281 | 3.560316 | 5.281675 | F | -6.052022 | 4.667884 | -1.605551 |
| H | -1.687431 | 2.893574 | 4.717459 | F | -4.771001 | 4.931673 | -2.800889 |
| H | 5.726353 | -2.995855 | -4.226644 | F | -5.114236 | 3.303126 | -2.242126 |
| H | 3.957562 | -2.784210 | -5.965408 | F | -6.715393 | -0.071681 | 4.130846 |
| H | 1.579743 | -3.147248 | -5.352175 | F | -5.725342 | -1.094894 | 3.071664 |
| H | 0.883699 | -1.603159 | 5.597041 | F | -5.751774 | -1.397521 | 4.800431 |
| H | 3.087074 | -0.580992 | 6.127936 | F | -6.198053 | 0.346573 | -3.523356 |
| H | 4.984832 | -0.846983 | 4.552170 | F | -5.082287 | 0.835028 | -2.240872 |
| F | 0.126901 | 3.742250 | 4.315330 | F | -5.020432 | 1.639004 | -3.814617 |
| F | 0.776021 | 4.643835 | 2.944981 | F | -6.380618 | -2.815338 | -0.174508 |
| F | 0.120054 | 3.026783 | 2.693857 | F | -5.375091 | -2.424237 | 1.229769 |
| F | -0.055638 | 1.071102 | 4.277169 | F | -5.313973 | -1.405919 | -0.217401 |
| F | -0.616783 | -0.530191 | 3.794068 | F | -0.242610 | -5.473276 | -0.201015 |
| F | -0.629182 | 0.784996 | 2.630278 | F | -0.154740 | -3.764017 | 0.224141 |
| F | -0.547518 | -2.790989 | 4.169084 | F | -0.868121 | -4.916894 | 1.355997 |
| F | -0.208310 | -2.689678 | 2.436100 | F | 6.374372 | -3.120828 | -1.914839 |
| F | 0.252607 | -4.123964 | 3.335096 | F | 5.190832 | -3.292398 | -0.600765 |
| F | 5.984559 | -1.916737 | 2.724587 | F | 5.652794 | -4.695045 | -1.545983 |
| F | 5.129460 | -3.194204 | 1.839314 | F | 6.681722 | 3.517194 | -2.479043 |
| F | 4.998088 | -1.513770 | 1.312009 | F | 5.508835 | 4.790486 | -2.105851 |
| F | -0.104122 | -3.718924 | -3.781436 | F | 5.659855 | 3.407758 | -1.031773 |
| F | 0.448912 | -4.657409 | -2.387387 | F | 6.384492 | 2.145382 | 2.413358 |
| F | 0.108472 | -2.937557 | -2.215026 | F | 5.237897 | 1.440798 | 1.262979 |
| F | 0.078321 | -1.573015 | -5.073208 | F | 5.467340 | 3.191457 | 1.313597 |
| F | -0.203458 | 0.167063 | -4.989386 | | | | |
| F | 0.028420 | -0.775469 | -3.498823 | 80 | | | |
| F | 0.315150 | 1.497201 | -3.466517 | 94 | | | |
| F | 0.830190 | 1.561140 | -1.778018 | E= | -2272.046943 | | |
| F | 0.489074 | 3.048665 | -2.662476 | C | 1.555267 | 3.111538 | -2.324349 |
| F | 0.253256 | 4.223256 | 0.764131 | C | 1.912365 | 3.040423 | -0.952648 |
| F | -0.295933 | 2.700234 | 0.045580 | C | 1.328887 | 3.921884 | -0.016068 |
| F | 0.025282 | 4.103523 | -0.972080 | C | 0.393322 | 4.873328 | -0.461954 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.034460 | 4.949760 | -1.809635 | C | -3.815008 | 2.836815 | 2.801501 |
| C | 0.612021 | 4.067753 | -2.732543 | C | -3.242748 | 3.907769 | 2.100593 |
| C | 2.977707 | 2.073009 | -0.526854 | C | -2.817784 | 3.725484 | 0.781080 |
| C | 2.675353 | 0.836926 | 0.086227 | C | -2.951770 | 2.480166 | 0.140539 |
| C | 3.717579 | -0.050408 | 0.446778 | C | -4.574448 | 0.431689 | 2.970939 |
| C | 5.050630 | 0.310905 | 0.204519 | C | -2.423938 | 2.317704 | -1.268456 |
| C | 5.356280 | 1.542016 | -0.389991 | C | -1.798245 | -3.060784 | -0.925758 |
| C | 4.323336 | 2.414055 | -0.750683 | C | -1.362422 | -3.301936 | -2.252413 |
| C | 1.267311 | 0.461136 | 0.348576 | C | -0.369144 | -4.271272 | -2.473218 |
| C | 0.550833 | 0.646177 | 1.486458 | C | 0.173179 | -5.000984 | -1.408213 |
| C | -0.846321 | 0.180875 | 1.467921 | C | -0.273635 | -4.765214 | -0.103062 |
| C | -1.274370 | -0.398532 | 0.314943 | C | -1.257350 | -3.797155 | 0.156132 |
| P | 0.209200 | -0.556774 | -0.783921 | C | -1.912418 | -2.509776 | -3.421017 |
| O | 0.058984 | -0.094381 | -2.330675 | C | -1.719196 | -3.563082 | 1.579853 |
| C | 3.408970 | -1.362163 | 1.101772 | H | -1.491326 | 0.339861 | 2.323266 |
| C | 3.141162 | -2.505719 | 0.319261 | H | 0.959910 | 1.128367 | 2.366250 |
| C | 2.855380 | -3.720938 | 0.969490 | H | 5.842166 | -0.377326 | 0.483691 |
| C | 2.827291 | -3.801619 | 2.363766 | H | 6.389645 | 1.817626 | -0.572373 |
| C | 3.096446 | -2.660252 | 3.133461 | H | 4.549196 | 3.370070 | -1.212569 |
| C | 3.395064 | -1.436629 | 2.516087 | H | -4.375307 | -3.378277 | -1.490122 |
| C | 3.168028 | -2.476961 | -1.196704 | H | -6.274325 | -1.815249 | -1.082428 |
| C | 3.714343 | -0.217324 | 3.357866 | H | -5.838263 | 0.388761 | -0.002189 |
| C | 1.674630 | 3.892992 | 1.459921 | H | 2.649756 | -4.601147 | 0.368352 |
| C | 2.155046 | 2.165869 | -3.344548 | H | 2.600324 | -4.744640 | 2.851184 |
| C | -2.640697 | -0.814598 | -0.047224 | H | 3.078634 | -2.721615 | 4.217757 |
| C | -3.723952 | 0.070954 | 0.198560 | H | -0.042853 | 5.559696 | 0.259032 |
| C | -5.021758 | -0.303579 | -0.181918 | H | -0.686121 | 5.690372 | -2.142716 |
| C | -5.266121 | -1.538069 | -0.793646 | H | 0.330934 | 4.120112 | -3.779965 |
| C | -4.199738 | -2.411051 | -1.029801 | H | -2.370929 | 4.548708 | 0.232862 |
| C | -2.887876 | -2.063308 | -0.669383 | H | -3.130455 | 4.874476 | 2.581419 |
| C | -3.539429 | 1.409236 | 0.850503 | H | -4.140276 | 2.973018 | 3.828930 |
| C | -3.973491 | 1.584200 | 2.187591 | H | 0.140060 | -5.333419 | 0.724557 |

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|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 0.934273 | -5.752276 | -1.596319 | C | -0.521718 | -1.235391 | 0.341297 |
| H | -0.021138 | -4.451630 | -3.485733 | O | -0.749477 | 0.306884 | -2.031339 |
| H | -1.464885 | -2.848659 | -4.359657 | C | 1.236528 | 2.469724 | -0.013090 |
| H | -2.999229 | -2.608303 | -3.505809 | C | 0.429315 | 3.581399 | -0.315006 |
| H | -1.678867 | -1.445565 | -3.303652 | C | 1.015502 | 4.798857 | -0.652577 |
| H | 1.875845 | 2.466221 | -4.358788 | C | 2.391353 | 4.934525 | -0.718478 |
| H | 3.247581 | 2.137885 | -3.283637 | C | 3.191993 | 3.841671 | -0.429790 |
| H | 1.778267 | 1.149801 | -3.181264 | C | 2.638689 | 2.615215 | -0.070781 |
| H | 4.065117 | -2.982419 | -1.574448 | C | -1.060325 | 3.530720 | -0.248601 |
| H | 2.293651 | -2.996136 | -1.604489 | C | -1.809706 | 3.510021 | -1.435999 |
| H | 3.175455 | -1.459621 | -1.596788 | C | -3.200418 | 3.502210 | -1.343624 |
| H | 3.519070 | -0.409749 | 4.416776 | C | -3.833026 | 3.529336 | -0.111981 |
| H | 4.767133 | 0.068902 | 3.252107 | C | -3.083748 | 3.556387 | 1.054349 |
| H | 3.122930 | 0.651862 | 3.050148 | C | -1.693699 | 3.560103 | 1.004355 |
| H | -1.408885 | -4.387715 | 2.227943 | C | -1.145713 | 3.457217 | -2.787608 |
| H | -1.284900 | -2.640135 | 1.981846 | C | -0.892621 | 3.587591 | 2.280751 |
| H | -2.808244 | -3.466087 | 1.638852 | C | 3.597363 | 1.508421 | 0.228583 |
| H | 1.944014 | 4.894481 | 1.812804 | C | 3.850080 | 0.516762 | -0.728571 |
| H | 0.806402 | 3.561419 | 2.042415 | C | 4.802628 | -0.457788 | -0.442097 |
| H | 2.510090 | 3.223359 | 1.678666 | C | 5.470544 | -0.471545 | 0.771767 |
| H | -4.640974 | 0.678108 | 4.034774 | C | 5.201233 | 0.505057 | 1.719188 |
| H | -5.582670 | 0.188186 | 2.617960 | C | 4.273183 | 1.509590 | 1.458233 |
| H | -3.976460 | -0.481242 | 2.864118 | C | 1.083808 | 0.284408 | 1.245316 |
| H | -2.548869 | 3.242571 | -1.839200 | C | 0.449853 | -1.044145 | 1.244042 |
| H | -1.347874 | 2.100858 | -1.255426 | C | -1.218417 | -2.501052 | 0.026333 |
| H | -2.915660 | 1.505274 | -1.809445 | C | -2.619917 | -2.580284 | 0.054457 |
| | | | | C | -3.253813 | -3.780529 | -0.256829 |
| 8OH | | | | C | -2.520112 | -4.902089 | -0.606897 |
| 95 | | | | C | -1.136841 | -4.826288 | -0.639304 |
| E: -2272.681347 | | | | C | -0.473867 | -3.642389 | -0.324965 |
| P | -0.754382 | 0.349303 | -0.536399 | C | 3.097898 | 0.483898 | -2.031584 |
| C | 0.644487 | 1.158445 | 0.324199 | C | 3.985713 | 2.563955 | 2.498452 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.467704 | -1.420908 | 0.459121 | H | -4.519552 | 0.208851 | 3.240135 |
| C | -3.590665 | -1.101964 | 1.819434 | H | 3.714389 | -4.600883 | 1.430455 |
| C | -4.417017 | -0.043305 | 2.189692 | H | 4.870525 | -3.806805 | -0.602472 |
| C | -5.116326 | 0.675236 | 1.233753 | H | 3.562112 | -2.918248 | -2.501481 |
| C | -4.990541 | 0.350086 | -0.107964 | H | 1.536534 | -2.471099 | -3.569927 |
| C | -4.167693 | -0.694951 | -0.517996 | H | 0.098588 | -3.345728 | -3.020660 |
| C | 1.018286 | -3.645034 | -0.390746 | H | 0.384668 | -1.699027 | -2.478105 |
| C | 1.664395 | -3.187173 | -1.548374 | H | -1.891678 | 3.531192 | -3.580741 |
| C | 3.053511 | -3.260492 | -1.605793 | H | -0.424808 | 4.267024 | -2.918736 |
| C | 3.788527 | -3.763006 | -0.542667 | H | -0.618292 | 2.507237 | -2.909749 |
| C | 3.139851 | -4.208475 | 0.597726 | H | 3.555603 | -0.222757 | -2.725952 |
| C | 1.750248 | -4.165557 | 0.684575 | H | 2.058776 | 0.173123 | -1.882097 |
| C | -2.857995 | -1.891343 | 2.873835 | H | 3.068502 | 1.468178 | -2.505317 |
| C | -4.005516 | -0.999091 | -1.985834 | H | 4.448694 | 2.303908 | 3.452139 |
| C | 0.880952 | -2.645646 | -2.714627 | H | 4.366911 | 3.542477 | 2.193429 |
| C | 1.053414 | -4.692418 | 1.914534 | H | 2.909988 | 2.686177 | 2.658841 |
| H | 0.804000 | -1.813935 | 1.919347 | H | 0.570689 | -5.653005 | 1.710917 |
| H | 1.893158 | 0.492719 | 1.933098 | H | 1.762956 | -4.839347 | 2.731060 |
| H | 4.272194 | 3.925623 | -0.480957 | H | 0.263531 | -4.018652 | 2.258384 |
| H | 2.837113 | 5.883996 | -0.991862 | H | -1.536212 | 3.798658 | 3.136440 |
| H | 0.369110 | 5.643720 | -0.863871 | H | -0.402210 | 2.624908 | 2.456370 |
| H | -0.546500 | -5.693243 | -0.915813 | H | -0.107561 | 4.346959 | 2.242584 |
| H | -3.022985 | -5.830599 | -0.851913 | H | -3.215896 | -1.630290 | 3.871284 |
| H | -4.336861 | -3.822671 | -0.214961 | H | -2.991367 | -2.966446 | 2.729946 |
| H | 5.013843 | -1.219718 | -1.182335 | H | -1.782955 | -1.691345 | 2.837510 |
| H | 6.200835 | -1.245430 | 0.980663 | H | -4.662856 | -0.363935 | -2.582072 |
| H | 5.718989 | 0.493229 | 2.672956 | H | -2.976527 | -0.815939 | -2.311516 |
| H | -3.581906 | 3.573506 | 2.017940 | H | -4.240187 | -2.041940 | -2.211451 |
| H | -4.915895 | 3.525606 | -0.059415 | H | -1.911618 | 0.906370 | 0.046232 |
| H | -3.789544 | 3.474430 | -2.254134 | | | | |
| H | -5.527572 | 0.923516 | -0.855772 | | | | |
| H | -5.758904 | 1.495206 | 1.535048 | | | | |

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|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| E= -4544.146046 | | | C | -3.798743 | 5.003518 | 2.134384 | |
| C | -2.239909 | -3.416480 | -2.365975 | C | -2.417573 | 4.864534 | 2.289291 |
| C | -3.335195 | -2.640346 | -2.794824 | C | -1.855101 | 3.650413 | 2.712841 |
| C | -4.652227 | -3.165786 | -2.736551 | C | -0.192677 | -2.851521 | 2.519591 |
| C | -4.851891 | -4.463944 | -2.241264 | C | -4.794415 | -2.116562 | 4.536501 |
| C | -3.766176 | -5.242435 | -1.820708 | C | -5.062048 | 1.567127 | 3.178472 |
| C | -2.472798 | -4.718084 | -1.887866 | C | -0.358339 | 3.551373 | 2.883933 |
| C | -3.157081 | -1.257106 | -3.355055 | C | -3.239313 | 2.458941 | -2.365944 |
| C | -2.932569 | -0.100585 | -2.551258 | C | -2.303383 | 3.507672 | -2.527523 |
| C | -3.084935 | 1.180450 | -3.139357 | C | -2.572797 | 4.761654 | -1.963573 |
| C | -3.294435 | 1.282991 | -4.528613 | C | -3.742784 | 4.984295 | -1.232676 |
| C | -3.403514 | 0.149199 | -5.333834 | C | -4.658382 | 3.945153 | -1.065359 |
| C | -3.366186 | -1.113849 | -4.734847 | C | -4.430576 | 2.680070 | -1.633163 |
| C | -2.736011 | -0.257586 | -1.088065 | C | -0.997491 | 3.293337 | -3.253250 |
| C | -3.623652 | -0.932128 | -0.328945 | C | -5.504393 | 1.623642 | -1.457897 |
| C | -3.452952 | -0.894829 | 1.128216 | C | -5.853805 | -2.346925 | -3.172140 |
| C | -2.424614 | -0.176678 | 1.624033 | C | -0.842084 | -2.849013 | -2.377588 |
| C | -2.200489 | 0.015542 | 3.076403 | P | -1.448799 | 0.481114 | 0.118718 |
| C | -2.120294 | -1.125356 | 3.929345 | O | -1.081971 | 2.015335 | -0.005762 |
| C | -1.821768 | -0.952115 | 5.288804 | O | -0.011126 | -0.455732 | 0.081062 |
| C | -1.663816 | 0.326717 | 5.834655 | P | 1.587304 | -0.607970 | -0.734365 |
| C | -1.901956 | 1.442827 | 5.029505 | C | 2.792158 | -0.914486 | 0.725128 |
| C | -2.194580 | 1.308462 | 3.658711 | C | 2.913351 | -2.072962 | 1.650974 |
| C | -2.501748 | -2.506177 | 3.471656 | C | 2.952604 | -3.419576 | 1.207630 |
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| C | -3.808874 | -2.969844 | 3.761458 | C | 3.116634 | -3.854127 | -0.223169 |
| C | -2.702523 | 2.551041 | 2.977195 | C | 2.135366 | -4.660325 | -0.847782 |
| C | -4.105912 | 2.687244 | 2.822752 | C | 2.403874 | -5.230764 | -2.102371 |
| C | -4.635247 | 3.915320 | 2.395475 | C | 3.642657 | -5.045389 | -2.723398 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.617185 | -4.264988 | -2.096453 | C | 3.644039 | 5.581603 | 1.576601 |
| C | 4.371932 | -3.658772 | -0.853185 | C | 2.288578 | 5.457560 | 1.253008 |
| C | 3.478774 | -0.452593 | 3.575733 | C | 1.875916 | 4.751997 | 0.108926 |
| C | 4.834402 | -0.208412 | 3.909351 | C | 5.307668 | 3.910978 | -1.419723 |
| C | 5.210192 | 1.073003 | 4.347243 | C | 0.418775 | 4.693384 | -0.276314 |
| C | 4.264876 | 2.101641 | 4.450776 | H | -4.490554 | -1.423758 | -0.749819 |
| C | 2.926802 | 1.846731 | 4.132799 | H | -4.178535 | -1.387812 | 1.761461 |
| C | 2.521121 | 0.572123 | 3.704681 | H | 4.592723 | 0.062214 | 1.366506 |
| C | 0.810293 | -4.954938 | -0.179116 | H | 4.263864 | 1.951414 | -0.262361 |
| C | 5.484232 | -2.868175 | -0.195774 | H | 2.501298 | 5.391782 | -2.943527 |
| C | 5.896869 | -1.279765 | 3.746716 | H | 2.161797 | 4.506655 | -5.251193 |
| C | 1.080271 | 0.299629 | 3.377983 | H | 2.138449 | 2.035073 | -5.594730 |
| C | 2.436829 | 1.118427 | -1.015875 | H | 3.270131 | -2.651850 | 5.011052 |
| C | 3.516118 | 1.176730 | -0.194343 | H | 3.105335 | -5.020859 | 4.236375 |
| C | 3.713031 | 0.080936 | 0.736612 | H | 3.086949 | -5.485174 | 1.792152 |
| C | 2.324471 | 2.058291 | -2.173331 | H | -1.738731 | -1.831907 | 5.919210 |
| C | 2.253495 | 1.562437 | -3.503560 | H | -1.420261 | 0.449534 | 6.884412 |
| C | 2.181141 | 2.449851 | -4.592375 | H | -1.901589 | 2.438125 | 5.463013 |
| C | 2.220240 | 3.830725 | -4.405035 | H | -3.519679 | -2.007498 | -5.331700 |
| C | 2.394570 | 4.324031 | -3.110341 | H | -3.560746 | 0.246600 | -6.402558 |
| C | 2.472314 | 3.469070 | -1.998047 | H | -3.417295 | 2.272133 | -4.958200 |
| C | 2.421307 | 0.117041 | -3.869934 | H | -1.323895 | -5.213630 | 1.766444 |
| C | 3.707391 | -0.471314 | -3.805271 | H | -3.638195 | -6.011703 | 2.205661 |
| C | 3.873649 | -1.788683 | -4.261112 | H | -5.208397 | -4.590737 | 3.509050 |
| C | 2.798293 | -2.509936 | -4.789096 | H | -5.711177 | 4.021312 | 2.289809 |
| C | 1.539593 | -1.909735 | -4.881285 | H | -4.220438 | 5.952472 | 1.818888 |
| C | 1.341587 | -0.595038 | -4.433837 | H | -1.765338 | 5.709595 | 2.090303 |
| C | 4.913989 | 0.295641 | -3.303644 | H | 6.250365 | 1.267367 | 4.592788 |
| C | -0.018170 | 0.047105 | -4.557314 | H | 4.570357 | 3.092783 | 4.770154 |
| C | 2.855859 | 4.156830 | -0.715466 | H | 2.191959 | 2.642033 | 4.203870 |
| C | 4.231423 | 4.355766 | -0.444245 | H | 1.644796 | -5.842811 | -2.581402 |
| C | 4.611406 | 5.042352 | 0.720677 | H | 3.850812 | -5.515190 | -3.679387 |

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|---|-----------|-----------|-----------|------------|-----------|-----------|-----------|
| H | 5.588767 | -4.135464 | -2.564481 | H | 0.946308 | 0.020565 | 2.326104 |
| H | -1.857390 | 5.567401 | -2.094673 | H | 0.693864 | -0.522293 | 3.985302 |
| H | -3.937409 | 5.959274 | -0.798151 | H | 0.446962 | -3.669392 | 2.193057 |
| H | -5.570078 | 4.112368 | -0.499226 | H | -0.159954 | -2.063549 | 1.756630 |
| H | -5.860034 | -4.864167 | -2.185130 | H | 0.247700 | -2.440123 | 3.429957 |
| H | -3.929325 | -6.246493 | -1.442276 | H | -5.782266 | -2.585877 | 4.557953 |
| H | -1.632226 | -5.320328 | -1.563888 | H | -4.466930 | -1.966876 | 5.570944 |
| H | 5.666942 | 5.171794 | 0.942861 | H | -4.898226 | -1.119002 | 4.095386 |
| H | 3.944782 | 6.118424 | 2.470843 | H | -6.783206 | -2.819875 | -2.841508 |
| H | 1.540768 | 5.932703 | 1.880825 | H | -5.822392 | -1.329942 | -2.764133 |
| H | 0.703911 | -2.461348 | -5.302020 | H | -5.897178 | -2.242657 | -4.261554 |
| H | 2.942595 | -3.529228 | -5.130413 | H | -6.096277 | 1.922988 | 3.163703 |
| H | 4.856160 | -2.247204 | -4.208476 | H | -4.983914 | 0.736009 | 2.469421 |
| H | 0.228014 | -5.651641 | -0.787015 | H | -4.852916 | 1.170495 | 4.178491 |
| H | 0.946172 | -5.411113 | 0.806239 | H | -6.495024 | 2.088007 | -1.425485 |
| H | 0.218981 | -4.045162 | -0.038495 | H | -5.499777 | 0.891373 | -2.270243 |
| H | -0.080736 | -3.622893 | -2.507189 | H | -5.361839 | 1.081314 | -0.515282 |
| H | -0.707936 | -2.113697 | -3.171546 | H | -0.491268 | 4.243777 | -3.437411 |
| H | -0.634799 | -2.335372 | -1.430918 | H | -0.330438 | 2.680779 | -2.636638 |
| H | -0.753893 | -0.659943 | -4.943929 | H | -1.120024 | 2.784920 | -4.212973 |
| H | -0.376216 | 0.414017 | -3.590227 | H | 6.262699 | 3.756645 | -0.907100 |
| H | -0.001898 | 0.909997 | -5.230869 | H | 5.046729 | 2.992318 | -1.953138 |
| H | 5.839548 | -0.215562 | -3.584557 | H | 5.459866 | 4.680236 | -2.186676 |
| H | 4.942168 | 1.308634 | -3.719987 | H | 6.896989 | -0.853773 | 3.869706 |
| H | 4.901356 | 0.390150 | -2.212039 | H | 5.778969 | -2.083651 | 4.480969 |
| H | -0.198976 | 5.288559 | 0.401689 | H | 5.842803 | -1.748910 | 2.756953 |
| H | 0.281226 | 5.087657 | -1.289164 | H | 6.438634 | -3.054526 | -0.696810 |
| H | 0.019715 | 3.673559 | -0.271603 | H | 5.282639 | -1.792828 | -0.242640 |
| H | 0.110720 | 4.531152 | 2.776114 | H | 5.594156 | -3.136787 | 0.860435 |
| H | -0.089401 | 3.161542 | 3.870837 | | | | |
| H | 0.067966 | 2.892743 | 2.119583 | 33A | | | |
| H | 0.462098 | 1.169883 | 3.577097 | 68 | | | |

| | | | | | | | |
|-----------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| E= -1431.315377 | | | C | -2.798646 | 2.112386 | -1.319739 | |
| C | -1.823965 | -1.085080 | -2.001272 | H | 3.287643 | -2.873042 | 1.734503 |
| C | -0.711776 | -0.645850 | -1.180789 | H | 1.787612 | -2.181874 | 1.164186 |
| C | -1.213084 | -0.009281 | -0.054157 | H | 2.921033 | -2.869753 | 0.026097 |
| C | -2.708225 | -0.009651 | -0.099581 | H | 5.409986 | -1.737163 | 1.281254 |
| C | -2.975199 | -0.729473 | -1.398206 | H | 5.043377 | -1.733873 | -0.427153 |
| P | 0.132732 | 0.496296 | 0.890379 | H | 5.423895 | -0.235734 | 0.387618 |
| O | 0.209228 | 1.214557 | 2.184203 | H | 3.821078 | -0.772847 | 2.876706 |
| C | 0.728857 | -0.700167 | -1.235780 | H | 3.834987 | 0.728582 | 1.983070 |
| C | 1.739196 | -1.219529 | -2.137203 | H | 2.321048 | -0.081679 | 2.306388 |
| C | 2.956470 | -0.953442 | -1.624412 | H | 3.101774 | 2.992390 | 0.710274 |
| C | 2.843957 | -0.219264 | -0.311347 | H | 1.966508 | 1.773792 | 1.238721 |
| C | 1.360902 | -0.106414 | -0.152350 | H | 3.677963 | 1.549941 | 1.510533 |
| C | -3.292164 | 1.371964 | -0.112173 | H | 4.593086 | 2.539694 | -1.179449 |
| H | -3.972728 | -0.920713 | -1.770734 | H | 5.169275 | 1.097245 | -0.379190 |
| H | -1.733683 | -1.611405 | -2.942121 | H | 4.521623 | 0.998172 | -1.999004 |
| C | 3.064941 | 1.253599 | -0.489788 | H | 2.193851 | 2.853503 | -1.560494 |
| H | 3.905550 | -1.218231 | -2.071118 | H | 2.122388 | 1.311981 | -2.380049 |
| H | 1.538236 | -1.734897 | -3.066921 | H | 1.058586 | 1.634904 | -1.032047 |
| C | 3.493279 | -0.988850 | 0.800461 | H | -3.215189 | 3.097938 | -1.328721 |
| C | -3.311666 | -1.216558 | 0.555578 | H | -1.731079 | 2.176663 | -1.287066 |
| C | 2.944139 | 1.941748 | 0.837562 | H | -3.097629 | 1.590727 | -2.204827 |
| C | 4.435451 | 1.489051 | -1.052161 | H | -5.205297 | 2.267408 | -0.166958 |
| C | 2.036216 | 1.802860 | -1.433206 | H | -5.087737 | 0.760197 | -1.043064 |
| C | 3.357896 | -0.223875 | 2.083616 | H | -5.140796 | 0.753688 | 0.703421 |
| C | 2.824460 | -2.324071 | 0.941413 | H | -3.289571 | 3.088813 | 1.119622 |
| C | 4.946803 | -1.188191 | 0.488164 | H | -3.225071 | 1.575094 | 1.990001 |
| C | -4.806993 | -1.138696 | 0.466487 | H | -1.805461 | 2.167538 | 1.161277 |
| C | -2.833096 | -2.455598 | -0.141379 | H | -3.263551 | -3.316525 | 0.325968 |
| C | -2.898352 | -1.262287 | 1.996786 | H | -3.127927 | -2.422978 | -1.169441 |
| C | -4.788754 | 1.281857 | -0.157976 | H | -1.766430 | -2.511140 | -0.077827 |
| C | -2.873029 | 2.103262 | 1.128604 | H | -3.328806 | -2.123214 | 2.464133 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -1.831686 | -1.317828 | 2.060338 | C | -4.548718 | 1.863449 | 0.590954 |
| H | -3.239732 | -0.378438 | 2.493948 | C | -3.111109 | -1.538608 | -1.836404 |
| H | -5.237447 | -1.999623 | 0.933834 | C | -3.225424 | -2.600799 | 0.381234 |
| H | -5.148373 | -0.254847 | 0.963649 | C | 5.090966 | -1.160275 | -0.367147 |
| H | -5.101824 | -1.106076 | -0.561575 | C | 3.226450 | -2.600487 | 0.381779 |

33AH

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E: -1431.944939

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| P | -0.000011 | -0.169949 | -1.068801 | H | -3.587743 | -3.459519 | -0.191454 |
| C | -1.307083 | -0.226573 | 0.179842 | H | -2.147426 | -2.719330 | 0.516411 |
| C | -0.734024 | -0.360315 | 1.395443 | H | -3.697675 | -2.634610 | 1.364852 |
| C | 0.734138 | -0.360733 | 1.395426 | H | -5.535619 | -2.097395 | -0.715872 |
| C | 1.307175 | -0.227550 | 0.179758 | H | -5.474777 | -0.974371 | 0.639100 |
| O | 0.000411 | 0.902131 | -2.108328 | H | -5.444805 | -0.367763 | -1.026727 |
| C | 2.811646 | -0.077363 | 0.313077 | H | -3.755546 | -2.298438 | -2.288565 |
| C | 2.947717 | -0.213245 | 1.824325 | H | -3.158272 | -0.652282 | -2.463228 |
| C | 1.762577 | -0.368443 | 2.429750 | H | -2.092826 | -1.928866 | -1.875331 |
| C | -2.811632 | -0.077404 | 0.313202 | H | -3.530269 | 2.708441 | -1.778864 |
| C | -2.947643 | -0.213722 | 1.824423 | H | -2.441968 | 1.371752 | -2.123935 |
| C | -1.762445 | -0.368753 | 2.429769 | H | -4.204788 | 1.104680 | -2.029656 |
| C | 3.231891 | 1.426792 | -0.082698 | H | -4.816998 | 2.857035 | 0.220650 |
| C | 2.152283 | 2.414384 | 0.408874 | H | -5.388634 | 1.204218 | 0.382259 |
| C | 3.562326 | -1.303265 | -0.383461 | H | -4.435269 | 1.942903 | 1.674900 |
| C | 3.111011 | -1.538992 | -1.836076 | H | -2.543280 | 3.432831 | 0.320887 |
| C | -3.232371 | 1.426643 | -0.082469 | H | -1.890626 | 2.250753 | 1.456853 |
| C | -2.153156 | 2.414631 | 0.409207 | H | -1.247797 | 2.359947 | -0.196818 |
| C | -3.561883 | -1.303440 | -0.383549 | H | 2.542398 | 3.432659 | 0.321381 |
| C | -5.090557 | -1.160824 | -0.366881 | H | 1.247329 | 2.360031 | -0.197764 |
| C | 4.547881 | 1.864019 | 0.591145 | H | 1.889166 | 2.249867 | 1.456275 |
| C | 3.359396 | 1.643264 | -1.596957 | H | 4.815940 | 2.857699 | 0.220937 |
| C | -3.359559 | 1.642895 | -1.596757 | H | 4.434042 | 1.943413 | 1.675059 |

| | | | | | | | |
|---------------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 5.388073 | 1.205064 | 0.382714 | C | -3.651844 | -1.620858 | 4.136554 |
| H | 3.530262 | 2.708827 | -1.778811 | C | -2.130395 | -3.175831 | 1.958380 |
| H | 4.204644 | 1.105069 | -2.029828 | C | -2.499501 | -3.603042 | 3.561892 |
| H | 2.441861 | 1.372407 | -2.124362 | C | -2.168652 | 2.315350 | -1.811244 |
| H | 3.588638 | -3.459271 | -0.190900 | C | -3.112440 | 2.930306 | -0.820743 |
| H | 3.699187 | -2.633990 | 1.365180 | C | -3.958901 | 4.234650 | -1.507906 |
| H | 2.148528 | -2.719138 | 0.517482 | C | -2.921352 | 2.060889 | -3.083522 |
| H | 3.755865 | -2.298243 | -2.288613 | C | -0.796634 | 3.460503 | -2.026197 |
| H | 2.093044 | -1.930197 | -1.874250 | C | -1.467498 | 4.953720 | -2.484720 |
| H | 3.156914 | -0.652653 | -2.462982 | H | -3.020920 | 2.923776 | -3.579014 |
| H | 5.536155 | -2.096631 | -0.716554 | C | 0.023735 | 3.703498 | -0.557201 |
| H | 5.444962 | -0.366892 | -1.026733 | C | 0.298959 | 2.965136 | -3.227983 |
| H | 5.475331 | -0.974148 | 0.638841 | O | 1.529323 | -1.657929 | 0.816718 |
| H | -0.000564 | -1.480811 | -1.602494 | C | 1.653000 | -0.399728 | -1.682194 |
| | | | | C | 1.634675 | -1.572468 | -2.617259 |
| {33A} ₂ | | | | C | 0.263123 | -2.150619 | -2.803230 |
| 136 | | | | C | 0.182977 | -2.876564 | -4.338346 |
| E= -2862.722465 | | | | C | -4.064193 | 1.720044 | -0.100027 |
| P | -1.611604 | 0.565260 | 0.439498 | C | -2.207769 | 3.699522 | 0.395759 |
| C | -2.376952 | -1.096078 | 0.448481 | C | -1.042494 | -1.105155 | 3.409309 |
| C | -3.027271 | -1.196855 | -0.735561 | C | -3.144852 | 0.597297 | 2.660703 |
| C | -3.817165 | -2.461642 | -0.573136 | C | -2.827443 | -4.383789 | 0.986288 |
| C | -3.974340 | -2.609653 | 1.110924 | C | -0.434576 | -3.141342 | 1.844315 |
| C | -2.797128 | -1.864261 | 1.666407 | C | 2.469291 | 0.640901 | -1.932309 |
| C | -2.041336 | 0.911404 | -1.298677 | C | 2.975929 | 1.410028 | -0.774165 |
| C | -2.847843 | -0.101766 | -1.689906 | C | 2.086665 | 2.433941 | 2.781932 |
| O | 0.048939 | 0.448400 | 0.513733 | C | 2.557808 | 2.167863 | 4.393523 |
| P | 1.397677 | -0.352826 | 0.120957 | C | 3.615289 | 0.164679 | 2.448811 |
| C | 2.606853 | 0.977227 | 0.441209 | C | 4.781542 | 0.561685 | 3.620237 |
| C | 3.167304 | 1.419782 | 1.760315 | C | 2.287793 | 4.088080 | 2.445222 |
| C | 4.074974 | 2.522138 | 1.301027 | C | 0.439234 | 2.064153 | 2.583869 |
| C | -2.660468 | -1.015240 | 2.895426 | C | 1.911228 | -0.933128 | -3.945703 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 2.840709 | -2.869944 | -2.297824 | H | -0.795558 | -3.344855 | -4.486627 |
| C | 2.484658 | -4.131134 | -3.380704 | H | 0.325707 | -2.144421 | -5.138057 |
| C | 4.425212 | -2.320263 | -2.575671 | H | 0.945385 | -3.651645 | -4.454877 |
| C | 2.683783 | -3.510648 | -0.731021 | H | -1.887017 | -1.250639 | -2.914240 |
| C | -0.055342 | -3.339610 | -1.630677 | H | -0.861888 | -0.428564 | -1.728858 |
| C | -0.873068 | -0.888841 | -2.719652 | H | -0.644045 | -0.111265 | -3.454943 |
| C | 2.332059 | -0.661773 | 3.197342 | H | -0.815296 | -0.360367 | 4.179043 |
| C | 4.315348 | -0.861884 | 1.288602 | H | -0.830639 | -2.093895 | 3.827230 |
| C | 2.707778 | 0.438155 | -3.399285 | H | -0.348845 | -0.961482 | 2.577403 |
| C | 3.886214 | 2.562734 | -0.469781 | H | -3.098372 | 1.135418 | 3.613752 |
| C | -3.381032 | 0.469321 | -2.970362 | H | -2.516463 | 1.121787 | 1.941048 |
| H | -2.105551 | -4.605859 | 3.760254 | H | -4.176646 | 0.642666 | 2.299002 |
| H | -2.036522 | -2.921633 | 4.280431 | H | -3.451431 | -1.063176 | 5.057732 |
| H | -3.574532 | -3.624801 | 3.755536 | H | -4.711110 | -1.488928 | 3.897812 |
| H | -2.223860 | -5.297135 | 1.011152 | H | -3.478008 | -2.678887 | 4.342774 |
| H | -3.823267 | -4.635702 | 1.363602 | H | 1.092693 | 3.709358 | -3.352329 |
| H | -2.937398 | -4.079354 | -0.055608 | H | 0.763586 | 2.013076 | -2.964452 |
| H | -0.036593 | -4.161891 | 1.843186 | H | -0.196066 | 2.835964 | -4.195016 |
| H | -0.055232 | -2.616055 | 0.968639 | H | -0.670996 | 5.691883 | -2.625673 |
| H | -0.023984 | -2.626048 | 2.718307 | H | -2.033700 | 4.890436 | -3.416900 |
| H | 5.151407 | -3.101031 | -2.326938 | H | -2.138277 | 5.337329 | -1.710241 |
| H | 4.572377 | -2.047573 | -3.625016 | H | 0.939902 | 4.280912 | -0.724388 |
| H | 4.634034 | -1.446032 | -1.954685 | H | -0.605396 | 4.261952 | 0.140747 |
| H | 3.413913 | -4.313567 | -0.601088 | H | 0.306116 | 2.765426 | -0.078372 |
| H | 2.859642 | -2.755831 | 0.035524 | H | -4.520124 | 4.761639 | -0.729257 |
| H | 1.684172 | -3.924459 | -0.570337 | H | -3.275290 | 4.954504 | -1.967614 |
| H | 3.236268 | -4.921403 | -3.280413 | H | -4.671920 | 3.916268 | -2.272420 |
| H | 1.509516 | -4.576663 | -3.162025 | H | -4.787741 | 2.155173 | 0.596809 |
| H | 2.481042 | -3.807305 | -4.423920 | H | -4.614483 | 1.135970 | -0.843185 |
| H | -1.074987 | -3.727801 | -1.718868 | H | -3.430291 | 1.031634 | 0.466818 |
| H | 0.634615 | -4.181106 | -1.744051 | H | -2.877823 | 4.058705 | 1.183972 |
| H | 0.077785 | -2.935114 | -0.624074 | H | -1.490475 | 3.016700 | 0.856167 |

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|-----------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -1.659309 | 4.562106 | 0.006425 | C | 1.195798 | 0.039790 | 0.143770 |
| H | 1.627967 | 4.673049 | 3.094963 | C | 2.688109 | 0.118039 | 0.210073 |
| H | 3.311471 | 4.429040 | 2.619211 | C | 2.948971 | -0.223747 | 1.656095 |
| H | 2.023751 | 4.318078 | 1.410379 | P | -0.143594 | 0.219676 | -0.920489 |
| H | -0.177742 | 2.694914 | 3.232280 | O | -0.214254 | 0.569712 | -2.358618 |
| H | 0.132372 | 2.232488 | 1.550287 | C | -0.747879 | -0.403301 | 1.436242 |
| H | 0.227893 | 1.022736 | 2.822731 | C | -1.760364 | -0.712887 | 2.427259 |
| H | 1.972923 | 2.796788 | 5.072521 | C | -2.973284 | -0.645027 | 1.844391 |
| H | 2.408282 | 1.125311 | 4.688210 | C | -2.855263 | -0.276255 | 0.386345 |
| H | 3.614652 | 2.409750 | 4.542833 | C | -1.374106 | -0.142957 | 0.225496 |
| H | 5.052107 | -0.335903 | 4.186065 | Si | 3.217027 | 1.479315 | -0.132231 |
| H | 5.695647 | 0.950609 | 3.162680 | H | 3.943130 | -0.266004 | 2.080685 |
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| H | 3.539266 | -1.224009 | 0.610051 | H | -3.922640 | -0.825599 | 2.330732 |
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| H | 1.794532 | -0.043756 | 3.920952 | Si | 3.492660 | -1.410733 | -0.295452 |
| H | 1.628907 | -1.001050 | 2.432671 | C | -3.066413 | 1.792913 | -1.335269 |
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| H | 4.149369 | 3.059461 | -1.380227 | C | 4.980736 | -1.247838 | -0.200096 |
| H | 4.563760 | 2.957631 | 2.147393 | C | 3.053333 | -2.528011 | 0.603815 |
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| H | -2.819748 | -2.923271 | 0.756405 | H | 5.294123 | -0.450847 | -0.841573 |
| H | -5.317411 | -2.271304 | -0.789455 | H | 5.250584 | -1.019862 | 0.809909 |
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| H | -3.822248 | -0.007846 | -2.091112 | E: -2437.735250 | | | |
| H | -2.269834 | -0.806134 | -2.167358 | C | 1.288940 | 0.184809 | 0.374944 |
| H | -3.268301 | 2.832087 | -1.491022 | C | 0.722986 | 0.190278 | 1.619814 |
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| H | -4.789690 | 2.824245 | 0.428696 | C | 2.758902 | 0.061980 | 0.481216 |
| H | -5.287881 | 1.198299 | 0.027234 | C | -0.746328 | 0.166901 | 1.609794 |
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| H | -2.415356 | 3.333639 | 0.749721 | C | -2.981473 | 0.140168 | 1.927758 |
| H | -2.305113 | 2.065468 | 1.946656 | C | -2.777110 | 0.068343 | 0.457134 |
| H | -1.219856 | 2.071062 | 0.577258 | C | -1.299777 | 0.089980 | 0.360392 |
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| H | 5.091580 | 2.442261 | -0.286128 | C | -2.479028 | -2.952816 | 0.790136 |
| H | 5.010188 | 1.213549 | 0.953513 | Si | -3.493812 | 1.656728 | -0.339666 |
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| H | 3.197057 | 1.121379 | -2.214629 | C | 1.984702 | -2.899536 | 0.336517 |
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| H | 1.991838 | -2.644209 | 0.535794 | C | -3.110446 | -1.879795 | -1.996740 |
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| H | 3.660149 | 2.519735 | -2.584587 | {33B}2 | | | |
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| H | 2.006994 | 2.444910 | -1.981864 | E= | -4874.297091 | | |
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| C | 2.620529 | 1.424629 | 2.467006 | C | -3.575640 | -3.336265 | -0.704509 |
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| Si | 1.082715 | 1.779965 | 3.547800 | C | -4.671964 | 0.428075 | -1.913069 |
| C | 1.631877 | 2.577674 | 5.161063 | C | -3.323826 | -0.045220 | 2.963780 |
| H | 4.076613 | 1.241844 | 4.201170 | C | -3.714470 | 2.728950 | 0.855899 |
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| C | 2.316458 | 3.910598 | 0.521470 | H | -0.280860 | -2.874946 | -1.208244 |
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| Si | -1.262023 | 3.840392 | -1.863371 | H | -3.106441 | -4.321059 | -0.728985 |
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| H | 1.297311 | 0.451752 | -4.671244 | H | -0.078543 | 2.358236 | -3.465407 |
| H | 0.882872 | -1.264475 | -4.590636 | H | -1.199687 | 5.695980 | -3.464578 |
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| H | 4.787653 | 0.520939 | -2.277725 | H | -5.630993 | 3.355685 | -2.508154 |
| H | 4.085012 | -0.876859 | -5.642702 | H | -4.443526 | 4.019376 | -3.641552 |
| H | 5.047310 | -1.798315 | -4.486628 | H | -5.429006 | 0.114338 | -2.638887 |
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| H | -0.297894 | 2.556184 | 1.637952 | H | -3.834619 | 0.588323 | 3.675966 |
| H | 4.658180 | 4.959873 | 2.544251 | H | -4.386674 | 3.032787 | 1.646843 |
| H | 3.182258 | 4.701000 | 3.469879 | H | -4.072445 | 4.236986 | -0.668834 |
| H | 4.614867 | 3.708660 | 3.790351 | | | | |
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| H | 0.118768 | 5.526206 | -0.661103 | C | -2.955790 | -0.001908 | 2.099774 |
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| C | 2.810170 | -0.028412 | 0.580831 | F | -1.914073 | -1.990612 | -1.398596 |
| C | 1.299092 | -0.110593 | 0.483370 | F | -3.565414 | 2.451086 | -1.841962 |
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| O | 0.000034 | -0.077284 | -2.130541 | F | -4.191150 | 0.809382 | -1.919681 |
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| C | 2.343205 | 2.499424 | 0.446376 | F | -5.479292 | 1.065865 | 0.375841 |
| C | 3.464657 | -1.379122 | 0.024919 | F | -4.652165 | 1.975664 | 1.645518 |
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| C | -2.343521 | 2.499413 | 0.446951 | F | -1.389862 | 2.445654 | -0.080429 |
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| C | 4.694540 | 1.793772 | 0.568881 | F | 2.141627 | 2.470807 | 1.519323 |
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33CH

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| C | -0.727751 | 0.005555 | -1.508705 | F | 3.481397 | 3.171578 | 1.686523 |
| C | -1.316806 | 0.081587 | -0.299426 | F | 2.231776 | 1.479450 | 2.016437 |
| C | -2.846050 | 0.019281 | -0.503633 | C | -2.265495 | -2.595808 | -0.159814 |
| C | -2.916100 | -0.068473 | -2.040369 | F | -1.379284 | -2.484418 | 0.815830 |
| C | -1.702101 | -0.104436 | -2.580579 | C | -3.844451 | -1.569503 | 1.490504 |
| P | -0.000023 | 0.290406 | 0.978042 | F | -5.070815 | -1.085243 | 1.662719 |
| O | -0.000032 | -0.493506 | 2.228102 | F | -2.812231 | -3.810459 | -0.072934 |
| C | -3.406211 | -1.479768 | -0.018352 | F | -1.611295 | -2.573427 | -1.316960 |
| C | -4.592103 | -2.038598 | -0.912570 | C | -5.044324 | 1.661395 | -0.398912 |
| F | -4.119648 | -2.612519 | -2.024866 | F | -5.814430 | 0.743271 | 0.154832 |
| C | -3.519740 | 1.479299 | -0.037714 | C | -3.396834 | 1.854172 | 1.501241 |
| C | -2.752233 | 2.670924 | -0.798452 | F | -2.231834 | 1.479669 | 2.016407 |
| F | -2.610869 | 2.471970 | -2.103076 | F | -5.509271 | 2.835904 | 0.024996 |
| C | 3.406213 | -1.479692 | -0.018387 | F | -5.217317 | 1.621015 | -1.725003 |
| C | 3.844327 | -1.569557 | 1.490509 | F | 5.293509 | -2.957205 | -0.257549 |
| F | 2.998069 | -0.889951 | 2.248726 | F | 4.119587 | -2.612295 | -2.024978 |
| C | 3.519751 | 1.479275 | -0.037660 | F | 3.860053 | -2.819932 | 1.944939 |
| C | 2.752346 | 2.670961 | -0.798442 | F | 5.070590 | -1.085150 | 1.662990 |
| F | 1.534372 | 2.849199 | -0.278592 | F | -3.860123 | -2.819810 | 1.945131 |
| C | 2.265612 | -2.595832 | -0.159962 | F | -2.998419 | -0.889686 | 2.248761 |
| F | 1.611425 | -2.573432 | -1.317113 | F | -5.293429 | -2.957348 | -0.257336 |
| C | 4.592104 | -2.038443 | -0.912681 | F | -5.448861 | -1.104308 | -1.312151 |
| F | 5.448786 | -1.104112 | -1.312333 | F | -3.481634 | 3.171652 | 1.686411 |
| F | 2.812491 | -3.810420 | -0.073150 | F | -4.368270 | 1.308137 | 2.218864 |
| | | | | F | -3.392974 | 3.828702 | -0.683492 |
| | | | | F | -1.534329 | 2.849233 | -0.278455 |
| | | | | F | 5.509387 | 2.835727 | 0.025429 |

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|---------------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| F | 5.814414 | 0.743087 | 0.155008 | C | -2.345007 | -2.080182 | -1.746702 |
| F | 3.393064 | 3.828746 | -0.683311 | C | 4.456901 | -0.917669 | 1.145565 |
| F | 2.611128 | 2.472104 | -2.103092 | C | 4.307791 | 0.541637 | 0.718485 |
| H | 3.848733 | -0.100067 | -2.574721 | C | 2.723241 | -0.514289 | 3.257865 |
| H | 1.478720 | -0.188115 | -3.634057 | C | 1.776805 | -1.375012 | 4.120956 |
| H | -3.848735 | -0.099974 | -2.574720 | C | -2.832525 | -0.558656 | 2.888521 |
| H | -1.478711 | -0.188151 | -3.634056 | C | -1.379566 | -0.516688 | 3.386210 |
| H | -0.000127 | 1.680939 | 1.127836 | C | -4.513035 | 0.934820 | 1.278179 |
| {33C} ₂ | | | | C | -4.445410 | 0.160856 | -0.046775 |
| 136 | | | | C | -0.528971 | 3.247737 | 1.134627 |
| E= -10007.8602808 | | | | C | -0.110039 | 2.670556 | -0.013029 |
| C | 2.913069 | -3.773088 | 1.991279 | C | 0.508185 | 3.755996 | -0.917150 |
| C | 1.967603 | -3.164174 | 1.066221 | C | 0.509414 | 4.926843 | 0.052501 |
| C | 2.037664 | -1.811517 | 1.117965 | C | -0.098206 | 4.635737 | 1.207817 |
| C | 3.209194 | -1.416293 | 2.037732 | C | 2.007432 | 3.425275 | -1.322778 |
| C | 3.603131 | -2.786086 | 2.571163 | C | 2.147124 | 2.023609 | -1.927517 |
| P | 1.127768 | -1.147707 | -0.327609 | C | -0.536148 | 4.157082 | -2.091944 |
| O | -0.082322 | -0.186443 | 0.368995 | C | -1.987347 | 4.119353 | -1.569584 |
| P | -0.973547 | 1.071322 | -0.146495 | O | -1.583254 | 0.825862 | -1.477920 |
| C | -1.988263 | 1.363151 | 1.341025 | C | 0.384900 | -4.081266 | -4.426997 |
| C | -3.171741 | 0.824487 | 2.157530 | C | 0.038309 | -1.692366 | -3.794447 |
| C | -3.240548 | 1.893075 | 3.240073 | C | -2.477385 | -4.178838 | -3.050436 |
| C | -2.300584 | 2.833344 | 3.094249 | C | -2.237368 | -4.249244 | -0.589798 |
| C | -1.536426 | 2.505531 | 1.900515 | C | 5.809844 | -1.082300 | 1.868414 |
| C | 1.114052 | -3.704777 | 0.025272 | C | 4.578468 | -1.751079 | -0.147219 |
| C | 0.430012 | -2.795509 | -0.716998 | C | 3.853860 | -0.045327 | 4.185999 |
| C | -0.187456 | -3.518875 | -1.931734 | C | 1.944357 | 0.735226 | 2.815828 |
| C | 0.245191 | -4.947983 | -1.643146 | C | -3.699655 | -0.815430 | 4.138513 |
| C | 0.977508 | -5.043451 | -0.528841 | C | -2.939541 | -1.776933 | 1.967375 |
| C | 0.537508 | -3.052363 | -3.287208 | C | 2.641429 | 4.430661 | -2.295865 |
| C | 2.060861 | -2.929213 | -3.062019 | C | 2.862751 | 3.466634 | -0.041222 |
| C | -1.786016 | -3.496246 | -1.861090 | C | -0.318971 | 5.603588 | -2.587851 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -0.471050 | 3.217950 | -3.304904 | F | -0.956753 | -1.760709 | -4.237483 |
| C | -5.758328 | 0.447143 | 2.034672 | F | 0.007896 | -0.932257 | -3.009837 |
| C | -4.765055 | 2.412866 | 0.909769 | F | 2.557098 | -2.869248 | -4.034936 |
| H | 4.357717 | -2.913182 | 3.335635 | F | 2.323436 | -2.025424 | -2.513048 |
| F | -3.544650 | -4.266103 | -2.825156 | F | 2.469337 | -3.793305 | -2.533124 |
| F | -2.391844 | -3.594311 | -3.967982 | F | 0.840849 | -3.666292 | -5.330809 |
| F | -2.102442 | -5.188001 | -3.239482 | F | 0.912131 | -5.010652 | -4.197551 |
| F | -3.303671 | -4.068000 | -0.426651 | F | -0.646070 | -4.323205 | -4.669493 |
| F | -2.093057 | -5.328160 | -0.674496 | F | 1.243095 | -0.738345 | 4.831673 |
| F | -1.702562 | -3.900130 | 0.295401 | F | 1.035127 | -1.890255 | 3.510107 |
| F | -3.431045 | -2.130956 | -1.628193 | F | 2.326579 | -2.125091 | 4.693503 |
| F | -1.942465 | -1.572159 | -0.875776 | F | 3.405765 | 0.425719 | 5.066355 |
| F | -2.141427 | -1.444919 | -2.602112 | F | 4.473421 | -0.872286 | 4.542475 |
| F | -5.608330 | 2.465735 | 0.215951 | F | 4.499879 | 0.699027 | 3.717186 |
| F | -5.014989 | 3.020037 | 1.781797 | F | 1.500061 | 1.209099 | 3.696681 |
| F | -3.903477 | 2.863164 | 0.413846 | F | 2.582243 | 1.478346 | 2.342419 |
| F | -5.378993 | 0.330020 | -0.592924 | F | 1.132021 | 0.496960 | 2.133862 |
| F | -3.629310 | 0.489252 | -0.690402 | F | 6.589174 | -0.615620 | 1.258378 |
| F | -4.350888 | -0.911941 | 0.096693 | F | 5.844464 | -0.614997 | 2.849298 |
| F | -6.644083 | 0.696424 | 1.442966 | F | 6.074856 | -2.136217 | 1.980468 |
| F | -5.759425 | -0.635338 | 2.172555 | F | 5.540062 | -1.525999 | -0.617755 |
| F | -5.874903 | 0.925152 | 3.010578 | F | 4.548754 | -2.824419 | 0.048956 |
| F | -2.499011 | -2.641925 | 2.472831 | F | 3.800358 | -1.507263 | -0.870641 |
| F | -3.971249 | -2.035187 | 1.723073 | F | 5.057074 | 0.774356 | -0.045030 |
| F | -2.384319 | -1.629031 | 1.042177 | F | 3.328660 | 0.730892 | 0.280140 |
| F | -3.466403 | -1.814441 | 4.518442 | F | 4.457467 | 1.238751 | 1.544212 |
| F | -3.469134 | -0.107828 | 4.938483 | F | 3.858601 | 3.068192 | -0.248657 |
| F | -4.770220 | -0.783492 | 3.951078 | F | 2.985501 | 4.486013 | 0.330346 |
| F | -1.209730 | -1.362401 | 4.057928 | F | 2.415104 | 2.867799 | 0.753796 |
| F | -0.677202 | -0.601772 | 2.559839 | F | 3.203521 | 1.812089 | -2.120012 |
| F | -1.156887 | 0.397301 | 3.942177 | F | 1.791884 | 1.254386 | -1.243708 |
| F | 0.718038 | -1.334780 | -4.574331 | F | 1.609552 | 1.902727 | -2.865131 |

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|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| F | 3.701959 | 4.183578 | -2.403825 | C | 1.291999 | 0.006827 | -0.634178 |
| F | 2.198606 | 4.394602 | -3.291659 | P | -0.007897 | 0.233063 | 0.550163 |
| F | 2.586739 | 5.457640 | -1.925665 | O | -0.041939 | -0.340583 | 1.937784 |
| F | -0.963233 | 5.770133 | -3.455924 | Si | 3.457578 | -1.625111 | -0.034660 |
| F | -0.607139 | 6.333717 | -1.827601 | C | 2.656768 | -3.003862 | -1.023634 |
| F | 0.700808 | 5.817474 | -2.898509 | Si | 3.450923 | 1.670562 | -0.000403 |
| F | -2.633824 | 4.601442 | -2.308707 | C | 3.394451 | 1.625825 | 1.873367 |
| F | -2.349052 | 3.099854 | -1.443759 | Si | -3.380508 | -1.665853 | -0.012367 |
| F | -2.101931 | 4.665799 | -0.630654 | C | -2.177757 | -2.978936 | -0.602212 |
| F | -1.291332 | 3.475731 | -3.982230 | Si | -3.532052 | 1.624602 | -0.029116 |
| F | 0.456515 | 3.330873 | -3.868625 | C | -5.394931 | 1.618325 | -0.271748 |
| F | -0.606456 | 2.175472 | -3.016793 | C | 5.323590 | -1.686783 | -0.258871 |
| H | -0.066742 | -5.781219 | -2.258569 | C | 3.040306 | -1.836876 | 1.777758 |
| H | 1.392487 | -5.946862 | -0.101423 | C | -3.383975 | -1.620737 | 1.858880 |
| H | 3.017819 | -4.833749 | 2.178236 | C | -5.101528 | -2.051467 | -0.661160 |
| H | -3.991205 | 1.878284 | 4.018013 | C | -3.150727 | 1.813891 | 1.798534 |
| H | -2.146155 | 3.699479 | 3.723756 | C | -2.767164 | 3.052161 | -0.975972 |
| H | -0.254962 | 5.301328 | 2.046037 | C | 5.211961 | 1.954552 | -0.587125 |
| H | 0.958352 | 5.878909 | -0.196101 | C | 2.359714 | 3.058213 | -0.637320 |

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E= -6009.660585

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -1.300515 | 0.050609 | -0.643771 | H | 3.944616 | 0.044938 | -2.674897 |
| C | -0.731923 | 0.043416 | -1.899575 | H | 1.644607 | 0.063263 | -3.943025 |
| C | -1.779617 | 0.001578 | -2.877756 | H | -3.946195 | -0.063456 | -2.686029 |
| C | -2.970347 | -0.019474 | -2.218326 | H | -1.644963 | -0.020967 | -3.950868 |
| C | -2.777480 | 0.012746 | -0.742419 | F | -3.141970 | 4.007394 | -0.595957 |
| C | 0.727659 | 0.035048 | -1.893753 | F | -1.678599 | 3.051425 | -0.870784 |
| C | 1.777542 | 0.056597 | -2.869497 | F | -2.998281 | 2.995253 | -2.042491 |
| C | 2.967153 | 0.052902 | -2.208335 | F | -5.804935 | 2.602835 | -0.026065 |
| C | 2.771209 | 0.033149 | -0.733179 | F | -5.674290 | 1.390832 | -1.304215 |
| | | | | F | -5.881821 | 0.888783 | 0.381230 |
| | | | | F | -3.275426 | 2.863716 | 2.082664 |
| | | | | F | -3.826873 | 1.221010 | 2.417846 |
| | | | | F | -2.130670 | 1.519522 | 2.058339 |

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|-----------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| F | -3.519065 | -2.637630 | 2.241592 | C | 0.742682 | 0.048112 | -1.678858 |
| F | -2.435424 | -1.239360 | 2.248829 | C | 1.760631 | 0.038655 | -2.689885 |
| F | -4.197170 | -1.008553 | 2.256870 | C | 2.965856 | 0.020134 | -2.077725 |
| F | -5.476507 | -2.967484 | -0.193907 | C | 2.792592 | 0.009886 | -0.574811 |
| F | -5.817842 | -1.254226 | -0.448718 | C | -0.720157 | 0.035421 | -1.679698 |
| F | -5.087097 | -2.213878 | -1.742558 | C | -1.282055 | 0.003894 | -0.438306 |
| F | -2.591345 | -3.979616 | -0.443829 | C | -2.776099 | -0.004674 | -0.589060 |
| F | -1.958535 | -2.865611 | -1.667625 | C | -2.940847 | 0.024388 | -2.091283 |
| F | -1.234216 | -2.913450 | -0.053866 | C | -1.732655 | 0.051646 | -2.696216 |
| F | 2.962474 | -3.978191 | -0.630313 | P | 0.010643 | 0.017697 | 0.853871 |
| F | 1.566694 | -2.943054 | -0.963558 | O | 0.042374 | -1.042250 | 1.883564 |
| F | 2.936605 | -2.960224 | -2.078990 | Si | -3.484831 | -1.671772 | -0.021444 |
| F | 5.683824 | -2.701690 | -0.063537 | C | -5.120269 | -2.058839 | -0.995699 |
| F | 5.628585 | -1.416887 | -1.273796 | F | -4.825977 | -2.529864 | -2.223216 |
| F | 5.835838 | -1.019213 | 0.439442 | Si | -3.408400 | 1.678330 | -0.002022 |
| F | 3.252975 | -2.870900 | 2.069243 | C | -2.622122 | 3.095890 | -1.074820 |
| F | 3.638189 | -1.185094 | 2.418228 | F | -3.132924 | 3.113949 | -2.317877 |
| F | 1.986519 | -1.635841 | 1.989715 | Si | 3.424799 | -1.694673 | -0.016309 |
| F | 2.826545 | 4.029910 | -0.449366 | C | 3.150447 | -2.190051 | 1.844110 |
| F | 2.194086 | 2.962648 | -1.714084 | F | 2.137252 | -3.041752 | 1.981986 |
| F | 1.382979 | 3.053730 | -0.146148 | Si | 3.463768 | 1.686786 | -0.016914 |
| F | 3.492094 | 2.641673 | 2.268833 | C | 2.268116 | 3.122657 | -0.549106 |
| F | 2.455877 | 1.208252 | 2.249897 | F | 1.218487 | 3.211380 | 0.290023 |
| F | 4.213749 | 1.030801 | 2.285552 | C | 2.582250 | -3.067303 | -1.101995 |
| F | 5.610347 | 2.866561 | -0.131512 | F | 3.078807 | -3.062790 | -2.354839 |
| F | 5.879735 | 1.131973 | -0.322002 | C | 5.319878 | -1.919291 | -0.351901 |
| F | 5.248998 | 2.084572 | -1.672345 | F | 6.059632 | -1.234464 | 0.533062 |
| | | | | F | 2.836655 | -4.275750 | -0.582041 |
| | | | | F | 1.252768 | -2.941771 | -1.202437 |
| | | | | C | 3.643142 | 1.881182 | 1.895109 |
| | | | | F | 4.618241 | 1.090839 | 2.369311 |
| | | | | C | 5.161629 | 2.149272 | -0.828323 |
| 33DH | | | | | | | |
| 69 | | | | | | | |
| E: -6010.291270 | | | | | | | |
| C | 1.299459 | 0.035636 | -0.435780 | | | | |

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|---|-----------|-----------|-----------|---------------------------|-----------|-----------|-----------|
| F | 4.971292 | 2.521991 | -2.109740 | H | 1.597453 | 0.044433 | -3.757680 |
| F | 3.941879 | 3.142188 | 2.231541 | H | -3.905941 | 0.037415 | -2.577855 |
| F | 2.501099 | 1.559179 | 2.524803 | H | -1.563099 | 0.085252 | -3.762508 |
| C | -2.295495 | -3.128425 | -0.489329 | H | -0.004374 | 1.343398 | 1.325915 |
| F | -1.277954 | -3.254931 | 0.359754 | | | | |
| C | -3.893466 | -1.805093 | 1.864069 | {33D} ₂ | | | |
| F | -4.720009 | -0.794665 | 2.216208 | 136 | | | |
| F | -2.989583 | -4.281390 | -0.467292 | E= -12019.3640216 | | | |
| F | -1.786146 | -2.992873 | -1.725846 | C | 3.777530 | -3.086304 | 1.756346 |
| C | -5.313177 | 1.971236 | -0.187416 | C | 2.943973 | -2.497376 | 0.750089 |
| F | -6.042222 | 1.174130 | 0.600700 | C | 2.459653 | -1.275797 | 1.131517 |
| C | -2.916495 | 2.057584 | 1.839726 | C | 3.133399 | -0.933388 | 2.465931 |
| F | -1.932138 | 2.972517 | 1.894613 | C | 3.901337 | -2.207979 | 2.769926 |
| F | -5.612689 | 3.239723 | 0.129962 | P | 1.674397 | -0.451257 | -0.348547 |
| F | -5.710536 | 1.774339 | -1.456802 | O | 0.066877 | -0.267844 | 0.105418 |
| F | 5.669583 | -3.208685 | -0.263093 | P | -1.245371 | 0.615627 | -0.204508 |
| F | 5.668891 | -1.500409 | -1.584064 | C | -2.279386 | 0.066372 | 1.230456 |
| F | 4.254887 | -2.801603 | 2.313182 | C | -3.111939 | -1.052680 | 1.822923 |
| F | 2.925340 | -1.127580 | 2.623435 | C | -3.322815 | -0.561545 | 3.244416 |
| F | -4.531250 | -2.953958 | 2.128184 | C | -2.813042 | 0.678553 | 3.394833 |
| F | -2.819846 | -1.749154 | 2.643189 | C | -2.214711 | 1.070337 | 2.154718 |
| F | -5.887382 | -2.965719 | -0.389552 | C | 2.678039 | -2.864362 | -0.626246 |
| F | -5.867286 | -0.952753 | -1.175801 | C | 1.835816 | -2.028288 | -1.305595 |
| F | -3.940087 | 2.520238 | 2.559660 | C | 1.824966 | -2.491244 | -2.759039 |
| F | -2.452497 | 0.952746 | 2.451898 | C | 2.808531 | -3.647058 | -2.739390 |
| F | -2.894375 | 4.285260 | -0.517614 | C | 3.267414 | -3.848714 | -1.489125 |
| F | -1.288964 | 3.005057 | -1.193062 | Si | 2.544220 | -1.224113 | -3.972143 |
| F | 5.747982 | 3.169458 | -0.193765 | C | 4.245526 | -0.563883 | -3.310923 |
| F | 6.026962 | 1.127202 | -0.840510 | Si | 0.222131 | -3.467970 | -3.116984 |
| F | 2.919403 | 4.293509 | -0.489853 | C | -1.443424 | -2.523590 | -2.854701 |
| F | 1.778929 | 2.999888 | -1.789574 | Si | 4.582147 | 0.220922 | 1.911505 |
| H | 3.933518 | -0.002175 | -2.558453 | C | 3.946305 | 1.863413 | 1.073090 |

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|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Si | 2.248339 | -0.489021 | 4.102533 | H | 4.499999 | -2.347385 | 3.658598 |
| C | 0.717178 | -1.441358 | 4.856802 | F | -0.749194 | -5.136089 | -5.042598 |
| Si | -2.531121 | -2.867418 | 1.887842 | F | -0.382211 | -3.136817 | -5.762569 |
| C | -0.611853 | -2.993543 | 1.687898 | F | 1.278264 | -4.499182 | -5.432509 |
| Si | -4.923710 | -0.668064 | 1.245026 | F | -1.056541 | -5.668835 | -2.189011 |
| C | -5.277870 | -0.892225 | -0.666810 | F | 0.979718 | -6.053059 | -2.801017 |
| C | -1.762581 | 2.364422 | 1.626813 | F | 0.583472 | -5.150092 | -0.884179 |
| C | -1.143788 | 2.317079 | 0.417780 | F | -2.478431 | -3.290463 | -3.224344 |
| C | -1.234665 | 3.693321 | -0.219328 | F | -1.633272 | -2.193744 | -1.564638 |
| C | -1.913166 | 4.488682 | 0.880834 | F | -1.479862 | -1.411525 | -3.585606 |
| C | -2.189036 | 3.700433 | 1.939632 | F | -6.717343 | 1.361721 | 1.143550 |
| Si | 0.439162 | 4.593874 | -0.381314 | F | -6.122211 | 0.857460 | 3.155162 |
| C | 1.786289 | 3.770488 | -1.507410 | F | -4.861654 | 2.105978 | 1.947924 |
| Si | -2.486748 | 3.708864 | -1.675131 | F | -6.042262 | 0.084699 | -1.164748 |
| C | -4.157920 | 2.835325 | -1.205238 | F | -4.147740 | -0.936548 | -1.376208 |
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| C | 2.997749 | -1.858883 | -5.753831 | F | -7.423885 | -1.647511 | 1.638829 |
| C | 1.363074 | 0.286928 | -4.170548 | F | -5.892838 | -3.177832 | 1.741159 |
| C | 0.086091 | -4.093839 | -4.950234 | F | -6.201670 | -1.843816 | 3.408471 |
| C | 0.185269 | -5.169583 | -2.160120 | F | -2.207632 | -4.937093 | 0.175081 |
| C | 5.874149 | 0.915184 | 3.203311 | F | -4.113437 | -4.999618 | 1.165805 |
| C | 5.820483 | -0.678899 | 0.688518 | F | -3.792145 | -3.604167 | -0.452681 |
| C | 3.471521 | -0.761118 | 5.603936 | F | -2.553004 | -4.982315 | 3.585456 |
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| C | -3.220492 | -4.172447 | 0.613827 | F | -0.113626 | -4.086719 | 2.276633 |
| C | 0.319490 | 6.409188 | -1.065067 | F | -0.243721 | -3.032152 | 0.405689 |
| C | 1.140909 | 4.915820 | 1.409438 | F | 0.000767 | -1.927992 | 2.232765 |
| C | -3.187323 | 5.492147 | -2.069876 | F | 2.020490 | 1.440534 | -4.326091 |
| C | -1.831332 | 3.073352 | -3.395686 | F | 0.530186 | 0.146817 | -5.208369 |
| C | -6.180512 | -1.905230 | 2.068206 | F | 0.612085 | 0.383703 | -3.059361 |
| C | -5.664041 | 1.034698 | 1.901551 | F | 4.817553 | 0.272142 | -4.183846 |

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| F | 4.106955 | 0.110502 | -2.160130 | F | -4.280040 | 5.338716 | -2.840240 |
| F | 5.108828 | -1.570930 | -3.095874 | F | -3.574282 | 6.163137 | -0.968745 |
| F | 3.724006 | -0.913913 | -6.372316 | F | -2.344361 | 6.283720 | -2.735811 |
| F | 3.752108 | -2.973060 | -5.705186 | F | -4.838700 | 2.497164 | -2.298924 |
| F | 1.944822 | -2.109288 | -6.531752 | F | -4.004598 | 1.719048 | -0.464361 |
| F | 0.745452 | -1.249476 | 6.188402 | F | -4.929211 | 3.663517 | -0.482750 |
| F | -0.456969 | -0.935730 | 4.446967 | F | -2.458036 | 2.004190 | -3.865329 |
| F | 0.720463 | -2.758251 | 4.644835 | F | -1.962532 | 4.046491 | -4.317299 |
| F | 3.243082 | 0.116119 | 6.584315 | F | -0.518899 | 2.798735 | -3.311037 |
| F | 3.298032 | -2.000446 | 6.102700 | H | 3.044001 | -4.232650 | -3.617169 |
| F | 4.772639 | -0.679289 | 5.287380 | H | 3.964394 | -4.617430 | -1.189187 |
| F | 0.950048 | 1.660466 | 5.213105 | H | 4.261885 | -4.049903 | 1.694183 |
| F | 2.554755 | 2.220127 | 3.878725 | H | -3.878825 | -1.115507 | 3.986884 |
| F | 0.695186 | 1.419478 | 3.079257 | H | -2.878299 | 1.284155 | 4.286453 |
| F | 6.700075 | 1.737163 | 2.531596 | H | -2.682808 | 4.013676 | 2.847576 |
| F | 5.309623 | 1.635676 | 4.182769 | H | -2.107545 | 5.548572 | 0.806437 |
| F | 6.644392 | -0.024438 | 3.761931 | | | | |
| F | 6.585397 | 0.246069 | 0.094948 | 33F | | | |
| F | 6.641508 | -1.487671 | 1.383605 | 152 | | | |
| F | 5.280702 | -1.425353 | -0.281560 | E: -3731.720817 | | | |
| F | 4.312626 | 1.913395 | -0.207873 | C | -1.676028 | 3.005358 | -0.647609 |
| F | 2.595061 | 1.951797 | 1.118464 | C | -2.756930 | 2.639214 | 0.146829 |
| F | 4.416203 | 2.957364 | 1.674242 | C | -3.253274 | 3.620608 | 1.021414 |
| F | 2.450842 | 5.171901 | 1.404747 | C | -2.659864 | 4.861249 | 1.153094 |
| F | 0.526457 | 5.998769 | 1.931492 | C | -1.542003 | 5.184228 | 0.393492 |
| F | 0.928166 | 3.905397 | 2.260165 | C | -1.069991 | 4.255892 | -0.513963 |
| F | 3.012261 | 4.111682 | -1.085771 | C | -3.598952 | 1.305337 | 0.080486 |
| F | 1.698251 | 2.432530 | -1.487596 | C | -3.894411 | 0.947669 | 1.559645 |
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| F | 1.426050 | 7.083174 | -0.708352 | C | -3.084400 | 0.929117 | 3.857797 |
| F | 0.238517 | 6.463159 | -2.397315 | C | -4.302531 | 0.445957 | 4.314492 |
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| C | -5.097986 | 0.419988 | 2.036375 | C | 7.009013 | 2.276076 | 0.897874 |
| C | -2.839581 | 0.004993 | -0.684180 | C | 5.625880 | 2.220797 | 0.774386 |
| C | -1.328764 | 0.046191 | -0.525946 | C | -2.493983 | -2.228007 | 0.832223 |
| C | -0.712835 | 0.095999 | -1.762323 | C | -1.433000 | -3.126563 | 0.663154 |
| C | -1.718129 | 0.186570 | -2.794063 | C | -0.695655 | -3.617501 | 1.735003 |
| C | -2.921429 | 0.136588 | -2.204229 | C | -1.012067 | -3.255695 | 3.033931 |
| C | -3.316734 | -1.625376 | -0.356682 | C | -2.092464 | -2.413217 | 3.234497 |
| C | -4.826912 | -1.722169 | -0.076726 | C | -2.811470 | -1.919511 | 2.156802 |
| C | -5.345643 | -2.652632 | 0.826293 | C | -3.078468 | -2.515281 | -1.633883 |
| C | -6.714495 | -2.790185 | 1.016675 | C | -4.122128 | -3.221300 | -2.238960 |
| C | -7.609767 | -2.018585 | 0.288132 | C | -3.925204 | -4.018659 | -3.364279 |
| C | -7.113836 | -1.134913 | -0.660487 | C | -2.670939 | -4.144160 | -3.932368 |
| C | -5.744700 | -1.005681 | -0.844416 | C | -1.610094 | -3.470121 | -3.340494 |
| P | -0.053996 | -0.046778 | 0.629471 | C | -1.813339 | -2.689185 | -2.216016 |
| O | -0.147201 | -0.008790 | 2.105608 | C | -4.830743 | 1.886299 | -0.705022 |
| C | 0.714271 | -0.002147 | -1.731379 | C | -6.068958 | 2.177552 | -0.129713 |
| C | 1.292558 | -0.005659 | -0.463190 | C | -7.097014 | 2.771617 | -0.855031 |
| C | 2.821462 | -0.071921 | -0.596710 | C | -6.916824 | 3.128226 | -2.180180 |
| C | 2.914556 | -0.289844 | -2.110445 | C | -5.662840 | 2.939022 | -2.746693 |
| C | 1.728927 | -0.196010 | -2.730395 | C | -4.642220 | 2.358449 | -2.011909 |
| C | 3.474484 | -1.327337 | 0.256863 | C | 3.378431 | -1.018211 | 1.768830 |
| C | 2.760865 | -2.709837 | 0.030798 | C | 4.284517 | -0.186309 | 2.432651 |
| C | 3.241441 | -3.771698 | 0.815478 | C | 4.151792 | 0.112182 | 3.779305 |
| C | 2.790100 | -5.067646 | 0.654490 | C | 3.087692 | -0.399884 | 4.510004 |
| C | 1.838207 | -5.362979 | -0.318188 | C | 2.167201 | -1.212667 | 3.869281 |
| C | 1.354755 | -4.334200 | -1.103730 | C | 2.320159 | -1.524257 | 2.524695 |
| C | 1.806116 | -3.025564 | -0.926796 | C | 4.919540 | -1.721734 | -0.202975 |
| C | 3.460737 | 1.522285 | -0.423543 | C | 5.095139 | -2.241991 | -1.493826 |
| C | 5.003355 | 1.529254 | -0.269903 | C | 6.328990 | -2.665216 | -1.956182 |
| C | 5.853133 | 0.909309 | -1.191513 | C | 7.438977 | -2.636682 | -1.119333 |
| C | 7.234356 | 0.967795 | -1.083406 | C | 7.268166 | -2.219851 | 0.188683 |
| C | 7.825678 | 1.650890 | -0.031743 | C | 6.027407 | -1.781549 | 0.640619 |

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| C | 3.068866 | 2.294775 | -1.730711 | H | -7.078845 | -3.512029 | 1.739043 |
| C | 3.954134 | 2.617866 | -2.757125 | H | -8.678016 | -2.119682 | 0.442650 |
| C | 3.519852 | 3.246728 | -3.921000 | H | -7.786526 | -0.533163 | -1.260750 |
| C | 2.185775 | 3.577609 | -4.088482 | H | -5.407501 | -0.322918 | -1.606862 |
| C | 1.299934 | 3.322005 | -3.048092 | H | -6.258149 | 1.971763 | 0.909909 |
| C | 1.744019 | 2.719852 | -1.883036 | H | -8.043778 | 2.961685 | -0.361549 |
| C | 2.834695 | 2.393935 | 0.700822 | H | -7.719780 | 3.583737 | -2.748152 |
| C | 2.990495 | 3.787654 | 0.593745 | H | -5.463444 | 3.271946 | -3.759213 |
| C | 2.433258 | 4.657024 | 1.513792 | H | -3.661791 | 2.308599 | -2.462128 |
| C | 1.684433 | 4.165986 | 2.580150 | H | -1.934451 | 1.567319 | 2.202019 |
| C | 1.542479 | 2.798555 | 2.716933 | H | -2.267492 | 1.109986 | 4.546311 |
| C | 2.127727 | 1.930420 | 1.796794 | H | -4.464053 | 0.261148 | 5.370678 |
| H | -3.852695 | 0.088317 | -2.744120 | H | -6.256445 | -0.222741 | 3.713066 |
| H | -1.530848 | 0.215706 | -3.858340 | H | -5.890974 | 0.145680 | 1.361725 |
| H | 3.849740 | -0.378902 | -2.632749 | H | -4.126922 | 3.406363 | 1.623115 |
| H | 1.565126 | -0.224362 | -3.798489 | H | -3.075142 | 5.577173 | 1.853478 |
| H | 1.404001 | -2.267927 | -1.573320 | H | -1.056412 | 6.147270 | 0.499041 |
| H | 0.606688 | -4.534596 | -1.862947 | H | -0.210207 | 4.499304 | -1.125210 |
| H | 1.483472 | -6.377899 | -0.455757 | H | -1.284325 | 2.332721 | -1.391689 |
| H | 3.191394 | -5.853493 | 1.284469 | H | 5.094946 | 0.269731 | 1.891935 |
| H | 3.998272 | -3.576397 | 1.565418 | H | 4.875524 | 0.768626 | 4.249449 |
| H | -0.954241 | -2.200119 | -1.790671 | H | 2.971900 | -0.155618 | 5.559933 |
| H | -0.609767 | -3.549567 | -3.753556 | H | 1.302422 | -1.595780 | 4.397784 |
| H | -2.516755 | -4.759514 | -4.811378 | H | 1.572599 | -2.156501 | 2.067275 |
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| H | -5.124839 | -3.170494 | -1.844212 | H | 7.842199 | 0.456734 | -1.820578 |
| H | -3.663159 | -1.304640 | 2.372422 | H | 8.904761 | 1.694191 | 0.061895 |
| H | -2.388546 | -2.117738 | 4.234420 | H | 7.442925 | 2.817389 | 1.731249 |
| H | -0.436612 | -3.636496 | 3.870492 | H | 5.027157 | 2.712218 | 1.528034 |
| H | 0.127844 | -4.293379 | 1.532831 | H | 4.238975 | -2.361854 | -2.143416 |
| H | -1.157670 | -3.495303 | -0.308360 | H | 6.415458 | -3.049137 | -2.966727 |
| H | -4.678074 | -3.284643 | 1.394283 | H | 8.407320 | -2.971816 | -1.473141 |

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|-----------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 8.103666 | -2.232284 | 0.879564 | C | -1.673450 | 0.345595 | -2.624881 |
| H | 5.948195 | -1.503568 | 1.678513 | C | -2.869374 | 0.503152 | -2.049104 |
| H | 3.555706 | 4.201137 | -0.232640 | C | 0.716152 | -0.150089 | -1.588254 |
| H | 2.573752 | 5.725002 | 1.388901 | C | 1.334240 | -0.021327 | -0.393530 |
| H | 1.222308 | 4.844753 | 3.287850 | C | 2.850172 | -0.156226 | -0.580295 |
| H | 0.969967 | 2.372350 | 3.532208 | C | 2.869956 | -0.542374 | -2.062428 |
| H | 2.004710 | 0.880555 | 1.976840 | C | 1.658952 | -0.504776 | -2.625814 |
| H | 5.006364 | 2.395297 | -2.668359 | C | 3.548683 | -1.339614 | 0.361672 |
| H | 4.241671 | 3.478721 | -4.696338 | C | 4.859286 | -1.924723 | -0.270292 |
| H | 1.844188 | 4.055782 | -4.999498 | C | 6.101403 | -1.950518 | 0.360329 |
| H | 0.256241 | 3.604527 | -3.139382 | C | 7.210771 | -2.547788 | -0.231520 |
| H | 1.048374 | 2.571757 | -1.070828 | C | 7.109963 | -3.159965 | -1.467942 |
| | | | | C | 5.860834 | -3.223363 | -2.076534 |
| 33FH | | | | C | 4.759789 | -2.642768 | -1.471306 |
| 153 | | | | C | 3.469420 | 1.453671 | -0.592422 |
| E: -3732.356263 | | | | C | 2.963430 | 2.099444 | -1.925826 |
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| C | -3.082530 | -2.392023 | 0.567720 | C | 3.229502 | 2.760415 | -4.248587 |
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| C | -1.809270 | -3.053969 | 2.523305 | P | 0.032439 | 0.258471 | 0.842423 |
| C | -3.548957 | -1.422596 | -0.556260 | O | 0.115867 | -0.428414 | 2.160858 |
| C | -3.033095 | -2.157259 | -1.841270 | C | -3.501741 | 1.339041 | 0.384824 |
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| C | -1.728883 | -2.667165 | -1.832134 | C | -7.302774 | 2.194485 | 0.255556 |
| C | -2.843874 | 0.169834 | -0.556762 | C | -6.079523 | 1.709565 | 0.708627 |
| C | -1.328729 | 0.008274 | -0.363606 | C | 2.708817 | -2.662626 | 0.487822 |
| C | -0.726558 | 0.025156 | -1.578293 | C | 1.529366 | -2.997811 | -0.163306 |

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| C | 0.897184 | -4.222951 | 0.056927 | C | -2.293392 | 0.912855 | 4.020858 |
| C | 1.442179 | -5.155153 | 0.917729 | C | -2.413220 | 1.350724 | 2.708544 |
| C | 2.647876 | -4.858637 | 1.546012 | C | -5.101970 | -1.352331 | -0.568663 |
| C | 3.265304 | -3.642676 | 1.326810 | C | -5.826571 | -0.682953 | -1.561844 |
| C | 3.757675 | -0.823123 | 1.807316 | C | -7.212396 | -0.665545 | -1.589088 |
| C | 2.845937 | -1.151722 | 2.814757 | C | -7.941945 | -1.317098 | -0.606701 |
| C | 2.972434 | -0.645868 | 4.102057 | C | -7.254955 | -1.986403 | 0.392554 |
| C | 4.026869 | 0.192620 | 4.430683 | C | -5.865274 | -2.007803 | 0.402993 |
| C | 4.948389 | 0.524124 | 3.447897 | H | 3.773648 | -0.723393 | -2.614993 |
| C | 4.810528 | 0.023540 | 2.161796 | H | 1.426699 | -0.665539 | -3.668789 |
| C | 5.021418 | 1.509735 | -0.577307 | H | -3.770069 | 0.705202 | -2.597899 |
| C | 5.706631 | 2.423772 | 0.233196 | H | -1.449555 | 0.422557 | -3.679358 |
| C | 7.091050 | 2.522186 | 0.219831 | H | -1.308673 | 2.347480 | -1.237438 |
| C | 7.849754 | 1.710955 | -0.612063 | H | -0.281076 | 4.549043 | -1.136808 |
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| C | 5.810170 | 0.709081 | -1.406223 | H | -3.088453 | 5.725450 | 1.871154 |
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| C | 1.976186 | 4.260280 | 2.428143 | H | 1.488690 | 3.526318 | -5.253310 |
| C | 1.932283 | 2.902698 | 2.683034 | H | 3.876691 | 2.858929 | -5.113003 |
| C | 2.407840 | 1.989863 | 1.744046 | H | 4.797026 | 1.975281 | -3.047561 |
| C | -2.756538 | 2.716154 | 0.303659 | H | 2.337627 | 0.948533 | 1.999999 |
| C | -3.249659 | 3.723170 | 1.148239 | H | 1.521744 | 2.520971 | 3.610941 |
| C | -2.682426 | 4.982411 | 1.194047 | H | 1.597679 | 4.973571 | 3.151256 |
| C | -1.597595 | 5.292011 | 0.378968 | H | 2.575736 | 5.753499 | 0.997091 |
| C | -1.121456 | 4.327537 | -0.488602 | H | 3.400165 | 4.151458 | -0.632630 |
| C | -1.701879 | 3.058864 | -0.532435 | H | 5.162860 | 3.051550 | 0.922848 |
| C | -3.435703 | 0.897950 | 1.870216 | H | 7.574613 | 3.238430 | 0.874742 |
| C | -4.342340 | -0.005719 | 2.427620 | H | 8.931234 | 1.783975 | -0.620860 |
| C | -4.246767 | -0.427698 | 3.743973 | H | 7.755493 | 0.140878 | -2.078304 |
| C | -3.214608 | 0.025906 | 4.552377 | H | 5.362965 | -0.026548 | -2.052542 |

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|---|-----------|-----------|-----------|---------------------------|-----------|-----------|-----------|
| H | 6.233801 | -1.518109 | 1.338333 | H | -1.788098 | -5.141267 | 3.026252 |
| H | 8.159570 | -2.527896 | 0.292944 | H | -1.149586 | -2.743604 | 3.324189 |
| H | 7.975557 | -3.617656 | -1.933176 | H | -1.979138 | -1.068921 | 1.853183 |
| H | 5.734596 | -3.756248 | -3.012481 | H | -4.826959 | -2.101172 | -3.035287 |
| H | 3.789488 | -2.784438 | -1.928222 | H | -3.864236 | -3.189521 | -4.973021 |
| H | 1.985872 | -1.764157 | 2.595498 | H | -1.497261 | -3.938643 | -4.966334 |
| H | 2.223845 | -0.905837 | 4.841362 | H | -0.148988 | -3.644223 | -2.887093 |
| H | 4.125616 | 0.588748 | 5.435237 | H | -1.144310 | -2.588325 | -0.928541 |
| H | 5.777015 | 1.187287 | 3.670261 | H | -0.025254 | 1.662947 | 0.931528 |
| H | 5.531322 | 0.331603 | 1.425955 | | | | |
| H | 4.201715 | -3.440160 | 1.832142 | {33F} ₂ | | | |
| H | 3.110024 | -5.577263 | 2.213601 | 304 | | | |
| H | 0.941440 | -6.099911 | 1.094899 | E= -7463.3172583 | | | |
| H | -0.040344 | -4.435683 | -0.444234 | C | -2.957718 | -6.036764 | -0.405653 |
| H | 1.071899 | -2.316392 | -0.856132 | C | -3.035420 | -4.635878 | -0.489855 |
| H | -5.126763 | -0.420571 | 1.821195 | C | -3.174857 | -3.951596 | 0.709050 |
| H | -4.971937 | -1.137487 | 4.125996 | C | -3.280045 | -4.629326 | 1.924478 |
| H | -3.124381 | -0.315862 | 5.577076 | C | -3.273882 | -6.008570 | 1.974893 |
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| H | -1.683258 | 2.061713 | 2.348378 | C | -2.984131 | -4.001437 | -1.920044 |
| H | -5.320983 | -0.147015 | -2.346336 | C | -4.024263 | -4.842880 | -2.754581 |
| H | -7.716362 | -0.118748 | -2.377169 | C | -5.158746 | -5.408123 | -2.158399 |
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| H | -7.795422 | -2.505981 | 1.175949 | C | -5.882026 | -6.391472 | -4.233629 |
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| H | -4.169424 | 2.641983 | -1.895307 | C | -3.853561 | -5.105730 | -4.111425 |
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| H | -6.046611 | 1.298572 | 1.704035 | C | -5.192478 | -1.548837 | -0.514934 |
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| H | -3.280664 | -5.752061 | 1.124560 | C | -4.026480 | 0.402351 | 0.534044 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -2.882659 | 0.858730 | 1.099356 | C | -5.960588 | -2.713383 | -4.121965 |
| C | -3.410297 | 1.955044 | 2.225372 | C | 2.997192 | 1.677038 | 0.499177 |
| C | -4.890571 | 1.879207 | 1.963198 | C | 2.365526 | 1.503027 | -0.678077 |
| C | -5.236673 | 0.998303 | 1.041364 | C | 2.781972 | 2.841935 | -1.550171 |
| C | -3.016559 | 3.568856 | 1.859545 | C | 3.208226 | 3.720763 | -0.386324 |
| C | -3.937451 | 4.580955 | 2.682088 | C | 3.438989 | 3.028212 | 0.723876 |
| C | -3.493032 | 5.395712 | 3.730105 | C | 4.380654 | 2.572932 | -2.211887 |
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| C | -5.661399 | 6.382338 | 4.089217 | C | 6.086260 | 2.834462 | -0.263957 |
| C | -6.130236 | 5.627304 | 3.026551 | C | 7.159732 | 2.394580 | 0.490161 |
| C | -5.282312 | 4.776138 | 2.334814 | C | 7.633692 | 1.091766 | 0.355524 |
| C | -3.308395 | 1.479984 | 3.869310 | C | 7.006850 | 0.252041 | -0.544350 |
| C | -1.940883 | 1.758164 | 4.537159 | C | 5.924669 | 0.708540 | -1.293782 |
| C | -1.064238 | 0.726214 | 4.872595 | C | 1.772002 | 3.574409 | -2.657106 |
| C | 0.030912 | 0.956206 | 5.695453 | C | 2.273835 | 3.444277 | -4.134960 |
| C | 0.329769 | 2.227255 | 6.156363 | C | 1.881671 | 2.319903 | -4.869973 |
| C | -0.454758 | 3.284850 | 5.730859 | C | 2.171313 | 2.161727 | -6.211710 |
| C | -1.562735 | 3.034746 | 4.940204 | C | 2.892171 | 3.137575 | -6.888284 |
| P | -1.629613 | -0.556611 | 0.504283 | C | 3.316491 | 4.251114 | -6.185838 |
| O | -0.090633 | 0.159180 | 0.126243 | C | 3.007178 | 4.399552 | -4.835883 |
| P | 1.471238 | -0.200381 | -0.318409 | C | 3.013787 | -1.934233 | 3.631942 |
| C | 2.599282 | -0.649336 | 1.146415 | C | 1.505790 | -2.114350 | 3.894769 |
| C | 3.332738 | 0.480907 | 1.251158 | C | 1.080992 | -2.167541 | 5.231796 |
| C | 4.627514 | 0.277675 | 1.843862 | C | -0.215665 | -2.511209 | 5.571482 |
| C | 4.734233 | -1.013963 | 2.127906 | C | -1.146174 | -2.783154 | 4.573910 |
| C | 3.451410 | -1.798615 | 1.931920 | C | -0.769832 | -2.625009 | 3.253868 |
| C | -3.609104 | -1.734024 | -3.504674 | C | 0.533677 | -2.270638 | 2.923138 |
| C | -4.654320 | -2.386747 | -4.496224 | C | 3.665787 | -3.264989 | 1.196396 |
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| C | -5.352107 | -2.838736 | -6.794363 | C | 2.298330 | -5.088881 | 2.443985 |
| C | -6.603431 | -3.262643 | -6.377694 | C | 1.180764 | -5.903231 | 2.561974 |
| C | -6.906293 | -3.164699 | -5.029114 | C | 0.160861 | -5.814244 | 1.635206 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.256433 | -4.870377 | 0.622123 | C | -0.493966 | -3.420055 | -2.224005 |
| C | 1.360174 | -4.042011 | 0.532442 | C | -3.658385 | -0.026248 | 4.189311 |
| C | -3.283424 | 4.004435 | 0.354015 | C | -3.674258 | -0.342906 | 5.562165 |
| C | -4.462087 | 3.759001 | -0.362057 | C | -4.196561 | -1.525656 | 6.044816 |
| C | -4.744386 | 4.386506 | -1.568294 | C | -4.760466 | -2.451996 | 5.170804 |
| C | -3.849902 | 5.278497 | -2.134746 | C | -4.724958 | -2.180060 | 3.817647 |
| C | -2.641816 | 5.483921 | -1.492157 | C | -4.150240 | -1.002338 | 3.335715 |
| C | -2.370529 | 4.852183 | -0.287513 | C | -4.501716 | 2.148449 | 4.711864 |
| C | -1.524304 | 3.831759 | 2.121772 | C | -4.359877 | 3.098236 | 5.718887 |
| C | -1.030749 | 5.127021 | 2.324739 | C | -5.443314 | 3.564638 | 6.462240 |
| C | 0.299162 | 5.363749 | 2.632372 | C | -6.716494 | 3.078676 | 6.245838 |
| C | 1.197329 | 4.309969 | 2.682721 | C | -6.882120 | 2.080336 | 5.292867 |
| C | 0.745608 | 3.037411 | 2.378255 | C | -5.799508 | 1.620206 | 4.567890 |
| C | -0.589457 | 2.805855 | 2.098023 | C | 5.128584 | 3.889715 | -2.627181 |
| O | 1.480765 | -1.196310 | -1.410176 | C | 6.467656 | 3.752490 | -3.034346 |
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| C | -1.312030 | -0.729808 | -3.534735 | C | 6.766688 | 6.132696 | -3.233051 |
| C | -0.021439 | -0.577340 | -4.003247 | C | 5.461696 | 6.299273 | -2.808142 |
| C | 0.445906 | -1.363988 | -5.044607 | C | 4.664443 | 5.194994 | -2.515892 |
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| C | -4.195433 | -0.272656 | -3.664240 | C | 3.614049 | -0.607877 | -4.215809 |
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| C | -5.503253 | 2.106545 | -4.506053 | C | 4.997458 | 1.749261 | -4.596978 |
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| C | -1.551515 | -4.298429 | -2.429002 | C | -1.830506 | 3.041148 | -3.798874 |
| C | -1.243120 | -5.532399 | -3.018312 | C | -2.418383 | 2.434576 | -2.698463 |
| C | 0.035176 | -5.836849 | -3.457274 | C | -1.647535 | 2.196249 | -1.586101 |
| C | 1.055542 | -4.911445 | -3.313804 | C | -0.297437 | 2.518504 | -1.556355 |
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|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 1.206402 | 6.054939 | -3.219568 | H | 5.368160 | 1.044280 | 2.009603 |
| C | 0.801569 | 7.337040 | -2.867585 | H | -6.237098 | 0.790826 | 0.688455 |
| C | 0.575258 | 7.665698 | -1.540968 | H | -5.571257 | 2.519611 | 2.484769 |
| C | 0.707850 | 6.669802 | -0.583760 | H | -5.546641 | -3.308095 | -1.632713 |
| C | 1.099207 | 5.388297 | -0.942496 | H | -6.135959 | -1.415548 | -0.004068 |
| C | 3.797021 | -3.102702 | 4.344546 | H | 4.666614 | -1.255736 | -0.513076 |
| C | 5.195629 | -3.173458 | 4.394831 | H | 5.687653 | -1.622726 | -2.740897 |
| C | 5.882044 | -4.157222 | 5.091630 | H | 5.516993 | -3.787262 | -3.860126 |
| C | 5.192641 | -5.130508 | 5.794745 | H | 4.277766 | -5.643790 | -2.740180 |
| C | 3.808415 | -5.090003 | 5.777332 | H | 3.339247 | -5.317973 | -0.526092 |
| C | 3.135934 | -4.102571 | 5.068376 | H | 5.494947 | 0.050994 | -2.024700 |
| C | 3.388331 | -0.605730 | 4.359865 | H | 7.352865 | -0.765711 | -0.691693 |
| C | 4.431407 | -0.475677 | 5.282118 | H | 8.485715 | 0.751765 | 0.933360 |
| C | 4.790440 | 0.757397 | 5.810704 | H | 7.647954 | 3.085795 | 1.168176 |
| C | 4.107414 | 1.904705 | 5.440260 | H | 5.804750 | 3.873909 | -0.181964 |
| C | 3.012477 | 1.780695 | 4.598724 | H | 5.500417 | 2.677615 | -4.815988 |
| C | 2.639972 | 0.541662 | 4.098538 | H | 5.550394 | 0.947580 | -6.496400 |
| C | 3.933289 | -3.254117 | -0.338899 | H | 4.345865 | -1.202812 | -6.151147 |
| C | 4.569004 | -2.216058 | -0.999620 | H | 3.077754 | -1.526264 | -4.014551 |
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| C | 5.056998 | -3.642903 | -2.889196 | H | 6.912568 | 2.767004 | -3.081269 |
| C | 4.367878 | -4.673233 | -2.265046 | H | 8.288912 | 4.671976 | -3.659059 |
| C | 3.823290 | -4.480656 | -1.009794 | H | 7.390598 | 6.989068 | -3.461688 |
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| C | 5.144344 | -5.333479 | 1.865842 | H | 3.648446 | 5.405040 | -2.229447 |
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| C | 7.550959 | -5.224315 | 2.008281 | H | 0.653884 | 8.075029 | -3.648289 |
| C | 7.477875 | -3.900085 | 1.595000 | H | 0.265711 | 8.665747 | -1.260241 |
| C | 6.250618 | -3.307815 | 1.352224 | H | 0.477266 | 6.874749 | 0.454112 |
| H | 3.485283 | 4.750750 | -0.502229 | H | 1.116723 | 4.632606 | -0.167151 |
| H | 3.900374 | 3.385865 | 1.632537 | H | 1.305586 | 1.550268 | -4.388970 |
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| H | 3.121626 | 3.026671 | -7.942200 | H | -0.647074 | -2.474696 | -1.724096 |
| H | 3.886490 | 5.029603 | -6.680805 | H | -2.231184 | -3.352027 | -5.437179 |
| H | 3.348244 | 5.301025 | -4.359806 | H | -0.009525 | -3.036414 | -6.313208 |
| H | -0.068130 | 3.845904 | -4.641215 | H | 1.439779 | -1.213129 | -5.444578 |
| H | -2.422620 | 3.287787 | -4.670738 | H | 0.621325 | 0.139611 | -3.516224 |
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| H | -2.112428 | 1.803996 | -0.700444 | H | -2.903009 | 0.133158 | -5.342064 |
| H | 0.243209 | 2.389300 | -0.631737 | H | -4.047922 | 2.122201 | -6.086178 |
| H | -1.394954 | 5.028211 | 0.126749 | H | -6.005439 | 3.011302 | -4.828925 |
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| H | 0.632249 | 6.378816 | 2.819417 | H | -7.893427 | -3.430488 | -4.668023 |
| H | 2.237127 | 4.487045 | 2.929459 | H | -6.286475 | -2.590862 | -3.105186 |
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| H | -0.697443 | -6.467947 | 1.689384 | H | 6.254874 | -2.309322 | 0.942119 |
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| H | 1.408140 | -3.316540 | -0.269143 | H | -0.501414 | -2.560342 | 6.616327 |
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|----------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 5.611156 | 0.810516 | 6.517592 | C | 4.098056 | 3.392527 | -2.724962 |
| H | 4.392043 | 2.873273 | 5.836271 | C | 3.044558 | 2.788763 | -2.029657 |
| H | 2.407075 | 2.646622 | 4.369608 | C | 1.747628 | 2.994232 | -2.522698 |
| H | 1.745002 | 0.460192 | 3.498131 | C | 1.516076 | 3.754012 | -3.660107 |
| H | -1.251991 | -0.284532 | 4.542116 | C | 2.579850 | 4.343126 | -4.334634 |
| H | 0.659399 | 0.123574 | 5.973533 | C | 3.871338 | 4.162642 | -3.861394 |
| H | 1.183669 | 2.386776 | 6.804101 | Si | 3.429043 | 1.733905 | -0.509562 |
| H | -0.225294 | 4.304383 | 6.020628 | C | 5.293761 | 1.737573 | -0.270973 |
| H | -2.160171 | 3.865587 | 4.639313 | C | 5.894517 | 2.596460 | 0.656558 |
| H | -3.306472 | 0.381544 | 6.277226 | C | 7.268840 | 2.587082 | 0.858237 |
| H | -4.194228 | -1.709451 | 7.113236 | C | 8.074413 | 1.718857 | 0.130133 |
| H | -5.215256 | -3.362824 | 5.543473 | C | 7.501216 | 0.875533 | -0.813726 |
| H | -5.158327 | -2.873121 | 3.106277 | C | 6.126377 | 0.893621 | -1.013504 |
| H | -4.152501 | -0.859917 | 2.275601 | C | 2.813876 | -0.099566 | -0.871219 |
| H | -3.396558 | 3.493763 | 5.983519 | C | 1.334373 | -0.016281 | -0.736794 |
| H | -5.265663 | 4.318426 | 7.221094 | C | 0.729097 | -0.045208 | -1.975390 |
| H | -7.558876 | 3.444137 | 6.821820 | C | 1.739921 | -0.225143 | -2.976429 |
| H | -7.856562 | 1.634647 | 5.127051 | C | 2.945008 | -0.281790 | -2.352024 |
| H | -5.971353 | 0.799210 | 3.886655 | P | 0.092530 | 0.206698 | 0.484156 |
| H | -3.197842 | -2.874798 | 0.727208 | O | 0.223871 | -0.220675 | 1.908564 |
| H | -3.361915 | -4.059390 | 2.839593 | C | -0.715862 | 0.087174 | -1.924049 |
| H | -3.371371 | -6.526563 | 2.922092 | C | -1.261733 | 0.031558 | -0.644624 |
| H | -3.058294 | -7.798120 | 0.794407 | C | -2.746552 | 0.193209 | -0.731047 |
| H | -2.826434 | -6.623172 | -1.302889 | C | -2.929668 | 0.452203 | -2.194931 |
| H | -2.979890 | -4.733157 | -4.615837 | C | -1.755102 | 0.351964 | -2.869944 |
| H | -4.576072 | -6.025908 | -5.899692 | Si | -3.489293 | 1.572145 | 0.382282 |
| H | -6.594654 | -6.978915 | -4.801183 | C | -5.275030 | 1.958808 | -0.085460 |
| H | -6.941775 | -6.567817 | -2.371324 | C | -5.530765 | 2.504259 | -1.350943 |
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| 152 | | | | C | -7.641826 | 2.183235 | 0.409346 |
| E=-4737.609321 | | | | C | -6.354216 | 1.825737 | 0.791872 |

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| Si | -3.525319 | -1.607415 | -0.540962 | C | -3.123024 | -2.550473 | -2.124051 |
| C | -2.826031 | -2.663703 | 0.845261 | C | -4.076110 | -2.905412 | -3.081664 |
| C | -3.077707 | -4.042050 | 0.745660 | C | -3.710805 | -3.581239 | -4.241950 |
| C | -2.611913 | -4.929193 | 1.704449 | C | -2.381725 | -3.914473 | -4.467445 |
| C | -1.858903 | -4.459664 | 2.775959 | C | -1.419775 | -3.583399 | -3.519152 |
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| C | -2.083742 | -2.214836 | 1.936554 | C | 2.416579 | -2.965674 | 0.403144 |
| Si | 3.617293 | -1.530451 | 0.171253 | C | 2.681051 | -3.866557 | 1.443265 |
| C | 4.116331 | -0.956202 | 1.896616 | C | 1.910714 | -5.006048 | 1.627750 |
| C | 3.169577 | -1.049761 | 2.926767 | C | 0.857111 | -5.276262 | 0.765553 |
| C | 3.474715 | -0.654289 | 4.222737 | C | 0.588814 | -4.409519 | -0.283934 |
| C | 4.735098 | -0.152934 | 4.522145 | C | 1.363779 | -3.268814 | -0.465080 |
| C | 5.683303 | -0.033118 | 3.513034 | C | 5.064318 | -2.307920 | -0.773336 |
| C | 5.374027 | -0.426946 | 2.216719 | C | 6.336653 | -2.506443 | -0.228560 |
| C | -2.593035 | 3.208633 | 0.113812 | C | 7.338734 | -3.153749 | -0.943529 |
| C | -2.950882 | 4.270130 | 0.956629 | C | 7.087653 | -3.632081 | -2.221817 |
| C | -2.431717 | 5.544044 | 0.773711 | C | 5.818698 | -3.482995 | -2.769355 |
| C | -1.537282 | 5.785892 | -0.264082 | C | 4.822977 | -2.838772 | -2.048346 |
| C | -1.172905 | 4.749552 | -1.112370 | C | 2.569034 | 2.465761 | 0.998574 |
| C | -1.697744 | 3.474391 | -0.923901 | C | 2.978992 | 2.189202 | 2.307153 |
| C | -3.302990 | 1.081948 | 2.183221 | C | 2.279714 | 2.679319 | 3.402387 |
| C | -4.169771 | 0.180648 | 2.816952 | C | 1.152508 | 3.468002 | 3.216210 |
| C | -3.944277 | -0.238529 | 4.119697 | C | 0.740678 | 3.780681 | 1.927109 |
| C | -2.832128 | 0.222376 | 4.815462 | C | 1.445072 | 3.287067 | 0.836733 |
| C | -1.956456 | 1.109189 | 4.205233 | H | 3.896348 | -0.384165 | -2.854697 |
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| C | -5.397230 | -1.494460 | -0.359982 | H | -3.897249 | 0.603959 | -2.652316 |
| C | -6.205023 | -0.892792 | -1.333821 | H | -1.629445 | 0.431407 | -3.940820 |
| C | -7.584395 | -0.842698 | -1.200579 | H | -1.407668 | 2.679630 | -1.600945 |
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| C | -7.415035 | -1.996821 | 0.899154 | H | -1.125250 | 6.778223 | -0.409178 |
| C | -6.032765 | -2.052342 | 0.754260 | H | -2.723862 | 6.348636 | 1.439482 |

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| H | -3.651188 | 4.098951 | 1.769422 | H | -4.624312 | -0.943583 | 4.584431 |
| H | 0.900021 | 2.541570 | -2.023747 | H | -2.644713 | -0.119298 | 5.827551 |
| H | 0.501363 | 3.883732 | -4.022339 | H | -1.070357 | 1.454556 | 4.725209 |
| H | 2.400696 | 4.939340 | -5.222559 | H | -1.492103 | 2.226242 | 2.449406 |
| H | 4.708772 | 4.619930 | -4.376766 | H | -5.757143 | -0.442280 | -2.212553 |
| H | 5.117264 | 3.261630 | -2.377083 | H | -8.181864 | -0.357453 | -1.963498 |
| H | 3.856435 | 1.583528 | 2.485185 | H | -9.270656 | -1.346777 | 0.032971 |
| H | 2.619023 | 2.431887 | 4.401985 | H | -7.883000 | -2.432803 | 1.774988 |
| H | 0.600468 | 3.845226 | 4.070638 | H | -5.439044 | -2.539168 | 1.521664 |
| H | -0.129484 | 4.405336 | 1.760102 | H | -4.708728 | 2.681242 | -2.038328 |
| H | 1.105575 | 3.563525 | -0.151860 | H | -6.985335 | 3.272122 | -2.728436 |
| H | 5.279952 | 3.270338 | 1.243657 | H | -8.883266 | 2.962842 | -1.161589 |
| H | 7.710983 | 3.254394 | 1.589748 | H | -8.462067 | 2.062778 | 1.108182 |
| H | 9.146254 | 1.703462 | 0.294471 | H | -6.199254 | 1.445233 | 1.793626 |
| H | 8.117702 | 0.192531 | -1.387088 | H | -3.639928 | -4.429825 | -0.099155 |
| H | 5.707033 | 0.214170 | -1.746472 | H | -2.823170 | -5.988761 | 1.607800 |
| H | 6.559648 | -2.165267 | 0.774014 | H | -1.473602 | -5.153417 | 3.515426 |
| H | 8.316741 | -3.288249 | -0.494376 | H | -0.993154 | -2.721965 | 3.704318 |
| H | 7.868781 | -4.134569 | -2.781520 | H | -1.858756 | -1.167056 | 2.066746 |
| H | 5.600867 | -3.878724 | -3.755243 | H | -5.121665 | -2.664733 | -2.922397 |
| H | 3.833065 | -2.760153 | -2.486520 | H | -4.468830 | -3.851186 | -4.969219 |
| H | 2.167574 | -1.403154 | 2.712622 | H | -2.097545 | -4.439880 | -5.372631 |
| H | 2.717588 | -0.728028 | 4.995226 | H | -0.379807 | -3.850258 | -3.676173 |
| H | 4.975308 | 0.153912 | 5.534481 | H | -1.040919 | -2.670173 | -1.623800 |
| H | 6.663590 | 0.377515 | 3.727833 | | | | |
| H | 6.123054 | -0.282629 | 1.448141 | 33GH | | | |
| H | 3.499441 | -3.673925 | 2.129530 | 153 | | | |
| H | 2.132280 | -5.680079 | 2.448003 | E: -4738.248811 | | | |
| H | 0.240476 | -6.155590 | 0.911416 | C | 1.821648 | 3.757193 | 0.743471 |
| H | -0.235463 | -4.621668 | -0.954091 | C | 2.527422 | 2.565903 | 0.963419 |
| H | 1.142779 | -2.604712 | -1.294303 | C | 2.422610 | 1.974147 | 2.228097 |
| H | -5.017730 | -0.228541 | 2.280703 | C | 1.620115 | 2.523687 | 3.219228 |

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|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.906925 | 3.688690 | 2.970411 | C | -2.078576 | -4.292122 | -4.024641 |
| C | 1.016832 | 4.309925 | 1.731899 | C | -1.215223 | -3.933011 | -2.996193 |
| Si | 3.478400 | 1.748790 | -0.441066 | C | -1.680544 | -3.157579 | -1.943328 |
| C | 2.842897 | -0.070112 | -0.767116 | C | 3.147655 | 2.698660 | -2.035470 |
| C | 1.357776 | -0.009145 | -0.637416 | C | 4.199968 | 3.145698 | -2.839954 |
| C | 0.772127 | -0.184820 | -1.858105 | C | 3.961022 | 3.760947 | -4.064779 |
| C | 1.782018 | -0.388482 | -2.854598 | C | 2.659384 | 3.936468 | -4.513362 |
| C | 2.985527 | -0.315888 | -2.235174 | C | 1.597294 | 3.509017 | -3.723685 |
| Si | 3.602817 | -1.610181 | 0.171949 | C | 1.841298 | 2.907044 | -2.497697 |
| C | 5.279977 | -2.136565 | -0.556416 | C | 5.320554 | 1.774334 | -0.088000 |
| C | 6.361361 | -2.421773 | 0.285689 | C | 5.825223 | 2.527783 | 0.977519 |
| C | 7.590111 | -2.836021 | -0.215838 | C | 7.179274 | 2.508940 | 1.288217 |
| C | 7.770597 | -2.993063 | -1.582273 | C | 8.055212 | 1.731588 | 0.538747 |
| C | 6.699099 | -2.768398 | -2.438401 | C | 7.576923 | 0.992598 | -0.536764 |
| C | 5.474733 | -2.358138 | -1.927944 | C | 6.223940 | 1.024314 | -0.848778 |
| P | 0.079726 | 0.280698 | 0.605996 | O | 0.182482 | -0.413987 | 1.924667 |
| C | -1.253375 | -0.025970 | -0.598428 | C | -5.228045 | 1.997007 | -0.304285 |
| C | -0.687193 | -0.076106 | -1.846907 | C | -5.403954 | 2.484845 | -1.606396 |
| C | -1.693588 | 0.118127 | -2.847341 | C | -6.659028 | 2.831531 | -2.085665 |
| C | -2.880677 | 0.290494 | -2.211753 | C | -7.772311 | 2.717037 | -1.260821 |
| C | -2.726803 | 0.148683 | -0.731666 | C | -7.615789 | 2.267685 | 0.042455 |
| Si | -3.475773 | 1.604937 | 0.269502 | C | -6.357057 | 1.914098 | 0.514290 |
| C | -3.368176 | 1.217031 | 2.103622 | C | -2.517295 | 3.198094 | -0.047419 |
| C | -4.284429 | 0.376440 | 2.749509 | C | -2.824423 | 4.297315 | 0.766270 |
| C | -4.126057 | 0.026096 | 4.082425 | C | -2.272807 | 5.548315 | 0.529523 |
| C | -3.030930 | 0.494153 | 4.798603 | C | -1.394683 | 5.728387 | -0.533312 |
| C | -2.106278 | 1.322688 | 4.177968 | C | -1.070323 | 4.651613 | -1.346269 |
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| Si | -3.539520 | -1.628878 | -0.450645 | C | -3.012360 | -2.579537 | 1.083181 |
| C | -3.006705 | -2.712445 | -1.895278 | C | -3.403054 | -3.929482 | 1.107568 |
| C | -3.863416 | -3.099027 | -2.930040 | C | -3.074089 | -4.756041 | 2.171759 |
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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -1.916979 | -2.929035 | 3.217679 | H | 4.794849 | 4.101286 | -4.668906 |
| C | -2.269432 | -2.098045 | 2.158586 | H | 5.225041 | 3.013420 | -2.509348 |
| C | -5.420135 | -1.461207 | -0.426618 | H | 2.941246 | 1.051760 | 2.444192 |
| C | -6.143181 | -0.935541 | -1.505702 | H | 1.541818 | 2.019173 | 4.175294 |
| C | -7.525772 | -0.832450 | -1.472448 | H | 0.264124 | 4.111955 | 3.735219 |
| C | -8.226464 | -1.250587 | -0.347882 | H | 0.459507 | 5.215440 | 1.525111 |
| C | -7.535292 | -1.777758 | 0.733690 | H | 1.878207 | 4.254610 | -0.217919 |
| C | -6.149415 | -1.885794 | 0.689747 | H | 5.147201 | 3.114421 | 1.588763 |
| C | 3.874641 | -1.187922 | 1.991112 | H | 7.549936 | 3.093613 | 2.122996 |
| C | 2.957017 | -1.541688 | 2.986519 | H | 9.109553 | 1.703897 | 0.791035 |
| C | 3.135028 | -1.140463 | 4.305548 | H | 8.249349 | 0.378127 | -1.124537 |
| C | 4.242881 | -0.384621 | 4.665212 | H | 5.874348 | 0.429277 | -1.684978 |
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| C | 4.994292 | -0.436682 | 2.381650 | H | 8.406912 | -3.037363 | 0.468408 |
| C | 2.446272 | -3.090161 | -0.042707 | H | 8.729879 | -3.309391 | -1.976848 |
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| C | 2.068963 | -5.338299 | -0.901438 | H | 4.649424 | -2.234690 | -2.618439 |
| C | 0.832405 | -5.391608 | -0.273110 | H | 2.072575 | -2.110987 | 2.739405 |
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| H | 3.940871 | -0.353843 | -2.736441 | H | 6.049753 | 0.552077 | 3.961128 |
| H | 1.614572 | -0.530457 | -3.913004 | H | 5.733701 | -0.138832 | 1.649017 |
| H | -3.834936 | 0.423549 | -2.700779 | H | 3.841254 | -4.209352 | -1.253053 |
| H | -1.537665 | 0.108630 | -3.916999 | H | 2.422954 | -6.183515 | -1.482023 |
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| H | -0.377302 | 4.786806 | -2.168402 | H | -0.566042 | -4.327647 | 0.967232 |
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| H | -2.531324 | 6.383771 | 1.170902 | H | -5.119862 | -0.041465 | 2.200667 |
| H | -3.514746 | 4.175883 | 1.596266 | H | -4.844743 | -0.633716 | 4.555205 |
| H | 1.000489 | 2.588433 | -1.892440 | H | -2.895350 | 0.205657 | 5.835110 |
| H | 0.576344 | 3.642171 | -4.066705 | H | -1.237405 | 1.678854 | 4.719491 |
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| H | -5.626659 | -0.590454 | -2.393836 | C | -3.772140 | 1.357826 | 3.479984 |
| H | -8.054243 | -0.408513 | -2.318397 | C | -3.509196 | 2.489029 | 2.718551 |
| H | -9.306887 | -1.163556 | -0.315863 | C | -3.631741 | 3.766829 | 3.263540 |
| H | -8.073645 | -2.111846 | 1.613910 | C | -4.014130 | 3.932676 | 4.584810 |
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| H | -6.767182 | 3.205001 | -3.098131 | C | -3.806482 | -0.732789 | 0.957309 |
| H | -8.754876 | 2.989953 | -1.629969 | C | -2.740117 | -0.139691 | 0.025709 |
| H | -8.476278 | 2.186588 | 0.697130 | C | -3.414680 | 0.460792 | -1.002567 |
| H | -6.265163 | 1.577283 | 1.539204 | C | -4.825700 | 0.446569 | -0.813456 |
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| H | -3.389560 | -5.793586 | 2.168132 | P | -1.116946 | 0.802513 | 0.062430 |
| H | -2.050098 | -4.901997 | 4.058457 | O | -0.901696 | 1.481488 | 1.362658 |
| H | -1.318461 | -2.523954 | 4.025446 | C | -2.669635 | 1.289087 | -1.929905 |
| H | -1.921326 | -1.077158 | 2.187879 | C | -1.537540 | 1.868847 | -1.417825 |
| H | -4.906049 | -2.799901 | -2.914063 | C | -1.234129 | 3.067691 | -2.304864 |
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| H | -0.181561 | -4.262035 | -2.997598 | Si | -4.366051 | -2.612596 | 0.446042 |
| H | -0.993963 | -2.901162 | -1.146863 | C | -5.092414 | -2.936818 | -1.305285 |
| H | -0.015422 | 1.684260 | 0.717233 | C | -5.067173 | -2.154623 | -2.462089 |
| | | | | C | -5.699049 | -2.549836 | -3.635480 |
| {33G} ₂ | | | | C | -6.378445 | -3.756586 | -3.697142 |
| 304 | | | | C | -6.407725 | -4.567526 | -2.570933 |
| E= -9475.178228 | | | | C | -5.780568 | -4.158529 | -1.402123 |
| C | -6.677170 | 0.204628 | 3.124442 | Si | -2.566781 | 4.526755 | -1.743668 |
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| C | -7.325122 | -1.796170 | 4.915179 | C | -0.850005 | 5.279798 | 1.971191 |
| C | -8.292325 | -0.876766 | 4.538009 | C | -1.084297 | 6.632629 | 2.172868 |
| C | -7.962636 | 0.130780 | 3.638659 | C | -1.738000 | 7.369102 | 1.192724 |
| Si | -3.897899 | -0.430975 | 2.887655 | C | -2.148205 | 6.754601 | 0.017260 |

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|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| Si | 0.420627 | 3.970070 | -2.793169 | C | 6.149186 | 0.318818 | 0.297382 |
| C | 0.609031 | 3.866647 | -4.680812 | Si | 2.133831 | -1.759083 | -3.967120 |
| C | 1.369912 | 4.825271 | -5.364073 | C | 0.359939 | -1.187800 | -4.142869 |
| C | 1.633808 | 4.709287 | -6.723559 | C | -0.145315 | -0.691646 | -5.352879 |
| C | 1.155028 | 3.616751 | -7.436067 | C | -1.512142 | -0.584637 | -5.572744 |
| C | 0.422187 | 2.640303 | -6.774645 | C | -2.403636 | -0.988630 | -4.585663 |
| C | 0.157346 | 2.765863 | -5.416482 | C | -1.922606 | -1.433689 | -3.366149 |
| O | 0.232349 | -0.039615 | -0.374172 | C | -0.559334 | -1.509364 | -3.145096 |
| P | 1.194589 | -1.253700 | 0.375742 | Si | 1.436842 | -4.598408 | -2.432666 |
| C | 2.239521 | -2.008622 | -1.005993 | C | 2.413280 | -5.714337 | -3.644689 |
| C | 3.468961 | -2.189164 | -0.431818 | C | 1.942693 | -6.125077 | -4.893177 |
| C | 4.368798 | -2.938995 | -1.245621 | C | 2.668257 | -7.001242 | -5.693932 |
| C | 3.699179 | -3.266823 | -2.364140 | C | 3.884626 | -7.502962 | -5.259588 |
| C | 2.275159 | -2.798090 | -2.331100 | C | 4.361689 | -7.137049 | -4.005742 |
| C | 3.661781 | -1.675583 | 0.886631 | C | 3.630314 | -6.266097 | -3.213070 |
| C | 2.758684 | -0.760342 | 1.379120 | C | 2.006013 | -2.361673 | 4.793569 |
| C | 3.328783 | -0.332400 | 2.755502 | C | 1.909082 | -2.805580 | 6.121127 |
| C | 4.507729 | -1.252072 | 2.904983 | C | 1.623909 | -4.127195 | 6.426301 |
| C | 4.684317 | -2.023406 | 1.820736 | C | 1.393795 | -5.038521 | 5.402578 |
| Si | 2.523385 | -0.568120 | 4.518024 | C | 1.454799 | -4.614108 | 4.084381 |
| C | 1.154298 | 0.634246 | 4.913381 | C | 1.771418 | -3.292971 | 3.784359 |
| C | 0.826767 | 0.927988 | 6.245605 | C | 3.857561 | -0.332155 | 5.856848 |
| C | -0.119960 | 1.894057 | 6.552743 | C | 4.698166 | -1.393590 | 6.220600 |
| C | -0.763735 | 2.583076 | 5.527858 | C | 5.649747 | -1.261536 | 7.221360 |
| C | -0.481921 | 2.271261 | 4.207115 | C | 5.781732 | -0.055158 | 7.897341 |
| C | 0.468254 | 1.304372 | 3.905541 | C | 4.958314 | 1.009221 | 7.562013 |
| Si | 4.400343 | 1.341206 | 2.540744 | C | 4.011908 | 0.867994 | 6.554838 |
| C | 5.743052 | 1.331683 | 1.169102 | C | 2.553894 | -2.824368 | -5.500354 |
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| C | 7.641470 | 2.642987 | 0.359523 | C | 1.973192 | -3.824079 | -7.649172 |
| C | 8.032311 | 1.607577 | -0.480415 | C | 3.269676 | -4.285370 | -7.814427 |
| C | 7.277783 | 0.444176 | -0.505995 | C | 4.220037 | -3.996665 | -6.843528 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.866677 | -3.267196 | -5.718956 | C | -5.282469 | 3.681981 | -2.304811 |
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| C | 5.658375 | 0.471197 | -4.304841 | C | -6.017641 | 3.538631 | 0.366595 |
| C | 5.191999 | 1.643339 | -4.887561 | C | -4.710287 | 3.849949 | 0.005709 |
| C | 3.827913 | 1.829117 | -5.059083 | C | -2.970249 | 5.804081 | -3.101075 |
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| C | -2.037354 | -4.524984 | -4.733581 | C | 0.493569 | 5.796837 | -2.276029 |
| C | -0.736005 | -4.363255 | -4.289382 | C | 0.972291 | 6.068294 | -0.987755 |
| C | 1.656941 | -5.614244 | -0.847266 | C | 1.142079 | 7.364958 | -0.531020 |
| C | 1.206054 | -6.939570 | -0.943529 | C | 0.831144 | 8.439478 | -1.355232 |
| C | 1.483230 | -7.877434 | 0.040389 | C | 0.366846 | 8.200367 | -2.639992 |
| C | 2.244003 | -7.518343 | 1.147631 | C | 0.211857 | 6.894679 | -3.092738 |
| C | 2.695370 | -6.211107 | 1.268354 | C | 2.031078 | 3.286729 | -2.144653 |
| C | 2.390915 | -5.270706 | 0.289061 | C | 3.143210 | 4.120560 | -2.347428 |
| C | 5.607556 | 1.693318 | 3.990758 | C | 4.429434 | 3.652916 | -2.156954 |
| C | 5.619748 | 2.930396 | 4.644914 | C | 4.629354 | 2.343716 | -1.739944 |
| C | 6.630759 | 3.280411 | 5.533266 | C | 3.543498 | 1.521067 | -1.492035 |
| C | 7.665256 | 2.397385 | 5.797795 | C | 2.250796 | 1.983862 | -1.710669 |
| C | 7.690690 | 1.171387 | 5.144650 | C | -2.949927 | -3.805558 | 0.738422 |
| C | 6.688639 | 0.838827 | 4.246252 | C | -3.189986 | -5.184511 | 0.811683 |
| C | 3.391274 | 2.924750 | 2.407139 | C | -2.192330 | -6.072380 | 1.188630 |
| C | 3.568156 | 3.792670 | 1.326627 | C | -0.920285 | -5.597345 | 1.479307 |
| C | 3.133278 | 5.111176 | 1.380703 | C | -0.653826 | -4.241860 | 1.364461 |
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| C | 2.235347 | 4.722610 | 3.571106 | C | -5.851748 | -3.225938 | 1.481657 |
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| C | -8.154127 | -4.286824 | 2.728629 | H | -4.494048 | 6.630490 | -1.812676 |
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| H | -2.176850 | 3.430522 | -4.343471 | H | -0.399332 | 1.975264 | -4.924880 |
| H | -3.857814 | 1.508528 | -3.802854 | H | 1.216693 | 5.249141 | -0.323196 |
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| H | -5.555921 | 0.898064 | -1.468189 | H | 0.954188 | 9.456249 | -0.998270 |
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| H | 4.104062 | -3.818419 | -3.195915 | H | -0.133687 | 6.748847 | -4.106116 |
| H | 5.139266 | -1.243897 | 3.777875 | H | 3.002672 | 5.145573 | -2.673410 |
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| H | -3.413332 | 4.640300 | 2.660706 | H | 3.699191 | 0.500680 | -1.164479 |
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| H | -4.389773 | 0.690107 | 5.440719 | H | 3.440134 | 2.750489 | -5.479218 |
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| H | -6.283134 | 3.493641 | 1.417408 | H | 6.721842 | 0.331780 | -4.142492 |
| H | -7.987632 | 3.069736 | -0.350518 | H | 5.158994 | -1.421418 | -3.462581 |
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| H | -0.753762 | 7.111996 | 3.088460 | H | -0.222291 | -1.894603 | -2.192784 |
| H | -0.331324 | 4.696065 | 2.720135 | H | 0.606436 | -2.753263 | -6.424510 |
| H | -1.080517 | 3.602158 | 0.694312 | H | 1.222204 | -4.021848 | -8.406421 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 3.542492 | -4.855141 | -8.695732 | H | -4.814132 | -4.713747 | 2.654112 |
| H | 5.242620 | -4.335871 | -6.963560 | H | -5.303421 | -2.449668 | 4.702506 |
| H | 4.649733 | -3.024571 | -5.011125 | H | -7.567419 | -2.581848 | 5.622296 |
| H | -3.502519 | -3.371038 | 3.158008 | H | -9.293951 | -0.936275 | 4.949854 |
| H | -2.381097 | -4.790282 | 4.786280 | H | -8.702561 | 0.870781 | 3.352908 |
| H | -1.031308 | -3.758580 | 6.598808 | H | -6.428390 | 1.032618 | 2.466501 |
| H | -0.748768 | -1.300707 | 6.664437 | H | -4.173567 | -5.581411 | 0.589579 |
| H | -1.848309 | 0.119825 | 5.012211 | H | -2.405509 | -7.134088 | 1.245483 |
| H | 1.332538 | 0.413037 | 7.056433 | H | -0.132969 | -6.286127 | 1.759847 |
| H | -0.352053 | 2.114286 | 7.589157 | H | 0.337934 | -3.862024 | 1.554818 |
| H | -1.501690 | 3.342541 | 5.756287 | H | -1.428293 | -2.300070 | 0.964986 |
| H | -1.004147 | 2.757389 | 3.397736 | H | -4.568919 | -1.199191 | -2.459737 |
| H | 0.674207 | 1.109242 | 2.861395 | H | -5.667200 | -1.900786 | -4.504003 |
| H | 2.545730 | 2.787996 | 4.389973 | H | -6.880889 | -4.060720 | -4.608728 |
| H | 1.703170 | 5.068324 | 4.450778 | H | -6.935010 | -5.514855 | -2.591388 |
| H | 2.129685 | 6.610529 | 2.551110 | H | -5.871613 | -4.802262 | -0.535127 |
| H | 3.323181 | 5.765942 | 0.538232 | H | -1.120486 | -5.344692 | -1.080046 |
| H | 4.084157 | 3.455695 | 0.438207 | H | -3.425360 | -5.622700 | -1.854834 |
| H | 6.279236 | 3.314029 | 1.843220 | H | -4.035873 | -5.111506 | -4.189701 |
| H | 8.213146 | 3.563632 | 0.395410 | H | -2.290982 | -4.277587 | -5.758482 |
| H | 8.910986 | 1.709291 | -1.107739 | H | -0.002176 | -3.982820 | -4.983009 |
| H | 7.553501 | -0.372125 | -1.165098 | H | 0.645307 | -7.254321 | -1.818466 |
| H | 5.580282 | -0.589330 | 0.214145 | H | 1.120696 | -8.893749 | -0.066822 |
| H | 4.838488 | 3.654340 | 4.455461 | H | 2.484641 | -8.252569 | 1.908755 |
| H | 6.604458 | 4.251462 | 6.016209 | H | 3.286990 | -5.913716 | 2.126890 |
| H | 8.452776 | 2.663855 | 6.494212 | H | 2.748864 | -4.261005 | 0.420586 |
| H | 8.502940 | 0.475451 | 5.323083 | H | 0.992370 | -5.769621 | -5.264766 |
| H | 6.782710 | -0.097041 | 3.707961 | H | 2.275541 | -7.284846 | -6.663961 |
| H | -7.270102 | -1.972027 | 0.441222 | H | 4.452231 | -8.183971 | -5.884318 |
| H | -9.240049 | -2.834187 | 1.574210 | H | 5.299138 | -7.540861 | -3.638936 |
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|---|----------|-----------|----------|
| H | 1.266566 | -5.316275 | 3.283578 |
| H | 1.162357 | -6.073159 | 5.631392 |
| H | 1.575108 | -4.444038 | 7.462710 |
| H | 2.091982 | -2.112701 | 6.935992 |
| H | 3.389004 | 1.720483 | 6.309257 |
| H | 5.061545 | 1.960098 | 8.071743 |
| H | 6.525642 | 0.055482 | 8.678611 |
| H | 6.285033 | -2.102686 | 7.476479 |
| H | 4.598208 | -2.353699 | 5.724160 |