Solid-state Inclusion of C_{60} and C_{70} in a Co-polymer Induced by Metal-Ligand Coordination of a Zn-Porphyrin Cage with a bis-pyridyl Perylene Derivative.

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Electronic Supplementary Information

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1. Figure S1:

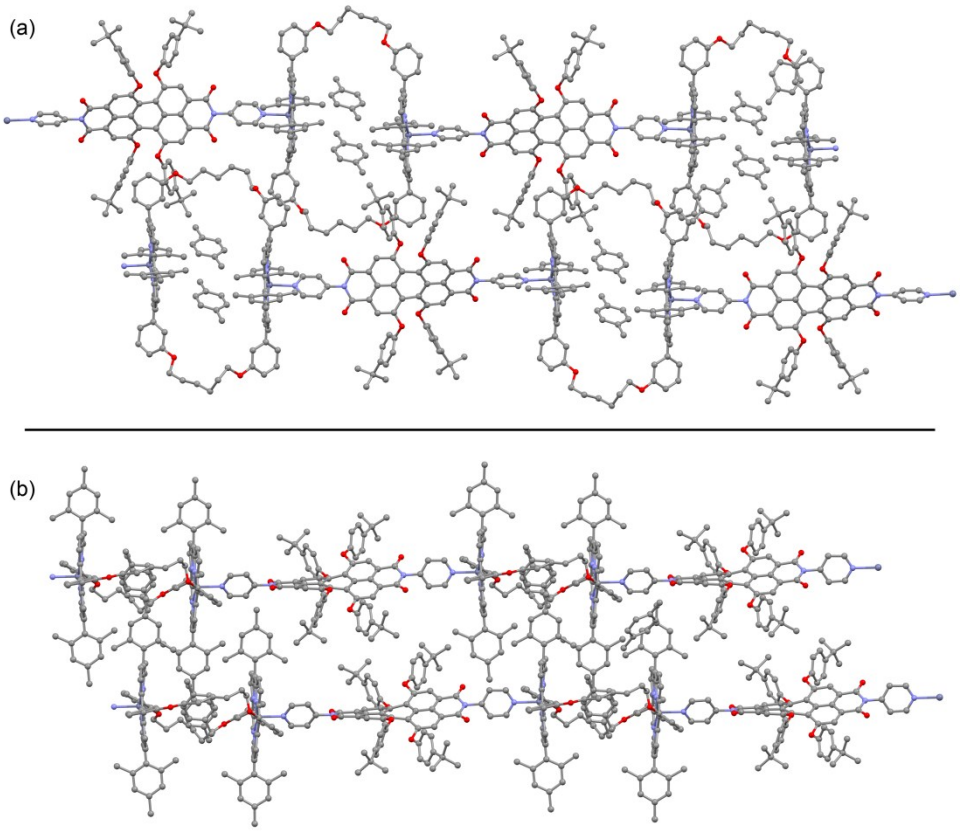

Fig. S1 2D Layers formed by the assembly of polymeric chains of **1** in an antiparallel (a) and parallel (b) mode. H-atoms and solvent molecules (apart from those encapsulated) are omitted for clarity.

2. Crystallographic details

Details on the procedure used for obtaining the refined structural model of compound 1

The refined structural model of compound **1** addresses the disorder encountered in the crystal for the atoms of one of its phenyl rings and the attached spacer chain in the Zn(II)-bisporphyrin macrocycle. The disorder was modelled considering two positions of the involved atoms in the fragment and assigning occupancies of 50% in each of the two sites. Restrains on the anisotropic thermal parameters, ADPs, were also applied to emulate an isotropic behavior of the disordered fragment. The assymetric unit of the crystal is completed by 8.5 *p*-xylene solvent molecules. The equivalent of 2.5 *p*-xylene molecules in the asymmetric unit displayed disordered postions. This disorder was modelled considering six sites for the *p*-xylene atoms with the following occupations

per site 75%, 50%, 50%, 25%, 25% and 25%. Restrains on the geometries and the ADPs of these disordered molecules were also applied.

Details on the procedure used for obtaining the refined structural model of compound 2

The asymmetric unit of the refined structural model of compound **2** is made up of half of the Zn(II)-bisporphyrin macrocycle and the axially coordinated bispyridyl perylene. Likewise, only half of the encapsulated C60 fullerene is included in the asymmetric unit that also contains 8 independent p-xylene molecules. One of the p-xylene solvent molecules in the asymmetric unit was modeled over two disordered positions with relative occupancies of 70:30. Restrains to the 30% occupancy sites in the solvent molecule were applied in order to preserve the geometry and covalent connectivity of its atoms.

Details on the procedure used for obtaining the refined structural model of compound 3

The asymmetric unit of the refined structural model of compound **3** is made up of half of the Zn(II)-bisporphyrin macrocycle and the axially coordinated bispyridyl perylene. Likewise, only half of the encapsulated C70 fullerene is included in the asymmetric unit that also contains 8 independent *p*-xylene molecules. The positions of the atoms in the solvent molecules and the molecular fragments are well defined except for those of the encapsulated C70 that exhitit evident disorder. The disorder of the C70 fullerene was modelled by considering two positions for the atoms in the half fragment of C70 and constraining them with respect to the isomer having the D_{5h} symmetry. This is the symmetry exhibited by the C70 isomer used to grow the crystals. The two positions of the C70 atoms were assigned a 50:50 occupancy. As a consequence of the symmetry operations involved in growing the crystal packing, the disorder model applied to the C70 produced four possible orientations of the C70 with respect to the Zn(II)-bisporphyrin macrocycle, Fig. S2. The geometry of the second orientation of the C70 fullerene was restrained to be identical to the first one (SAME instruction). In order to avoid correlation between the ADPs of all the C70 fullerene atoms, certain restrains were applied. On the one hand, the ADPs of the atoms were restrained to behave isotropically (ISOR). On the other hand, the ADPs of the atoms were restrained to be identical to the ADPs of the neighboring atoms (SIMU). Additionally, rigid bond restrains were also applied (DELU).

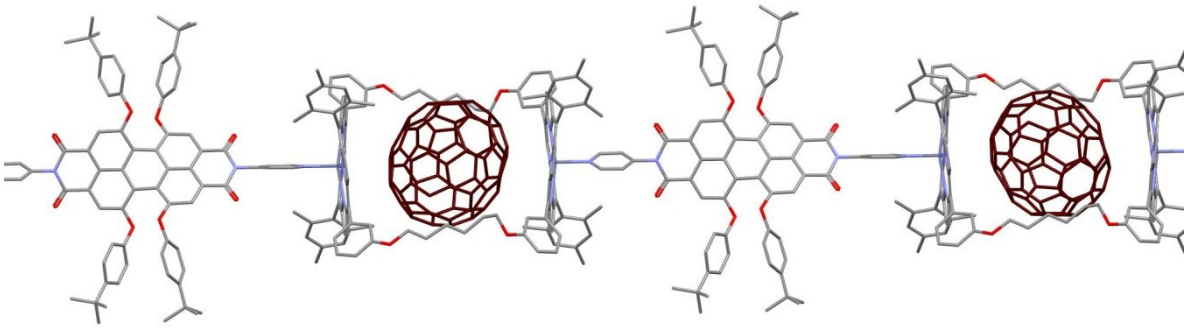

Fig. S2. Section of the crystal structure of compond **3** showing two orientations (atom positioning) of the C70 fullerenes after appling the corresponding symmetry operation.

3. Cartesian coordinates:

Zn-porphyrin···C_{60}_CC

C	1.2540553	-2.8137986	2.9625811
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Zn-porphyrin···C_{60}_5R

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Zn-porphyrin···C_{60}_6R

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C	5.3333036	2.8627447	0.0000000
C	4.0954992	3.5159601	0.0000000
C	3.2428670	3.4584773	1.1762485
C	3.6599367	2.7500130	2.3083962
C	3.4142245	0.7267166	3.4849998
C	2.7604387	-0.5106998	3.4846497
C	3.4617196	-1.7027028	3.0344499
C	4.7892760	-1.6118866	2.6021495
C	5.2223204	-2.3484726	1.4263518
C	6.1691603	-1.5185369	0.6993947
C	6.1691603	-1.5185369	-0.6993947
C	6.3206237	-0.2685934	-1.4263529
C	4.9449182	2.0703117	-2.3076403
C	4.7928068	0.8201601	-3.0344170
C	5.4679836	-0.3264841	-2.6024689
C	4.7892760	-1.6118866	-2.6021495
C	5.2223204	-2.3484726	-1.4263518
C	4.3106702	-3.1469387	-0.7270312
C	4.3106702	-3.1469387	0.7270312

C	2.9322680	-3.2431241	1.1769454
C	2.5155173	-2.5345886	2.3096475
C	2.7139660	1.9193509	3.0357798
C	1.3802672	-0.6059953	3.0390201
C	6.4666731	0.9339823	0.7268390

Zn-porphyrin···C_{70}_CC

C	1.2513709	-2.8237190	3.3534145
C	2.5198969	-3.4960377	3.1579161
C	3.4807408	-2.5232359	3.1103356
C	2.8036343	-1.2543393	3.2846496
N	1.4567119	-1.4688399	3.4429929
C	0.0000000	-3.4504248	3.3571454
C	3.4218412	0.0000000	3.2305088
C	2.8036343	1.2543393	3.2846496
C	3.4807408	2.5232359	3.1103356
C	2.5198969	3.4960377	3.1579161
C	1.2513709	2.8237190	3.3534145
N	1.4567119	1.4688399	3.4429929
C	0.0000000	3.4504248	3.3571454
C	-1.2513709	2.8237190	3.3534145
C	-2.5198969	3.4960377	3.1579161
C	-3.4807408	2.5232359	3.1103356
C	-2.8036343	1.2543393	3.2846496
N	-1.4567119	1.4688399	3.4429929

C	-3.4218412	0.0000000	3.2305088
C	-2.8036343	-1.2543393	3.2846496
C	-3.4807408	-2.5232359	3.1103356
C	-2.5198969	-3.4960377	3.1579161
C	-1.2513709	-2.8237190	3.3534145
N	-1.4567119	-1.4688399	3.4429929
H	2.6472764	-4.5696390	3.0447682
H	4.5492567	-2.6446594	2.9518231
H	0.0000000	-4.5371755	3.2608830
H	4.5027351	0.0000000	3.0816167
H	4.5492567	2.6446594	2.9518231
H	2.6472764	4.5696390	3.0447682
H	0.0000000	4.5371755	3.2608830
H	-2.6472764	4.5696390	3.0447682
H	-4.5492567	2.6446594	2.9518231
H	-4.5027351	0.0000000	3.0816167
H	-4.5492567	-2.6446594	2.9518231
H	-2.6472764	-4.5696390	3.0447682
Zn	0.0000000	0.0000000	3.7507492
C	0.0000000	1.1585777	6.5688518
C	0.0000000	-1.1585777	6.5688518
C	0.0000000	1.2032862	7.9615930
H	0.0000000	2.0629946	5.9573885
C	0.0000000	-1.2032862	7.9615930
H	0.0000000	-2.0629946	5.9573885
H	0.0000000	2.1637222	8.4764365
H	0.0000000	-2.1637222	8.4764365

N	0.0000000	0.0000000	5.8896645
C	0.0000000	0.0000000	8.6699271
H	0.0000000	0.0000000	9.7606172
C	1.4236327	3.2237363	-0.9156663
C	0.6971617	2.4428296	0.0662265
C	0.7268681	3.9702621	-1.8735101
C	-0.6971617	2.4428296	0.0662265
C	-1.4137093	1.2071393	0.2880398
C	-0.7326601	0.0000000	0.5925254
C	-1.4137093	-1.2071393	0.2880398
C	2.3017163	3.2222517	-3.6215093
C	3.0150226	2.4449333	-2.6279998
C	1.1750025	3.9688508	-3.2553265
C	2.5858070	2.4453011	-1.3018086
C	2.5836515	1.2090207	-0.5483152
C	3.0973268	0.0000000	-1.0954434
C	2.5836515	-1.2090207	-0.5483152
C	0.7326601	0.0000000	0.5925254
C	1.4137093	1.2071393	0.2880398
C	1.4137093	-1.2071393	0.2880398
C	0.0000000	3.2216974	-5.2940679
C	1.1648861	2.4429987	-5.6631276
C	0.0000000	3.9682635	-4.1085407
C	2.2924157	2.4429779	-4.8432687
C	3.0085702	1.2081550	-4.6080729
C	2.6451415	0.0000000	-5.2651346
C	3.0085702	-1.2081550	-4.6080729

C	3.5483397	0.0000000	-2.4934889
C	3.4548926	1.2085428	-3.2390752
C	3.4548926	-1.2085428	-3.2390752
C	-2.3017163	3.2222517	-3.6215093
C	-2.2924157	2.4429779	-4.8432687
C	-1.1750025	3.9688508	-3.2553265
C	-1.1648861	2.4429987	-5.6631276
C	-0.7197081	1.2078490	-6.2711667
C	-1.4565353	0.0000000	-6.1283910
C	-0.7197081	-1.2078490	-6.2711667
C	1.4565353	0.0000000	-6.1283910
C	0.7197081	1.2078490	-6.2711667
C	0.7197081	-1.2078490	-6.2711667
C	-1.4236327	3.2237363	-0.9156663
C	-2.5858070	2.4453011	-1.3018086
C	-0.7268681	3.9702621	-1.8735101
C	-3.0150226	2.4449333	-2.6279998
C	-3.4548926	1.2085428	-3.2390752
C	-3.5483397	0.0000000	-2.4934889
C	-3.4548926	-1.2085428	-3.2390752
C	-2.6451415	0.0000000	-5.2651346
C	-3.0085702	1.2081550	-4.6080729
C	-3.0085702	-1.2081550	-4.6080729
C	-3.0973268	0.0000000	-1.0954434
C	-2.5836515	1.2090207	-0.5483152
C	-2.5836515	-1.2090207	-0.5483152
C	-2.3017163	-3.2222517	-3.6215093

C	-3.0150226	-2.4449333	-2.6279998
C	-2.5858070	-2.4453011	-1.3018086
C	-1.1750025	-3.9688508	-3.2553265
C	0.0000000	-3.2216974	-5.2940679
C	-1.1648861	-2.4429987	-5.6631276
C	-2.2924157	-2.4429779	-4.8432687
C	0.0000000	-3.9682635	-4.1085407
C	2.3017163	-3.2222517	-3.6215093
C	2.2924157	-2.4429779	-4.8432687
C	1.1648861	-2.4429987	-5.6631276
C	1.1750025	-3.9688508	-3.2553265
C	1.4236327	-3.2237363	-0.9156663
C	2.5858070	-2.4453011	-1.3018086
C	3.0150226	-2.4449333	-2.6279998
C	0.7268681	-3.9702621	-1.8735101
C	-1.4236327	-3.2237363	-0.9156663
C	-0.6971617	-2.4428296	0.0662265
C	0.6971617	-2.4428296	0.0662265
C	-0.7268681	-3.9702621	-1.8735101

Zn-porphyrin···C_{70}_6R

C	2.9464861	1.9208914	-2.8120490
C	2.5160302	3.1301669	-3.4838438
C	2.3615716	4.0868581	-2.5184701
C	2.6905934	3.4641651	-1.2527647
N	3.0578723	2.1572887	-1.4640268
C	3.1556150	0.6837199	-3.4331377

C	2.5570684	4.0728928	0.0000000
C	2.6905934	3.4641651	1.2527647
C	2.3615716	4.0868581	2.5184701
C	2.5160302	3.1301669	3.4838438
C	2.9464861	1.9208914	2.8120490
N	3.0578723	2.1572887	1.4640268
C	3.1556150	0.6837199	3.4331377
C	3.4671171	-0.5319107	2.8121260
C	3.5710097	-1.8111683	3.4844175
C	3.8193060	-2.7477416	2.5185169
C	3.8608839	-2.0451576	1.2528039
N	3.6614585	-0.7023869	1.4639270
C	3.9870916	-2.6552336	0.0000000
C	3.8608839	-2.0451576	-1.2528039
C	3.8193060	-2.7477416	-2.5185169
C	3.5710097	-1.8111683	-3.4844175
C	3.4671171	-0.5319107	-2.8121260
N	3.6614585	-0.7023869	-1.4639270
H	2.3362514	3.2215547	-4.5519657
H	2.0273091	5.1138373	-2.6409236
H	3.0123250	0.6531916	-4.5143525
H	2.2394761	5.1164710	0.0000000
H	2.0273091	5.1138373	2.6409236
H	2.3362514	3.2215547	4.5519657
H	3.0123250	0.6531916	4.5143525
H	3.4479486	-1.9676710	4.5530957
H	3.9351816	-3.8215684	2.6410205

H	4.1242348	-3.7375943	0.0000000
H	3.9351816	-3.8215684	-2.6410205
H	3.4479486	-1.9676710	-4.5530957
Zn	3.6578014	0.7920626	0.0000000
C	6.4276766	1.3082238	1.1585307
C	6.4276766	1.3082238	-1.1585307
C	7.8035730	1.5242902	1.2034569
H	5.8230614	1.2106452	2.0623545
C	7.8035730	1.5242902	-1.2034569
H	5.8230614	1.2106452	-2.0623545
H	8.3123203	1.6032558	2.1638191
H	8.3123203	1.6032558	-2.1638191
N	5.7569746	1.2015480	0.0000000
C	8.5034172	1.6327550	0.0000000
H	9.5813203	1.7991802	0.0000000
C	-4.0107846	-4.1611968	1.4228135
C	-3.8067211	-3.3174399	2.5825539
C	-2.9110689	-4.6779858	0.7262677
C	-2.5136732	-3.0252670	3.0140192
C	-2.1891237	-1.6861280	3.4563934
C	-3.1817070	-0.6709573	3.5473768
C	-2.7217387	0.6722789	3.4562209
C	-4.0107846	-4.1611968	-1.4228135
C	-5.1414978	-3.6178798	-0.6969972
C	-2.9110689	-4.6779858	-0.7262677
C	-5.1414978	-3.6178798	0.6969972
C	-5.6389707	-2.4642314	1.4144986

C	-6.2153883	-1.3562459	0.7344401
C	-6.1714120	-0.1078627	1.4143309
C	-4.5437189	-0.9787264	3.0915926
C	-4.8131590	-2.2779591	2.5790360
C	-5.3453241	0.0787594	2.5787323
C	-1.3719589	-3.5660632	-2.3027807
C	-2.5136732	-3.0252670	-3.0140192
C	-1.5639207	-4.3748423	-1.1756750
C	-3.8067211	-3.3174399	-2.5825539
C	-4.8131590	-2.2779591	-2.5790360
C	-4.5437189	-0.9787264	-3.0915926
C	-5.3453241	0.0787594	-2.5787323
C	-6.2153883	-1.3562459	-0.7344401
C	-5.6389707	-2.4642314	-1.4144986
C	-6.1714120	-0.1078627	-1.4143309
C	0.2599696	-3.1990995	0.0000000
C	0.4454186	-2.3567676	-1.1665121
C	-0.7302926	-4.1873882	0.0000000
C	-0.3500672	-2.5376590	-2.2961095
C	-0.8529608	-1.3848298	-3.0132073
C	-0.4817976	-0.0610942	-2.6483636
C	-1.3858565	0.9747959	-3.0136487
C	-3.1817070	-0.6709573	-3.5473768
C	-2.1891237	-1.6861280	-3.4563934
C	-2.7217387	0.6722789	-3.4562209
C	-1.3719589	-3.5660632	2.3027807
C	-0.3500672	-2.5376590	2.2961095

C	-1.5639207	-4.3748423	1.1756750
C	0.4454186	-2.3567676	1.1665121
C	0.7538211	-1.0174605	0.7192960
C	0.3480776	0.1265754	1.4556346
C	0.2248563	1.3345534	0.7192144
C	0.3480776	0.1265754	-1.4556346
C	0.7538211	-1.0174605	-0.7192960
C	0.2248563	1.3345534	-0.7192144
C	-0.4817976	-0.0610942	2.6483636
C	-0.8529608	-1.3848298	3.0132073
C	-1.3858565	0.9747959	3.0136487
C	-1.1597957	3.0922771	0.0000000
C	-0.6296001	2.4115258	1.1667228
C	-1.4269324	2.2320946	2.2964862
C	-2.4797458	3.5584564	0.0000000
C	-2.7918067	2.7210337	-2.3028853
C	-1.4269324	2.2320946	-2.2964862
C	-0.6296001	2.4115258	-1.1667228
C	-3.3131387	3.3689996	-1.1756684
C	-5.4307709	2.1239485	-1.4227157
C	-4.8834171	1.4498189	-2.5822921
C	-3.5901811	1.7417829	-3.0137661
C	-4.6596182	3.0633550	-0.7262089
C	-5.4307709	2.1239485	1.4227157
C	-6.2182093	1.1474267	0.6969047
C	-6.2182093	1.1474267	-0.6969047
C	-4.6596182	3.0633550	0.7262089

C	-2.7918067	2.7210337	2.3028853
C	-3.5901811	1.7417829	3.0137661
C	-4.8834171	1.4498189	2.5822921
C	-3.3131387	3.3689996	1.1756684

Zn-porphyrin···bispyridyl perylene bisimide

C	2.0044459	-2.3423845	-7.5696688
C	2.0738796	-3.7900462	-7.5967377
H	2.9915283	-4.3723642	-7.6173899
C	0.7852064	-4.2481219	-7.5982384
H	0.4411436	-5.2788826	-7.6200594
C	-0.0748494	-3.0818085	-7.5718845
C	-1.4758695	-3.1072340	-7.5682721
C	-2.3440820	-2.0071311	-7.5679395
C	-3.7904440	-2.0750762	-7.5926713
H	-4.3734586	-2.9921745	-7.6191006
C	-4.2491501	-0.7848263	-7.5907235
H	-5.2802772	-0.4418350	-7.6157580
C	-3.0847389	0.0756174	-7.5649291
C	-3.1065150	1.4771296	-7.5639931
C	-1.0637031	0.4218958	14.0867403
H	-1.9214428	0.7640533	14.6716831
C	-1.1185590	0.4414786	12.6911045
H	-2.0030613	0.7981696	12.1648781
C	0.0000000	-0.0000000	11.9909490
C	-0.0518155	-1.2511171	9.8950868
C	-1.0878830	-0.3910038	-4.4154513

H	-1.9408610	-0.6992872	-5.0214293
C	-1.1344093	-0.4045013	-3.0248036
H	-2.0304124	-0.7328213	-2.5022315
C	0.0000000	0.0000000	-2.3228990
C	-0.2146596	-1.2369647	-0.2267410
C	-0.2202019	-1.2052390	1.2650492
C	-0.4672962	-2.3907293	1.9340541
H	-0.6763617	-3.3040349	1.3784833
C	-0.5983232	-2.4299430	3.3650826
C	-0.2066010	-1.2137904	4.1292172
C	-0.0000000	0.0000000	3.4199719
C	0.0000000	0.0000000	1.9680216
C	-0.0000000	0.0000000	6.2436516
C	0.0475847	-2.5009874	6.3000554
C	-0.0702588	-2.4338131	7.7318010
H	-0.0652680	-3.3703729	8.2883977
C	-0.0476274	-1.2236963	8.4006690
C	-0.0662871	-1.2289837	5.5347913
C	-0.0000000	0.0000000	7.6964277
N	0.6915796	-1.9444168	-7.5555840
N	-1.9465414	-0.6924411	-7.5461073
N	0.0000000	0.0000000	14.7864922
N	-0.0000000	0.0000000	10.5456541
N	-0.0000000	0.0000000	-5.0992145
N	-0.0000000	0.0000000	-0.8828534
O	-0.0968145	-2.2902580	10.5335630
O	-0.3821488	-2.2637294	-0.8648343

O	-1.1181420	-3.4266834	3.9108809
O	0.3366805	-3.5870148	5.7546628
Zn	-0.0000000	0.0000000	-7.2726284
C	-2.0044459	2.3423845	-7.5696688
C	-2.0738796	3.7900462	-7.5967377
H	-2.9915283	4.3723642	-7.6173899
C	-0.7852064	4.2481219	-7.5982384
H	-0.4411436	5.2788826	-7.6200594
C	0.0748494	3.0818085	-7.5718845
C	1.4758695	3.1072340	-7.5682721
C	2.3440820	2.0071311	-7.5679395
C	3.7904440	2.0750762	-7.5926713
H	4.3734586	2.9921745	-7.6191006
C	4.2491501	0.7848263	-7.5907235
H	5.2802772	0.4418350	-7.6157580
C	3.0847389	-0.0756174	-7.5649291
C	3.1065150	-1.4771296	-7.5639931
N	-0.6915796	1.9444168	-7.5555840
N	1.9465414	0.6924411	-7.5461073
C	1.0878830	0.3910038	-4.4154513
H	1.9408610	0.6992872	-5.0214293
C	1.1344093	0.4045013	-3.0248036
H	2.0304124	0.7328213	-2.5022315
C	0.2146596	1.2369647	-0.2267410
C	0.2202019	1.2052390	1.2650492
C	0.4672962	2.3907293	1.9340541
H	0.6763617	3.3040349	1.3784833

C	0.5983232	2.4299430	3.3650826
C	0.2066010	1.2137904	4.1292172
C	0.0662871	1.2289837	5.5347913
O	0.3821488	2.2637294	-0.8648343
O	1.1181420	3.4266834	3.9108809
C	1.0637031	-0.4218958	14.0867403
H	1.9214428	-0.7640533	14.6716831
C	1.1185590	-0.4414786	12.6911045
H	2.0030613	-0.7981696	12.1648781
C	0.0518155	1.2511171	9.8950868
C	-0.0475847	2.5009874	6.3000554
C	0.0702588	2.4338131	7.7318010
H	0.0652680	3.3703729	8.2883977
C	0.0476274	1.2236963	8.4006690
O	0.0968145	2.2902580	10.5335630
O	-0.3366805	3.5870148	5.7546628
H	1.9433048	4.0933459	-7.5817102
H	-1.9433048	-4.0933459	-7.5817102
H	4.0916317	-1.9467718	-7.5767281
H	-4.0916317	1.9467718	-7.5767281