

Application of Superhalogens in the Design of Organic Superconductors

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Cartesian co-ordinates of (TMTSF)₂X systems

Format:	Atom	X	Y	Z (unit = Å)
X = PF₆				
C	6.871738000000	0.704548000000	0.000853000000	
C	6.167151000000	-0.341210000000	0.522273000000	
Se	7.821722000000	0.612921000000	-1.646363000000	
Se	7.002233000000	2.406979000000	0.843060000000	
Se	5.216746000000	-0.251532000000	2.159786000000	
Se	6.024591000000	-2.032642000000	-0.321529000000	
C	8.412791000000	2.436337000000	-1.596286000000	
C	8.066643000000	3.194817000000	-0.543911000000	
C	4.885999000000	-2.790459000000	1.006062000000	
C	4.542550000000	-2.031340000000	2.063997000000	
C	9.229035000000	2.849335000000	-2.790971000000	
H	9.583018000000	3.875413000000	-2.696438000000	
H	10.104500000000	2.204026000000	-2.910964000000	
H	8.639779000000	2.781640000000	-3.710554000000	
C	8.410648000000	4.640295000000	-0.306526000000	
H	9.058023000000	5.030380000000	-1.091315000000	
H	7.508065000000	5.258425000000	-0.278810000000	
H	8.929251000000	4.769225000000	0.648300000000	
C	3.596431000000	-2.405384000000	3.169638000000	
H	2.590820000000	-2.054448000000	2.925003000000	
H	3.550418000000	-3.487831000000	3.292254000000	
H	3.903763000000	-1.970279000000	4.124441000000	
C	4.398106000000	-4.176942000000	0.697343000000	
H	4.028380000000	-4.668145000000	1.597310000000	
H	3.570975000000	-4.122032000000	-0.014866000000	
H	5.193349000000	-4.796475000000	0.273421000000	
C	-6.155198000000	0.366609000000	-0.350061000000	
C	-7.480124000000	0.491091000000	-0.087102000000	
Se	-5.419178000000	-1.020567000000	-1.428374000000	
Se	-4.829190000000	1.558025000000	0.321328000000	
Se	-8.216259000000	1.884138000000	0.993412000000	
Se	-8.805626000000	-0.709779000000	-0.758505000000	
C	-3.600463000000	-0.438710000000	-1.244557000000	
C	-3.350117000000	0.652388000000	-0.501300000000	
C	-10.277341000000	0.179760000000	0.095273000000	
C	-10.029371000000	1.272843000000	0.832606000000	
C	-2.602422000000	-1.307927000000	-1.956033000000	

H	-1.622914000000	-0.836975000000	-2.000737000000
H	-2.469388000000	-2.260008000000	-1.435403000000
H	-2.928338000000	-1.520162000000	-2.978743000000
C	-2.011682000000	1.271028000000	-0.211325000000
H	-1.203306000000	0.704618000000	-0.668679000000
H	-1.971878000000	2.302614000000	-0.576524000000
H	-1.818638000000	1.285522000000	0.865252000000
C	-11.026640000000	2.116399000000	1.579405000000
H	-11.010740000000	3.150883000000	1.222434000000
H	-12.041227000000	1.738065000000	1.457588000000
H	-10.802523000000	2.133798000000	2.650477000000
C	-11.611910000000	-0.466615000000	-0.159939000000
H	-12.419254000000	0.073051000000	0.334361000000
H	-11.835893000000	-0.495340000000	-1.230811000000
H	-11.624712000000	-1.497542000000	0.207132000000
P	0.974180000000	-1.859510000000	-0.101281000000
F	0.161948000000	-2.923871000000	-1.042706000000
F	0.630413000000	-0.647165000000	-1.164217000000
F	-0.406452000000	-1.523990000000	0.720324000000
F	1.794190000000	-0.791611000000	0.846910000000
F	1.328502000000	-3.061986000000	0.967728000000
F	2.361340000000	-2.187314000000	-0.921066000000

X = BO₂

C	-9.233079454615	-0.009844027342	0.096393392535
C	-7.879279477549	-0.017517193657	-0.036712121715
Se	-10.348818833098	1.388390510506	-0.565713038007
Se	-10.213044439588	-1.396980586580	0.964646716517
Se	-6.762698389733	-1.407579604703	0.621310347159
Se	-6.895791653794	1.361233848477	-0.899321351493
C	-11.985553374874	0.593866474178	0.044410273080
C	-11.928427420819	-0.581783187957	0.689549171613
C	-5.174169461125	0.554965887297	-0.630730278995
C	-5.117789721076	-0.624559098585	0.016142314433
C	-13.214275271082	1.401550153836	-0.275058879510
H	-14.118731742724	0.911910345952	0.084654332939
H	-13.164139430980	2.392080257836	0.187468542075
H	-13.319323728478	1.546368800377	-1.354654958164
C	-13.078951207411	-1.374561648461	1.247942682830
H	-14.032420816703	-0.881816856026	1.060111646931
H	-13.123601384479	-2.371091542943	0.797984680908
H	-12.977329596045	-1.505096462233	2.329716517954
C	-3.897048833804	-1.439804731715	0.335342847497
H	-3.952319492424	-2.417945240535	-0.154548019007
H	-2.975746205527	-0.946462318246	0.009103052402

H	-3.824888477845	-1.615110390843	1.413968107625
C	-4.030512934697	1.349871021205	-1.193784682877
H	-3.062808462698	0.880802275070	-0.989299497016
H	-4.136327259741	1.455109463816	-2.278899806653
H	-4.017166915140	2.357436986592	-0.764804330752
C	7.879264554750	0.017498075435	-0.035847594736
C	9.233171690209	0.010334565761	0.096228608327
Se	6.895609193478	-1.361845201661	-0.897322913612
Se	6.762694950081	1.407349661313	0.622626834319
Se	10.213336915853	1.398191497587	0.963099852042
Se	10.348876566336	-1.387791958120	-0.566164775458
C	5.173890457713	-0.556272679930	-0.627362864863
C	5.117570779281	0.623424473770	0.019216711534
C	11.985745095792	-0.592799811597	0.042983471726
C	11.928721378781	0.583094891354	0.687684001730
C	4.030035828489	-1.351835729328	-1.189081916416
H	3.062359408176	-0.882875353402	-0.984188348597
H	4.135104124739	-1.457781978260	-2.274199146317
H	4.017234020107	-2.359119659117	-0.759414422341
C	3.896741186026	1.438132145308	0.339430785668
H	2.975411273371	0.944637662174	0.013492791629
H	3.825094063206	1.612858847484	1.418190280600
H	3.951454763881	2.416543518796	-0.149974478688
C	13.079344915284	1.376197843347	1.245406076978
H	12.978561626516	1.506276389912	2.327315122182
H	14.032886281011	0.883964569517	1.056594332759
H	13.123166771204	2.372916532397	0.795788336028
C	13.214436934732	-1.400531831597	-0.276482355727
H	14.119121852192	-0.909766564248	0.081117258230
H	13.165336059493	-2.390195566605	0.188016019332
H	13.318195469665	-1.547378560528	-1.355925174066
B	-0.000176553982	-0.001215955522	-0.597986515944
O	1.260003955277	0.008602389287	-0.593578935136
O	-1.260358699830	-0.011059470435	-0.600070442410

X = AuF₆

C	5.534900000000	0.311480000000	-0.497655000000
C	5.069399000000	-0.796166000000	0.183239000000
Se	4.379990000000	1.509212000000	-1.411436000000
Se	7.361747000000	0.803635000000	-0.583743000000
Se	6.134621000000	-1.849305000000	1.328882000000
Se	3.257461000000	-1.336726000000	0.053600000000
C	5.803260000000	2.615229000000	-2.055784000000
C	7.068072000000	2.336187000000	-1.693765000000
C	3.448349000000	-2.691210000000	1.374833000000

C	4.676734000000	-2.926209000000	1.897822000000
C	5.341562000000	3.756783000000	-2.923106000000
H	6.169635000000	4.403075000000	-3.212746000000
H	4.868324000000	3.385135000000	-3.836778000000
H	4.604178000000	4.371909000000	-2.399310000000
C	8.318885000000	3.089109000000	-2.057966000000
H	8.094547000000	3.945702000000	-2.692836000000
H	8.829351000000	3.461344000000	-1.164383000000
H	9.022830000000	2.449378000000	-2.598957000000
C	5.003696000000	-3.942127000000	2.963746000000
H	4.725082000000	-3.573012000000	3.955950000000
H	4.467440000000	-4.876688000000	2.789486000000
H	6.070693000000	-4.174681000000	2.984680000000
C	2.183876000000	-3.376159000000	1.804741000000
H	2.400919000000	-4.225001000000	2.454371000000
H	1.553912000000	-2.658440000000	2.338895000000
H	1.600094000000	-3.702902000000	0.943650000000
C	-5.129880000000	0.797459000000	0.170670000000
C	-5.318762000000	-0.397299000000	-0.501207000000
Se	-6.549701000000	1.935164000000	0.680566000000
Se	-3.406095000000	1.403218000000	0.668959000000
Se	-3.897041000000	-1.553250000000	-0.984466000000
Se	-7.026320000000	-1.028167000000	-1.025573000000
C	-5.404127000000	3.215989000000	1.493905000000
C	-4.069637000000	2.983912000000	1.487192000000
C	-6.371256000000	-2.636490000000	-1.825208000000
C	-5.041854000000	-2.846803000000	-1.802646000000
C	-6.082270000000	4.427235000000	2.074380000000
H	-6.417163000000	5.110243000000	1.286378000000
H	-6.958137000000	4.153033000000	2.669069000000
H	-5.397395000000	4.975159000000	2.721918000000
C	-3.035129000000	3.905980000000	2.086006000000
H	-3.025027000000	4.864702000000	1.558690000000
H	-3.255309000000	4.097034000000	3.140282000000
H	-2.039600000000	3.463713000000	2.014204000000
C	-4.306969000000	-4.036761000000	-2.362965000000
H	-3.794295000000	-4.586576000000	-1.568289000000
H	-4.982578000000	-4.726385000000	-2.868272000000
H	-3.547300000000	-3.721748000000	-3.083867000000
C	-7.437162000000	-3.524095000000	-2.408616000000
H	-7.004332000000	-4.416715000000	-2.859102000000
H	-8.145004000000	-3.849314000000	-1.639975000000
H	-8.006770000000	-3.002625000000	-3.183990000000
F	-1.572740000000	-1.011708000000	1.275450000000
F	-1.215878000000	0.218736000000	-1.158920000000
F	-0.977909000000	1.886277000000	1.243958000000

F	1.415168000000	1.025550000000	-0.398510000000
F	1.049796000000	-0.248340000000	2.075316000000
F	0.851162000000	-1.867083000000	-0.279872000000
Au	-0.075305000000	0.014658000000	0.459210000000

X = B₂F₇

C	5.362070000000	-0.410527000000	-0.008658000000
C	4.529528000000	0.657549000000	-0.080823000000
Se	6.017192000000	-1.346121000000	-1.541394000000
Se	6.007932000000	-1.135184000000	1.638144000000
Se	3.874011000000	1.587231000000	1.446899000000
Se	3.891388000000	1.390798000000	-1.718905000000
C	7.094826000000	-2.574683000000	-0.531988000000
C	7.090869000000	-2.486017000000	0.806503000000
C	2.877711000000	2.795421000000	-0.894457000000
C	2.869820000000	2.878542000000	0.445930000000
C	7.864930000000	-3.550129000000	-1.380208000000
H	8.437515000000	-4.247055000000	-0.768807000000
H	7.191636000000	-4.137067000000	-2.012615000000
H	8.565581000000	-3.028994000000	-2.039980000000
C	7.855283000000	-3.340397000000	1.781049000000
H	8.456300000000	-4.091652000000	1.269386000000
H	8.530146000000	-2.731851000000	2.390885000000
H	7.176324000000	-3.862184000000	2.462760000000
C	2.114493000000	3.857081000000	1.299459000000
H	2.767948000000	4.307396000000	2.052852000000
H	1.682547000000	4.656995000000	0.701031000000
H	1.289020000000	3.354125000000	1.810469000000
C	2.139784000000	3.669211000000	-1.869240000000
H	1.622270000000	4.480291000000	-1.360210000000
H	2.825253000000	4.101109000000	-2.605305000000
H	1.381366000000	3.087895000000	-2.400731000000
C	-5.222732000000	-1.196359000000	0.050512000000
C	-3.890386000000	-1.481889000000	0.120026000000
Se	-6.276101000000	-0.733872000000	1.564181000000
Se	-6.209844000000	-1.191161000000	-1.574540000000
Se	-2.831634000000	-1.904210000000	-1.394292000000
Se	-2.897448000000	-1.456581000000	1.733742000000
C	-7.866855000000	-0.382837000000	0.554689000000
C	-7.839001000000	-0.576137000000	-0.773978000000
C	-1.211578000000	-1.740511000000	0.893708000000
C	-1.183315000000	-1.930839000000	-0.439351000000
C	-9.024244000000	0.105804000000	1.382605000000
H	-9.926500000000	0.213813000000	0.781375000000
H	-9.247361000000	-0.590651000000	2.196463000000

H	-8.801170000000	1.078849000000	1.830549000000
C	-8.957894000000	-0.349821000000	-1.754041000000
H	-9.884002000000	-0.082310000000	-1.246170000000
H	-8.711266000000	0.458314000000	-2.449311000000
H	-9.150443000000	-1.249551000000	-2.346216000000
C	0.043492000000	-2.084719000000	-1.294086000000
H	0.324605000000	-1.112640000000	-1.709992000000
H	0.883182000000	-2.462209000000	-0.709309000000
H	-0.127384000000	-2.779931000000	-2.120455000000
C	-0.022320000000	-1.644303000000	1.808006000000
H	0.831741000000	-2.184861000000	1.398007000000
H	0.262719000000	-0.595192000000	1.929595000000
H	-0.239496000000	-2.062618000000	2.794371000000
B	-1.474857000000	4.656036000000	0.143083000000
F	-2.277342000000	1.460591000000	-0.190201000000
F	-0.223156000000	1.490861000000	0.850251000000
F	-0.350749000000	1.181710000000	-1.423654000000
F	-0.823200000000	3.260298000000	-0.555117000000
F	-2.641635000000	4.818503000000	-0.521263000000
F	-1.568189000000	4.340833000000	1.459503000000
F	-0.490379000000	5.552482000000	-0.170163000000
B	-0.941632000000	1.759016000000	-0.306526000000

X = BF₄

C	-3.657792000000	0.770557000000	-0.032206000000
C	-2.429088000000	1.322611000000	-0.114797000000
Se	-4.579963000000	0.477452000000	1.623777000000
Se	-4.672246000000	0.204640000000	-1.558203000000
Se	-1.508827000000	1.623692000000	-1.762048000000
Se	-1.415573000000	1.886206000000	1.403002000000
C	-6.212287000000	-0.113841000000	0.790551000000
C	-6.250919000000	-0.226935000000	-0.544074000000
C	-0.031046000000	2.738615000000	0.370476000000
C	-0.070221000000	2.625964000000	-0.965439000000
C	-7.326951000000	-0.387587000000	1.763326000000
H	-8.205705000000	-0.794244000000	1.262968000000
H	-7.015140000000	-1.107890000000	2.526371000000
H	-7.629252000000	0.527996000000	2.281256000000
C	-7.419742000000	-0.653308000000	-1.390089000000
H	-8.263753000000	-0.970461000000	-0.777836000000
H	-7.759127000000	0.166368000000	-2.031078000000
H	-7.149101000000	-1.489224000000	-2.043021000000
C	0.896270000000	3.201267000000	-1.961942000000
H	0.416200000000	3.984085000000	-2.558675000000
H	1.776653000000	3.613631000000	-1.472829000000

H	1.250690000000	2.424900000000	-2.646519000000
C	0.993370000000	3.457781000000	1.200562000000
H	1.749163000000	3.934889000000	0.579987000000
H	0.519119000000	4.222346000000	1.824095000000
H	1.521224000000	2.762374000000	1.859959000000
C	2.887727000000	-1.488459000000	0.113938000000
C	1.580127000000	-1.904360000000	0.091517000000
Se	3.985795000000	-1.417143000000	-1.419419000000
Se	3.770390000000	-0.915902000000	1.680146000000
Se	0.496349000000	-2.025675000000	1.641611000000
Se	0.666900000000	-2.394933000000	-1.495653000000
C	5.497831000000	-0.707788000000	-0.516029000000
C	5.408996000000	-0.497430000000	0.812083000000
C	-0.950506000000	-2.892269000000	-0.608278000000
C	-1.023823000000	-2.734583000000	0.725345000000
C	6.655683000000	-0.330834000000	-1.398278000000
H	7.604664000000	-0.481943000000	-0.880564000000
H	6.679173000000	-0.926041000000	-2.314127000000
H	6.570999000000	0.727968000000	-1.660308000000
C	6.446180000000	0.149274000000	1.684109000000
H	7.425462000000	0.119863000000	1.205887000000
H	6.174175000000	1.196636000000	1.844821000000
H	6.525633000000	-0.350170000000	2.653803000000
C	-2.209823000000	-3.021155000000	1.604820000000
H	-2.720759000000	-2.095031000000	1.888513000000
H	-2.934539000000	-3.653835000000	1.092167000000
H	-1.909041000000	-3.535106000000	2.521745000000
C	-2.042527000000	-3.382147000000	-1.520061000000
H	-2.817022000000	-3.905702000000	-0.959513000000
H	-2.518764000000	-2.545585000000	-2.041410000000
H	-1.652688000000	-4.071883000000	-2.273243000000
B	4.363356000000	2.786032000000	-0.108555000000
F	5.637109000000	2.598884000000	-0.687142000000
F	3.850492000000	4.054604000000	-0.439015000000
F	3.476664000000	1.786831000000	-0.597222000000
F	4.462419000000	2.655259000000	1.298700000000

X = BH₄

C	3.571038000000	0.600283000000	0.063859000000
C	2.360333000000	1.193950000000	0.086441000000
Se	4.536540000000	0.214991000000	-1.548690000000
Se	4.513308000000	0.050115000000	1.641690000000
Se	1.396083000000	1.579461000000	1.692799000000
Se	1.413425000000	1.738233000000	-1.483808000000
C	6.130933000000	-0.367069000000	-0.638460000000

C	6.121294000000	-0.435189000000	0.699508000000
C	-0.006957000000	2.620276000000	-0.526861000000
C	-0.011496000000	2.555721000000	0.812421000000
C	7.273862000000	-0.691094000000	-1.561584000000
H	8.126543000000	-1.097587000000	-1.017789000000
H	6.975077000000	-1.429736000000	-2.312282000000
H	7.611352000000	0.201979000000	-2.096808000000
C	7.252593000000	-0.849288000000	1.600619000000
H	8.110742000000	-1.204204000000	1.030103000000
H	7.585187000000	-0.012078000000	2.222256000000
H	6.944274000000	-1.655294000000	2.274188000000
C	-0.998006000000	3.195462000000	1.749142000000
H	-0.572884000000	4.100319000000	2.196825000000
H	-1.925375000000	3.454281000000	1.235394000000
H	-1.259322000000	2.514877000000	2.565426000000
C	-0.990267000000	3.337237000000	-1.408324000000
H	-1.905691000000	3.589918000000	-0.871195000000
H	-0.550219000000	4.256755000000	-1.809199000000
H	-1.280596000000	2.712472000000	-2.258642000000
C	-3.465212000000	-0.887490000000	-0.047147000000
C	-2.209175000000	-1.438165000000	-0.120081000000
Se	-4.413543000000	-0.667557000000	1.570809000000
Se	-4.403359000000	-0.228857000000	-1.541783000000
Se	-1.260646000000	-1.662283000000	-1.745414000000
Se	-1.233740000000	-2.019720000000	1.397617000000
C	-5.920078000000	0.167585000000	0.774360000000
C	-5.920052000000	0.348048000000	-0.560847000000
C	0.291092000000	-2.603440000000	0.402563000000
C	0.279041000000	-2.451281000000	-0.932761000000
C	-6.946095000000	0.697451000000	1.735977000000
H	-7.941892000000	0.686121000000	1.289658000000
H	-6.986864000000	0.110105000000	2.656374000000
H	-6.695514000000	1.733531000000	1.985807000000
C	-6.942566000000	1.105113000000	-1.356131000000
H	-7.906545000000	1.111216000000	-0.845830000000
H	-6.595282000000	2.138674000000	-1.461969000000
H	-7.087578000000	0.671850000000	-2.349304000000
C	1.383195000000	-2.796118000000	-1.893667000000
H	1.912277000000	-1.894466000000	-2.218291000000
H	2.113796000000	-3.460895000000	-1.433108000000
H	0.992739000000	-3.296425000000	-2.784044000000
C	1.412705000000	-3.150546000000	1.241960000000
H	2.149303000000	-3.667360000000	0.627068000000
H	1.930444000000	-2.344990000000	1.772271000000
H	1.042117000000	-3.860292000000	1.986734000000
B	-4.380109000000	3.288474000000	-0.058854000000

H	-4.551227000000	3.171512000000	-1.275656000000
H	-5.472470000000	3.302201000000	0.508189000000
H	-3.717112000000	2.334922000000	0.356894000000
H	-3.776111000000	4.332545000000	0.165798000000

X = ClO₄

C	3.893436000000	-0.695217000000	-0.000504000000
C	2.668396000000	-1.260650000000	-0.000653000000
Se	4.858587000000	-0.253590000000	1.596949000000
Se	4.858307000000	-0.252041000000	-1.597688000000
Se	1.703900000000	-1.703971000000	-1.590055000000
Se	1.704198000000	-1.705445000000	1.588508000000
C	6.466251000000	0.259791000000	0.669680000000
C	6.466140000000	0.260412000000	-0.670198000000
C	0.305664000000	-2.659710000000	0.669216000000
C	0.305558000000	-2.659096000000	-0.671384000000
C	7.608846000000	0.611556000000	1.583056000000
H	8.469179000000	0.981476000000	1.025518000000
H	7.316520000000	1.387628000000	2.297610000000
H	7.932180000000	-0.260312000000	2.160318000000
C	7.608552000000	0.613130000000	-1.583428000000
H	8.469378000000	0.981438000000	-1.025587000000
H	7.931083000000	-0.257883000000	-2.162423000000
H	7.316409000000	1.390693000000	-2.296444000000
C	-0.677500000000	-3.329707000000	-1.588103000000
H	-0.188160000000	-4.116100000000	-2.172180000000
H	-1.506707000000	-3.766927000000	-1.034756000000
H	-1.107685000000	-2.607780000000	-2.288927000000
C	-0.677319000000	-3.330992000000	1.585502000000
H	-1.505904000000	-3.768887000000	1.031773000000
H	-0.187713000000	-4.117004000000	2.169863000000
H	-1.108421000000	-2.609345000000	2.286054000000
C	-2.974818000000	1.548471000000	0.000238000000
C	-1.651235000000	1.913090000000	0.000826000000
Se	-3.975997000000	1.267535000000	-1.573400000000
Se	-3.976943000000	1.265877000000	1.572951000000
Se	-0.642737000000	2.181176000000	1.582292000000
Se	-0.642188000000	2.184591000000	-1.579718000000
C	-5.571071000000	0.760153000000	-0.675178000000
C	-5.571456000000	0.759340000000	0.673214000000
C	0.942133000000	2.745763000000	-0.670225000000
C	0.941883000000	2.744327000000	0.674576000000
C	-6.684815000000	0.287885000000	-1.566740000000
H	-7.652439000000	0.407953000000	-1.077466000000
H	-6.713669000000	0.843523000000	-2.507472000000

H	-6.534958000000	-0.774189000000	-1.785390000000
C	-6.685650000000	0.286030000000	1.563641000000
H	-7.652823000000	0.404513000000	1.073112000000
H	-6.534620000000	-0.775731000000	1.783002000000
H	-6.716363000000	0.842106000000	2.504064000000
C	2.089569000000	3.098957000000	1.579692000000
H	2.539377000000	2.199020000000	2.011022000000
H	2.871156000000	3.628115000000	1.034887000000
H	1.762798000000	3.740662000000	2.402331000000
C	2.090084000000	3.102446000000	-1.574185000000
H	2.872093000000	3.629195000000	-1.027660000000
H	2.539195000000	2.203592000000	-2.008488000000
H	1.763794000000	3.747081000000	-2.394730000000
Cl	-4.328130000000	-2.762315000000	0.000276000000
O	-5.178414000000	-2.598055000000	-1.221420000000
O	-3.250868000000	-1.711769000000	-0.001023000000
O	-3.685508000000	-4.112336000000	-0.001382000000
O	-5.174420000000	-2.599075000000	1.224882000000

X = NO₃

C	-3.147817000000	-1.444085000000	-0.220699000000
C	-3.062474000000	-0.189609000000	-0.725378000000
Se	-4.462174000000	-1.981675000000	1.060714000000
Se	-1.973689000000	-2.867721000000	-0.723586000000
Se	-1.741949000000	0.349452000000	-1.988075000000
Se	-4.238490000000	1.230916000000	-0.237072000000
C	-3.757352000000	-3.756160000000	1.275813000000
C	-2.709586000000	-4.129320000000	0.526626000000
C	-3.393019000000	2.541208000000	-1.353626000000
C	-2.340661000000	2.166730000000	-2.101444000000
C	-4.486281000000	-4.581055000000	2.301591000000
H	-4.096877000000	-5.597747000000	2.348586000000
H	-4.393547000000	-4.139472000000	3.298671000000
H	-5.553536000000	-4.643742000000	2.067509000000
C	-2.012607000000	-5.462719000000	0.530964000000
H	-2.494459000000	-6.163656000000	1.212159000000
H	-2.018084000000	-5.911595000000	-0.467332000000
H	-0.967916000000	-5.359628000000	0.840660000000
C	-1.506581000000	3.036048000000	-3.000222000000
H	-1.224535000000	2.503597000000	-3.913249000000
H	-2.050278000000	3.936756000000	-3.283116000000
H	-0.600337000000	3.361022000000	-2.478513000000
C	-3.978077000000	3.920241000000	-1.236098000000
H	-3.676908000000	4.545545000000	-2.075607000000
H	-5.070989000000	3.885151000000	-1.204169000000
H	-3.611242000000	4.412064000000	-0.328598000000

C	2.780250000000	0.508675000000	0.763144000000
C	3.635768000000	-0.390710000000	0.204074000000
Se	0.956721000000	0.130683000000	1.135547000000
Se	3.271711000000	2.285820000000	1.228259000000
Se	5.461858000000	-0.002859000000	-0.184747000000
Se	3.132794000000	-2.166484000000	-0.276870000000
C	0.572947000000	1.842951000000	1.863378000000
C	1.560257000000	2.761834000000	1.903820000000
C	4.867397000000	-2.653581000000	-0.941442000000
C	5.849504000000	-1.740741000000	-0.902165000000
C	-0.839328000000	2.073901000000	2.323570000000
H	-1.205962000000	3.018338000000	1.904892000000
H	-1.508488000000	1.274135000000	2.000466000000
H	-0.888918000000	2.129313000000	3.416102000000
C	1.424107000000	4.152127000000	2.455064000000
H	0.418746000000	4.528578000000	2.256711000000
H	1.612224000000	4.160819000000	3.534784000000
H	2.126839000000	4.839356000000	1.980431000000
C	7.270875000000	-1.906489000000	-1.367156000000
H	7.974055000000	-1.752265000000	-0.542970000000
H	7.445118000000	-2.903094000000	-1.771652000000
H	7.514748000000	-1.181227000000	-2.149422000000
C	4.949298000000	-4.063367000000	-1.460693000000
H	5.949140000000	-4.296896000000	-1.825342000000
H	4.702984000000	-4.785870000000	-0.676448000000
H	4.248091000000	-4.219354000000	-2.286336000000
N	-0.853398000000	5.007907000000	-0.243905000000
O	-1.242276000000	5.776766000000	-1.142652000000
O	-1.485149000000	4.937503000000	0.852368000000
O	0.159123000000	4.277329000000	-0.418136000000