Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Designing Dithienonaphthalene Based Acceptor Materials with Promising Photovoltaic Parameters for Organic Solar Cells

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Cartesian Coordinates

Reference Compound R

Symbol	X	Y	Z
C	0.8179470	1.6951040	0.0010690
C	0.6606810	0.2851200	-0.0001720
C	-0.6606860	-0.2851790	-0.0005770
C	-1.7625120	0.6202810	0.0003000
C	-1.5695060	2.0094820	0.0015220
C	-0.2731690	2.5446890	0.0019110
C	1.7625070	-0.6203390	-0.0010520
C	1.5695010	-2.0095410	-0.0022470
C	0.2731640	-2.5447470	-0.0025970
C	-0.8179520	-1.6951630	-0.0017830
C	-3.1942140	0.3989680	0.0002420
C	-3.8795580	1.6139180	0.0013770
C	-2.8972800	2.7717180	0.0022910
C	-5.6836400	0.1415010	0.0003330
C	-5.2693640	1.4810290	0.0014490
C	3.1942110	-0.3990260	-0.0009520
C	3.8795530	-1.6139750	-0.0020720
C	2.8972780	-2.7717740	-0.0030430
C	5.6836390	-0.1415630	-0.0009120
C	5.2693630	-1.4810870	-0.0020740

C	**-6.9468970**	**-0.5078990**	**0.0001530**
C	**6.9468890**	**0.5078610**	**-0.0005300**
C	**-8.2475870**	**-0.0413680**	**0.0005090**
C	**8.2475930**	**0.0413650**	**-0.0005820**
C	**-9.4523930**	**-0.8870550**	**0.0002550**
C	**-10.6321110**	**0.0175780**	**-0.0001290**
C	**-10.1798700**	**1.3480590**	**0.0003160**
C	**-8.7001830**	**1.3772490**	**0.0008050**
C	**9.4523760**	**0.8870840**	**-0.0002410**
C	**10.6321190**	**-0.0175130**	**0.0023480**
C	**10.1799210**	**-1.3480060**	**0.0024150**
C	**8.7002370**	**-1.3772450**	**0.0003140**
C	**-12.0106100**	**-0.2298980**	**-0.0007980**
C	**-12.8852300**	**0.8607950**	**-0.0009540**
C	**-12.4166170**	**2.1802910**	**-0.0004470**
C	**-11.0444580**	**2.4341850**	**0.0001910**
C	**12.0106080**	**0.2300130**	**0.0044490**
C	**12.8852630**	**-0.8606500**	**0.0064730**
C	**12.4166940**	**-2.1801610**	**0.0063900**
C	**11.0445450**	**-2.4341020**	**0.0043410**
O	**8.0257000**	**-2.4014930**	**-0.0003000**
C	**9.5335220**	**2.2689550**	**-0.0025850**
O	**-8.0256010**	**2.4014700**	**0.0012960**
C	**-9.5335730**	**-2.2689240**	**0.0005660**
C	**-10.7715670**	**-2.9841830**	**0.0002300**
N	**-11.7527360**	**-3.6124270**	**-0.0000350**
C	**-8.4090700**	**-3.1514380**	**0.0013490**
N	**-7.5235240**	**-3.9093310**	**0.0019520**

C	**8.4089910**	**3.1514270**	**-0.0062800**
N	**7.5234980**	**3.9093740**	**-0.0093660**
C	**10.7714950**	**2.9842480**	**-0.0018780**
N	**11.7526030**	**3.6125860**	**-0.0013580**
C	**-3.0470490**	**3.6448040**	**-1.2646950**
C	**-3.0468610**	**3.6426080**	**1.2708160**
C	**3.0468500**	**-3.6426140**	**-1.2715960**
C	**3.0470540**	**-3.6449140**	**1.2639140**
H	**1.8161670**	**2.1196890**	**0.0013660**
H	**-0.1207330**	**3.6198880**	**0.0028620**
H	**0.1207280**	**-3.6199470**	**-0.0034960**
H	**-1.8161710**	**-2.1197480**	**-0.0020750**
H	**-5.9962500**	**2.2816430**	**0.0022180**
H	**5.9962360**	**-2.2817120**	**-0.0028390**
H	**-6.8498070**	**-1.5875940**	**-0.0004450**
H	**6.8497710**	**1.5875510**	**0.0000450**
H	**-12.4152520**	**-1.2320950**	**-0.0012160**
H	**-13.9547180**	**0.6738930**	**-0.0014910**
H	**-13.1244510**	**3.0034790**	**-0.0005600**
H	**-10.6432290**	**3.4425100**	**0.0005710**
H	**12.4152140**	**1.2322230**	**0.0046190**
H	**13.9547440**	**-0.6737130**	**0.0081470**
H	**13.1245530**	**-3.0033260**	**0.0079560**
H	**10.6433540**	**-3.4424420**	**0.0042410**
H	**-4.0304730**	**4.1245190**	**-1.2810210**
H	**-2.9422280**	**3.0452710**	**-2.1729410**
H	**-2.2872170**	**4.4324970**	**-1.2828260**
H	**-4.0302870**	**4.1222830**	**1.2881090**

H	**-2.2870370**	**4.4302790**	**1.2902010**
H	**-2.9419040**	**3.0414970**	**2.1780010**
H	**4.0302750**	**-4.1222910**	**-1.2889260**
H	**2.9418810**	**-3.0414740**	**-2.1787620**
H	**2.2870240**	**-4.4302840**	**-1.2910030**
H	**4.0304780**	**-4.1246270**	**1.2802050**
H	**2.2872220**	**-4.4326080**	**1.2820200**
H	**2.9422430**	**-3.0454110**	**2.1721800**
S	**4.2641370**	**0.9443710**	**0.0001130**
S	**-4.2641400**	**-0.9444320**	**-0.0007560**

Designed molecule H1.

Symbol	**X**	**Y**	**Z**
C	**0.7668300**	**1.7187520**	**0.0004210**
C	**0.6518020**	**0.3047030**	**-0.0003990**
C	**-0.6518040**	**-0.3047290**	**-0.0006230**
C	**-1.7801100**	**0.5675920**	**0.0000100**
C	**-1.6287810**	**1.9621080**	**0.0008190**
C	**-0.3489830**	**2.5356520**	**0.0010260**
C	**1.7801090**	**-0.5676180**	**-0.0010290**
C	**1.6287800**	**-1.9621340**	**-0.0018350**
C	**0.3489820**	**-2.5356780**	**-0.0020290**
C	**-0.7668310**	**-1.7187780**	**-0.0014350**
C	**-3.2042440**	**0.3037170**	**0.0000300**
C	**-3.9257430**	**1.4982020**	**0.0008190**
C	**-2.9784360**	**2.6847470**	**0.0013890**
C	**-5.6844300**	**-0.0282890**	**0.0001890**
C	**-5.3103420**	**1.3237030**	**0.0009210**

C	**3.2042430**	**-0.3037420**	**-0.0010020**
C	**3.9257410**	**-1.4982260**	**-0.0017790**
C	**2.9784370**	**-2.6847720**	**-0.0024170**
C	**5.6844300**	**0.0282600**	**-0.0010230**
C	**5.3103420**	**-1.3237280**	**-0.0017960**
C	**-6.9266930**	**-0.7147950**	**0.0001020**
C	**6.9266900**	**0.7147800**	**-0.0007930**
C	**-8.2415280**	**-0.2874450**	**0.0004210**
C	**8.2415300**	**0.2874460**	**-0.0008700**
C	**-9.4190780**	**-1.1697800**	**0.0002540**
C	**-10.6247450**	**-0.3019960**	**0.0003480**
C	**-10.2132930**	**1.0403490**	**0.0007120**
C	**-8.7351230**	**1.1155710**	**0.0008140**
C	**9.4190740**	**1.1697890**	**-0.0006780**
C	**10.6247480**	**0.3020140**	**0.0009360**
C	**10.2133050**	**-1.0403340**	**0.0010120**
C	**8.7351390**	**-1.1155700**	**-0.0002960**
C	**-11.9947390**	**-0.5970820**	**0.0001400**
C	**-12.8869940**	**0.4672560**	**0.0003030**
C	**-12.4565050**	**1.8025030**	**0.0006830**
C	**-11.1042130**	**2.1064620**	**0.0008870**
C	**11.9947400**	**0.5971100**	**0.0021950**
C	**12.8870020**	**-0.4672210**	**0.0034600**
C	**12.4565230**	**-1.8024710**	**0.0034580**
C	**11.1042340**	**-2.1064400**	**0.0022240**
O	**8.0966950**	**-2.1621920**	**-0.0006210**
C	**9.4613590**	**2.5530230**	**-0.0021580**
O	**-8.0966640**	**2.1621850**	**0.0011380**

C	**-9.4613750**	**-2.5530120**	**0.0001590**
C	**-10.6813800**	**-3.2979220**	**0.0000310**
N	**-11.6527910**	**-3.9410480**	**-0.0000280**
C	**-8.3121790**	**-3.4027730**	**0.0002670**
N	**-7.4044750**	**-4.1337980**	**0.0003260**
C	**8.3121520**	**3.4027660**	**-0.0045220**
N	**7.4044740**	**4.1338210**	**-0.0064790**
C	**10.6813530**	**3.2979500**	**-0.0016550**
N	**11.6527260**	**3.9411330**	**-0.0012580**
C	**-3.1541060**	**3.5525730**	**-1.2659600**
C	**-3.1538260**	**3.5511090**	**1.2697830**
C	**3.1538350**	**-3.5510840**	**-1.2708370**
C	**3.1540970**	**-3.5526480**	**1.2649060**
H	**1.7518410**	**2.1731320**	**0.0005740**
H	**-0.2284970**	**3.6148510**	**0.0016510**
H	**0.2284960**	**-3.6148770**	**-0.0026380**
H	**-1.7518420**	**-2.1731590**	**-0.0016030**
H	**-6.0598970**	**2.1030400**	**0.0014560**
H	**6.0598890**	**-2.1030740**	**-0.0023270**
H	**-6.7981770**	**-1.7912140**	**-0.0003350**
H	**6.7981590**	**1.7911960**	**-0.0003960**
H	**-12.3971640**	**-1.6004500**	**-0.0001540**
H	**-10.7579330**	**3.1339020**	**0.0011750**
H	**12.3971570**	**1.6004800**	**0.0022830**
H	**10.7579630**	**-3.1338830**	**0.0022140**
H	**-4.1511470**	**4.0032370**	**-1.2821050**
H	**-3.0318460**	**2.9562870**	**-2.1741510**
H	**-2.4179300**	**4.3623380**	**-1.2843390**

H	**-4.1508680**	**4.0017420**	**1.2866620**
H	**-2.4176540**	**4.3608600**	**1.2889310**
H	**-3.0313590**	**2.9537690**	**2.1772540**
H	**4.1508750**	**-4.0017230**	**-1.2877340**
H	**3.0313750**	**-2.9537150**	**-2.1782890**
H	**2.4176610**	**-4.3608330**	**-1.2900230**
H	**4.1511420**	**-4.0033010**	**1.2810370**
H	**2.4179270**	**-4.3624200**	**1.2832420**
H	**3.0318220**	**-2.9563930**	**2.1731150**
S	**4.2328380**	**1.0710760**	**-0.0002980**
S	**-4.2328390**	**-1.0711030**	**-0.0006030**
F	**14.2041880**	**-0.2311220**	**0.0047410**
F	**13.3799030**	**-2.7704970**	**0.0046980**
F	**-13.3798800**	**2.7705350**	**0.0008350**
F	**-14.2041820**	**0.2311670**	**0.0000970**

Designed molecule H2

Symbol	**X**	**Y**	**Z**
C	**0.7376890**	**1.7310980**	**0.0003720**
C	**0.6463970**	**0.3153790**	**-0.0005140**
C	**-0.6464000**	**-0.3154070**	**-0.0007460**
C	**-1.7890370**	**0.5385430**	**-0.0000670**
C	**-1.6611450**	**1.9360910**	**0.0008050**
C	**-0.3910210**	**2.5302670**	**0.0010300**
C	**1.7890350**	**-0.5385700**	**-0.0011980**
C	**1.6611430**	**-1.9361190**	**-0.0020540**
C	**0.3910190**	**-2.5302950**	**-0.0022430**
C	**-0.7376910**	**-1.7311260**	**-0.0016060**

C	**-3.2072520**	**0.2512670**	**-0.0000620**
C	**-3.9493030**	**1.4358690**	**0.0008030**
C	**-3.0215840**	**2.6375790**	**0.0014230**
C	**-5.6805820**	**-0.1223770**	**0.0001240**
C	**-5.3283430**	**1.2384480**	**0.0009200**
C	**3.2072510**	**-0.2512950**	**-0.0011960**
C	**3.9493000**	**-1.4358960**	**-0.0020270**
C	**3.0215830**	**-2.6376050**	**-0.0026900**
C	**5.6805840**	**0.1223440**	**-0.0012190**
C	**5.3283430**	**-1.2384760**	**-0.0020440**
C	**-6.9069960**	**-0.8278200**	**0.0000370**
C	**6.9069920**	**0.8278020**	**-0.0009700**
C	**-8.2332120**	**-0.4215170**	**0.0004470**
C	**8.2332130**	**0.4215140**	**-0.0010690**
C	**-9.3929060**	**-1.3231410**	**0.0002950**
C	**-10.6168170**	**-0.4735790**	**0.0004410**
C	**-10.2254700**	**0.8741600**	**0.0008600**
C	**-8.7432380**	**0.9702640**	**0.0009380**
C	**9.3929010**	**1.3231460**	**-0.0009330**
C	**10.6168180**	**0.4735920**	**0.0005730**
C	**10.2254820**	**-0.8741500**	**0.0006520**
C	**8.7432520**	**-0.9702660**	**-0.0005080**
C	**-11.9790210**	**-0.7841230**	**0.0002300**
C	**-12.9147690**	**0.2639060**	**0.0004650**
C	**-12.4975670**	**1.6213890**	**0.0009230**
C	**-11.1289500**	**1.9223970**	**0.0011140**
C	**11.9790190**	**0.7841490**	**0.0017680**
C	**12.9147760**	**-0.2638700**	**0.0029740**

C	**12.4975860**	**-1.6213570**	**0.0029530**
C	**11.1289730**	**-1.9223770**	**0.0017680**
O	**8.1269700**	**-2.0294590**	**-0.0008520**
C	**9.4168800**	**2.7062400**	**-0.0024040**
O	**-8.1269420**	**2.0294500**	**0.0013130**
C	**-9.4168960**	**-2.7062350**	**0.0001680**
C	**-10.6242770**	**-3.4712600**	**0.0000140**
N	**-11.5837410**	**-4.1317530**	**-0.0000810**
C	**-8.2529430**	**-3.5359580**	**0.0002350**
N	**-7.3299700**	**-4.2472820**	**0.0002790**
C	**8.2529130**	**3.5359400**	**-0.0046540**
N	**7.3299730**	**4.2473050**	**-0.0065190**
C	**10.6242490**	**3.4712840**	**-0.0020130**
N	**11.5836750**	**4.1318310**	**-0.0017080**
C	**-3.2109980**	**3.5024990**	**-1.2662110**
C	**-3.2106780**	**3.5009270**	**1.2701810**
C	**3.2106600**	**-3.5009050**	**-1.2714790**
C	**3.2110130**	**-3.5025760**	**1.2649140**
H	**1.7147660**	**2.2022530**	**0.0005440**
H	**-0.2877490**	**3.6111100**	**0.0017130**
H	**0.2877470**	**-3.6111380**	**-0.0028770**
H	**-1.7147680**	**-2.2022800**	**-0.0017660**
H	**-6.0901250**	**2.0057560**	**0.0015070**
H	**6.0901130**	**-2.0057950**	**-0.0025960**
H	**-6.7617540**	**-1.9020430**	**-0.0004920**
H	**6.7617360**	**1.9020210**	**-0.0005300**
H	**-12.3468540**	**-1.8003330**	**-0.0001220**
H	**-10.7795070**	**2.9488560**	**0.0014520**

H	**12.3468420**	**1.8003620**	**0.0018390**
H	**10.7795410**	**-2.9488410**	**0.0017430**
H	**-4.2146020**	**3.9380780**	**-1.2815020**
H	**-3.0799230**	**2.9088060**	**-2.1748390**
H	**-2.4875820**	**4.3234910**	**-1.2841470**
H	**-4.2142760**	**3.9364900**	**1.2862560**
H	**-2.4872560**	**4.3218950**	**1.2889590**
H	**-3.0793800**	**2.9061020**	**2.1780350**
H	**4.2142590**	**-3.9364640**	**-1.2875910**
H	**3.0793440**	**-2.9060500**	**-2.1793110**
H	**2.4872400**	**-4.3218740**	**-1.2902720**
H	**4.2146160**	**-3.9381560**	**1.2801700**
H	**2.4875970**	**-4.3235680**	**1.2828320**
H	**3.0799530**	**-2.9089130**	**2.1735630**
S	**4.2101410**	**1.1406840**	**-0.0004460**
S	**-4.2101440**	**-1.1407120**	**-0.0007520**
C	**14.3113810**	**0.0585000**	**0.0042520**
N	**15.4402680**	**0.3363460**	**0.0052900**
C	**13.4569240**	**-2.6846150**	**0.0041590**
N	**14.2109030**	**-3.5697780**	**0.0051250**
C	**-13.4568960**	**2.6846550**	**0.0011940**
N	**-14.2108660**	**3.5698270**	**0.0014250**
C	**-14.3113770**	**-0.0584520**	**0.0002220**
N	**-15.4402670**	**-0.3362880**	**0.0000170**

Designed Molecule H3

Symbol	**X**	**Y**	**Z**
C	**-1.1164450**	**-1.0849680**	**-0.0004350**

C	**-0.8257050**	**0.3038660**	**-0.0000970**
C	**0.5439430**	**0.7457090**	**0.0000200**
C	**1.5547910**	**-0.2604660**	**-0.0001600**
C	**1.2304780**	**-1.6251710**	**-0.0004870**
C	**-0.1108580**	**-2.0343610**	**-0.0006390**
C	**-1.8374390**	**1.3094830**	**0.0001170**
C	**-1.5116230**	**2.6738920**	**0.0003510**
C	**-0.1705170**	**3.0837470**	**0.0004090**
C	**0.8348770**	**2.1341670**	**0.0002650**
C	**3.0006580**	**-0.1763600**	**-0.0001060**
C	**3.5676230**	**-1.4515230**	**-0.0003970**
C	**2.4795550**	**-2.5104020**	**-0.0006430**
C	**5.5030780**	**-0.1567010**	**-0.0000610**
C	**4.9630950**	**-1.4514530**	**-0.0003820**
C	**-3.2847530**	**1.2218790**	**0.0001080**
C	**-3.8451360**	**2.4990360**	**0.0003090**
C	**-2.7602200**	**3.5605040**	**0.0005270**
C	**-5.7719360**	**1.1677320**	**0.0002690**
C	**-5.2363920**	**2.4709470**	**0.0004020**
C	**2.5455520**	**-3.3925210**	**-1.2685220**
C	**2.5454700**	**-3.3929720**	**1.2669420**
C	**-2.8244690**	**4.4431670**	**-1.2670080**
C	**-2.8244850**	**4.4425460**	**1.2685140**
H	**-2.1504910**	**-1.4124810**	**-0.0005740**
H	**-0.3650390**	**-3.0901420**	**-0.0009250**
H	**0.0837040**	**4.1395420**	**0.0005550**
H	**1.8689170**	**2.4620330**	**0.0003190**
H	**5.6109410**	**-2.3172920**	**-0.0005590**

H	**-5.8842870**	**3.3412160**	**0.0005210**
H	**3.4786410**	**-3.9639900**	**-1.2852590**
H	**2.4985510**	**-2.7848870**	**-2.1762080**
H	**1.7138970**	**-4.1039540**	**-1.2873780**
H	**3.4785740**	**-3.9644190**	**1.2835600**
H	**1.7138260**	**-4.1044240**	**1.2854540**
H	**2.4983680**	**-2.7856520**	**2.1748310**
H	**-3.7549880**	**5.0191990**	**-1.2835260**
H	**-2.7803960**	**3.8357010**	**-2.1749170**
H	**-1.9908230**	**5.1521450**	**-1.2866810**
H	**-3.7550300**	**5.0185250**	**1.2853180**
H	**-1.9908580**	**5.1515330**	**1.2884940**
H	**-2.7803700**	**3.8346210**	**2.1761110**
S	**-4.4635170**	**-0.0380290**	**0.0000710**
S	**4.1931120**	**1.0593980**	**0.0002100**
C	**6.8219330**	**0.3670460**	**-0.0000640**
C	**8.0743250**	**-0.2196770**	**-0.0001340**
C	**8.3936020**	**-1.6843640**	**0.0004000**
C	**9.8677320**	**-1.7716250**	**0.0008730**
C	**10.4277790**	**-0.4560930**	**0.0005230**
C	**9.3404960**	**0.5341990**	**-0.0002910**
C	**10.7915990**	**-2.7735070**	**0.0015790**
C	**11.8007200**	**-0.4655020**	**0.0009690**
O	**7.6190940**	**-2.6335930**	**0.0004480**
C	**9.5605470**	**1.9012830**	**-0.0012200**
C	**8.5400640**	**2.8983350**	**-0.0024230**
N	**7.7285950**	**3.7352840**	**-0.0034260**
C	**10.8884950**	**2.4264920**	**-0.0011110**

N	**11.9742260**	**2.8495440**	**-0.0009980**
H	**10.6367800**	**-3.8430310**	**0.0019160**
H	**12.5002020**	**0.3567570**	**0.0008790**
S	**12.3924950**	**-2.0990440**	**0.0019010**
C	**-7.1755450**	**0.9687590**	**0.0002150**
C	**-7.9942820**	**-0.1421530**	**0.0001160**
C	**-7.5336730**	**-1.5593770**	**-0.0001170**
C	**-8.7591700**	**-2.3835960**	**-0.0003110**
C	**-9.9048840**	**-1.5247960**	**-0.0002200**
C	**-9.4636960**	**-0.1210220**	**0.0001010**
C	**-9.0582770**	**-3.7130630**	**-0.0005620**
C	**-11.0879400**	**-2.2205910**	**-0.0004060**
O	**-6.3751140**	**-1.9581660**	**-0.0001160**
C	**-10.3333980**	**0.9559690**	**0.0004030**
C	**-9.9288980**	**2.3239800**	**0.0008760**
N	**-9.6166520**	**3.4471400**	**0.0012660**
C	**-11.7467940**	**0.7546680**	**0.0002770**
N	**-12.8989220**	**0.5802410**	**0.0001630**
H	**-8.3898600**	**-4.5622410**	**-0.0006730**
H	**-12.1049720**	**-1.8582150**	**-0.0004160**
S	**-10.7821710**	**-3.9310510**	**-0.0006460**
H	**-7.6883630**	**1.9249360**	**0.0003150**
H	**6.8325440**	**1.4518850**	**-0.0000260**

Designed Molecule H4

Symbol	**X**	**Y**	**Z**
C	**0.7006060**	**1.6794520**	**0.4794170**
C	**0.6395520**	**0.3157820**	**0.0936650**

C	**-0.6396270**	**-0.3160130**	**-0.0934380**
C	**-1.8001230**	**0.4837820**	**0.1240560**
C	**-1.7019320**	**1.8308940**	**0.5030390**
C	**-0.4453870**	**2.4268810**	**0.6811280**
C	**1.8000470**	**-0.4840120**	**-0.1238270**
C	**1.7018580**	**-1.8311200**	**-0.5028180**
C	**0.4453140**	**-2.4271110**	**-0.6809010**
C	**-0.7006810**	**-1.6796840**	**-0.4791830**
C	**-3.2124440**	**0.1794410**	**0.0339510**
C	**-3.9777310**	**1.3050860**	**0.3393320**
C	**-3.0777690**	**2.4805030**	**0.6745420**
C	**-5.6725470**	**-0.2216530**	**-0.1419600**
C	**-5.3517940**	**1.0877180**	**0.2399970**
C	**3.2123730**	**-0.1796680**	**-0.0337350**
C	**3.9776560**	**-1.3053130**	**-0.3391180**
C	**3.0776930**	**-2.4807290**	**-0.6743300**
C	**5.6724710**	**0.2214550**	**0.1420900**
C	**5.3517280**	**-1.0879380**	**-0.2397940**
C	**-6.9043330**	**-0.9145130**	**-0.2765120**
C	**6.9042320**	**0.9143790**	**0.2765030**
C	**-8.2187930**	**-0.4833810**	**-0.2956500**
C	**8.2187430**	**0.4834050**	**0.2955140**
C	**-9.3493240**	**-1.3697930**	**0.0496960**
C	**-10.4386140**	**-0.4910180**	**0.5122140**
C	**-10.0825720**	**0.8568750**	**0.2507860**
C	**-8.7720830**	**0.8704660**	**-0.4186260**
C	**9.3491780**	**1.3699930**	**-0.0496760**
C	**10.4386450**	**0.4913830**	**-0.5121110**

C	**10.0827100**	**-0.8565910**	**-0.2509930**
C	**8.7721730**	**-0.8704180**	**0.4182810**
C	**-11.6603030**	**-0.7877250**	**1.1228880**
C	**-12.5069270**	**0.2631130**	**1.4804660**
C	**-12.1515610**	**1.5905790**	**1.2264690**
C	**-10.9416220**	**1.9000020**	**0.6028290**
C	**11.6604150**	**0.7883060**	**-1.1225110**
C	**12.5072090**	**-0.2623940**	**-1.4801100**
C	**12.1519510**	**-1.5899430**	**-1.2263760**
C	**10.9419220**	**-1.8995820**	**-0.6030090**
C	**9.4133340**	**2.7457780**	**0.0581390**
C	**-9.4135810**	**-2.7456010**	**-0.0580930**
C	**-10.5613220**	**-3.5069020**	**0.3238770**
N	**-11.4758870**	**-4.1613570**	**0.6274010**
C	**-8.3658540**	**-3.5510850**	**-0.6026810**
N	**-7.5286070**	**-4.2335600**	**-1.0395360**
C	**8.3654420**	**3.5513510**	**0.6023390**
N	**7.5280970**	**4.2339750**	**1.0387670**
C	**10.5612500**	**3.5071150**	**-0.3232910**
N	**11.4759680**	**4.1615540**	**-0.6263800**
C	**-3.2787090**	**3.6453550**	**-0.3226450**
C	**-3.2919610**	**2.9717750**	**2.1244470**
C	**3.2918880**	**-2.9719980**	**-2.1242330**
C	**3.2786290**	**-3.6455900**	**0.3228510**
H	**1.6672630**	**2.1504400**	**0.6221790**
H	**-0.3659360**	**3.4690410**	**0.9754680**
H	**0.3658640**	**-3.4692730**	**-0.9752330**
H	**-1.6673370**	**-2.1506770**	**-0.6219290**

H	**-6.1078060**	**1.8299730**	**0.4603220**
H	**6.1077320**	**-1.8301850**	**-0.4601460**
H	**-6.7807530**	**-1.9922310**	**-0.2754710**
H	**6.7805780**	**1.9920880**	**0.2756050**
H	**-11.9558630**	**-1.8067270**	**1.3309970**
H	**-10.6816270**	**2.9329990**	**0.4144900**
H	**11.9559230**	**1.8073770**	**-1.3303860**
H	**10.6819530**	**-2.9326230**	**-0.4148360**
H	**-4.2854780**	**4.0624930**	**-0.2230530**
H	**-3.1504190**	**3.3099020**	**-1.3547770**
H	**-2.5615050**	**4.4482410**	**-0.1257580**
H	**-4.3038040**	**3.3710720**	**2.2459480**
H	**-2.5859490**	**3.7715490**	**2.3684120**
H	**-3.1530760**	**2.1600170**	**2.8436060**
H	**4.3037280**	**-3.3713030**	**-2.2457290**
H	**3.1530110**	**-2.1602390**	**-2.8433920**
H	**2.5858710**	**-3.7717670**	**-2.3682020**
H	**4.2854080**	**-4.0627110**	**0.2232860**
H	**2.5614450**	**-4.4484860**	**0.1259300**
H	**3.1502880**	**-3.3101550**	**1.3549820**
S	**4.1884280**	**1.1769680**	**0.3652020**
S	**-4.1885030**	**-1.1772050**	**-0.3649360**
H	**-12.8205610**	**2.3940990**	**1.5176420**
H	**-13.4520130**	**0.0407880**	**1.9655560**
H	**13.4523450**	**-0.0398950**	**-1.9650230**
H	**12.8211060**	**-2.3933300**	**-1.5175530**
C	**-8.2791070**	**1.8976760**	**-1.2014070**
C	**8.2792340**	**-1.8978060**	**1.2008210**

C	**-8.9031540**	**3.1815420**	**-1.2796240**
N	**-9.3752360**	**4.2442810**	**-1.3482840**
C	**-7.1659420**	**1.7495860**	**-2.0823250**
N	**-6.2732070**	**1.6689960**	**-2.8259590**
C	**8.9032820**	**-3.1817010**	**1.2785220**
N	**9.3755120**	**-4.2444120**	**1.3466230**
C	**7.1662030**	**-1.7498680**	**2.0819290**
N	**6.2735270**	**-1.6694500**	**2.8256480**