**Designing and Theoretical study of fluorinated small molecule donor materials for organic solar cells**

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Supporting information (SI-1) is cartesian coordinates of internally optimized geometries of all molecules (reference **R**, and architecture molecules **D-1**, **D-2**, **D-3** and **D-4** along X, Y and Z axis at MPW1PW91/6-31G (d, p) level of density functional theory(DFT).

**Cartesian coordinates of Reference Molecule R**

|  |  |  |  |
| --- | --- | --- | --- |
| **Symbol** | **X** | **Y** | **Z** |
| C | -1.2092630 | 0.7118650 | -0.0887310 |
| C | -1.1728340 | -0.7076350 | -0.0191400 |
| C | 0.0094470 | -1.4469100 | -0.0404820 |
| C | 1.2113560 | -0.7108510 | -0.1237920 |
| C | 1.1749200 | 0.7086890 | -0.1936820 |
| C | -0.0073340 | 1.4480030 | -0.1717200 |
| S | -2.7839510 | -1.3795450 | 0.0326000 |
| S | 2.7860770 | 1.3806360 | -0.2432100 |
| C | -0.0178780 | -2.9118060 | 0.0197620 |
| C | 0.0190680 | 2.9130250 | -0.2294440 |
| C | 2.5513680 | -1.2024390 | -0.0950690 |
| C | -2.5493230 | 1.2033630 | -0.1182630 |
| C | -3.4972300 | 0.2209830 | -0.0602930 |
| C | 3.4993930 | -0.2201840 | -0.1538360 |
| C | -0.6534600 | -3.7042780 | 0.9385990 |
| C | -0.4986550 | -5.0804210 | 0.6423030 |
| C | 0.2293340 | -5.3700090 | -0.4744860 |
| C | 0.6541690 | 3.7083300 | -1.1462800 |
| C | 0.4962860 | 5.0836340 | -0.8476390 |
| C | -0.2333820 | 5.3696210 | 0.2690810 |
| S | 0.7471650 | -3.8880140 | -1.2054790 |
| S | -0.7489490 | 3.8853930 | 0.9968890 |
| F | -1.0290920 | -6.0318890 | 1.4204250 |
| F | 1.0250550 | 6.0376610 | -1.6237400 |
| C | 0.5552950 | -6.7153440 | -1.0259380 |
| H | 1.6343890 | -6.8862610 | -1.0727090 |
| H | 0.1195270 | -7.4780790 | -0.3790380 |
| H | 0.1503900 | -6.8527680 | -2.0324960 |
| C | -0.5623670 | 6.7131450 | 0.8232480 |
| H | -0.1544690 | 6.8507230 | 1.8285870 |
| H | -1.6418910 | 6.8797810 | 0.8746610 |
| H | -0.1316990 | 7.4783420 | 0.1758170 |
| H | -1.1884040 | -3.3312300 | 1.8014220 |
| H | -2.7941060 | 2.2541990 | -0.1996130 |
| H | 2.7958730 | -2.2534520 | -0.0147000 |
| H | 1.1909520 | 3.3380350 | -2.0091490 |
| C | -9.6386170 | 1.2897510 | -0.1369750 |
| C | -9.5994860 | -0.1328450 | -0.1269310 |
| C | -8.4149540 | -0.8695130 | -0.1005040 |
| C | -7.2175300 | -0.1229950 | -0.0989470 |
| C | -7.2560070 | 1.3002040 | -0.1023310 |
| C | -8.4375530 | 2.0368090 | -0.1134590 |
| S | -11.2067970 | -0.8141030 | -0.1244500 |
| S | -5.6451490 | 1.9756760 | -0.0555390 |
| C | -8.4380850 | -2.3358470 | -0.0708550 |
| C | -8.4171100 | 3.5031130 | -0.0999590 |
| C | -5.8772720 | -0.6129220 | -0.0948040 |
| C | -10.9745870 | 1.7751620 | -0.1733510 |
| C | -11.9266620 | 0.7855500 | -0.1664540 |
| C | -4.9311550 | 0.3727310 | -0.0682850 |
| C | -9.0879310 | -3.1869920 | -0.9272740 |
| C | -8.9372450 | -4.5563170 | -0.5829390 |
| C | -8.1800220 | -4.7594670 | 0.5372870 |
| C | -7.7437120 | 4.3453380 | -0.9469700 |
| C | -7.9118010 | 5.7186940 | -0.6274030 |
| C | -8.7055730 | 5.9342760 | 0.4649860 |
| S | -7.6425910 | -3.2447910 | 1.1854970 |
| S | -9.2563130 | 4.4261910 | 1.1173490 |
| C | -7.8180320 | -6.0527130 | 1.1897950 |
| H | -8.1978150 | -6.1115940 | 2.2138420 |
| H | -8.2486530 | -6.8812920 | 0.6248120 |
| H | -6.7349400 | -6.1996550 | 1.2304970 |
| C | -9.0965910 | 7.2351040 | 1.0849610 |
| H | -8.7583750 | 7.3095830 | 2.1224880 |
| H | -10.1808610 | 7.3789410 | 1.0807550 |
| H | -8.6470030 | 8.0575900 | 0.5258160 |
| H | -9.6390600 | -2.8380880 | -1.7916130 |
| H | -11.2319460 | 2.8255060 | -0.2105610 |
| H | -5.6325510 | -1.6666360 | -0.1221530 |
| H | -7.1650760 | 3.9861770 | -1.7887960 |
| C | 7.2200440 | 0.1230660 | -0.1415050 |
| C | 7.2583190 | -1.3001650 | -0.1433800 |
| C | 8.4397360 | -2.0369390 | -0.1334030 |
| C | 9.6411750 | -1.2902240 | -0.1382440 |
| C | 9.6022140 | 0.1323500 | -0.1309610 |
| C | 8.4175850 | 0.8692710 | -0.1242260 |
| S | 5.6468400 | -1.9755440 | -0.1312630 |
| S | 11.2094540 | 0.8132730 | -0.1041400 |
| C | 8.4191120 | -3.5032070 | -0.1166940 |
| C | 8.4411560 | 2.3357210 | -0.0971620 |
| C | 10.9773910 | -1.7760680 | -0.1523290 |
| C | 5.8799370 | 0.6131610 | -0.1550770 |
| C | 4.9332630 | -0.3722770 | -0.1439340 |
| C | 11.9294860 | -0.7866530 | -0.1318570 |
| C | 7.7620440 | -4.3480510 | -0.9738030 |
| C | 7.9237910 | -5.7203840 | -0.6465240 |
| C | 8.6962080 | -5.9324400 | 0.4617480 |
| C | 9.1028390 | 3.1841730 | -0.9471830 |
| C | 8.9483340 | 4.5544960 | -0.6086120 |
| C | 8.1763020 | 4.7609650 | 0.5008380 |
| S | 9.2345860 | -4.4222840 | 1.1195080 |
| S | 7.6294970 | 3.2483610 | 1.1459970 |
| C | 9.0735390 | -7.2311020 | 1.0945890 |
| H | 8.7087720 | -7.3035460 | 2.1232320 |
| H | 8.6397260 | -8.0557460 | 0.5262460 |
| H | 10.1577740 | -7.3730600 | 1.1186280 |
| C | 7.8058550 | 6.0562550 | 1.1444740 |
| H | 8.1693780 | 6.1171130 | 2.1742860 |
| H | 6.7224240 | 6.2046060 | 1.1674320 |
| H | 8.2464510 | 6.8828830 | 0.5843470 |
| H | 7.1997250 | -3.9913550 | -1.8276710 |
| H | 5.6358570 | 1.6672210 | -0.1733540 |
| H | 11.2349250 | -2.8265760 | -0.1834390 |
| H | 9.6652130 | 2.8326700 | -1.8031880 |
| H | 9.3918240 | 5.3669880 | -1.1712640 |
| H | 7.4870760 | -6.5309070 | -1.2174130 |
| H | -9.3729430 | -5.3705360 | -1.1491700 |
| H | -7.4643140 | 6.5272550 | -1.1927090 |
| C | -14.3758990 | 0.1663990 | -0.2145260 |
| C | -15.7560110 | 0.6890210 | -0.2546440 |
| C | -16.1539430 | -1.6397020 | -0.2322550 |
| N | -16.6668370 | -0.3747670 | -0.2614940 |
| S | -14.3902190 | -1.5859760 | -0.1896850 |
| S | -17.0058800 | -3.0404330 | -0.2350080 |
| O | -16.0870130 | 1.8563740 | -0.2791060 |
| C | -13.3335310 | 1.0291850 | -0.2037210 |
| H | -13.6274690 | 2.0764850 | -0.2270600 |
| C | 14.3794120 | -0.1682980 | -0.1411390 |
| C | 15.7597790 | -0.6914800 | -0.1589530 |
| C | 16.1582340 | 1.6371020 | -0.1322580 |
| N | 16.6710240 | 0.3719470 | -0.1524000 |
| S | 14.3940310 | 1.5840880 | -0.1175210 |
| S | 17.0106740 | 3.0374950 | -0.1226250 |
| O | 16.0906630 | -1.8589810 | -0.1772230 |
| C | 13.3366980 | -1.0307200 | -0.1461900 |
| H | 13.6306460 | -2.0781330 | -0.1637400 |
| C | -18.0942270 | -0.1229440 | -0.2986430 |
| H | -18.5709080 | -0.5534760 | 0.5829530 |
| H | -18.5293820 | -0.5785990 | -1.1890340 |
| H | -18.2243370 | 0.9575720 | -0.3170170 |
| C | 18.0987120 | 0.1195050 | -0.1670500 |
| H | 18.5478790 | 0.5741390 | -1.0509850 |
| H | 18.5618190 | 0.5506400 | 0.7214570 |
| H | 18.2286110 | -0.9610820 | -0.1823920 |

**Cartesian coordinates of Designed Molecule D-1**

|  |  |  |  |
| --- | --- | --- | --- |
| **Symbol** | **X** | **Y** | **Z** |
| C | -1.1949890 | 0.7853660 | -0.1585160 |
| C | -1.1541280 | -0.6348010 | -0.1027780 |
| C | 0.0303660 | -1.3701490 | -0.1319520 |
| C | 1.2293790 | -0.6285280 | -0.2089280 |
| C | 1.1883180 | 0.7916640 | -0.2655520 |
| C | 0.0039380 | 1.5269990 | -0.2357530 |
| S | -2.7628110 | -1.3126450 | -0.0559970 |
| S | 2.7966560 | 1.4700400 | -0.3089440 |
| C | 0.0081350 | -2.8355070 | -0.0852330 |
| C | 0.0253190 | 2.9924920 | -0.2798440 |
| C | 2.5708990 | -1.1155720 | -0.1848220 |
| C | -2.5362830 | 1.2727470 | -0.1819590 |
| C | -3.4807090 | 0.2863390 | -0.1327340 |
| C | 3.5151360 | -0.1289620 | -0.2343370 |
| C | -0.6244810 | -3.6381320 | 0.8268870 |
| C | -0.4649840 | -5.0110630 | 0.5185100 |
| C | 0.2636860 | -5.2882010 | -0.6011250 |
| C | 0.6561890 | 3.7979600 | -1.1907710 |
| C | 0.4944960 | 5.1699920 | -0.8794630 |
| C | -0.2339480 | 5.4434670 | 0.2413010 |
| S | 0.7761470 | -3.7981030 | -1.3192530 |
| S | -0.7433570 | 3.9511420 | 0.9567130 |
| F | -0.9919740 | -5.9707760 | 1.2881060 |
| F | 1.0188650 | 6.1323510 | -1.6477030 |
| C | 0.5934660 | -6.6273890 | -1.1651080 |
| H | 1.6730350 | -6.7941350 | -1.2149010 |
| H | 0.1613190 | -7.3974290 | -0.5245160 |
| H | 0.1875490 | -6.7570310 | -2.1722520 |
| C | -0.5653210 | 6.7807520 | 0.8089750 |
| H | -0.1543360 | 6.9102250 | 1.8140970 |
| H | -1.6451550 | 6.9433680 | 0.8656960 |
| H | -0.1394400 | 7.5533370 | 0.1672190 |
| H | -1.1598930 | -3.2747810 | 1.6935810 |
| H | -2.7841510 | 2.3236180 | -0.2532850 |
| H | 2.8187620 | -2.1665570 | -0.1145190 |
| H | 1.1921380 | 3.4373020 | -2.0582550 |
| C | -9.6218260 | 1.3440840 | -0.1835030 |
| C | -9.5802350 | -0.0790070 | -0.2032420 |
| C | -8.3950200 | -0.8141340 | -0.1938230 |
| C | -7.1995580 | -0.0643300 | -0.1783260 |
| C | -7.2401270 | 1.3594580 | -0.1524160 |
| C | -8.4219230 | 2.0944610 | -0.1462540 |
| S | -11.1853050 | -0.7649300 | -0.2128640 |
| S | -5.6306820 | 2.0361280 | -0.0914090 |
| C | -8.4158080 | -2.2806570 | -0.1926230 |
| C | -8.4053110 | 3.5596970 | -0.1019380 |
| C | -5.8592480 | -0.5520270 | -0.1843720 |
| C | -10.9565120 | 1.8272260 | -0.2074770 |
| C | -11.9078890 | 0.8342190 | -0.2190920 |
| C | -4.9148230 | 0.4351850 | -0.1378090 |
| C | -9.0601360 | -3.1159310 | -1.0688490 |
| C | -8.9096850 | -4.4912330 | -0.7495370 |
| C | -8.1583210 | -4.7145140 | 0.3709520 |
| C | -7.7292570 | 4.4205020 | -0.9282900 |
| C | -7.9032490 | 5.7864110 | -0.5822570 |
| C | -8.7036290 | 5.9779220 | 0.5099980 |
| S | -7.6257440 | -3.2118470 | 1.0504090 |
| S | -9.2536500 | 4.4557260 | 1.1291590 |
| C | -7.7992230 | -6.0192450 | 1.0017320 |
| H | -8.1882020 | -6.0983440 | 2.0208940 |
| H | -8.2228050 | -6.8376830 | 0.4171230 |
| H | -6.7162550 | -6.1644160 | 1.0493820 |
| C | -9.1006560 | 7.2646030 | 1.1549940 |
| H | -8.7694380 | 7.3168610 | 2.1960430 |
| H | -10.1850360 | 7.4069430 | 1.1465580 |
| H | -8.6485390 | 8.0993950 | 0.6166740 |
| H | -9.6057000 | -2.7517610 | -1.9305080 |
| H | -11.2158710 | 2.8777670 | -0.2215240 |
| H | -5.6129190 | -1.6045310 | -0.2335730 |
| H | -7.1455120 | 4.0802890 | -1.7744600 |
| C | 7.2329630 | 0.2306890 | -0.2180820 |
| C | 7.2776760 | -1.1931290 | -0.2249110 |
| C | 8.4617240 | -1.9246820 | -0.2141590 |
| C | 9.6595120 | -1.1700080 | -0.2133800 |
| C | 9.6134180 | 0.2529040 | -0.2003440 |
| C | 8.4260540 | 0.9841270 | -0.1948740 |
| S | 5.6694740 | -1.8756190 | -0.2163880 |
| S | 11.2162100 | 0.9434960 | -0.1659140 |
| C | 8.4500830 | -3.3904300 | -0.2012260 |
| C | 8.4422990 | 2.4505220 | -0.1619940 |
| C | 10.9962170 | -1.6485820 | -0.2268950 |
| C | 5.8915890 | 0.7146410 | -0.2312300 |
| C | 4.9494200 | -0.2758840 | -0.2244950 |
| C | 11.9442550 | -0.6530570 | -0.1981650 |
| C | 7.7920540 | -4.2366670 | -1.0567770 |
| C | 7.9664500 | -5.6085680 | -0.7358370 |
| C | 8.7487780 | -5.8190860 | 0.3660890 |
| C | 9.0937330 | 3.3052180 | -1.0138580 |
| C | 8.9341120 | 4.6734460 | -0.6694000 |
| C | 8.1684310 | 4.8716540 | 0.4460890 |
| S | 9.2812860 | -4.3078140 | 1.0255270 |
| S | 7.6340460 | 3.3539610 | 1.0896460 |
| C | 9.1398980 | -7.1168520 | 0.9921360 |
| H | 8.7835590 | -7.1943390 | 2.0232660 |
| H | 8.7074920 | -7.9427470 | 0.4247160 |
| H | 10.2251850 | -7.2509180 | 1.0074360 |
| C | 7.7954530 | 6.1624240 | 1.0972590 |
| H | 8.1674880 | 6.2219040 | 2.1240530 |
| H | 6.7113880 | 6.3035840 | 1.1300700 |
| H | 8.2258210 | 6.9937210 | 0.5361920 |
| H | 7.2218570 | -3.8815330 | -1.9060870 |
| H | 5.6429250 | 1.7676440 | -0.2453960 |
| H | 11.2595070 | -2.6976750 | -0.2614450 |
| H | 9.6507540 | 2.9597420 | -1.8758870 |
| H | 9.3685400 | 5.4904960 | -1.2324600 |
| H | 7.5317070 | -6.4202320 | -1.3064520 |
| H | -9.3409350 | -5.2952330 | -1.3334050 |
| H | -7.4549920 | 6.6073780 | -1.1286210 |
| C | -14.3575470 | 0.2196340 | -0.2670030 |
| C | -15.7228410 | 0.7445260 | -0.2789190 |
| C | -16.1291760 | -1.6176630 | -0.3455670 |
| N | -16.6583030 | -0.3326890 | -0.2236220 |
| S | -14.3719250 | -1.5331110 | -0.2894240 |
| S | -16.9271180 | -3.0147460 | -0.5891940 |
| O | -16.0783060 | 1.9007000 | -0.3126220 |
| C | -13.3102550 | 1.0816440 | -0.2449290 |
| H | -13.6001220 | 2.1302730 | -0.2468270 |
| C | 14.3938670 | -0.0348050 | -0.1765670 |
| C | 15.7626460 | -0.5613100 | -0.2016850 |
| C | 16.1444660 | 1.8041230 | -0.1199510 |
| N | 16.6879490 | 0.5242940 | -0.1039480 |
| S | 14.3964370 | 1.7187890 | -0.1261400 |
| S | 16.9813580 | 3.2083330 | -0.1128180 |
| O | 16.1051870 | -1.7120540 | -0.3193470 |
| C | 13.3477470 | -0.8968930 | -0.2065360 |
| H | 13.6407250 | -1.9442190 | -0.2396530 |
| C | -17.9985170 | 0.0235030 | -0.2338160 |
| H | -18.1917160 | 0.9390840 | -0.7813950 |
| C | 18.0625540 | 0.3570800 | -0.1972150 |
| H | 18.5699270 | 1.1173210 | -0.7803060 |
| C | 18.7821070 | -0.6301960 | 0.3842900 |
| C | -19.0200320 | -0.5840470 | 0.4132010 |
| C | -20.3393110 | -0.0619830 | 0.2201110 |
| C | -18.8933480 | -1.6331630 | 1.3733510 |
| C | 20.1843740 | -0.6965890 | 0.1030570 |
| C | 18.2831660 | -1.5669850 | 1.3407330 |
| N | -21.4084540 | 0.3588790 | 0.0608640 |
| N | -18.8433400 | -2.4207470 | 2.2241080 |
| N | 21.3200050 | -0.7531010 | -0.1263190 |
| N | 17.9409360 | -2.2990830 | 2.1726440 |

**Cartesian coordinates of Designed Molecule D-2**

|  |  |  |  |
| --- | --- | --- | --- |
| **Symbol** | **X** | **Y** | **Z** |
| C | -1.1744350 | 0.8771450 | -0.1457580 |
| C | -1.1366830 | -0.5418080 | -0.0646980 |
| C | 0.0474000 | -1.2782860 | -0.0490580 |
| C | 1.2491550 | -0.5393260 | -0.1054480 |
| C | 1.2112300 | 0.8796340 | -0.1870260 |
| C | 0.0272330 | 1.6161460 | -0.2024500 |
| S | -2.7469890 | -1.2174140 | -0.0500830 |
| S | 2.8211220 | 1.5558730 | -0.1975140 |
| C | 0.0221740 | -2.7427030 | 0.0213160 |
| C | 0.0517060 | 3.0807080 | -0.2704260 |
| C | 2.5890260 | -1.0268570 | -0.0353810 |
| C | -2.5141670 | 1.3650520 | -0.2140450 |
| C | -3.4609130 | 0.3806000 | -0.1734570 |
| C | 3.5355360 | -0.0420640 | -0.0747330 |
| C | -0.6355930 | -3.5301010 | 0.9288760 |
| C | -0.4694610 | -4.9079480 | 0.6470020 |
| C | 0.2886720 | -5.2037000 | -0.4479620 |
| C | 0.7083230 | 3.8706070 | -1.1767570 |
| C | 0.5398320 | 5.2477240 | -0.8926170 |
| C | -0.2187620 | 5.5402530 | 0.2029990 |
| S | 0.8219700 | -3.7257500 | -1.1759250 |
| S | -0.7495080 | 4.0603280 | 0.9285630 |
| F | -1.0180570 | -5.8549700 | 1.4176410 |
| F | 1.0862630 | 6.1970030 | -1.6619570 |
| C | 0.6324580 | -6.5521430 | -0.9806770 |
| H | 1.7126610 | -6.7218960 | -0.9941710 |
| H | 0.1785630 | -7.3112160 | -0.3420180 |
| H | 0.2578070 | -6.6966240 | -1.9978650 |
| C | -0.5646790 | 6.8870740 | 0.7385350 |
| H | -0.1858220 | 7.0317530 | 1.7541460 |
| H | -1.6453750 | 7.0528610 | 0.7578870 |
| H | -0.1163890 | 7.6483800 | 0.0985570 |
| H | -1.1938470 | -3.1524530 | 1.7747800 |
| H | -2.7589320 | 2.4146920 | -0.3097970 |
| H | 2.8337850 | -2.0764950 | 0.0608960 |
| H | 1.2674470 | 3.4954210 | -2.0231890 |
| C | -9.5986180 | 1.4413190 | -0.3982430 |
| C | -9.5584630 | 0.0184160 | -0.3858280 |
| C | -8.3743650 | -0.7171490 | -0.3326730 |
| C | -7.1783360 | 0.0313110 | -0.3045770 |
| C | -7.2179870 | 1.4549140 | -0.3105010 |
| C | -8.3991100 | 2.1906110 | -0.3490830 |
| S | -11.1644230 | -0.6651680 | -0.4177360 |
| S | -5.6096940 | 2.1320480 | -0.2256250 |
| C | -8.3969140 | -2.1834120 | -0.3025750 |
| C | -8.3809900 | 3.6566580 | -0.3368850 |
| C | -5.8383830 | -0.4571290 | -0.2674030 |
| C | -10.9327170 | 1.9252770 | -0.4642340 |
| C | -11.8843430 | 0.9339520 | -0.4762820 |
| C | -4.8943350 | 0.5300330 | -0.2188510 |
| C | -9.0250360 | -3.0351910 | -1.1745600 |
| C | -8.8816450 | -4.4042480 | -0.8262880 |
| C | -8.1518340 | -4.6063760 | 0.3122370 |
| C | -7.6860130 | 4.4983380 | -1.1670990 |
| C | -7.8647940 | 5.8718240 | -0.8546910 |
| C | -8.6880260 | 6.0881570 | 0.2156530 |
| S | -7.6315480 | -3.0911400 | 0.9730190 |
| S | -9.2539250 | 4.5805450 | 0.8558130 |
| C | -7.8052180 | -5.8990110 | 0.9742080 |
| H | -8.2132510 | -5.9589130 | 1.9872520 |
| H | -8.2180110 | -6.7283780 | 0.3972500 |
| H | -6.7233820 | -6.0434330 | 1.0450150 |
| C | -9.0980020 | 7.3893550 | 0.8223710 |
| H | -8.7941320 | 7.4634890 | 1.8704220 |
| H | -10.1814170 | 7.5339600 | 0.7823220 |
| H | -8.6295880 | 8.2113480 | 0.2782450 |
| H | -9.5544930 | -2.6869880 | -2.0526600 |
| H | -11.1902500 | 2.9753830 | -0.5078940 |
| H | -5.5919190 | -1.5105790 | -0.2871720 |
| H | -7.0848670 | 4.1388830 | -1.9928750 |
| C | 7.2521160 | 0.3146570 | 0.0526520 |
| C | 7.2957340 | -1.1088640 | 0.0529790 |
| C | 8.4786830 | -1.8411880 | 0.1010770 |
| C | 9.6767370 | -1.0887550 | 0.1344230 |
| C | 9.6317470 | 0.3338650 | 0.1407060 |
| C | 8.4451060 | 1.0663030 | 0.1082080 |
| S | 5.6872180 | -1.7900520 | 0.0151240 |
| S | 11.2337180 | 1.0222620 | 0.2211790 |
| C | 8.4639810 | -3.3072300 | 0.1184620 |
| C | 8.4624580 | 2.5327830 | 0.1352740 |
| C | 11.0137890 | -1.5687560 | 0.1635000 |
| C | 5.9117430 | 0.7997000 | -0.0031890 |
| C | 4.9688580 | -0.1895760 | -0.0208380 |
| C | 11.9609790 | -0.5746970 | 0.2174410 |
| C | 7.8335490 | -4.1552860 | -0.7554990 |
| C | 7.9924730 | -5.5265710 | -0.4231200 |
| C | 8.7356570 | -5.7347520 | 0.7057940 |
| C | 9.1449610 | 3.3829570 | -0.6965160 |
| C | 8.9759950 | 4.7528750 | -0.3633760 |
| C | 8.1720770 | 4.9571490 | 0.7236800 |
| S | 9.2498440 | -4.2220040 | 1.3768280 |
| S | 7.6125140 | 3.4430440 | 1.3541940 |
| C | 9.0999430 | -7.0312160 | 1.3505870 |
| H | 8.7020230 | -7.1058280 | 2.3666900 |
| H | 8.6899360 | -7.8583100 | 0.7683800 |
| H | 10.1835860 | -7.1666190 | 1.4102550 |
| C | 7.7781740 | 6.2514300 | 1.3552770 |
| H | 8.1072310 | 6.3124260 | 2.3965560 |
| H | 6.6942950 | 6.3975650 | 1.3422930 |
| H | 8.2354210 | 7.0791330 | 0.8103530 |
| H | 7.2930890 | -3.8015730 | -1.6245930 |
| H | 5.6645200 | 1.8528400 | -0.0288680 |
| H | 11.2766590 | -2.6182000 | 0.1402760 |
| H | 9.7316740 | 3.0332260 | -1.5368200 |
| H | 9.4317660 | 5.5666950 | -0.9141230 |
| H | 7.5746120 | -6.3392520 | -1.0048820 |
| H | -9.3024010 | -5.2190270 | -1.4028780 |
| H | -7.4036760 | 6.6800990 | -1.4092710 |
| C | -14.3325090 | 0.3177200 | -0.5694560 |
| C | -15.7015300 | 0.8410100 | -0.6294920 |
| C | -16.1070600 | -1.5120960 | -0.6381940 |
| N | -16.6321180 | -0.2285640 | -0.5812740 |
| S | -14.3522230 | -1.4336780 | -0.5512940 |
| S | -16.8942110 | -2.9278000 | -0.8344240 |
| O | -16.0510740 | 1.9978850 | -0.7015950 |
| C | -13.2875660 | 1.1797750 | -0.5416890 |
| H | -13.5779150 | 2.2277990 | -0.5739880 |
| C | 14.4083570 | 0.0468890 | 0.3055440 |
| C | 15.7814770 | -0.4783410 | 0.3439660 |
| C | 16.1563820 | 1.8801650 | 0.4247010 |
| N | 16.6992830 | 0.6103070 | 0.3582600 |
| S | 14.4063420 | 1.7990780 | 0.3587390 |
| S | 16.9927080 | 3.2820770 | 0.5325220 |
| O | 16.1135820 | -1.6373270 | 0.3994350 |
| C | 13.3663450 | -0.8167500 | 0.2530160 |
| H | 13.6615410 | -1.8636670 | 0.2379430 |
| C | -17.9816570 | 0.1184140 | -0.6695040 |
| H | -18.1718590 | 0.9293620 | -1.3635400 |
| C | 18.0757580 | 0.4371240 | 0.5011010 |
| H | 18.5330300 | 1.0898680 | 1.2364650 |
| C | 18.8213660 | -0.4623020 | -0.1700760 |
| C | -18.9951020 | -0.4274030 | 0.0283570 |
| C | -20.3217720 | -0.0042150 | -0.2912770 |
| C | -18.8124280 | -1.3548970 | 1.1890400 |
| C | 20.1895180 | -0.6051790 | 0.2164720 |
| C | 18.3365390 | -1.2402450 | -1.3525250 |
| N | -21.3951300 | 0.3508260 | -0.5531670 |
| N | 21.3003270 | -0.7091810 | 0.5358240 |
| O | 17.3903430 | -0.9263870 | -2.0323070 |
| O | 19.1245370 | -2.2897620 | -1.5812330 |
| O | -17.8136630 | -1.3993880 | 1.8644430 |
| O | -19.9163950 | -2.0665010 | 1.4050690 |
| C | 18.7673160 | -3.0788350 | -2.7178720 |
| C | -19.8578330 | -2.9515550 | 2.5264430 |
| H | 19.5051790 | -3.8762730 | -2.7625540 |
| H | 17.7634880 | -3.4870330 | -2.5930970 |
| H | 18.7967650 | -2.4743720 | -3.6255650 |
| H | -19.6683360 | -2.3916490 | 3.4433320 |
| H | -20.8301980 | -3.4365690 | 2.5655190 |
| H | -19.0643520 | -3.6865480 | 2.3856930 |

**Cartesian coordinates of Designed Molecule D-3**

|  |  |  |  |
| --- | --- | --- | --- |
| **Symbol** | **X** | **Y** | **Z** |
| C | -1.2282750 | 0.8551710 | -0.4354240 |
| C | -1.2393180 | -0.5653350 | -0.3768810 |
| C | -0.0828310 | -1.3438870 | -0.4103890 |
| C | 1.1426050 | -0.6476730 | -0.4936420 |
| C | 1.1536060 | 0.7727800 | -0.5536870 |
| C | -0.0028830 | 1.5513210 | -0.5208440 |
| S | -2.8715460 | -1.1832450 | -0.3180850 |
| S | 2.7860310 | 1.3910730 | -0.6024420 |
| C | -0.1585890 | -2.8074070 | -0.3604310 |
| C | 0.0726410 | 3.0149240 | -0.5691300 |
| C | 2.4653870 | -1.1839060 | -0.4717730 |
| C | -2.5510780 | 1.3916560 | -0.4504600 |
| C | -3.5309380 | 0.4410380 | -0.3922090 |
| C | 3.4454990 | -0.2332310 | -0.5251960 |
| C | -0.8140730 | -3.5851240 | 0.5570410 |
| C | -0.7057480 | -4.9634920 | 0.2505650 |
| C | 0.0058410 | -5.2687570 | -0.8726530 |
| C | 0.7279280 | 3.7940860 | -1.4856390 |
| C | 0.6181270 | 5.1720530 | -1.1778700 |
| C | -0.0941730 | 5.4753990 | -0.0544930 |
| S | 0.5669720 | -3.7993380 | -1.5969760 |
| S | -0.6540530 | 4.0048470 | 0.6682340 |
| F | -1.2620030 | -5.9024700 | 1.0255530 |
| F | 1.1732750 | 6.1124620 | -1.9519800 |
| C | 0.2844590 | -6.6199990 | -1.4354820 |
| H | 1.3571630 | -6.8247640 | -1.4918550 |
| H | -0.1703980 | -7.3729110 | -0.7902330 |
| H | -0.1322680 | -6.7375270 | -2.4397180 |
| C | -0.3742980 | 6.8256430 | 0.5100840 |
| H | 0.0460680 | 6.9436850 | 1.5127530 |
| H | -1.4473170 | 7.0271260 | 0.5714810 |
| H | 0.0758530 | 7.5802300 | -0.1365310 |
| H | -1.3310900 | -3.2010980 | 1.4259630 |
| H | -2.7610220 | 2.4507610 | -0.5213040 |
| H | 2.6746080 | -2.2431480 | -0.4001870 |
| H | 1.2459540 | 3.4114190 | -2.3545620 |
| C | -9.6307090 | 1.7218110 | -0.3701790 |
| C | -9.6412910 | 0.2984920 | -0.3948360 |
| C | -8.4831490 | -0.4791350 | -0.4022500 |
| C | -7.2608170 | 0.2259700 | -0.3993510 |
| C | -7.2494810 | 1.6497700 | -0.3692060 |
| C | -8.4039750 | 2.4271270 | -0.3462620 |
| S | -11.2703890 | -0.3277390 | -0.3834120 |
| S | -5.6158320 | 2.2676950 | -0.3254590 |
| C | -8.5571610 | -1.9439550 | -0.4039780 |
| C | -8.3326450 | 3.8907540 | -0.2972520 |
| C | -5.9388050 | -0.3100180 | -0.4221120 |
| C | -10.9479580 | 2.2535030 | -0.3734980 |
| C | -11.9343530 | 1.2963290 | -0.3744600 |
| C | -4.9587620 | 0.6418830 | -0.3835500 |
| C | -9.2436720 | -2.7533180 | -1.2723020 |
| C | -9.1392330 | -4.1339160 | -0.9573280 |
| C | -8.3810820 | -4.3869180 | 0.1521690 |
| C | -7.6381000 | 4.7294540 | -1.1308740 |
| C | -7.7560170 | 6.0994720 | -0.7772010 |
| C | -8.5319650 | 6.3156200 | 0.3279820 |
| S | -7.7847760 | -2.9062010 | 0.8265480 |
| S | -9.1282940 | 4.8122480 | 0.9499750 |
| C | -8.0612310 | -5.7053090 | 0.7756670 |
| H | -8.4358510 | -5.7712070 | 1.8011460 |
| H | -8.5252400 | -6.5062620 | 0.1974790 |
| H | -6.9838650 | -5.8915610 | 0.8050530 |
| C | -8.8720630 | 7.6134600 | 0.9831680 |
| H | -8.5230660 | 7.6499880 | 2.0191010 |
| H | -9.9506370 | 7.7947200 | 0.9923390 |
| H | -8.3986370 | 8.4334910 | 0.4403880 |
| H | -9.7881910 | -2.3674510 | -2.1250800 |
| H | -11.1693310 | 3.3126690 | -0.3796080 |
| H | -5.7312020 | -1.3706160 | -0.4764320 |
| H | -7.0802410 | 4.3712460 | -1.9870160 |
| C | 7.1754190 | -0.0160180 | -0.5101920 |
| C | 7.1648670 | -1.4398970 | -0.4879560 |
| C | 8.3195950 | -2.2166850 | -0.4565880 |
| C | 9.5460810 | -1.5109940 | -0.4628850 |
| C | 9.5559770 | -0.0877470 | -0.4805760 |
| C | 8.3975590 | 0.6894420 | -0.4972300 |
| S | 5.5314990 | -2.0596600 | -0.4713550 |
| S | 11.1848130 | 0.5390460 | -0.4475830 |
| C | 8.2484480 | -3.6806530 | -0.4156190 |
| C | 8.4718980 | 2.1543160 | -0.4946260 |
| C | 10.8638310 | -2.0422540 | -0.4520240 |
| C | 5.8530990 | 0.5190900 | -0.5379130 |
| C | 4.8733430 | -0.4335710 | -0.5133220 |
| C | 11.8494910 | -1.0849140 | -0.4357140 |
| C | 7.5677550 | -4.5160490 | -1.2636330 |
| C | 7.6805660 | -5.8875890 | -0.9138550 |
| C | 8.4387220 | -6.1082760 | 0.2026140 |
| C | 9.1677830 | 2.9644740 | -1.3547150 |
| C | 9.0598770 | 4.3448270 | -1.0397980 |
| C | 8.2895810 | 4.5968810 | 0.0614540 |
| S | 9.0245270 | -4.6071870 | 0.8402090 |
| S | 7.6861400 | 3.1155280 | 0.7283110 |
| C | 8.7679130 | -7.4087040 | 0.8581960 |
| H | 8.3980860 | -7.4508010 | 1.8866750 |
| H | 8.3066970 | -8.2268260 | 0.3022070 |
| H | 9.8463640 | -7.5884630 | 0.8879650 |
| C | 7.9611300 | 5.9150140 | 0.6810150 |
| H | 8.3187200 | 5.9797190 | 1.7126440 |
| H | 6.8835850 | 6.1023220 | 0.6925810 |
| H | 8.4353280 | 6.7159780 | 0.1111620 |
| H | 7.0234610 | -4.1541890 | -2.1269550 |
| H | 5.6450600 | 1.5803290 | -0.5752980 |
| H | 11.0854830 | -3.1013620 | -0.4599530 |
| H | 9.7214360 | 2.5794070 | -2.2019490 |
| H | 9.5344820 | 5.1317010 | -1.6133310 |
| H | 7.2199900 | -6.6917450 | -1.4748420 |
| H | -9.6079760 | -4.9203680 | -1.5362330 |
| H | -7.2862640 | 6.9057030 | -1.3275150 |
| C | -14.4052030 | 0.7704980 | -0.3895070 |
| C | -15.7524330 | 1.3455270 | -0.3849680 |
| C | -16.2429740 | -0.9926820 | -0.4205390 |
| N | -16.7274570 | 0.3041000 | -0.3272840 |
| S | -14.4861400 | -0.9774300 | -0.4152080 |
| S | -17.0903330 | -2.3786840 | -0.5964040 |
| O | -16.0616290 | 2.5135220 | -0.4188220 |
| C | -13.3286460 | 1.5936930 | -0.3790990 |
| H | -13.5810510 | 2.6518370 | -0.3719250 |
| C | 14.3193330 | -0.5547990 | -0.4026730 |
| C | 15.6694950 | -1.1269020 | -0.3636280 |
| C | 16.1607710 | 1.2124060 | -0.4042910 |
| N | 16.6334040 | -0.0898870 | -0.2758620 |
| S | 14.4010720 | 1.1948570 | -0.4234280 |
| S | 17.0101600 | 2.5880830 | -0.6010230 |
| O | 15.9816320 | -2.2965250 | -0.3786590 |
| C | 13.2448370 | -1.3799340 | -0.4172230 |
| H | 13.4992300 | -2.4377100 | -0.4102690 |
| C | -18.0567180 | 0.6998520 | -0.3650380 |
| H | -18.2090710 | 1.6039840 | -0.9496950 |
| C | 17.9729150 | -0.4784890 | -0.2771510 |
| H | 18.1746820 | -1.2942700 | -0.9608640 |
| C | -19.1625820 | 0.1483240 | 0.1738030 |
| C | 18.9175320 | 0.0420770 | 0.5327930 |
| C | -20.4793910 | 0.6450040 | -0.3645760 |
| C | 18.6278040 | 0.8203140 | 1.7824950 |
| C | 20.3579530 | -0.2415020 | 0.5055850 |
| C | -19.4650960 | -0.9028720 | 1.1418010 |
| C | -19.0689620 | -2.2767330 | 3.1396970 |
| C | -17.4041670 | -0.6930490 | 2.4415600 |
| C | 20.4504720 | -1.2707960 | -1.7311930 |
| C | 22.4672950 | -1.0381720 | -0.4783650 |
| N | -19.3761270 | -3.0743100 | 3.9264030 |
| N | -16.3927410 | -0.1743930 | 2.6811180 |
| N | 19.9896590 | -1.6426730 | -2.7308300 |
| N | 23.6135930 | -1.2268400 | -0.4754310 |
| O | -20.6520720 | 1.6126710 | -1.0730170 |
| O | 17.5480640 | 1.1929560 | 2.1866340 |
| C | -18.6660530 | -1.3004670 | 2.1819210 |
| C | 21.0568660 | -0.8286190 | -0.5180590 |
| C | -20.8818910 | -1.2675290 | 0.9509280 |
| C | -21.4881860 | -0.3268080 | 0.1018740 |
| C | -22.8351540 | -0.3803310 | -0.2192000 |
| C | -23.5922060 | -1.4181090 | 0.3141650 |
| C | -22.9964740 | -2.3702620 | 1.1462320 |
| C | -21.6457270 | -2.3081440 | 1.4800060 |
| H | -23.2657970 | 0.3710300 | -0.8711600 |
| H | -24.6485510 | -1.4954600 | 0.0822210 |
| H | -23.5984150 | -3.1797170 | 1.5441480 |
| H | -21.2143500 | -3.0613210 | 2.1252290 |
| C | 22.2330160 | 0.2740780 | 2.2595790 |
| C | 22.4757280 | 0.8873960 | 3.4853760 |
| C | 21.4571250 | 1.5174250 | 4.2063890 |
| C | 20.1585090 | 1.5402010 | 3.7101260 |
| C | 19.9196330 | 0.9326000 | 2.4880640 |
| C | 20.9320040 | 0.2996230 | 1.7507890 |
| H | 23.0446720 | -0.2087790 | 1.7335660 |
| H | 23.4822560 | 0.8727910 | 3.8884570 |
| H | 21.6849160 | 1.9875700 | 5.1565480 |
| H | 19.3436950 | 2.0155920 | 4.2440590 |

**Cartesian coordinates of Designed Molecule D-4**

|  |  |  |  |
| --- | --- | --- | --- |
| **Symbol** | **X** | **Y** | **Z** |
| C | -1.2979630 | -0.5107090 | -0.0833510 |
| C | -1.2499290 | 0.9102120 | -0.0593560 |
| C | -0.0609290 | 1.6373230 | -0.0202810 |
| C | 1.1343070 | 0.8872190 | 0.0151390 |
| C | 1.0869960 | -0.5334620 | -0.0138320 |
| C | -0.1016980 | -1.2603750 | -0.0728420 |
| S | -2.8537940 | 1.5983200 | -0.1078410 |
| S | 2.6929630 | -1.2195740 | 0.0051090 |
| C | -0.0739220 | 3.1041470 | -0.0204630 |
| C | -0.0866650 | -2.7264530 | -0.1213080 |
| C | 2.4761480 | 1.3682130 | 0.0863650 |
| C | -2.6418720 | -0.9912940 | -0.1162810 |
| C | -3.5804920 | 0.0014340 | -0.1399610 |
| C | 3.4165580 | 0.3769210 | 0.0867120 |
| C | -0.7506060 | 3.9387210 | 0.8291880 |
| C | -0.5599390 | 5.3004980 | 0.4903360 |
| C | 0.2353600 | 5.5380680 | -0.5923890 |
| C | 0.5407370 | -3.5880860 | 0.7391380 |
| C | 0.3708190 | -4.9383410 | 0.3474290 |
| C | -0.3607560 | -5.1408890 | -0.7861620 |
| S | 0.7741080 | 4.0231840 | -1.2350660 |
| S | -0.8625450 | -3.6059240 | -1.4110290 |
| F | -1.1210500 | 6.2871880 | 1.2000610 |
| F | 0.8907210 | -5.9473020 | 1.0569670 |
| C | 0.6107030 | 6.8567390 | -1.1761160 |
| H | 0.2616710 | 6.9601660 | -2.2073310 |
| H | 0.1532480 | 7.6499760 | -0.5831070 |
| H | 1.6932750 | 7.0109130 | -1.1722320 |
| C | -0.7016610 | -6.4400580 | -1.4315140 |
| H | -0.2902350 | -6.5135590 | -2.4421050 |
| H | -1.7826840 | -6.5903560 | -1.4987020 |
| H | -0.2829560 | -7.2525450 | -0.8359210 |
| H | -1.3400040 | 3.6057270 | 1.6726950 |
| H | -2.8957990 | -2.0431580 | -0.1215570 |
| H | 2.7265600 | 2.4192060 | 0.1470650 |
| H | 1.0804710 | -3.2820400 | 1.6250040 |
| C | -9.7283280 | -1.0033600 | -0.3508130 |
| C | -9.6697590 | 0.4155200 | -0.4450630 |
| C | -8.4785930 | 1.1405730 | -0.4055070 |
| C | -7.2941790 | 0.3842540 | -0.2750820 |
| C | -7.3515860 | -1.0353580 | -0.1813030 |
| C | -8.5396040 | -1.7604990 | -0.2221790 |
| S | -11.2663650 | 1.1143060 | -0.5453950 |
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| C | -8.4824410 | 2.6040990 | -0.4939160 |
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| C | -11.0706220 | -1.4709740 | -0.3453940 |
| C | -12.0085540 | -0.4724730 | -0.4466970 |
| C | -5.0155300 | -0.1361650 | -0.1712310 |
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| C | -8.8228070 | -5.6847560 | -0.5501400 |
| S | -7.7307210 | 3.6010310 | 0.7219080 |
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| C | -7.8711110 | 6.4023940 | 0.4999450 |
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| H | -8.7941250 | -7.8074650 | -0.4601450 |
| H | -9.6001960 | 2.9814380 | -2.3008280 |
| H | -11.3437520 | -2.5141910 | -0.2567200 |
| H | -5.6891760 | 1.9039500 | -0.3656720 |
| H | -7.4039400 | -3.6021360 | 1.6627470 |
| C | 7.1296850 | 0.0120410 | 0.2888760 |
| C | 7.1742040 | 1.4355710 | 0.3011800 |
| C | 8.3565290 | 2.1669260 | 0.3699840 |
| C | 9.5518100 | 1.4129560 | 0.4461500 |
| C | 9.5072020 | -0.0097520 | 0.4262770 |
| C | 8.3221820 | -0.7409400 | 0.3414650 |
| S | 5.5705010 | 2.1187770 | 0.1865000 |
| S | 11.1096360 | -0.6989800 | 0.4977050 |
| C | 8.3444790 | 3.6329910 | 0.3619200 |
| C | 8.3403630 | -2.2071640 | 0.3078230 |
| C | 10.8848320 | 1.8920160 | 0.5518320 |
| C | 5.7891040 | -0.4713340 | 0.2207990 |
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| S | 9.2526140 | 4.5562370 | -0.8048010 |
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| C | 9.1067800 | 7.3655190 | -0.7687880 |
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| C | -15.8307490 | -0.3471440 | -0.5713620 |
| C | -16.1852250 | 2.0020700 | -0.7907520 |
| N | -16.7345010 | 0.7483580 | -0.6400540 |
| S | -14.4328620 | 1.9115800 | -0.7399310 |
| S | -17.0171770 | 3.3996230 | -0.9833530 |
| O | -16.1761970 | -1.5028780 | -0.5551080 |
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| H | -13.7229670 | -1.7429210 | -0.3828690 |
| C | 14.2753390 | 0.2745590 | 0.7555030 |
| C | 15.6411490 | 0.7959420 | 0.8747590 |
| C | 16.0430230 | -1.5536170 | 0.8797620 |
| N | 16.5768250 | -0.2787630 | 0.8655850 |
| S | 14.2904810 | -1.4761950 | 0.7138450 |
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| O | 15.9826310 | 1.9532030 | 0.9601690 |
| C | 13.2331700 | 1.1391850 | 0.6996010 |
| H | 13.5242760 | 2.1861060 | 0.7533720 |
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| O | 20.5086740 | 1.1258030 | 1.3839670 |
| C | -19.2363990 | -2.0660880 | 3.2913800 |
| C | 22.6481680 | 0.1326540 | -0.1638950 |
| H | -19.4464090 | -3.1329000 | 3.2077420 |
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| H | -18.1992790 | -1.8983540 | 3.5752200 |
| H | 23.3315750 | -0.6623640 | 0.1369370 |
| H | 22.9310330 | 0.4809310 | -1.1579970 |
| H | 22.6739570 | 0.9522070 | 0.5518250 |
| O | -17.2915020 | -0.5914800 | 1.8991320 |