

## Designing Triazatruxene-based Donor Materials with Promising Photovoltaic Parameters for Organic Solar Cells

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### Optimized Cartesian Co-ordinates of compounds

#### Reference Molecule (R)

Symbol	X	Y	Z
C	7.92744700	-1.03169600	0.14824400
C	6.85093600	-1.89021800	-0.18584600
C	7.15407000	-3.16334500	-0.69389200
C	8.47770200	-3.57893100	-0.77632600
C	9.52123400	-2.73511800	-0.37741100
C	9.25756500	-1.44586800	0.07024400
N	7.43572800	0.23195800	0.47510100

C	6.04788400	0.20631400	0.34773700
C	5.64210100	-1.10755300	-0.01399500
C	5.11480000	1.27253000	0.43495400
C	3.81261800	1.03088000	-0.07159800
C	3.33078100	-0.28294600	-0.28389000
C	4.25871000	-1.34809700	-0.18413900
C	5.12419500	2.65910700	0.87814600
C	3.89059800	3.22050800	0.45563000
N	3.10780400	2.23334000	-0.13949000
C	2.01475700	-0.88522300	-0.41234400
C	2.22400400	-2.28866700	-0.41261800
N	3.57862500	-2.56493400	-0.26725000
C	0.69746800	-0.41299300	-0.41454400
C	-0.38378900	-1.30194500	-0.48006300
C	-0.13008100	-2.68792200	-0.53162000
C	1.16193500	-3.18917400	-0.48521800
C	5.96149300	3.45036600	1.67948400
C	5.62623900	4.77563600	1.93583800
C	4.44995600	5.33297900	1.42165300
C	3.56239700	4.55533800	0.68562300
C	4.00823600	-3.80550900	0.39115800
C	3.63982900	-3.86120000	1.87719600
C	2.13747500	2.55802600	-1.19063100
C	2.77528900	3.19399600	-2.43038600
C	8.28735600	1.41147800	0.30038700
C	8.50310800	1.79229500	-1.16744200
H	6.37696300	-3.81308000	-1.07258900

H	8.70417800	-4.56294100	-1.17023700
H	10.54725400	-3.07837800	-0.44223600
H	10.07131300	-0.78283100	0.33650300
H	0.49082000	0.64032500	-0.29374700
H	-0.95966100	-3.37861300	-0.62220200
H	1.33182400	-4.25859300	-0.50626200
H	6.84238500	3.03503100	2.14977900
H	6.27742100	5.37837800	2.55823700
H	4.20975700	6.36978900	1.62664200
H	2.62569400	4.97123600	0.33428000
H	3.56403800	-4.64355600	-0.15158200
H	5.08285800	-3.89636200	0.28661900
H	3.99268100	-4.80171200	2.30918400
H	4.11263400	-3.04016200	2.42063600
H	2.56067300	-3.79884700	2.02913200
H	1.64199900	1.63762600	-1.48279600
H	1.37444400	3.21783800	-0.76681500
H	2.00446400	3.39826000	-3.17879300
H	3.27557600	4.13404900	-2.19155800
H	3.50909900	2.51717800	-2.87412400
H	7.84495500	2.24582900	0.83029200
H	9.24083800	1.20200100	0.78957900
H	9.15141800	2.67056200	-1.23163400
H	8.97056600	0.97907100	-1.72630600
H	7.55215600	2.03806300	-1.64501100
C	-1.77328100	-0.79433400	-0.47928200
C	-2.11890200	0.39857600	-1.13727400

C	-2.80212000	-1.48784300	0.18332200
C	-3.41991600	0.87081100	-1.12867600
H	-1.36070700	0.94351700	-1.68675800
C	-4.10526500	-1.01979400	0.19181800
H	-2.56720000	-2.39646100	0.72448700
C	-4.45221900	0.17704800	-0.46567200
H	-3.65879200	1.78886300	-1.65490200
H	-4.85178600	-1.59156100	0.72707800
C	-5.78391900	0.74183200	-0.51125900
C	-6.95938700	0.32373400	0.01057300
H	-5.87699700	1.67378700	-1.06415400
C	-8.18631500	1.12078300	-0.20142100
S	-7.33540800	-1.11071400	0.97437300
N	-9.28073800	0.49758900	0.43659900
O	-8.29098500	2.16520200	-0.80447100
C	-9.04939400	-0.68289500	1.09687100
C	-10.60506000	1.05546400	0.27900400
S	-10.14591900	-1.59758000	1.91444000
C	-11.33126100	0.44715600	-0.92924200
H	-11.17571700	0.87886200	1.19275000
H	-10.48846300	2.12924900	0.11283700
O	-10.82492000	-0.29169300	-1.71667600
O	-12.61905700	0.84688100	-1.05838300
H	-12.88131900	1.41596500	-0.32437400

**M1**

<b>Symbol</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
C	8.46283100	-0.92631800	-0.02231900
C	7.39945800	-1.81859200	-0.30578400
C	7.71845800	-3.08218800	-0.82779400
C	9.04913800	-3.45630700	-0.97137200
C	10.08306600	-2.57976300	-0.62094800
C	9.80025600	-1.29874900	-0.16176600
N	7.94763600	0.32206200	0.32636900
C	6.55739600	0.25339600	0.26441400
C	6.17609800	-1.07363400	-0.07775000
C	5.59686700	1.29025100	0.39633200
C	4.28068200	1.00821500	-0.04903500
C	3.83089200	-0.32056400	-0.23790000
C	4.79457100	-1.35643300	-0.18144200
C	5.58358200	2.67679300	0.84013000
C	4.31464000	3.19888000	0.47667200
N	3.53595600	2.18733700	-0.08279600
C	2.52976700	-0.96287100	-0.30153200
C	2.78147700	-2.36040100	-0.30871100
N	4.14731100	-2.59410000	-0.22844600
C	1.20131700	-0.53089600	-0.24089600
C	0.14479700	-1.45313700	-0.25018100
C	0.43778000	-2.83185600	-0.30984900
C	1.74457600	-3.29321600	-0.32713400
C	6.43247400	3.49406400	1.60227200
C	6.06780300	4.80791400	1.87592500

C	4.85145600	5.32764600	1.41851300
C	3.95523000	4.52251400	0.72396000
C	4.64842700	-3.82239600	0.40221200
C	4.36028900	-3.89093300	1.90525200
C	2.51021800	2.48188100	-1.08984300
C	3.07245900	3.13738000	-2.35563100
C	8.75425500	1.52725200	0.11542700
C	8.89603700	1.91187900	-1.36036300
H	6.94568700	-3.75629600	-1.17111900
H	9.28785900	-4.43313900	-1.37569400
H	11.11518600	-2.89089900	-0.73320800
H	10.60425500	-0.61014500	0.06634200
H	0.97081100	0.51634000	-0.11186300
H	-0.37306300	-3.54832200	-0.35929900
H	1.94570300	-4.35694900	-0.35522200
H	7.34716800	3.10687300	2.03009200
H	6.72800700	5.43109500	2.46788200
H	4.58836300	6.35619900	1.63634000
H	2.99032500	4.90866200	0.41803000
H	4.20197300	-4.67250300	-0.11943100
H	5.71823000	-3.88005300	0.24103600
H	4.76423100	-4.82047600	2.31552800
H	4.83541700	-3.05628600	2.42535900
H	3.28917200	-3.86234700	2.11387900
H	2.03148000	1.54625500	-1.36139400
H	1.74672100	3.11771300	-0.63173200
H	2.26332000	3.31743500	-3.06888900

H	3.55264900	4.09278000	-2.13766400
H	3.80709100	2.48419200	-2.83223200
H	8.30853100	2.34825600	0.66299100
H	9.73342700	1.34832800	0.56433200
H	9.51391000	2.80938000	-1.45204900
H	9.36418100	1.11256500	-1.93834800
H	7.91880400	2.12789800	-1.79755900
C	-1.25504800	-0.98874400	-0.18330400
C	-1.66114600	0.21366700	-0.79070600
C	-2.23741600	-1.72726800	0.50373200
C	-2.97142900	0.64635000	-0.71810500
H	-0.94135300	0.80028400	-1.34812400
C	-3.55252700	-1.30340200	0.57131300
H	-1.95267800	-2.63352900	1.02400000
C	-3.96412500	-0.10457600	-0.04921900
H	-3.25335900	1.57678100	-1.19884700
H	-4.24713800	-1.89680100	1.14941200
C	-5.30220400	0.43957900	-0.05057900
C	-6.49628500	-0.09950000	0.32524900
H	-5.34470900	1.44190300	-0.45095900
C	-7.80297400	0.55497000	0.27631100
S	-6.70992900	-1.78600800	0.83746300
N	-8.82714100	-0.36725000	0.46676900
C	-8.44745000	-1.66559100	0.80187900
C	-10.24405600	-0.09731500	0.22541500
S	-9.43405000	-2.93667300	1.14722700
C	-10.52959100	0.06941600	-1.27695700

H	-10.77586600	-0.99923400	0.54115000
H	-10.59337300	0.72244700	0.84427500
O	-9.94092500	-0.56169600	-2.10526100
O	-11.54697500	0.89230400	-1.58706600
H	-11.69140100	1.54847700	-0.88814500
C	-8.02455900	1.92617200	0.11738100
C	-6.97641900	2.87600200	-0.02495500
N	-6.16954800	3.69781200	-0.14115200
C	-9.29913600	2.55361300	0.12809700
N	-10.32340100	3.09442900	0.13872000

## M2

Symbol	X	Y	Z
C	8.76829500	-0.75138200	0.18233900
C	7.75641400	-1.67189600	-0.18632300
C	8.15078100	-2.90533600	-0.72857600
C	9.50050700	-3.22594600	-0.81042100
C	10.48005800	-2.32429600	-0.37720600
C	10.12450200	-1.07014100	0.10493300
N	8.18791700	0.46519500	0.54084600
C	6.80663300	0.34814200	0.40062300
C	6.49511600	-0.97987300	-0.00273100
C	5.80140900	1.34448400	0.51122400
C	4.52275300	1.02895800	-0.01365600
C	4.13467800	-0.30832200	-0.26772300
C	5.13300000	-1.30958600	-0.19071900
C	5.71132500	2.71464300	0.99536000



C	4.44470000	3.20155300	0.57888100
N	3.73616900	2.18066900	-0.05223100
C	2.86436000	-0.99533700	-0.42245700
C	3.16957700	-2.38149100	-0.45955400
N	4.53748200	-2.56777200	-0.31191300
C	1.51858400	-0.61474200	-0.42068900
C	0.50034600	-1.57404900	-0.51670900
C	0.84899400	-2.93803200	-0.60432100
C	2.17175400	-3.35035200	-0.56408400
C	6.48604000	3.53745100	1.82733000
C	6.05742500	4.82773400	2.11991300
C	4.84865200	5.31735300	1.61210900
C	4.02246600	4.50268100	0.84550700
C	5.04988300	-3.79649800	0.30901800
C	4.68441900	-3.92256100	1.79136200
C	2.75581900	2.46945700	-1.10472400
C	3.35991600	3.18392600	-2.31831800
C	8.95845700	1.70509800	0.41330000
C	9.16274200	2.14593700	-1.03925800
H	7.42374300	-3.59561400	-1.13400600
H	9.79758700	-4.17978200	-1.23066200
H	11.52779900	-2.59390000	-0.44219200
H	10.88832800	-0.36064200	0.39785500
H	1.24096700	0.41833300	-0.27121200
H	0.07037100	-3.68206900	-0.71996900
H	2.41473700	-4.40452900	-0.61375100
H	7.39035100	3.17032600	2.29316600

H	6.66059300	5.45512100	2.76581900
H	4.53538300	6.32821200	1.84583700
H	3.06144400	4.86299300	0.49852100
H	4.66412800	-4.64522100	-0.26104000
H	6.12819700	-3.81087600	0.20482800
H	5.09934100	-4.85006200	2.19524500
H	5.10037500	-3.08891500	2.36135900
H	3.60335500	-3.93778200	1.94197800
H	2.32746500	1.52624400	-1.42901900
H	1.94558700	3.06302600	-0.67066300
H	2.58375400	3.35824700	-3.06876500
H	3.79286000	4.14801300	-2.04631500
H	4.14203600	2.57213900	-2.77377300
H	8.45426500	2.48997600	0.96309800
H	9.91879400	1.54573600	0.90787800
H	9.74996700	3.06790400	-1.06801000
H	9.69069100	1.38480200	-1.61725900
H	8.20224700	2.34148200	-1.52094000
C	-0.91821400	-1.16168700	-0.50931800
C	-1.33707500	0.03649600	-1.11697100
C	-1.90748500	-1.95712900	0.09859800
C	-2.66522900	0.42063800	-1.10490000
H	-0.61216900	0.65370100	-1.63353200
C	-3.23732200	-1.57428500	0.11759100
H	-1.62168400	-2.88290000	0.58281200
C	-3.65375600	-0.36306100	-0.47210800
H	-2.95873200	1.34371700	-1.59364500

H	-3.95787200	-2.23925800	0.57576800
C	-5.01434500	0.11924000	-0.49058000
C	-6.09220800	-0.24661100	0.25377800
H	-5.19078200	0.93384700	-1.18522400
C	-7.40704700	0.36728600	0.12810000
S	-6.05191300	-1.27192100	1.69756700
N	-8.14123700	0.19722100	1.29534800
C	-7.59113000	-0.64900700	2.25751000
C	-9.51873900	0.65713800	1.45995200
S	-8.24134300	-1.06855300	3.70801800
C	-10.48396000	-0.11467000	0.54054800
H	-9.80130400	0.40594500	2.48491200
H	-9.57252000	1.73537800	1.34685500
O	-10.39373500	-1.29691100	0.38008900
O	-11.48478300	0.61060300	0.01156100
H	-11.25069800	1.55253900	-0.02567700
C	-7.84669300	1.06737300	-0.99557200
C	-8.82125900	2.09000200	-0.91129800
N	-9.63163600	2.91308000	-0.80853400
C	-7.39812300	0.81519300	-2.39722200
O	-7.45689900	1.64613900	-3.27187200
O	-7.01319300	-0.45909500	-2.60087000
C	-6.60800900	-0.77560400	-3.94554000
H	-5.75397300	-0.16519100	-4.24419200
H	-6.33830600	-1.82873500	-3.92282700
H	-7.43027900	-0.60260000	-4.64048700

**M3**

<b>Symbol</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
C	9.49964200	-0.56939600	0.01911300
C	8.51784500	-1.57788200	-0.14358000
C	8.94516600	-2.86283200	-0.51385900
C	10.30327800	-3.13511700	-0.62698000
C	11.25721900	-2.13670200	-0.39609700
C	10.86429600	-0.83901000	-0.09014800
N	8.87767200	0.66237200	0.22211300
C	7.49828600	0.46649400	0.18351800
C	7.23439800	-0.91972600	0.00707800
C	6.45049800	1.42424900	0.19863400
C	5.16413300	0.97640300	-0.19554400
C	4.83192300	-0.39926100	-0.21840000
C	5.88290500	-1.33275100	-0.04785000
C	6.31569500	2.84810100	0.47054400
C	5.00598300	3.20971500	0.05910800
N	4.31923500	2.07381400	-0.36481200
C	3.59192300	-1.15595700	-0.19258600
C	3.96557300	-2.51615500	-0.03540500
N	5.34809700	-2.61861600	0.05889100
C	2.22973400	-0.83776900	-0.17210600
C	1.25907200	-1.84309300	-0.06293900
C	1.67240300	-3.18747500	0.04004600
C	3.01515500	-3.53143400	0.06752000
C	7.08916600	3.82328200	1.11868400
C	6.61097500	5.12423300	1.23373300

C	5.35422300	5.47655300	0.72865300
C	4.53230100	4.51750300	0.14664000
C	5.95287300	-3.71084700	0.83248800
C	5.66771600	-3.61829000	2.33488200
C	3.27074500	2.15215000	-1.38787300
C	3.77170300	2.69474200	-2.73057600
C	9.57586300	1.89867400	-0.13989500
C	9.67821900	2.11758200	-1.65240300
H	8.23341700	-3.63747800	-0.76445900
H	10.62583100	-4.12925300	-0.91397000
H	12.31244100	-2.36867500	-0.48226300
H	11.60553500	-0.06116000	0.04470300
H	1.90634700	0.19279300	-0.16742400
H	0.92702000	-3.97221300	0.08472200
H	3.30916300	-4.56909500	0.16607100
H	8.03388100	3.57232100	1.58142200
H	7.21400000	5.87006100	1.73850300
H	5.00221200	6.49737200	0.82185000
H	3.53749700	4.77782100	-0.19456400
H	5.58383000	-4.65461800	0.42351800
H	7.02417300	-3.69485700	0.67117000
H	6.14903000	-4.45215900	2.85319400
H	6.06780300	-2.68826600	2.74468500
H	4.59752900	-3.65608300	2.54670500
H	2.87620800	1.15217900	-1.53780900
H	2.45426800	2.76965300	-1.00155600
H	2.94947800	2.71345900	-3.45138600

H	4.16516300	3.70831700	-2.63662900
H	4.56133200	2.05539800	-3.13206600
H	9.06325500	2.73751200	0.31420600
H	10.56866700	1.85820700	0.31287900
H	10.21614100	3.04733400	-1.85723300
H	10.21122400	1.29838600	-2.13923400
H	8.68430000	2.19659700	-2.09809100
C	-0.17856200	-1.50004200	-0.04175700
C	-0.69149900	-0.43668200	-0.80622100
C	-1.08722200	-2.21773400	0.75768200
C	-2.03667400	-0.11707600	-0.77817400
H	-0.02639600	0.12711400	-1.44910500
C	-2.43595900	-1.90744700	0.78101100
H	-0.71897000	-3.00794000	1.40066400
C	-2.95464200	-0.85571200	-0.00192300
H	-2.40318300	0.70484500	-1.38366700
H	-3.07776400	-2.45816200	1.45621900
C	-4.34480500	-0.47021200	-0.05510300
C	-5.46203800	-1.14630200	0.32231500
H	-4.52096100	0.50501200	-0.48899900
C	-6.82120500	-0.64197100	0.17093500
S	-5.50254200	-2.86525200	0.76409000
N	-7.72907500	-1.71373700	0.16049800
C	-7.21797700	-2.96911800	0.44688800
C	-9.16756400	-1.58907300	-0.00683400
S	-8.06029400	-4.38666500	0.55846100
C	-9.58008100	-1.64253600	-1.48386300

H	-9.62303900	-2.43205100	0.51785300
H	-9.51533800	-0.66520700	0.45354000
O	-8.80821700	-1.64154600	-2.39439500
O	-10.91582300	-1.67507300	-1.68548600
H	-11.39772600	-1.70281500	-0.84945800
C	-7.15817000	0.69877700	0.06031500
C	-6.41883400	1.80291700	0.70406100
C	-8.26514100	3.00795300	-0.21087400
O	-5.40248500	1.76525700	1.36958500
S	-9.24928000	4.27600500	-0.60531100
S	-8.59221400	1.36696400	-0.76028700
N	-7.11383200	3.02509700	0.51840800
C	-6.57889300	4.25008400	1.13481700
C	-7.10695200	4.46500300	2.55184300
H	-6.85483400	5.07773400	0.48234300
H	-5.49538800	4.13635900	1.14234800
H	-6.68492400	5.38550100	2.96320600
H	-8.19448600	4.55904500	2.55457900
H	-6.81609500	3.63765100	3.20186200

#### M4

Symbol	X	Y	Z
C	9.74030600	-0.62549900	-0.03524400
C	8.76577500	-1.62760700	-0.26595600
C	9.20325300	-2.88451100	-0.71288200
C	10.56360200	-3.14140500	-0.83379800
C	11.50993300	-2.15378300	-0.53506500

C	11.10724500	-0.87984400	-0.15211700
N	9.10981800	0.58802900	0.23926900
C	7.73251400	0.38755100	0.18093700
C	7.47752300	-0.98713400	-0.08252200
C	6.67943800	1.33662300	0.25136400
C	5.39774000	0.90864500	-0.17848900
C	5.07384600	-0.46503400	-0.28905700
C	6.12877600	-1.40172500	-0.16919200
C	6.53517600	2.73908500	0.61449200
C	5.22574400	3.11950200	0.22067300
N	4.54790200	2.00970600	-0.28108900
C	3.83822900	-1.22818500	-0.31478500
C	4.21878000	-2.59475100	-0.23436600
N	5.59834300	-2.69476500	-0.13907100
C	2.47555400	-0.91947000	-0.28378400
C	1.50871800	-1.93559500	-0.23554700
C	1.92955900	-3.28260900	-0.20558700
C	3.27305300	-3.61990400	-0.19378700
C	7.30000500	3.67359300	1.32943700
C	6.81308900	4.96101900	1.52770400
C	5.55630000	5.33842500	1.04096000
C	4.74301000	4.41552700	0.39252200
C	6.20959600	-3.83274200	0.56056600
C	5.92383100	-3.84000800	2.06552600
C	3.50305500	2.14920200	-1.30129400
C	4.00434500	2.78769300	-2.60105200
C	9.80314400	1.84861300	-0.04016100



C	9.91682300	2.15977000	-1.53552100
H	8.49823200	-3.64629400	-1.01637000
H	10.89404200	-4.11384500	-1.17991900
H	12.56703000	-2.37397800	-0.62841100
H	11.84273800	-0.10755200	0.03551100
H	2.14777400	0.10751700	-0.21981300
H	1.18963900	-4.07349800	-0.20942600
H	3.57264700	-4.65976400	-0.15426400
H	8.24387300	3.39793000	1.77966800
H	7.40860500	5.67529600	2.08425100
H	5.19692700	6.34824400	1.20106900
H	3.74767300	4.69179000	0.06588600
H	5.84582800	-4.74933100	0.08982100
H	7.28057600	-3.79957100	0.40066700
H	6.41064700	-4.70276900	2.52823600
H	6.31802600	-2.93625900	2.53528200
H	4.85403100	-3.89860400	2.27455000
H	3.11941000	1.15811100	-1.52237000
H	2.67918000	2.73111200	-0.87728400
H	3.18490600	2.84849600	-3.32269700
H	4.38733100	3.79602100	-2.43559800
H	4.80187400	2.18517700	-3.04195400
H	9.28079000	2.65481600	0.45955600
H	10.79211200	1.78652500	0.41846300
H	10.45020500	3.10355000	-1.67845300
H	10.45938700	1.37520500	-2.06676600
H	8.92619700	2.25980600	-1.98434300

C	0.07319600	-1.60275900	-0.20294600
C	-0.43611100	-0.47433800	-0.87529100
C	-0.84430200	-2.39528500	0.51693000
C	-1.78090400	-0.16511000	-0.83824100
H	0.23394500	0.14794300	-1.45539100
C	-2.19178700	-2.09390100	0.55273100
H	-0.48025500	-3.23706100	1.09273500
C	-2.70680800	-0.97511100	-0.14067700
H	-2.14404700	0.70508200	-1.37437700
H	-2.83952000	-2.70238700	1.16998000
C	-4.08942700	-0.59486700	-0.17148200
C	-5.21401700	-1.28398900	0.19461300
H	-4.28053500	0.39854000	-0.56453900
C	-6.54626100	-0.73786300	0.10717700
S	-5.29783100	-3.01833300	0.54288600
N	-7.50060400	-1.74255100	0.15330600
C	-7.03866500	-3.03532500	0.36253100
C	-8.93708300	-1.51103400	0.21562000
S	-7.96769100	-4.38962000	0.49504800
C	-9.62286200	-1.85594300	-1.11578900
H	-9.33364300	-2.10526700	1.03984200
H	-9.11013700	-0.45630000	0.43305100
O	-9.08826300	-1.71120200	-2.17503700
O	-10.90418900	-2.25830200	-1.01474500
H	-11.13326200	-2.46125700	-0.09950100
C	-6.85795800	0.61959100	-0.09048400
C	-6.26473100	1.75121300	0.55508700

C	-7.42645000	2.82460200	-1.19425900
S	-7.97761300	4.03160700	-2.18212400
S	-7.94156600	1.16679600	-1.39553200
N	-6.53973200	2.93211500	-0.13741300
C	-6.08610600	4.28327700	0.26734600
C	-7.00947400	4.93671300	1.29351600
H	-6.07088200	4.86743900	-0.65168300
H	-5.06793800	4.20491000	0.63533000
H	-6.61432100	5.92294800	1.54782300
H	-8.01295300	5.06445300	0.88403500
H	-7.06907700	4.35572900	2.21448500
C	-5.72624300	0.52249500	2.60769900
N	-5.80471200	-0.41191200	3.28918500
C	-4.83404900	2.70940900	2.39909400
N	-4.15579800	3.49336300	2.91844200
C	-5.62937700	1.69412600	1.81423900

## M5

<b>Symbol</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
C	9.89485900	-0.63438400	0.00527800
C	8.93179800	-1.65015100	-0.21266500
C	9.38545700	-2.91428300	-0.62157600
C	10.74928100	-3.16272800	-0.71742600
C	11.68342600	-2.15992300	-0.43104600
C	11.26534100	-0.88011800	-0.08637500
N	9.25091600	0.58053500	0.23962800
C	7.87634700	0.36756200	0.16765600

C	7.63601500	-1.01603500	-0.06306800
C	6.81466800	1.30962200	0.19716200
C	5.54268000	0.85833700	-0.23687000
C	5.23139600	-0.52002200	-0.31267000
C	6.29216800	-1.44451300	-0.15612300
C	6.65370000	2.72157200	0.51488900
C	5.34738100	3.07889800	0.08995900
N	4.68469400	1.94822500	-0.38523200
C	4.00219700	-1.29302400	-0.33317800
C	4.39249600	-2.65422100	-0.21633700
N	5.77103700	-2.74072500	-0.10092200
C	2.63750600	-0.99356700	-0.32104200
C	1.67657500	-2.01531900	-0.26025500
C	2.10832700	-3.35846900	-0.19978300
C	3.45369500	-3.68538700	-0.16524300
C	7.40020300	3.68446500	1.21124800
C	6.90121700	4.97395100	1.36029300
C	5.64994900	5.32614100	0.84172600
C	4.85340400	4.37632400	0.21147600
C	6.38200700	-3.85794900	0.63195500
C	6.07613400	-3.83388300	2.13275000
C	3.65956200	2.04689100	-1.43019300
C	4.18485900	2.63618600	-2.74352700
C	9.93933100	1.83918700	-0.05969400
C	10.07006600	2.11715500	-1.56015100
H	8.69100800	-3.68938900	-0.91544700
H	11.09228200	-4.14075800	-1.03426700

H	12.74342700	-2.37356600	-0.50433500
H	11.99206400	-0.09728400	0.09132700
H	2.30407100	0.03286100	-0.28187300
H	1.37553900	-4.15576100	-0.19707500
H	3.76013000	-4.72197000	-0.10066500
H	8.33887600	3.43099500	1.68463000
H	7.48314900	5.71029100	1.90222700
H	5.28185600	6.33837700	0.96190600
H	3.86217500	4.63485900	-0.14128900
H	6.03182300	-4.78766500	0.17697300
H	7.45466400	-3.81933100	0.48549100
H	6.56334300	-4.68220200	2.62096900
H	6.45712100	-2.91683300	2.58739100
H	5.00413700	-3.89646000	2.32897200
H	3.27969000	1.04776800	-1.62004500
H	2.82783600	2.64404300	-1.04426100
H	3.37938200	2.66862500	-3.48247700
H	4.56427900	3.65047400	-2.60887500
H	4.99079000	2.01826900	-3.14606200
H	9.40572000	2.65289000	0.41524100
H	10.92270400	1.79411500	0.41260600
H	10.59974600	3.06066200	-1.71776800
H	10.62398000	1.32410400	-2.06648800
H	9.08471800	2.20096300	-2.02367100
C	0.23894700	-1.69345600	-0.24537900
C	-0.27088800	-0.56138000	-0.91289800
C	-0.68401500	-2.50162600	0.45094700

C	-1.61817200	-0.26395500	-0.89326500
H	0.40135600	0.07278700	-1.47730300
C	-2.03446100	-2.21436000	0.46654400
H	-0.32319100	-3.34751000	1.02249800
C	-2.54971600	-1.09106500	-0.22105700
H	-1.98204500	0.60938200	-1.42326500
H	-2.68600000	-2.84262000	1.05920600
C	-3.93204500	-0.72282600	-0.28087500
C	-5.06212400	-1.41432800	0.07851800
H	-4.12445400	0.26565300	-0.68486300
C	-6.38989000	-0.88760800	-0.06474400
S	-5.15127000	-3.13269700	0.49906000
N	-7.34380700	-1.86708700	0.04731100
C	-6.89470600	-3.15551900	0.32775200
C	-8.77436300	-1.59894700	0.07150100
S	-7.83298300	-4.49139500	0.52249000
C	-9.43036700	-1.93238000	-1.27483100
H	-9.20498500	-2.17897400	0.88807200
H	-8.91746400	-0.53820900	0.28511100
O	-8.83948800	-1.89789600	-2.31375800
O	-10.74849300	-2.20282000	-1.21575600
H	-11.04519900	-2.29557400	-0.30194900
C	-6.70014500	0.47043000	-0.34750600
C	-6.20296500	1.55825600	0.38799200
C	-7.14502500	2.68996300	-1.44573900
S	-7.58955600	3.92984800	-2.44978200
S	-7.58914800	1.02174200	-1.78097000

N	-6.43993400	2.76884900	-0.26023200
C	-6.26077900	4.09112600	0.38111900
C	-7.44954400	4.46158100	1.26721400
H	-6.15287500	4.80335700	-0.43581900
H	-5.32962600	4.06531400	0.93337300
H	-7.27339400	5.44469800	1.71111300
H	-8.37072800	4.51499100	0.68375400
H	-7.58007100	3.74234400	2.07758700
C	-5.70958900	1.42025100	1.72544900
C	-6.34822000	0.45215900	2.53851200
N	-6.92336800	-0.33482800	3.16949600
C	-4.51279200	2.03350300	2.28001000
O	-4.15269600	1.97773900	3.43455900
O	-3.74530100	2.64045300	1.30911800
C	-2.52341700	3.22618900	1.78528600
H	-2.72213700	3.96553300	2.56298200
H	-1.86419900	2.45839400	2.19340700
H	-2.06777700	3.69785100	0.91621600