

## A DFT insight into the properties of CrI<sub>3</sub> fullerenes

Andrey N. Enyashin

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### xyz-file for the monolayer CrI<sub>3</sub>

8  
siesta: Etot = -7970.063167 eV  
Cr 3.383417 1.953417 10.000049  
Cr 6.766849 3.906842 9.999951  
I 5.601202 2.018111 8.430590  
I 8.985330 3.841709 8.430581  
I 5.714004 5.860677 8.430584  
I 4.549064 3.842148 11.569410  
I 1.164936 2.018550 11.569419  
I 4.436262 -0.000418 11.569416  
#  
6.766844000 0.000000000 0.000000000  
3.383422000 5.860258807 0.000000000  
0.000000000 0.000000000 20.000000000

xyz-file for tetrahedral fullerene (CrI<sub>3</sub>)<sub>12</sub>

48

siesta: Etot = -47796.120163 eV

|    |           |           |           |
|----|-----------|-----------|-----------|
| Cr | 30.009167 | 26.713269 | 33.703447 |
| Cr | 25.787989 | 30.379980 | 27.377903 |
| Cr | 27.937475 | 26.912269 | 26.711017 |
| Cr | 25.719489 | 32.142682 | 31.319580 |
| Cr | 27.772739 | 30.346325 | 34.417194 |
| Cr | 31.994622 | 34.161660 | 28.206247 |
| Cr | 27.885580 | 34.097804 | 28.139541 |
| Cr | 34.154158 | 32.271528 | 31.424238 |
| Cr | 32.092150 | 30.397072 | 34.488380 |
| Cr | 32.249356 | 27.002257 | 26.748088 |
| Cr | 34.236919 | 30.552387 | 27.472561 |
| Cr | 30.090337 | 25.036032 | 29.928646 |
| I  | 26.595003 | 29.815224 | 30.010048 |
| I  | 28.259871 | 27.113945 | 29.488050 |
| I  | 28.196587 | 28.420497 | 32.421577 |
| I  | 31.539000 | 32.958427 | 30.689499 |
| I  | 28.330404 | 32.900923 | 30.650410 |
| I  | 29.934630 | 31.502177 | 33.061035 |
| I  | 31.606158 | 31.506159 | 27.396276 |
| I  | 28.392195 | 31.447369 | 27.359568 |
| I  | 30.059385 | 28.747049 | 26.834350 |
| I  | 31.855473 | 27.178905 | 29.523279 |
| I  | 33.401342 | 29.937457 | 30.087901 |
| I  | 31.794604 | 28.482915 | 32.462829 |
| I  | 26.769429 | 32.986460 | 33.880711 |
| I  | 25.146023 | 30.094798 | 33.282632 |
| I  | 33.026470 | 33.083076 | 33.951842 |
| I  | 34.767333 | 30.257517 | 33.395871 |
| I  | 29.897121 | 35.820191 | 29.272419 |
| I  | 29.968589 | 34.460300 | 26.184412 |
| I  | 26.944234 | 29.083236 | 25.079759 |
| I  | 25.257136 | 27.560050 | 27.567865 |
| I  | 33.193761 | 29.205569 | 25.145585 |
| I  | 31.748138 | 24.897554 | 32.285590 |
| I  | 28.377241 | 24.831446 | 32.250785 |
| I  | 34.876388 | 27.739142 | 27.671048 |
| I  | 34.182879 | 34.806940 | 30.006417 |
| I  | 34.251907 | 33.302557 | 26.576248 |
| I  | 36.121740 | 31.664909 | 29.381325 |
| I  | 28.099880 | 27.723405 | 35.645783 |
| I  | 29.917132 | 30.934156 | 36.314662 |
| I  | 31.848809 | 27.780387 | 35.693025 |
| I  | 30.127701 | 25.959819 | 25.059883 |
| I  | 28.256054 | 24.254449 | 27.827671 |
| I  | 32.004248 | 24.325314 | 27.864643 |
| I  | 25.638073 | 34.659935 | 29.904060 |
| I  | 23.825205 | 31.444754 | 29.245061 |
| I  | 25.701569 | 33.141091 | 26.475331 |

xyz-file for tetrahedral fullerene (CrI<sub>3</sub>)<sub>48</sub>

192

siesta: Etot = -191232.224106 eV

|    |           |           |           |
|----|-----------|-----------|-----------|
| Cr | 29.914537 | 19.579597 | 25.961158 |
| Cr | 30.001058 | 25.191024 | 40.083469 |
| Cr | 20.425238 | 34.311950 | 26.160949 |
| Cr | 21.934943 | 30.936537 | 25.032673 |
| Cr | 25.690480 | 24.565678 | 23.522384 |
| Cr | 27.942062 | 21.471103 | 23.061829 |
| Cr | 20.431068 | 35.771340 | 29.895989 |
| Cr | 22.260647 | 28.215164 | 28.478294 |
| Cr | 24.255032 | 24.832640 | 27.651453 |
| Cr | 21.992977 | 34.084166 | 32.995337 |
| Cr | 22.289261 | 29.753936 | 32.402708 |
| Cr | 26.345159 | 22.798950 | 30.713222 |
| Cr | 24.280705 | 27.851814 | 35.319827 |
| Cr | 26.363968 | 24.284512 | 34.439827 |
| Cr | 25.773790 | 30.525284 | 38.445007 |
| Cr | 28.030978 | 28.578472 | 40.890249 |
| Cr | 37.623154 | 37.580827 | 26.972837 |
| Cr | 33.805754 | 38.070461 | 26.793925 |
| Cr | 26.260653 | 38.079457 | 26.809906 |
| Cr | 22.444325 | 37.648359 | 26.995585 |
| Cr | 39.629656 | 35.656268 | 29.882837 |
| Cr | 32.055553 | 37.792048 | 30.775601 |
| Cr | 28.038683 | 37.816219 | 30.796657 |
| Cr | 38.072738 | 34.011194 | 32.993075 |
| Cr | 34.163150 | 35.799765 | 33.841750 |
| Cr | 25.923186 | 35.820822 | 33.854570 |
| Cr | 32.155710 | 33.902640 | 36.757428 |
| Cr | 27.931393 | 33.928451 | 36.760345 |
| Cr | 34.313100 | 30.469165 | 38.444973 |
| Cr | 32.031859 | 28.553817 | 40.883621 |
| Cr | 32.031448 | 35.125616 | 24.086849 |
| Cr | 28.016232 | 35.148492 | 24.090727 |
| Cr | 34.118479 | 31.568406 | 23.214646 |
| Cr | 25.871941 | 31.598753 | 23.228441 |
| Cr | 32.079347 | 28.200261 | 22.392307 |
| Cr | 27.855510 | 28.214997 | 22.394987 |
| Cr | 31.947727 | 21.460487 | 23.063889 |
| Cr | 34.210863 | 24.556863 | 23.519860 |
| Cr | 38.062926 | 30.848171 | 25.029837 |
| Cr | 39.606342 | 34.206597 | 26.151009 |
| Cr | 35.679462 | 24.753354 | 27.638145 |
| Cr | 37.701313 | 28.123793 | 28.437712 |
| Cr | 29.926187 | 20.527720 | 29.706740 |
| Cr | 33.560926 | 22.766127 | 30.695122 |
| Cr | 37.717228 | 29.680552 | 32.358722 |
| Cr | 33.576851 | 24.252913 | 34.424787 |
| Cr | 35.718078 | 27.788834 | 35.276717 |
| Cr | 29.995292 | 23.260553 | 36.737636 |
| I  | 21.288618 | 33.446592 | 28.655348 |
| I  | 22.998456 | 30.676335 | 27.927134 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 24.599319 | 27.506724 | 27.257433 |
| I | 26.576256 | 24.592397 | 26.434068 |
| I | 28.178598 | 21.725186 | 25.816376 |
| I | 23.006503 | 31.938887 | 31.110947 |
| I | 23.805789 | 28.289018 | 30.705604 |
| I | 25.561846 | 25.297362 | 29.979502 |
| I | 28.280463 | 22.942125 | 28.926452 |
| I | 24.631282 | 30.072016 | 33.756564 |
| I | 25.556674 | 26.598400 | 33.275092 |
| I | 28.079656 | 24.165781 | 32.320892 |
| I | 26.614209 | 28.512017 | 36.337228 |
| I | 28.301889 | 25.613138 | 35.615211 |
| I | 28.251932 | 26.853331 | 38.724050 |
| I | 36.975497 | 36.319301 | 29.360245 |
| I | 33.634682 | 36.326183 | 29.269442 |
| I | 30.033020 | 36.540368 | 29.441266 |
| I | 26.434280 | 36.366380 | 29.291793 |
| I | 23.088895 | 36.384058 | 29.371444 |
| I | 35.344290 | 34.687952 | 31.769554 |
| I | 31.811521 | 35.710141 | 32.494220 |
| I | 28.270708 | 35.716317 | 32.499701 |
| I | 24.720880 | 34.736758 | 31.779014 |
| I | 33.524033 | 33.224571 | 34.501413 |
| I | 30.039167 | 34.041056 | 35.065614 |
| I | 26.538511 | 33.244382 | 34.516164 |
| I | 31.743487 | 31.311495 | 36.984748 |
| I | 28.297917 | 31.324525 | 37.008167 |
| I | 30.032849 | 29.816430 | 39.438509 |
| I | 36.966924 | 35.025013 | 26.087875 |
| I | 33.628589 | 35.078990 | 26.171818 |
| I | 30.022330 | 35.130930 | 25.940930 |
| I | 26.413037 | 35.125420 | 26.188031 |
| I | 23.077977 | 35.092829 | 26.099638 |
| I | 35.325094 | 32.181575 | 25.467847 |
| I | 31.775253 | 32.429432 | 24.270312 |
| I | 28.225944 | 32.450285 | 24.276662 |
| I | 24.679259 | 32.229736 | 25.481973 |
| I | 33.481862 | 29.239784 | 24.490755 |
| I | 29.979698 | 29.462011 | 23.539597 |
| I | 26.488454 | 29.268232 | 24.504617 |
| I | 31.692505 | 26.146718 | 23.995796 |
| I | 28.254478 | 26.161304 | 23.994083 |
| I | 29.953852 | 23.371678 | 23.271228 |
| I | 31.708664 | 21.687936 | 25.814341 |
| I | 33.349726 | 24.541211 | 26.425748 |
| I | 35.352900 | 27.437166 | 27.237214 |
| I | 36.996392 | 30.595248 | 27.893014 |
| I | 38.731201 | 33.347585 | 28.639954 |
| I | 31.621643 | 22.922196 | 28.922974 |
| I | 34.386039 | 25.241136 | 29.966582 |
| I | 36.173337 | 28.217695 | 30.676926 |
| I | 37.005205 | 31.863522 | 31.079662 |
| I | 31.850139 | 24.138163 | 32.320668 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 34.402418 | 26.551636 | 33.253721 |
| I | 35.380163 | 30.014818 | 33.731453 |
| I | 31.656873 | 25.582197 | 35.630878 |
| I | 33.398726 | 28.473277 | 36.321787 |
| I | 31.776076 | 26.833598 | 38.727224 |
| I | 32.967390 | 31.187282 | 40.748390 |
| I | 34.681320 | 28.250548 | 40.051118 |
| I | 36.683753 | 29.583414 | 37.226148 |
| I | 34.541096 | 33.260816 | 38.110696 |
| I | 36.633798 | 35.231897 | 35.074494 |
| I | 38.770540 | 31.552510 | 34.180304 |
| I | 40.468111 | 33.668601 | 31.655685 |
| I | 38.748191 | 36.606612 | 32.360948 |
| I | 21.337093 | 36.693536 | 32.378255 |
| I | 19.581307 | 33.783611 | 31.680143 |
| I | 21.260406 | 31.657383 | 34.213257 |
| I | 23.441450 | 35.287925 | 35.083734 |
| I | 25.542285 | 33.308145 | 38.132149 |
| I | 23.361900 | 29.675100 | 37.258593 |
| I | 25.369954 | 28.312740 | 40.060397 |
| I | 27.116237 | 31.220630 | 40.762848 |
| I | 24.257733 | 38.159350 | 24.916734 |
| I | 24.261322 | 39.441311 | 28.138254 |
| I | 27.935426 | 37.926593 | 24.552026 |
| I | 32.127314 | 37.896574 | 24.537567 |
| I | 32.146667 | 39.509612 | 28.553200 |
| I | 35.807308 | 38.097578 | 24.902001 |
| I | 35.830647 | 39.388626 | 28.125780 |
| I | 25.282206 | 21.862131 | 23.866738 |
| I | 27.032032 | 23.510214 | 21.361824 |
| I | 23.309829 | 24.808260 | 24.991475 |
| I | 25.472418 | 26.830664 | 21.838789 |
| I | 21.228816 | 28.345015 | 25.852147 |
| I | 23.389918 | 30.373034 | 22.699945 |
| I | 21.299189 | 33.270629 | 23.711549 |
| I | 19.561296 | 31.638797 | 26.231754 |
| I | 28.255737 | 23.363034 | 38.864597 |
| I | 31.729036 | 23.346723 | 38.871997 |
| I | 27.812342 | 22.064982 | 35.415845 |
| I | 32.151876 | 22.033333 | 35.418797 |
| I | 32.098750 | 20.490404 | 31.506200 |
| I | 27.774433 | 20.515919 | 31.517012 |
| I | 28.181912 | 19.093406 | 28.113863 |
| I | 31.644847 | 19.066855 | 28.114589 |
| I | 40.454488 | 31.523966 | 26.214675 |
| I | 38.718814 | 33.173468 | 23.700421 |
| I | 36.589458 | 30.308760 | 22.688189 |
| I | 38.739512 | 28.240597 | 25.824385 |
| I | 36.615468 | 24.733573 | 24.974766 |
| I | 34.458383 | 26.791462 | 21.826041 |
| I | 34.604469 | 21.842258 | 23.867882 |
| I | 32.873539 | 23.473845 | 21.353216 |
| I | 20.401929 | 29.168270 | 30.375309 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 21.819500 | 27.694225 | 34.132355 |
| I | 21.795904 | 25.518125 | 28.624769 |
| I | 24.490910 | 22.200665 | 28.672397 |
| I | 24.736077 | 22.697044 | 32.917103 |
| I | 24.515718 | 25.242410 | 36.356656 |
| I | 25.913297 | 38.343337 | 32.588213 |
| I | 27.088976 | 36.473932 | 36.242168 |
| I | 30.060169 | 39.257946 | 31.944417 |
| I | 30.042323 | 34.415068 | 38.571144 |
| I | 33.014230 | 36.447290 | 36.241043 |
| I | 34.190332 | 38.315805 | 32.546807 |
| I | 25.867993 | 34.319179 | 22.439828 |
| I | 27.015062 | 30.431628 | 21.032794 |
| I | 30.017946 | 35.396550 | 22.251241 |
| I | 34.148070 | 34.278500 | 22.420151 |
| I | 32.951481 | 30.406821 | 21.027738 |
| I | 29.968048 | 27.336414 | 20.726343 |
| I | 39.584139 | 29.062413 | 30.327641 |
| I | 38.146323 | 25.423394 | 28.595624 |
| I | 35.407876 | 22.130475 | 28.652106 |
| I | 35.180575 | 22.640766 | 32.897582 |
| I | 38.171845 | 27.612109 | 34.088927 |
| I | 35.449141 | 25.180323 | 36.331214 |
| I | 27.942094 | 39.523495 | 28.563857 |
| I | 28.125906 | 25.996679 | 42.015510 |
| I | 30.035727 | 29.161006 | 42.782784 |
| I | 31.890787 | 25.972285 | 42.015163 |
| I | 18.445851 | 35.178897 | 27.973426 |
| I | 20.353688 | 36.956234 | 25.242537 |
| I | 20.360891 | 38.335554 | 28.747072 |
| I | 39.707877 | 36.849869 | 25.220616 |
| I | 41.591787 | 35.054243 | 27.951541 |
| I | 39.717814 | 38.230457 | 28.726390 |
| I | 28.034364 | 18.831745 | 24.011015 |
| I | 31.802982 | 18.806492 | 24.011486 |
| I | 29.940200 | 20.609230 | 21.275599 |

xyz-file for tetrahedral fullerene (CrI<sub>3</sub>)<sub>108</sub>

432

siesta: Etot = -430310.338565 eV

|    |           |           |           |
|----|-----------|-----------|-----------|
| Cr | 30.027235 | 17.816769 | 32.685507 |
| Cr | 30.007069 | 21.560324 | 43.440302 |
| Cr | 29.992885 | 23.384730 | 46.872367 |
| Cr | 14.690060 | 37.982493 | 24.653701 |
| Cr | 16.285888 | 34.665289 | 23.519457 |
| Cr | 20.346173 | 28.407123 | 22.226269 |
| Cr | 22.316606 | 25.215257 | 21.441940 |
| Cr | 25.869272 | 18.786391 | 19.602167 |
| Cr | 28.133661 | 15.685565 | 19.124588 |
| Cr | 14.655900 | 39.401825 | 28.389695 |
| Cr | 16.678679 | 31.898338 | 26.959582 |
| Cr | 18.658448 | 28.606351 | 26.045372 |
| Cr | 22.490675 | 22.369341 | 24.466874 |
| Cr | 24.459519 | 19.020158 | 23.751788 |
| Cr | 16.210650 | 37.685679 | 31.488664 |
| Cr | 16.632139 | 33.397522 | 30.847115 |
| Cr | 19.881508 | 26.432424 | 29.174254 |
| Cr | 21.864721 | 23.161281 | 28.343164 |
| Cr | 26.526253 | 17.034547 | 26.781576 |
| Cr | 18.625881 | 31.600481 | 33.744705 |
| Cr | 19.863362 | 27.878026 | 32.908178 |
| Cr | 23.853323 | 21.275145 | 31.243422 |
| Cr | 26.570017 | 18.437528 | 30.465686 |
| Cr | 20.258773 | 34.022602 | 36.698337 |
| Cr | 21.828210 | 26.039165 | 35.737284 |
| Cr | 23.826673 | 22.685780 | 34.893274 |
| Cr | 22.184376 | 32.210017 | 39.475573 |
| Cr | 22.391633 | 28.047742 | 39.176581 |
| Cr | 26.535094 | 21.156656 | 37.433592 |
| Cr | 24.316187 | 26.071285 | 41.997872 |
| Cr | 26.435024 | 22.595601 | 41.114488 |
| Cr | 25.678250 | 28.685275 | 45.202466 |
| Cr | 27.939516 | 26.746422 | 47.676950 |
| Cr | 43.282146 | 41.471132 | 25.673778 |
| Cr | 39.438113 | 41.912426 | 25.473877 |
| Cr | 31.876930 | 41.500780 | 25.512194 |
| Cr | 28.040745 | 41.499795 | 25.507002 |
| Cr | 20.497632 | 41.917104 | 25.396048 |
| Cr | 16.634724 | 41.406148 | 25.503864 |
| Cr | 45.291174 | 39.567695 | 28.570295 |
| Cr | 37.629118 | 41.481016 | 29.426735 |
| Cr | 33.681997 | 41.452619 | 29.265640 |
| Cr | 26.212147 | 41.453226 | 29.249675 |
| Cr | 22.263949 | 41.451251 | 29.342048 |
| Cr | 43.710233 | 37.796387 | 31.613181 |
| Cr | 39.712409 | 39.472162 | 32.425004 |
| Cr | 31.881821 | 40.233029 | 32.639789 |
| Cr | 27.974072 | 40.222673 | 32.632677 |
| Cr | 20.157772 | 39.416276 | 32.312628 |
| Cr | 37.786473 | 37.512307 | 35.257314 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Cr | 33.862713 | 38.339030 | 35.541093 |
| Cr | 25.964041 | 38.292417 | 35.511923 |
| Cr | 22.044962 | 37.459607 | 35.163290 |
| Cr | 39.620394 | 34.114967 | 36.790927 |
| Cr | 31.908558 | 36.465449 | 38.359720 |
| Cr | 27.922029 | 36.450269 | 38.346593 |
| Cr | 37.688409 | 32.258699 | 39.553504 |
| Cr | 34.038590 | 33.942335 | 40.666686 |
| Cr | 25.789813 | 33.923707 | 40.617596 |
| Cr | 31.984890 | 32.135910 | 43.500860 |
| Cr | 27.832029 | 32.086369 | 43.473574 |
| Cr | 34.172966 | 28.779609 | 45.207232 |
| Cr | 31.948355 | 26.807187 | 47.668268 |
| Cr | 37.690975 | 38.912465 | 22.779841 |
| Cr | 33.746926 | 38.954789 | 22.794586 |
| Cr | 26.238608 | 38.913164 | 22.780228 |
| Cr | 22.283487 | 38.824188 | 22.725813 |
| Cr | 39.801583 | 35.432622 | 21.915379 |
| Cr | 31.963763 | 35.761581 | 21.143789 |
| Cr | 28.039109 | 35.730810 | 21.107048 |
| Cr | 20.204053 | 35.340775 | 21.821016 |
| Cr | 37.913893 | 32.061758 | 21.097328 |
| Cr | 33.989318 | 32.432553 | 20.313480 |
| Cr | 26.055823 | 32.363915 | 20.293387 |
| Cr | 22.124881 | 31.975793 | 21.060197 |
| Cr | 32.057636 | 29.145464 | 19.482849 |
| Cr | 28.049284 | 29.107478 | 19.483313 |
| Cr | 34.212857 | 25.755290 | 19.502631 |
| Cr | 25.962197 | 25.691551 | 19.492381 |
| Cr | 32.171610 | 22.475504 | 18.648427 |
| Cr | 28.019757 | 22.442259 | 18.629564 |
| Cr | 32.151485 | 15.673123 | 19.129254 |
| Cr | 34.399505 | 18.820573 | 19.660553 |
| Cr | 37.847827 | 25.296902 | 21.484626 |
| Cr | 39.741215 | 28.511899 | 22.314393 |
| Cr | 43.736049 | 34.783314 | 23.697446 |
| Cr | 45.303173 | 38.141285 | 24.823885 |
| Cr | 30.103205 | 13.770519 | 22.029359 |
| Cr | 35.731732 | 19.082028 | 23.801285 |
| Cr | 37.672865 | 22.440856 | 24.539597 |
| Cr | 41.356088 | 28.771921 | 26.146163 |
| Cr | 43.349646 | 32.052783 | 27.078068 |
| Cr | 30.086755 | 14.699191 | 25.787913 |
| Cr | 33.646999 | 17.068522 | 26.787155 |
| Cr | 38.221736 | 23.249642 | 28.428545 |
| Cr | 40.142521 | 26.550334 | 29.259649 |
| Cr | 43.338129 | 33.529325 | 30.956958 |
| Cr | 33.514649 | 18.465635 | 30.480586 |
| Cr | 36.206850 | 21.327993 | 31.310601 |
| Cr | 40.131518 | 28.005019 | 32.993948 |
| Cr | 41.337239 | 31.730293 | 33.841288 |
| Cr | 36.192599 | 22.742466 | 34.958625 |
| Cr | 38.167317 | 26.113307 | 35.807233 |

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| Cr | 30.012931 | 19.214002 | 36.261353 |
| Cr | 33.478338 | 21.177183 | 37.476776 |
| Cr | 37.566634 | 28.127671 | 39.211491 |
| Cr | 33.560865 | 22.620727 | 41.148045 |
| Cr | 35.606040 | 26.155540 | 42.012887 |
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| I  | 17.406756 | 34.364710 | 26.483479 |
| I  | 19.058555 | 31.248869 | 25.758828 |
| I  | 21.045466 | 28.098921 | 24.933151 |
| I  | 22.987936 | 24.981948 | 24.151013 |
| I  | 24.855485 | 21.710163 | 23.374239 |
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| I  | 28.370418 | 15.913573 | 21.882885 |
| I  | 17.291052 | 35.615739 | 29.610069 |
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| I  | 28.193876 | 22.572509 | 39.010241 |
| I  | 26.591455 | 26.699451 | 43.142296 |
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| I | 35.430642 | 26.705631 | 21.690687 |
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| I | 28.352872 | 13.285902 | 24.174591 |
| I | 31.830733 | 13.279383 | 24.196037 |
| I | 46.143411 | 37.549025 | 30.332599 |
| I | 44.337170 | 40.422826 | 31.062873 |
| I | 42.177602 | 38.920709 | 33.678383 |
| I | 44.402045 | 35.360170 | 32.811220 |
| I | 42.182025 | 33.488023 | 35.788132 |
| I | 40.112520 | 36.868459 | 36.586426 |
| I | 38.503387 | 34.890284 | 39.208564 |
| I | 40.230939 | 31.995852 | 38.473296 |
| I | 38.528801 | 29.995055 | 40.994677 |
| I | 36.471667 | 33.380750 | 41.834855 |
| I | 34.382530 | 31.560369 | 44.869977 |
| I | 36.554484 | 27.954560 | 43.961636 |
| I | 34.604788 | 26.574686 | 46.807137 |
| I | 32.828331 | 29.465939 | 47.525393 |
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| I | 17.726907 | 33.361966 | 35.663475 |
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| I | 19.651478 | 31.909823 | 38.398411 |

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| I | 25.447930 | 31.460904 | 44.825860 |
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| I | 38.066064 | 21.785117 | 33.239660 |
| I | 38.091181 | 23.544354 | 36.773088 |
| I | 38.032800 | 25.983476 | 40.831491 |
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| I | 40.284403 | 25.572122 | 34.190683 |
| I | 39.721596 | 27.315912 | 37.731614 |
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| I | 42.015515 | 27.334085 | 31.109712 |
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| I | 43.775418 | 29.386268 | 27.241854 |
| I | 43.761680 | 31.446278 | 32.630102 |
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| I | 29.886639 | 32.652302 | 45.294538 |
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| I | 25.725659 | 36.589793 | 40.001044 |
| I | 23.720904 | 38.448258 | 37.100398 |
| I | 21.324026 | 40.040127 | 34.671170 |
| I | 20.174039 | 41.979055 | 31.146454 |
| I | 24.249406 | 42.840491 | 30.541718 |
| I | 25.985589 | 40.819724 | 34.429825 |
| I | 27.665131 | 39.016754 | 37.500230 |
| I | 29.905119 | 37.087806 | 40.128912 |
| I | 32.784260 | 34.663783 | 42.977233 |

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| I | 34.090131 | 36.615474 | 40.032472 |
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| I | 27.956587 | 42.501002 | 31.089366 |
| I | 31.916408 | 42.504343 | 31.086321 |
| I | 33.844331 | 40.855785 | 34.459561 |
| I | 36.081306 | 38.515287 | 37.161124 |
| I | 38.520953 | 40.094072 | 34.773519 |
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| I | 32.984752 | 24.687178 | 17.314351 |
| I | 30.060254 | 28.406152 | 17.747367 |
| I | 27.786203 | 31.563262 | 18.359673 |
| I | 26.072533 | 34.947744 | 19.362646 |
| I | 24.266864 | 39.088558 | 20.902210 |
| I | 27.990299 | 38.456465 | 20.717643 |
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| I | 36.227312 | 31.499763 | 19.009631 |
| I | 33.942931 | 35.016427 | 19.397245 |
| I | 31.997742 | 38.481472 | 20.735318 |
| I | 35.726696 | 39.137607 | 20.933981 |
| I | 38.642143 | 34.311399 | 19.741032 |
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| I | 21.913761 | 25.890628 | 40.771931 |
| I | 24.468704 | 20.208362 | 35.901884 |
| I | 21.917109 | 23.467632 | 36.701017 |
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| I | 17.993096 | 27.184851 | 31.020784 |
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| I | 21.971235 | 20.612268 | 29.357283 |
| I | 24.893178 | 16.928031 | 28.936115 |
| I | 24.662630 | 16.402314 | 24.769193 |
| I | 22.028318 | 19.692341 | 24.726038 |
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| I | 18.279361 | 26.055861 | 26.972818 |
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| I | 14.775815 | 32.793705 | 28.828274 |
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| I | 29.934508 | 27.373307 | 49.555253 |

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| I | 30.146831 | 14.832684 | 17.339143 |
| I | 32.002906 | 13.018057 | 20.074360 |
| I | 28.234965 | 13.032341 | 20.059537 |
| I | 14.523880 | 41.999103 | 27.270788 |
| I | 14.539185 | 40.665741 | 23.757586 |
| I | 12.700540 | 38.791446 | 26.468939 |

xyz-file for tetrahedral fullerene (CrI<sub>3</sub>)<sub>192</sub>

768

siesta: Etot = -765032.367398 eV

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| Cr | 30.000463 | 18.737875 | 49.792522 |
| Cr | 8.799223  | 43.492481 | 27.671455 |
| Cr | 10.863066 | 36.024475 | 25.796250 |
| Cr | 12.921814 | 32.810068 | 24.753482 |
| Cr | 16.874252 | 26.585492 | 22.953137 |
| Cr | 18.840364 | 23.347495 | 21.940698 |
| Cr | 22.490182 | 17.024299 | 19.872235 |
| Cr | 24.406171 | 13.683324 | 18.912951 |
| Cr | 10.403110 | 41.580324 | 30.664655 |
| Cr | 10.849936 | 37.314357 | 29.772760 |
| Cr | 13.948314 | 30.371101 | 27.747839 |
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| I | 34.052975 | 38.767859 | 42.443980 |
| I | 32.368943 | 36.600293 | 45.105285 |
| I | 29.966438 | 34.464139 | 47.427390 |
| I | 27.046747 | 31.775373 | 49.989082 |
| I | 29.977996 | 29.719829 | 52.227918 |
| I | 32.897081 | 31.787734 | 50.000886 |
| I | 34.234566 | 33.905474 | 47.190487 |
| I | 36.316877 | 35.899897 | 44.380268 |
| I | 38.564571 | 37.644642 | 41.876192 |
| I | 40.102377 | 39.812091 | 39.149737 |
| I | 42.034670 | 41.956829 | 36.360921 |
| I | 44.406543 | 43.680584 | 34.014916 |
| I | 45.561038 | 45.849242 | 30.569442 |
| I | 6.819767  | 43.016751 | 25.724026 |
| I | 8.692071  | 46.140130 | 26.689125 |
| I | 8.696227  | 44.973729 | 23.105466 |
| I | 31.880258 | 21.040238 | 55.329564 |
| I | 29.980057 | 24.147104 | 56.302542 |
| I | 28.107832 | 21.021701 | 55.329624 |
| I | 51.267660 | 45.008710 | 23.149029 |
| I | 51.264447 | 46.189025 | 26.725664 |
| I | 53.159626 | 43.073972 | 25.768628 |
| I | 30.047980 | 9.751254  | 12.229461 |
| I | 28.159921 | 7.798378  | 14.848586 |
| I | 31.930786 | 7.800803  | 14.851204 |

xyz-file for octahedral fullerene (CrI<sub>3</sub>)<sub>24</sub>

96

siesta: Etot = -95605.563114 eV

|    |           |           |           |
|----|-----------|-----------|-----------|
| Cr | 28.040759 | 23.641765 | 29.999949 |
| Cr | 31.958992 | 23.641702 | 30.000181 |
| Cr | 25.844003 | 25.843998 | 33.104927 |
| Cr | 27.789597 | 27.789617 | 35.889366 |
| Cr | 25.842936 | 25.843554 | 26.894951 |
| Cr | 27.789526 | 27.789679 | 24.110743 |
| Cr | 23.641701 | 31.959176 | 30.000014 |
| Cr | 23.641705 | 28.041045 | 29.999905 |
| Cr | 25.843835 | 34.156229 | 33.105087 |
| Cr | 27.789541 | 32.210508 | 35.889182 |
| Cr | 25.843960 | 34.156478 | 26.895145 |
| Cr | 27.789780 | 32.210436 | 24.110724 |
| Cr | 31.959105 | 36.358174 | 30.000066 |
| Cr | 28.040929 | 36.358210 | 30.000077 |
| Cr | 34.156613 | 34.156259 | 33.105267 |
| Cr | 32.210450 | 32.210551 | 35.889285 |
| Cr | 34.156794 | 34.156253 | 26.895037 |
| Cr | 32.210797 | 32.210244 | 24.110597 |
| Cr | 36.357989 | 28.040719 | 30.000056 |
| Cr | 36.358320 | 31.958683 | 30.000065 |
| Cr | 34.156099 | 25.843466 | 33.104947 |
| Cr | 32.209998 | 27.789609 | 35.889614 |
| Cr | 34.156651 | 25.842018 | 26.895176 |
| Cr | 32.210166 | 27.789505 | 24.110692 |
| I  | 28.336165 | 25.965626 | 31.675377 |
| I  | 31.664090 | 25.965534 | 31.675348 |
| I  | 30.000370 | 27.631296 | 34.035304 |
| I  | 28.335775 | 25.965685 | 28.324757 |
| I  | 31.664489 | 25.965504 | 28.324467 |
| I  | 30.000020 | 27.630896 | 25.964617 |
| I  | 25.965695 | 31.664307 | 31.675493 |
| I  | 25.965654 | 28.336272 | 31.675332 |
| I  | 27.631380 | 30.000121 | 34.035146 |
| I  | 25.965613 | 31.664157 | 28.324791 |
| I  | 25.965495 | 28.335825 | 28.324608 |
| I  | 27.630994 | 30.000069 | 25.964640 |
| I  | 31.664022 | 34.034436 | 31.675410 |
| I  | 28.336007 | 34.034481 | 31.675384 |
| I  | 30.000023 | 32.368774 | 34.035154 |
| I  | 31.664332 | 34.034394 | 28.324642 |
| I  | 28.335735 | 34.034332 | 28.324578 |
| I  | 30.000099 | 32.369050 | 25.964922 |
| I  | 34.034381 | 28.335867 | 31.675354 |
| I  | 34.034581 | 31.663960 | 31.675371 |
| I  | 32.368798 | 30.000052 | 34.035336 |
| I  | 34.034327 | 28.335523 | 28.324716 |
| I  | 34.034465 | 31.664050 | 28.324596 |
| I  | 32.369012 | 29.999778 | 25.964490 |
| I  | 25.101492 | 32.419782 | 24.833155 |
| I  | 27.580487 | 34.899037 | 24.832936 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 34.898391 | 27.580612 | 35.167027 |
| I | 32.419179 | 25.101393 | 35.167379 |
| I | 32.419151 | 25.100885 | 24.832330 |
| I | 34.898455 | 27.580149 | 24.832928 |
| I | 27.580695 | 34.898587 | 35.167276 |
| I | 25.101633 | 32.419409 | 35.167166 |
| I | 27.580373 | 25.101718 | 35.166961 |
| I | 34.898933 | 32.419396 | 24.832647 |
| I | 32.419694 | 34.898500 | 24.832655 |
| I | 25.101522 | 27.580649 | 35.166785 |
| I | 34.898625 | 32.419215 | 35.167454 |
| I | 27.580093 | 25.101517 | 24.832834 |
| I | 32.419513 | 34.898738 | 35.167171 |
| I | 25.100966 | 27.580808 | 24.832512 |
| I | 29.999464 | 22.689961 | 31.752282 |
| I | 30.000054 | 37.309788 | 31.751860 |
| I | 29.999371 | 22.689980 | 28.247878 |
| I | 30.000088 | 37.309977 | 28.247871 |
| I | 37.310031 | 29.999280 | 31.752253 |
| I | 22.690059 | 30.000460 | 31.752104 |
| I | 37.310134 | 29.999246 | 28.247535 |
| I | 22.689853 | 30.000670 | 28.247639 |
| I | 26.052542 | 36.697150 | 31.939598 |
| I | 23.302983 | 33.947610 | 31.939696 |
| I | 23.303054 | 33.947558 | 28.060349 |
| I | 26.052409 | 36.697389 | 28.060298 |
| I | 23.302812 | 26.052987 | 31.939303 |
| I | 26.052543 | 23.302871 | 31.939211 |
| I | 26.052309 | 23.302445 | 28.060536 |
| I | 23.302243 | 26.052716 | 28.060406 |
| I | 33.947081 | 23.302522 | 31.939493 |
| I | 36.697206 | 26.052572 | 31.939236 |
| I | 36.697428 | 26.052268 | 28.060473 |
| I | 33.947295 | 23.301711 | 28.060544 |
| I | 36.697330 | 33.947096 | 31.939438 |
| I | 33.947649 | 36.697027 | 31.939660 |
| I | 33.947707 | 36.697266 | 28.060265 |
| I | 36.697323 | 33.947282 | 28.060319 |
| I | 32.748847 | 29.999829 | 37.527054 |
| I | 30.000148 | 27.251209 | 37.527089 |
| I | 27.251192 | 29.999867 | 37.526966 |
| I | 29.999873 | 32.748743 | 37.526946 |
| I | 30.000025 | 27.251221 | 22.472862 |
| I | 32.748980 | 29.999873 | 22.472618 |
| I | 29.999653 | 32.748818 | 22.472831 |
| I | 27.251086 | 29.999936 | 22.472820 |

xyz-file for octahedral fullerene (CrI<sub>3</sub>)<sub>96</sub>

384

siesta: Etot = -382497.202217 eV

|    |           |           |           |
|----|-----------|-----------|-----------|
| Cr | 22.392374 | 18.242944 | 29.999972 |
| Cr | 26.158419 | 17.914925 | 29.999391 |
| Cr | 33.845995 | 17.919068 | 29.994917 |
| Cr | 37.607747 | 18.252386 | 29.999348 |
| Cr | 20.327217 | 20.324729 | 32.921891 |
| Cr | 28.035567 | 19.135986 | 33.474805 |
| Cr | 31.964467 | 19.138363 | 33.473248 |
| Cr | 22.036328 | 22.035889 | 35.817920 |
| Cr | 26.052826 | 21.144044 | 36.290640 |
| Cr | 33.948210 | 21.146131 | 36.290958 |
| Cr | 28.019040 | 23.106812 | 39.082153 |
| Cr | 31.981984 | 23.106792 | 39.081596 |
| Cr | 25.882131 | 25.882797 | 41.265862 |
| Cr | 27.931680 | 27.931577 | 43.708577 |
| Cr | 20.329055 | 20.328032 | 27.079252 |
| Cr | 28.039136 | 19.139001 | 26.526385 |
| Cr | 31.966058 | 19.137614 | 26.523523 |
| Cr | 22.036613 | 22.036013 | 24.181936 |
| Cr | 26.051590 | 21.146876 | 23.709042 |
| Cr | 33.949141 | 21.150103 | 23.708900 |
| Cr | 28.019572 | 23.105466 | 20.917783 |
| Cr | 31.983230 | 23.106690 | 20.917149 |
| Cr | 25.882527 | 25.882526 | 18.734849 |
| Cr | 27.931706 | 27.931799 | 16.291322 |
| Cr | 18.243166 | 37.607151 | 29.999853 |
| Cr | 17.915491 | 33.841361 | 30.000674 |
| Cr | 17.911841 | 26.156582 | 30.001766 |
| Cr | 18.247362 | 22.393893 | 30.001271 |
| Cr | 20.324910 | 39.672761 | 32.920781 |
| Cr | 19.138933 | 31.962832 | 33.474066 |
| Cr | 19.136468 | 28.033909 | 33.474904 |
| Cr | 22.035256 | 37.963939 | 35.817439 |
| Cr | 21.144491 | 33.947702 | 36.290173 |
| Cr | 21.148910 | 26.051653 | 36.290625 |
| Cr | 23.106991 | 31.981941 | 39.081328 |
| Cr | 23.107752 | 28.018230 | 39.081371 |
| Cr | 25.882320 | 34.117299 | 41.265807 |
| Cr | 27.932265 | 32.068700 | 43.708544 |
| Cr | 20.325401 | 39.672603 | 27.078199 |
| Cr | 19.137970 | 31.964144 | 26.526197 |
| Cr | 19.139070 | 28.035359 | 26.525455 |
| Cr | 22.036205 | 37.963038 | 24.181513 |
| Cr | 21.145888 | 33.948179 | 23.710584 |
| Cr | 21.148997 | 26.050860 | 23.710538 |
| Cr | 23.106496 | 31.981351 | 20.918165 |
| Cr | 23.107464 | 28.017835 | 20.920646 |
| Cr | 25.883883 | 34.117699 | 18.734781 |
| Cr | 27.931924 | 32.067860 | 16.292673 |
| Cr | 37.606741 | 41.757228 | 29.999971 |
| Cr | 33.841367 | 42.085580 | 29.999170 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Cr | 26.155606 | 42.088287 | 29.999269 |
| Cr | 22.393918 | 41.750355 | 30.000657 |
| Cr | 39.672026 | 39.673651 | 32.920565 |
| Cr | 31.962877 | 40.862369 | 33.473786 |
| Cr | 28.034021 | 40.864663 | 33.474390 |
| Cr | 37.964624 | 37.963066 | 35.817910 |
| Cr | 33.947682 | 38.856202 | 36.288892 |
| Cr | 26.050610 | 38.852728 | 36.289789 |
| Cr | 31.980667 | 36.899241 | 39.082323 |
| Cr | 28.017001 | 36.894371 | 39.082214 |
| Cr | 34.117144 | 34.117653 | 41.264503 |
| Cr | 32.069580 | 32.068125 | 43.710318 |
| Cr | 39.673680 | 39.674604 | 27.078077 |
| Cr | 31.963493 | 40.862092 | 26.525153 |
| Cr | 28.035484 | 40.860487 | 26.525428 |
| Cr | 37.963673 | 37.964195 | 24.183009 |
| Cr | 33.947474 | 38.853526 | 23.709743 |
| Cr | 26.051299 | 38.852237 | 23.710125 |
| Cr | 31.981673 | 36.890610 | 20.920412 |
| Cr | 28.017353 | 36.891639 | 20.919520 |
| Cr | 34.116652 | 34.117904 | 18.734115 |
| Cr | 32.069017 | 32.068919 | 16.289134 |
| Cr | 41.764132 | 22.393408 | 29.999202 |
| Cr | 42.086617 | 26.157545 | 30.002702 |
| Cr | 42.087467 | 33.843833 | 30.000707 |
| Cr | 41.749885 | 37.607243 | 30.000053 |
| Cr | 39.671257 | 20.329010 | 32.920857 |
| Cr | 40.861064 | 28.036118 | 33.474162 |
| Cr | 40.860259 | 31.964577 | 33.474077 |
| Cr | 37.964592 | 22.037873 | 35.818373 |
| Cr | 38.852076 | 26.051967 | 36.289909 |
| Cr | 38.849774 | 33.948643 | 36.289291 |
| Cr | 36.891173 | 28.019068 | 39.079451 |
| Cr | 36.886475 | 31.985861 | 39.075423 |
| Cr | 34.117810 | 25.882673 | 41.265328 |
| Cr | 32.067953 | 27.931414 | 43.708349 |
| Cr | 39.687010 | 20.329711 | 27.077886 |
| Cr | 40.866209 | 28.035676 | 26.525232 |
| Cr | 40.866386 | 31.965969 | 26.525140 |
| Cr | 37.963091 | 22.034329 | 24.182363 |
| Cr | 38.856473 | 26.052335 | 23.710822 |
| Cr | 38.852910 | 33.949059 | 23.709585 |
| Cr | 36.893875 | 28.018849 | 20.918323 |
| Cr | 36.894453 | 31.982732 | 20.916484 |
| Cr | 34.117325 | 25.882161 | 18.732991 |
| Cr | 32.069996 | 27.931251 | 16.286915 |
| I  | 22.817612 | 20.374880 | 31.723219 |
| I  | 26.315327 | 20.196093 | 31.725062 |
| I  | 29.999523 | 20.076582 | 31.857685 |
| I  | 33.680698 | 20.199509 | 31.719461 |
| I  | 37.167015 | 20.362239 | 31.741256 |
| I  | 24.479424 | 22.045346 | 34.327838 |
| I  | 28.150632 | 21.574292 | 34.647086 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 31.851546 | 21.576702 | 34.646596 |
| I | 35.517951 | 22.049963 | 34.327730 |
| I | 26.354480 | 23.730141 | 37.030295 |
| I | 29.999303 | 23.431480 | 37.275529 |
| I | 33.642453 | 23.732963 | 37.029974 |
| I | 28.166675 | 25.734350 | 39.546473 |
| I | 31.832942 | 25.734946 | 39.547045 |
| I | 30.000046 | 27.567323 | 41.911495 |
| I | 22.813739 | 20.385189 | 28.289148 |
| I | 26.319042 | 20.198953 | 28.278577 |
| I | 30.003955 | 20.075505 | 28.142223 |
| I | 33.690944 | 20.195318 | 28.274221 |
| I | 37.214587 | 20.408914 | 28.306826 |
| I | 24.482336 | 22.046649 | 25.674256 |
| I | 28.152171 | 21.576151 | 25.353237 |
| I | 35.521610 | 22.044275 | 25.674176 |
| I | 26.357732 | 23.733935 | 22.968973 |
| I | 30.000104 | 23.432633 | 22.723392 |
| I | 33.646636 | 23.734792 | 22.966166 |
| I | 28.167326 | 25.732500 | 20.454170 |
| I | 31.833755 | 25.732801 | 20.453514 |
| I | 30.002162 | 27.582265 | 18.090387 |
| I | 20.382753 | 37.185745 | 31.712114 |
| I | 20.197356 | 33.682371 | 31.723756 |
| I | 20.075076 | 29.995062 | 31.857489 |
| I | 20.196797 | 26.313973 | 31.724565 |
| I | 20.382853 | 22.811760 | 31.713847 |
| I | 22.045448 | 35.519481 | 34.326519 |
| I | 21.575626 | 31.848557 | 34.647493 |
| I | 21.574499 | 28.149635 | 34.647049 |
| I | 22.045649 | 24.478860 | 34.326076 |
| I | 23.729891 | 33.645296 | 37.030783 |
| I | 23.432321 | 29.998533 | 37.276122 |
| I | 23.734884 | 26.355915 | 37.031007 |
| I | 25.734068 | 31.834342 | 39.545139 |
| I | 25.735473 | 28.167102 | 39.546513 |
| I | 27.572099 | 30.000424 | 41.910392 |
| I | 20.375665 | 37.182151 | 28.277647 |
| I | 20.197931 | 33.683763 | 28.277368 |
| I | 20.076419 | 29.998976 | 28.141794 |
| I | 20.199107 | 26.317659 | 28.278939 |
| I | 20.376776 | 22.817898 | 28.278076 |
| I | 22.046169 | 35.520642 | 25.673842 |
| I | 21.575468 | 31.850330 | 25.352570 |
| I | 21.576789 | 28.148346 | 25.354154 |
| I | 22.046954 | 24.480158 | 25.675879 |
| I | 23.730979 | 33.643030 | 22.969848 |
| I | 23.431868 | 29.999646 | 22.725014 |
| I | 23.734033 | 26.356007 | 22.970986 |
| I | 25.732576 | 31.834533 | 20.454322 |
| I | 25.735404 | 28.166168 | 20.454499 |
| I | 27.556697 | 29.999848 | 18.083907 |
| I | 37.177002 | 39.630809 | 31.727033 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 33.682153 | 39.802630 | 31.722146 |
| I | 29.994123 | 39.926007 | 31.858092 |
| I | 26.315512 | 39.803014 | 31.723693 |
| I | 22.816116 | 39.623648 | 31.722044 |
| I | 35.520605 | 37.954023 | 34.326807 |
| I | 31.849454 | 38.425698 | 34.647640 |
| I | 28.149419 | 38.427129 | 34.646393 |
| I | 24.478614 | 37.954485 | 34.325852 |
| I | 33.643880 | 36.271532 | 37.030692 |
| I | 30.000060 | 36.570741 | 37.276712 |
| I | 26.355859 | 36.266770 | 37.031493 |
| I | 31.832647 | 34.273118 | 39.546407 |
| I | 28.167035 | 34.267476 | 39.546704 |
| I | 30.000989 | 32.432004 | 41.911562 |
| I | 37.190691 | 39.610864 | 28.292367 |
| I | 33.684382 | 39.803411 | 28.275363 |
| I | 29.998790 | 39.924749 | 28.143604 |
| I | 26.314920 | 39.800759 | 28.278933 |
| I | 22.812196 | 39.614648 | 28.287115 |
| I | 35.520263 | 37.954804 | 25.672968 |
| I | 31.849861 | 38.424710 | 25.353462 |
| I | 28.149651 | 38.424170 | 25.353417 |
| I | 24.479919 | 37.953511 | 25.674854 |
| I | 33.644407 | 36.268265 | 22.971449 |
| I | 29.998882 | 36.566157 | 22.725004 |
| I | 26.354644 | 36.266738 | 22.970319 |
| I | 31.833468 | 34.264985 | 20.455196 |
| I | 28.168085 | 34.264725 | 20.454613 |
| I | 30.001705 | 32.416870 | 18.091801 |
| I | 39.602497 | 22.797645 | 31.690694 |
| I | 39.802481 | 26.313739 | 31.723992 |
| I | 39.922844 | 30.001412 | 31.856306 |
| I | 39.799356 | 33.683938 | 31.721521 |
| I | 39.606590 | 37.192543 | 31.706717 |
| I | 37.956643 | 24.479272 | 34.323904 |
| I | 38.422836 | 28.149014 | 34.645453 |
| I | 38.422656 | 31.850479 | 34.644578 |
| I | 37.954360 | 35.521251 | 34.325344 |
| I | 36.266608 | 26.354612 | 37.029455 |
| I | 36.563679 | 30.001209 | 37.272893 |
| I | 36.262693 | 33.646292 | 37.026376 |
| I | 34.265868 | 28.166436 | 39.545358 |
| I | 34.262170 | 31.834945 | 39.542841 |
| I | 32.429144 | 30.000260 | 41.911021 |
| I | 39.652353 | 22.833720 | 28.254663 |
| I | 39.804126 | 26.318796 | 28.276707 |
| I | 39.929356 | 30.003179 | 28.141188 |
| I | 39.804478 | 33.684219 | 28.275934 |
| I | 39.629773 | 37.180268 | 28.271645 |
| I | 37.954804 | 24.479175 | 25.672564 |
| I | 38.429093 | 31.850672 | 25.352597 |
| I | 37.953747 | 35.520904 | 25.673902 |
| I | 36.270553 | 26.356456 | 22.971381 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 36.569953 | 30.000761 | 22.723702 |
| I | 36.267034 | 33.642827 | 22.969271 |
| I | 34.267280 | 28.166017 | 20.453651 |
| I | 34.266462 | 31.833864 | 20.452901 |
| I | 32.444619 | 29.998929 | 18.083678 |
| I | 38.429383 | 28.152161 | 25.351792 |
| I | 31.853195 | 21.575799 | 25.354349 |
| I | 27.898049 | 16.888838 | 31.931307 |
| I | 32.104697 | 16.892973 | 31.929470 |
| I | 35.808392 | 17.014147 | 31.728231 |
| I | 21.838314 | 19.376023 | 35.060075 |
| I | 30.004032 | 18.171307 | 35.087428 |
| I | 32.322187 | 20.499684 | 38.375402 |
| I | 38.171065 | 19.377970 | 35.066753 |
| I | 23.762027 | 21.030173 | 37.775936 |
| I | 27.678509 | 20.500091 | 38.375239 |
| I | 36.237335 | 21.033699 | 37.776391 |
| I | 25.870310 | 23.137722 | 40.761754 |
| I | 34.129215 | 23.139248 | 40.761849 |
| I | 27.651365 | 25.191480 | 43.293561 |
| I | 21.846162 | 19.378345 | 24.946657 |
| I | 27.898691 | 16.890377 | 28.066196 |
| I | 32.112362 | 16.889481 | 28.063237 |
| I | 35.814964 | 17.048896 | 28.250009 |
| I | 23.763367 | 21.029780 | 22.224334 |
| I | 27.679589 | 20.498843 | 21.625963 |
| I | 33.967109 | 18.601104 | 24.724586 |
| I | 36.239277 | 21.028722 | 22.223022 |
| I | 32.325619 | 20.499703 | 21.623636 |
| I | 25.870340 | 23.136583 | 19.237282 |
| I | 34.129576 | 23.137069 | 19.234453 |
| I | 27.657581 | 25.195273 | 16.710084 |
| I | 17.028663 | 35.806021 | 31.739237 |
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| I | 16.888476 | 27.892932 | 31.934130 |
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| I | 19.379573 | 21.842226 | 35.053370 |
| I | 21.029407 | 36.237145 | 37.775624 |
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| I | 27.893306 | 43.111331 | 31.933003 |
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| I | 41.399328 | 33.965774 | 35.271752 |
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| I | 29.998468 | 37.436086 | 40.892668 |
| I | 33.966096 | 41.403987 | 35.265355 |
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| I | 33.964435 | 41.403418 | 24.729279 |
| I | 30.000634 | 37.430660 | 19.111022 |
| I | 22.569075 | 29.998138 | 19.109361 |
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| I | 18.597319 | 33.966125 | 24.731280 |
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| I | 30.003389 | 18.171508 | 24.910563 |
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| I | 39.584131 | 17.757754 | 31.883911 |
| I | 39.581027 | 17.749875 | 28.106503 |
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| I | 42.252659 | 20.428163 | 31.893669 |

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| I | 29.999497 | 32.677519 | 14.544144 |
| I | 17.750134 | 39.576588 | 28.114776 |
| I | 17.747348 | 39.573639 | 31.888257 |
| I | 20.418824 | 42.246986 | 31.887584 |
| I | 20.420760 | 42.247867 | 28.109642 |
| I | 17.753144 | 20.419172 | 28.112499 |
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| I | 17.750780 | 20.421890 | 31.890667 |
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| I | 39.573469 | 42.253914 | 28.108771 |
| I | 42.246072 | 39.581792 | 28.114923 |
| I | 42.249826 | 39.576283 | 31.890690 |

xyz-file for octahedral fullerene (CrI<sub>3</sub>)<sub>216</sub>

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siesta: Etot = -860668.487771 eV

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| Cr | 20.399359 | 12.186696 | 29.999044 |
| Cr | 28.084206 | 12.270888 | 29.999470 |
| Cr | 31.918830 | 12.271090 | 30.000052 |
| Cr | 39.602024 | 12.186465 | 30.003398 |
| Cr | 43.398079 | 12.466258 | 29.999565 |
| Cr | 14.537457 | 14.535708 | 32.928702 |
| Cr | 22.296579 | 13.476507 | 33.440710 |
| Cr | 26.193508 | 13.484462 | 33.394623 |
| Cr | 33.808321 | 13.484326 | 33.394850 |
| Cr | 37.704082 | 13.477538 | 33.440284 |
| Cr | 16.307424 | 16.306640 | 35.797699 |
| Cr | 20.322722 | 15.459468 | 36.220283 |
| Cr | 28.068147 | 15.175978 | 36.370813 |
| Cr | 31.934432 | 15.176834 | 36.370868 |
| Cr | 39.678202 | 15.459100 | 36.219908 |
| Cr | 22.232872 | 17.431908 | 38.996043 |
| Cr | 26.125119 | 17.127682 | 39.117108 |
| Cr | 33.877405 | 17.128587 | 39.117775 |
| Cr | 37.768444 | 17.431960 | 38.995454 |
| Cr | 20.171607 | 20.169724 | 41.168302 |
| Cr | 28.049963 | 19.040277 | 41.871621 |
| Cr | 31.949778 | 19.040813 | 41.870533 |
| Cr | 22.116157 | 22.116515 | 43.880983 |
| Cr | 26.052241 | 21.255945 | 44.385384 |
| Cr | 33.948323 | 21.255147 | 44.385618 |
| Cr | 28.024305 | 23.157486 | 47.163181 |
| Cr | 31.975611 | 23.157593 | 47.163787 |
| Cr | 25.883046 | 25.889297 | 49.407194 |
| Cr | 27.927594 | 27.927886 | 51.880392 |
| Cr | 14.537698 | 14.536119 | 27.070156 |
| Cr | 22.297571 | 13.473533 | 26.557894 |
| Cr | 26.195066 | 13.484466 | 26.603128 |
| Cr | 33.810145 | 13.483812 | 26.604037 |
| Cr | 37.705424 | 13.474326 | 26.557276 |
| Cr | 16.307506 | 16.308066 | 24.200637 |
| Cr | 20.322617 | 15.460381 | 23.786231 |
| Cr | 28.069131 | 15.176722 | 23.628127 |
| Cr | 31.934178 | 15.177005 | 23.629179 |
| Cr | 39.677950 | 15.459667 | 23.778367 |
| Cr | 22.229978 | 17.433965 | 21.009023 |
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| Cr | 33.876287 | 17.129777 | 20.881951 |
| Cr | 37.767427 | 17.433158 | 21.005863 |
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| Cr | 28.047807 | 19.039881 | 18.128809 |
| Cr | 31.950365 | 19.039312 | 18.127172 |
| Cr | 22.117006 | 22.116824 | 16.118309 |
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| Cr | 28.025127 | 23.157973 | 12.836506 |
| Cr | 31.974912 | 23.157901 | 12.837120 |
| Cr | 25.887752 | 25.883624 | 10.592586 |
| Cr | 27.926696 | 27.926712 | 8.120716  |
| Cr | 12.466399 | 43.398194 | 30.000549 |
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| Cr | 12.271844 | 28.084324 | 30.000360 |
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| Cr | 12.466182 | 16.600764 | 29.999948 |
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| Cr | 13.476159 | 37.705110 | 33.440796 |
| Cr | 13.484148 | 33.811775 | 33.394450 |
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| Cr | 13.475544 | 22.296311 | 33.439883 |
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| Cr | 15.459493 | 39.678594 | 36.217462 |
| Cr | 15.178143 | 31.935906 | 36.371912 |
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| Cr | 15.460130 | 20.323091 | 36.217553 |
| Cr | 17.433317 | 37.769750 | 38.992775 |
| Cr | 17.132253 | 33.878788 | 39.119324 |
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| Cr | 17.432588 | 22.230852 | 38.993788 |
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| Cr | 19.041554 | 31.950344 | 41.871333 |
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| Cr | 22.115847 | 37.883676 | 43.881494 |
| Cr | 21.255284 | 33.949102 | 44.387176 |
| Cr | 21.254571 | 26.051736 | 44.386967 |
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| Cr | 23.158044 | 28.025085 | 47.163521 |
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| Cr | 13.476624 | 37.705037 | 26.559446 |
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| Cr | 13.483580 | 26.193693 | 26.603883 |
| Cr | 13.476668 | 22.295357 | 26.556775 |
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| Cr | 21.254520 | 33.948084 | 15.612498 |

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| Cr | 23.157752 | 31.976250 | 12.836428 |
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| Cr | 25.887178 | 34.116921 | 10.591649 |
| Cr | 27.927179 | 32.073025 | 8.120588  |
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| Cr | 31.919921 | 47.729431 | 30.000233 |
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| Cr | 22.297592 | 46.521981 | 26.561647 |
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| Cr | 38.743820 | 33.947635 | 44.386216 |
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| Cr | 36.842615 | 31.975215 | 47.163124 |
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| Cr | 32.073445 | 27.927014 | 51.881156 |
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| Cr | 46.523181 | 22.296015 | 26.559065 |
| Cr | 46.515653 | 26.193524 | 26.605554 |
| Cr | 46.517188 | 33.809240 | 26.604105 |
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| Cr | 39.829254 | 20.170974 | 18.832634 |
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| Cr | 40.959283 | 31.949425 | 18.130219 |

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| Cr | 37.883271 | 22.116537 | 16.118668 |
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| Cr | 36.842600 | 31.975912 | 12.836591 |
| Cr | 34.113521 | 25.883530 | 10.591720 |
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| I | 39.429740 | 27.679348 | 46.460785 |
| I | 47.093868 | 39.694434 | 35.237719 |
| I | 45.182700 | 38.066092 | 38.297819 |
| I | 43.337269 | 35.934708 | 40.844506 |
| I | 41.352151 | 33.981883 | 43.642596 |
| I | 39.429314 | 32.320360 | 46.458963 |
| I | 37.425086 | 30.000137 | 48.969401 |
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| I | 35.943428 | 43.336681 | 40.843909 |
| I | 33.984047 | 41.354378 | 43.644236 |
| I | 32.320509 | 39.430022 | 46.461926 |
| I | 29.999921 | 37.414267 | 48.975029 |
| I | 35.751507 | 47.493813 | 35.035656 |
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| I | 26.133909 | 45.432154 | 38.183602 |

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| I | 39.689443 | 12.904859 | 35.240717 |
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| I | 35.751462 | 12.507530 | 35.034578 |
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| I | 14.572141 | 33.869673 | 38.182525 |
| I | 12.700937 | 31.972985 | 35.227295 |
| I | 16.665177 | 35.940185 | 40.843213 |
| I | 18.646512 | 33.981754 | 43.642881 |
| I | 16.474691 | 32.062126 | 41.023628 |
| I | 14.427210 | 30.001822 | 38.117191 |
| I | 12.700695 | 28.032692 | 35.226464 |
| I | 12.507324 | 24.250725 | 35.033591 |
| I | 14.570636 | 26.130899 | 38.182468 |
| I | 16.473664 | 27.938843 | 41.023403 |
| I | 18.432548 | 30.000726 | 43.671448 |
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| I | 22.575468 | 29.999857 | 48.969928 |
| I | 20.569956 | 27.678782 | 46.461303 |
| I | 18.646552 | 26.017727 | 43.642955 |
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| I | 14.819069 | 21.934701 | 38.293318 |
| I | 12.905286 | 20.308944 | 35.235311 |
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| I | 29.999917 | 32.652642 | 53.623414 |
| I | 27.297102 | 29.999661 | 53.623960 |
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| I | 14.635182 | 48.033013 | 31.890179 |
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| I | 11.963922 | 14.637634 | 28.103717 |
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| I | 45.347954 | 11.953502 | 31.907901 |
| I | 45.371508 | 11.971260 | 28.116646 |
| I | 48.045895 | 14.651333 | 28.091356 |

xyz-file for icosahedral fullerene (CrI<sub>3</sub>)<sub>60</sub>

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siesta: Etot = -239036.557967 eV

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| Cr | 23.103813 | 16.641799 | 30.173155 |
| Cr | 26.895853 | 16.642064 | 30.172983 |
| Cr | 21.018674 | 19.519731 | 32.350714 |
| Cr | 22.912568 | 22.121252 | 34.344525 |
| Cr | 21.020588 | 15.967798 | 26.607261 |
| Cr | 22.917547 | 15.356016 | 23.392449 |
| Cr | 16.470583 | 24.225757 | 30.172859 |
| Cr | 17.645005 | 20.617572 | 30.172782 |
| Cr | 18.552624 | 27.102823 | 32.348354 |
| Cr | 21.624933 | 26.101586 | 34.344079 |
| Cr | 15.179573 | 25.997257 | 26.608598 |
| Cr | 15.179349 | 24.002448 | 23.391251 |
| Cr | 21.625254 | 32.872798 | 30.171326 |
| Cr | 18.551485 | 30.652321 | 30.172732 |
| Cr | 24.999911 | 31.766276 | 32.353478 |
| Cr | 24.999922 | 28.542383 | 34.342357 |
| Cr | 22.917339 | 34.643687 | 26.607449 |
| Cr | 21.020401 | 34.032247 | 23.392937 |
| Cr | 31.448865 | 30.652490 | 30.172583 |
| Cr | 28.374903 | 32.872975 | 30.171025 |
| Cr | 31.447225 | 27.103011 | 32.348010 |
| Cr | 28.374629 | 26.101636 | 34.343948 |
| Cr | 33.526650 | 29.962588 | 26.606214 |
| Cr | 32.350055 | 31.575707 | 23.390201 |
| Cr | 32.355194 | 20.617693 | 30.172471 |
| Cr | 33.530122 | 24.225187 | 30.172918 |
| Cr | 28.981401 | 19.519493 | 32.350853 |
| Cr | 27.086664 | 22.121294 | 34.344343 |
| Cr | 32.349789 | 18.424336 | 26.609837 |
| Cr | 33.526804 | 20.037509 | 23.393767 |
| Cr | 26.896355 | 33.358242 | 19.826823 |
| Cr | 23.103731 | 33.358244 | 19.826883 |
| Cr | 28.981450 | 30.480749 | 17.649049 |
| Cr | 27.087114 | 27.878378 | 15.655679 |
| Cr | 28.979433 | 34.031246 | 23.392737 |
| Cr | 27.082685 | 34.643626 | 26.607406 |
| Cr | 33.529502 | 25.773795 | 19.827501 |
| Cr | 32.355415 | 29.382030 | 19.827151 |
| Cr | 31.447258 | 22.897303 | 17.651777 |
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| Cr | 34.820365 | 24.002716 | 23.391305 |
| Cr | 34.820472 | 25.997370 | 26.608741 |
| Cr | 28.374655 | 17.127131 | 19.828704 |
| Cr | 31.448083 | 19.347552 | 19.827889 |
| Cr | 25.000151 | 18.234487 | 17.646181 |
| Cr | 24.999942 | 21.457445 | 15.657698 |
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| Cr | 28.979373 | 15.967761 | 26.607188 |
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| Cr | 18.552687 | 22.896692 | 17.651889 |
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| Cr | 16.473118 | 20.037986 | 23.393985 |
| Cr | 17.650390 | 18.424215 | 26.610404 |
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| Cr | 16.470404 | 25.774314 | 19.827187 |
| Cr | 21.018313 | 30.480569 | 17.649435 |
| Cr | 22.912778 | 27.878378 | 15.655867 |
| Cr | 17.650044 | 31.575969 | 23.390176 |
| Cr | 16.472995 | 29.962536 | 26.606528 |
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| I  | 23.040288 | 14.195598 | 25.907699 |
| I  | 23.108033 | 19.394673 | 30.522523 |
| I  | 26.891952 | 19.394652 | 30.522664 |
| I  | 24.999667 | 21.998791 | 32.503036 |
| I  | 23.108744 | 17.550966 | 27.536244 |
| I  | 26.890905 | 17.551140 | 27.536011 |
| I  | 24.999914 | 16.950623 | 24.323533 |
| I  | 19.092409 | 25.071469 | 30.527710 |
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| I  | 23.240337 | 27.421600 | 32.499714 |
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| I | 16.501717 | 18.322740 | 29.125272 |
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| I | 27.951115 | 24.038830 | 36.135942 |
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| I | 31.675341 | 31.088382 | 17.761789 |
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| I | 18.324359 | 31.088548 | 17.761942 |
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| I | 21.276012 | 35.156960 | 20.874491 |
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| I | 16.021429 | 24.000828 | 17.761048 |
| I | 14.196813 | 24.595830 | 20.874159 |
| I | 16.021284 | 25.998951 | 32.239034 |
| I | 14.197157 | 25.403837 | 29.125377 |
| I | 14.199255 | 28.509814 | 27.206291 |
| I | 16.020760 | 31.021766 | 29.123550 |
| I | 17.145645 | 29.473287 | 32.238742 |

xyz-file for icosahedral fullerene (CrI<sub>3</sub>)<sub>240</sub>

960

siesta: Etot = -956274.439793 eV

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| Cr | 26.168877 | 13.670280 | 40.115768 |
| Cr | 33.829311 | 13.670703 | 40.116455 |
| Cr | 37.622432 | 13.744295 | 40.066518 |
| Cr | 20.259525 | 16.605078 | 42.279086 |
| Cr | 28.059115 | 16.394007 | 42.377295 |
| Cr | 31.941733 | 16.394394 | 42.376766 |
| Cr | 22.132738 | 19.214750 | 44.347925 |
| Cr | 26.145991 | 19.027611 | 44.405861 |
| Cr | 33.852006 | 19.027795 | 44.406578 |
| Cr | 28.080087 | 21.707264 | 46.424188 |
| Cr | 31.909443 | 21.707544 | 46.424313 |
| Cr | 25.969926 | 24.500321 | 48.389521 |
| Cr | 27.915857 | 27.175673 | 50.336487 |
| Cr | 20.256934 | 13.027658 | 36.523656 |
| Cr | 28.055944 | 12.751392 | 36.683593 |
| Cr | 31.938483 | 12.749143 | 36.682534 |
| Cr | 22.135879 | 12.310511 | 33.281223 |
| Cr | 26.148540 | 12.129931 | 33.412765 |
| Cr | 33.850281 | 12.124269 | 33.412292 |
| Cr | 28.076054 | 11.510310 | 30.109265 |
| Cr | 31.912338 | 11.510493 | 30.108556 |
| Cr | 25.968476 | 11.064485 | 26.726861 |
| Cr | 27.920544 | 10.561267 | 23.507517 |
| Cr | 12.168389 | 32.251881 | 40.067850 |
| Cr | 13.260419 | 28.597589 | 40.116741 |
| Cr | 15.645344 | 21.300091 | 40.114478 |
| Cr | 16.883296 | 17.707845 | 40.065203 |
| Cr | 14.247356 | 35.140664 | 42.278920 |
| Cr | 16.406550 | 27.641483 | 42.404611 |
| Cr | 17.611097 | 23.956031 | 42.399266 |
| Cr | 17.281742 | 34.139388 | 44.353054 |
| Cr | 18.316902 | 30.273597 | 44.446507 |
| Cr | 20.697199 | 22.954913 | 44.449720 |
| Cr | 21.454560 | 29.258684 | 46.500755 |
| Cr | 22.610364 | 25.608032 | 46.508209 |
| Cr | 23.495634 | 32.148293 | 48.398480 |
| Cr | 26.618172 | 31.133003 | 50.345268 |
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| Cr | 14.228045 | 20.815294 | 33.398582 |
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| Cr | 13.026280 | 22.486310 | 30.102714 |
| Cr | 10.770709 | 28.010072 | 26.720357 |
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| Cr | 17.299810 | 40.971781 | 40.106843 |
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| Cr | 29.999957 | 46.584716 | 42.279601 |
| Cr | 23.536269 | 42.201294 | 42.397836 |
| Cr | 20.412597 | 39.933257 | 42.398787 |
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| Cr | 26.630448 | 41.192989 | 44.435255 |
| Cr | 20.412939 | 36.664627 | 44.432983 |
| Cr | 26.630856 | 37.904549 | 46.486327 |
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| Cr | 25.969602 | 48.935837 | 33.273060 |
| Cr | 22.637324 | 46.698747 | 33.394498 |
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| Cr | 20.713058 | 46.061300 | 30.096087 |
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| Cr | 39.586498 | 39.933168 | 42.398825 |
| Cr | 36.463212 | 42.200088 | 42.396975 |
| Cr | 42.716164 | 34.140592 | 44.352903 |
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| Cr | 36.503583 | 32.146948 | 48.397413 |
| Cr | 33.381142 | 31.132451 | 50.344907 |
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| Cr | 37.866289 | 19.214616 | 44.347884 |
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| Cr | 32.084036 | 27.174702 | 50.334921 |
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| Cr | 17.302048 | 19.028294 | 19.893529 |
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| Cr | 20.413587 | 20.066351 | 17.601156 |
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| I | 32.939715 | 29.079565 | 52.136036 |
| I | 39.478235 | 11.950420 | 39.054165 |
| I | 39.454196 | 13.856170 | 42.154945 |
| I | 42.426317 | 15.995837 | 42.131652 |
| I | 44.246521 | 15.394682 | 39.044128 |
| I | 42.445657 | 12.859566 | 37.116133 |
| I | 28.170143 | 11.351874 | 17.865654 |
| I | 27.070514 | 9.815336  | 20.978015 |
| I | 29.999717 | 8.844127  | 22.903647 |
| I | 32.927178 | 9.815875  | 20.979299 |
| I | 31.830508 | 11.350958 | 17.863772 |
| I | 27.059468 | 30.922185 | 7.861065  |
| I | 28.168260 | 27.449195 | 7.851604  |
| I | 31.829597 | 27.449529 | 7.852458  |
| I | 32.939323 | 30.921089 | 7.863030  |
| I | 29.998748 | 33.086306 | 7.863218  |
| I | 48.287562 | 25.968450 | 17.855657 |
| I | 47.165454 | 22.489577 | 17.867824 |
| I | 48.284517 | 20.953904 | 20.984256 |
| I | 50.111527 | 23.459523 | 22.897449 |
| I | 50.106093 | 26.553200 | 20.962405 |
| I | 50.111637 | 36.539798 | 37.101382 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 50.106159 | 33.446811 | 39.037228 |
| I | 48.287446 | 34.031974 | 42.143513 |
| I | 47.165400 | 37.510698 | 42.131275 |
| I | 48.284344 | 39.045948 | 39.014914 |
| I | 44.247564 | 44.602050 | 20.954710 |
| I | 42.446508 | 47.137726 | 22.881661 |
| I | 39.481424 | 48.045030 | 20.941873 |
| I | 39.449662 | 46.144590 | 17.837711 |
| I | 42.422937 | 44.005232 | 17.870068 |