Supporting Information

Molecular Triads Composed of Ferrocene, C₆₀ and Nitroaromatic Entities: Electrochemical, Computational and Photochemical Investigations

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1. Cartesian Coordinates and Total Energy of the Computed Molecules

Compound 1: 2-ferrocenyl fulleropyrrolidine

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%mem=120MB
%chk=fera-3bh
#P opt B3LYP/3-21G* scf=conver=7 int(ultrafine) opt optcyc=10
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[1] ferrocenyl-fulleropyrrolidine
RMS Force = .000119
E(RB+HF-LYP) = -4048.253906 au
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C	1	1.439293				
C	1	1.438530	2	107.935370		
C	3	2.049095	1	69.485327	2	58.936333
Fe	1	1.076697	2	126.110722	4	123.668890
H	2	1.439154	1	108.056088	3	-0.054857
C	6	1.438414	2	107.947237	1	0.053405
C	4	2.037429	3	120.621147	1	80.653192
C	8	1.440323	4	69.425596	3	-160.893012
C	9	1.443558	8	107.589640	4	-58.511208
C	10	1.437644	9	108.212750	8	-0.487841
C	11	1.437967	10	107.926799	9	0.360607
H	2	1.076958	1	126.099979	3	176.530064
H	3	1.076794	1	125.958505	2	-177.625552
H	6	1.076775	2	126.008506	1	177.530959
H	11	1.076815	10	126.039546	9	-177.871115
H	12	1.076969	11	125.940787	10	-178.414886
H	8	1.075644	4	127.936547	3	-40.652421
H	10	1.077419	9	125.871873	8	-177.496061
H	7	1.076794	6	125.931612	2	177.643192
C	9	1.503268	8	126.894640	4	125.275579
N	21	1.444729	9	115.179788	8	-22.584281
C	21	1.616322	9	111.483642	8	93.937602
H	21	1.096690	9	108.981939	8	-147.311372
C	23	1.598502	21	105.028978	9	-107.776191
C	22	1.442888	21	113.104811	9	88.921649
C	23	1.535424	21	108.939299	9	129.707583
C	23	1.534633	21	114.362460	9	18.314464
H	26	1.098895	22	114.235284	21	-82.586350
H	26	1.093804	22	111.577262	21	153.882614
C	25	1.533901	23	114.705525	21	126.197688
C	25	1.535510	23	114.265076	21	-118.559568
C	27	1.442407	23	109.938151	21	-102.748303
C	27	1.371705	23	124.736943	21	103.413848
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C	28	1.443635	23	109.898428	21	99.081026
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C	31	1.372554	25	124.115048	23	-12.087770
C	31	1.442225	25	110.017609	23	140.315027
C	35	1.452757	28	120.128291	23	-150.053398
C	33	1.394322	27	120.912159	23	-156.481324
C	36	1.394457	28	121.174990	23	155.710072
C	38	1.453250	32	120.028800	25	-150.442749
C	40	1.453148	31	119.912410	25	150.361716
C	39	1.394564	32	120.965495	25	156.015839
C	42	1.394952	35	120.617998	28	-1.148217
C	37	1.458047	34	108.369870	27	-141.852423
C	41	1.394760	31	121.030758	25	-155.763361
C	46	1.457878	40	108.332862	31	-142.370440
C	37	1.395160	34	120.567044	27	1.830982
C	43	1.460419	33	119.827689	27	139.131470
C	53	1.389623	43	120.007667	33	0.855325
C	45	1.395075	38	120.548661	32	-1.589348
C	47	1.460835	39	119.857371	32	-139.241291
C	56	1.389481	47	120.071520	39	-0.967159
C	46	1.395351	40	120.589074	31	1.236507
C	51	1.390409	46	120.192182	40	143.789327
C	48	1.457988	42	119.974052	35	138.726337
C	49	1.390789	37	120.156034	34	143.718686
C	52	1.457672	37	119.968557	34	-138.671899
C	53	1.458724	43	107.718452	33	-141.560825
C	54	1.458247	53	120.034627	43	-137.901819
C	55	1.457834	45	119.960208	38	138.652209
C	56	1.458618	47	107.764386	39	141.569971
C	60	1.391360	48	120.075012	42	0.946578
C	65	1.391326	55	120.087691	45	0.850878
C	63	1.391060	53	119.923428	43	142.303775
C	64	1.391350	54	119.962061	53	0.162451
C	62	1.391395	52	120.077279	37	-0.849082
C	58	1.458171	46	119.987697	40	-138.682731
C	72	1.391188	58	120.035781	46	-0.760379
C	57	1.458525	56	120.036825	47	137.880836
C	66	1.391288	56	119.942514	47	-142.363482
C	70	1.458411	64	119.970660	54	138.020073
C	76	1.391327	70	119.948016	64	-0.074065
C	71	1.456587	62	120.052824	52	138.154865
C	68	1.456424	65	120.027407	55	-138.164408
C	78	1.391391	71	120.095122	62	-0.046708
C	74	1.391080	57	119.977899	56	-0.010296
C	73	1.456533	72	120.078454	58	138.193662
C	79	1.391257	68	120.109725	65	0.034113
C	80	1.459159	78	119.978485	71	-138.100636
C	82	1.391503	73	120.088657	72	-0.159337
C	84	1.390822	80	120.060977	78	-0.341171
H	22	1.010194	21	122.425220	9	-102.745151

Compound 2: N(3,5-Dinitrobenzoyl)-2-ferrocenyl-fullerpyrrolidine

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%mem=120MB
%chk=ferb-3bm
#P B3LYP/3-21G* scf=conver=7 int(ultrafine) opt optcyc=12
[2] ferrocenyl-dinitrobenzoyl-fulleropyrrolidine
RMS FORCE = .000151
E(RB+HF-LYP) = -4797.443835 au
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C	1	1.439219			
C	3	2.048811	1	69.482237	2
Fe	1	1.076814	2	125.969327	4
H	2	1.437449	1	107.821904	3
C	6	1.438875	2	108.177125	1
C	4	2.035109	3	120.507179	1
C	8	1.443837	4	69.047272	3
C	9	1.444967	8	107.563834	4
C	10	1.436826	9	108.151813	8
C	11	1.437298	10	108.049609	9
H	2	1.077156	1	125.962525	3
H	3	1.076806	1	126.068701	2
H	6	1.076817	2	125.803368	1
H	11	1.076650	10	125.944222	9
H	12	1.076685	11	125.968454	10
H	8	1.076244	4	128.011009	3
H	10	1.077087	9	125.832508	8
H	7	1.076811	6	126.041537	2
C	9	1.495882	8	128.084581	4
C	21	1.482304	9	112.510518	8
C	21	1.596324	9	113.397436	8
C	21	1.091989	9	110.573147	8
C	23	1.600083	21	105.483490	9
C	22	1.473656	21	110.236693	9
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C	23	1.538493	21	109.245184	9
C	23	1.536516	21	113.847203	9
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C	37	1.452665	28	119.963900	23
C	34	1.371063	25	124.434490	23
C	34	1.443405	25	109.654337	23
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C	33	1.440921	25	109.980306	23
C	38	1.452860	29	120.149413	23
C	36	1.394553	28	120.767591	23
C	39	1.394276	29	121.126392	23
C	41	1.391430	35	119.243186	27
C	40	1.386095	35	119.472659	27
C	40	1.080208	35	120.357078	27
H	41	1.079633	35	122.849123	27
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C	45	1.452708	33	119.819600	25
C	44	1.394550	34	120.896648	25
C	47	1.394464	38	120.583346	29
C	42	1.458032	37	108.383623	28
C	46	1.394456	33	120.827111	25
C	55	1.457515	45	108.321681	33
C	42	1.394612	37	120.480727	28
C	48	1.460438	36	119.869942	28
C	62	1.389290	48	120.009208	36
C	50	1.384274	41	122.197668	35
N	50	1.465411	41	118.741527	35
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C	56	1.461289	44	119.911696	34
C	68	1.389246	56	120.095048	44
C	55	1.394989	45	120.497709	33
C	60	1.389892	55	120.174275	45
C	57	1.458079	47	119.994856	38
C	58	1.390117	42	120.148645	37
C	61	1.457814	42	119.987325	37
C	62	1.458692	48	107.746063	36
C	63	1.458611	62	120.061490	48
H	64	1.078568	50	121.305949	41
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C	66	1.279571	51	116.740649	40
O	66	1.280403	51	116.698448	40
O	65	1.279042	50	116.962925	41
C	65	1.282418	50	116.610377	41
C	68	1.458656	56	107.747430	44
C	72	1.391203	57	120.082336	47
C	78	1.391168	67	120.015292	54
C	75	1.391035	62	119.946335	48
C	76	1.391162	63	119.945106	62
C	74	1.391191	61	120.050043	42
C	70	1.458223	55	120.001578	45
C	89	1.391004	70	119.992259	55
C	69	1.458643	68	120.083489	56
C	83	1.391170	68	119.935125	56

C	87	1.458411	76	120.001788	63	138.010230
C	93	1.391282	87	119.953114	76	-0.084527
C	88	1.456288	74	120.066835	61	138.173372
C	85	1.456355	78	120.084617	67	-138.155043
C	95	1.391328	88	120.070381	74	-0.120964
C	91	1.391099	69	119.933055	68	-0.083754
C	90	1.456309	89	120.090844	70	138.146613
C	96	1.391284	85	120.055007	78	0.195758
C	97	1.459313	95	119.963115	88	-138.069688
C	99	1.391320	90	120.051697	89	-0.230335
C	101	1.390606	97	120.059774	95	-0.307343

Compound 3: N(2,4-dinitrophenyl)-2-Ferrocenyl-fulleropyrrolidine

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%mem=120MB
%chk=ferf-3bl
#P B3LYP/3-21G* opt scf=conver=7 int(ultrafine) optcyc=25
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[3] ferrocenyl-dinitrophenyl-fulleropyrrolidine (anti)
RMS FORCE = 0.000003
E(RB+HF-LYP) = -4684.724903 au
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O 1

C	1	1.439121				
C	1	1.438159	2	107.930664		
Fe	3	2.047332	1	69.492073	2	59.211060
H	1	1.076626	2	126.003937	4	122.509464
C	2	1.438574	1	108.078967	3	-0.235651
C	6	1.438645	2	107.946608	1	0.189036
C	4	2.034396	3	119.175423	1	80.524466
C	8	1.443818	4	69.185077	3	-161.752014
C	9	1.445712	8	107.775090	4	-58.554589
C	10	1.437136	9	107.979902	8	-0.615658
C	8	1.436582	4	69.622157	3	78.792428
H	2	1.075816	1	125.584955	3	177.001050
H	3	1.076696	1	125.937873	2	-177.671115
H	6	1.076893	2	126.072368	1	177.466345
H	11	1.076709	10	125.890652	9	-177.934707
H	12	1.076652	8	125.706423	4	-122.464431
H	8	1.075336	4	124.777687	3	-41.887852
H	10	1.077058	9	126.054771	8	-176.776390
H	7	1.076783	6	125.966245	2	177.611731
C	9	1.500225	8	127.871986	4	127.299243
N	21	1.481279	9	111.888119	8	-19.934829
C	21	1.594900	9	113.603533	8	96.124780
H	21	1.090084	9	109.515982	8	-142.935887
C	23	1.600064	21	105.012607	9	-102.764983
C	22	1.474616	21	109.336240	9	86.008860
C	23	1.538783	21	109.036217	9	134.778378
C	23	1.535249	21	114.137235	9	23.336433
H	26	1.088516	22	112.047741	21	-79.697491
H	26	1.090355	22	110.519565	21	158.041641
C	25	1.534932	23	114.740185	21	126.135556
C	25	1.539267	23	114.313429	21	-118.482442
C	22	2.428244	21	97.862364	9	-115.634349
C	27	1.441594	23	109.808950	21	-102.569113
C	27	1.370646	23	124.743238	21	103.407805
C	28	1.372591	23	124.028791	21	-109.619547
C	28	1.443924	23	109.785690	21	99.331700
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C	33	1.375852	22	150.913518	21	168.619680
C	35	1.452993	27	119.895024	23	151.140469
C	32	1.371021	25	124.581545	23	12.029080
C	32	1.442934	25	109.694312	23	-140.616647
C	31	1.372093	25	123.939799	23	-12.010183
C	31	1.441340	25	109.944943	23	140.300041
C	36	1.452665	28	120.092133	23	-149.829185
C	34	1.394505	27	120.730628	23	-156.454488
C	37	1.394162	28	121.135187	23	155.467487
C	39	1.399078	33	119.766100	22	-7.188282
C	38	1.425841	22	123.663300	21	153.998451
H	39	1.080086	33	121.919991	22	170.624066
C	41	1.452536	32	120.124622	25	-150.316826
C	43	1.452795	31	119.839961	25	150.338009
C	42	1.394612	32	120.853132	25	155.778252
C	45	1.394590	36	120.613615	28	-0.858476
C	40	1.457694	35	108.347685	27	-141.911001
C	44	1.394690	31	120.890333	25	-155.660424
C	45	1.457756	36	108.494648	28	142.981835
C	40	1.395008	35	120.440805	27	1.629906
C	46	1.460586	34	119.856459	27	139.066597

C	59	1.389134	46	119.982469	34	0.705083
C	48	1.375551	39	120.339551	33	-2.101037
N	48	1.451333	39	119.888814	33	178.685936
N	49	1.457880	38	123.525295	22	-14.498744
C	51	1.394825	41	120.421775	32	-1.271159
C	53	1.460967	42	119.906989	32	-139.308511
C	65	1.389014	53	120.061989	42	-0.776458
C	52	1.394793	43	120.534808	31	1.069407
C	57	1.389941	45	120.211274	36	-143.827650
C	54	1.458065	45	120.004028	36	138.825233
C	55	1.390102	40	120.110128	35	143.559197
C	58	1.457615	40	119.988118	35	-138.652154
C	59	1.458792	46	107.703239	34	-141.685048
C	60	1.458331	59	120.063102	46	-137.877564
H	61	1.077819	48	120.299751	39	-177.873837
C	64	1.457952	51	119.995147	41	138.640657
O	63	1.293693	49	118.758159	38	-20.537733
O	63	1.282976	49	117.258265	38	163.610845
O	62	1.284199	48	117.259282	39	-179.458137
O	62	1.285831	48	116.772150	39	0.420459
C	65	1.458670	53	107.751913	42	141.700116
C	69	1.391331	54	120.043390	45	0.830253
C	75	1.391112	64	120.052293	51	0.677796
C	72	1.391108	59	119.900284	46	142.251407
C	73	1.391179	60	119.926079	59	0.207639
C	71	1.391009	58	120.018914	40	-0.673969
C	67	1.458062	52	120.017723	43	-138.777243
C	86	1.391288	67	120.015622	52	-0.625246
C	66	1.458795	65	120.073447	53	137.871490
C	80	1.390994	65	119.944890	53	-142.304159
C	84	1.458357	73	119.969761	60	137.975777
C	90	1.391245	84	119.981235	73	-0.001041
C	85	1.456371	71	120.068726	58	138.183266
C	82	1.456299	75	120.097374	64	-138.231672
C	92	1.391455	85	120.042085	71	-0.172858
C	88	1.391115	66	119.939141	65	-0.103068
C	87	1.456246	86	120.077198	67	138.172741
C	93	1.391380	82	120.023516	75	0.241692
C	94	1.459047	92	119.976628	85	-138.026567
C	96	1.391358	87	120.048334	86	-0.269116
C	98	1.390683	94	120.057319	92	-0.316696
H	33	1.080039	22	89.806338	21	-21.541129

Compound 4: N(3,5-dinitrobenzyl)-2-Ferrocenyl-fulleropyrroline

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%mem=120MB
%chk=FERc-3bu
#P B3LYP/3-21G* scf=conver=7 int(ultrafine) opt optcyc=17
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[4] ferrocenyl-dinitrobenzyl-fulleropyrrolidina
RMS FORCE = .000116
E(RB+HF-LYP) = -4723.821620 au
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C	1	1.439817				
C	1	1.437687	2	107.808346		
Fe	3	2.050249	1	69.750241	2	58.806398
H	1	1.076998	2	126.807934	4	124.403734
C	2	1.439607	1	108.122932	3	0.051420
C	6	1.438676	2	107.909828	1	-0.019371
C	4	2.036337	3	120.761674	1	81.055100
C	8	1.443342	4	69.497171	3	-162.044362
C	9	1.443820	8	107.525906	4	-58.287187
C	10	1.437081	9	108.239115	8	-0.819886
C	11	1.437324	10	107.985022	9	0.598944
H	2	1.076990	1	126.016239	3	176.957563
H	3	1.076759	1	125.730871	2	-177.734878
H	6	1.076908	2	126.106656	1	177.475688
H	11	1.076721	10	125.931437	9	-177.947774
H	12	1.076690	11	125.949698	10	-178.730934
H	8	1.075447	4	127.539083	3	-41.471839
H	10	1.076871	9	125.866877	8	-177.451090
H	7	1.076793	6	125.961193	2	177.762187
C	9	1.500085	8	127.933253	4	127.265653
N	21	1.479453	9	112.216811	8	-19.488698
C	21	1.620221	9	112.247612	8	98.904572
H	21	1.093560	9	109.537739	8	-141.057513
C	23	1.596764	21	104.489987	9	-105.350375
C	22	1.477620	21	107.132603	9	88.964193
C	22	1.483740	21	117.641048	9	-139.788506
C	23	1.536590	21	109.986137	9	131.854616
C	23	1.533442	21	113.987236	9	20.033281
H	26	1.091194	22	109.875025	21	-79.807714
H	26	1.091246	22	111.014840	21	158.911093
C	25	1.532035	23	114.826518	21	125.409524
C	25	1.538725	23	114.527604	21	-119.126384
C	27	1.525441	22	110.538067	21	148.891358
C	28	1.443427	23	109.925085	21	-102.856893
C	28	1.372383	23	124.699651	21	103.866622

C	29	1.373049	23	124.179603	21	-108.106524
C	29	1.444029	23	109.975325	21	100.247752
C	34	1.395624	27	121.406409	22	153.862420
C	34	1.397133	27	119.406746	22	-28.437380
C	36	1.453222	28	120.083230	23	150.834343
C	33	1.373253	25	124.426785	23	11.195206
C	33	1.444613	25	109.753377	23	-140.601210
C	32	1.372144	25	123.992874	23	-12.563278
C	32	1.440731	25	110.177987	23	140.619750
C	37	1.452360	29	120.132271	23	-150.188024
C	35	1.394681	28	120.896657	23	-156.183610
C	38	1.394187	29	121.136599	23	155.717435
C	40	1.387792	34	119.722350	27	-176.844580
C	39	1.392772	34	119.468874	27	177.094575
H	39	1.081268	34	122.385809	27	-3.082278
H	40	1.078541	34	119.421634	27	3.633592
C	42	1.452977	33	120.252712	25	-149.918646
C	44	1.452424	32	119.786409	25	150.771601
C	43	1.394858	33	120.969525	25	155.352423
C	46	1.394788	37	120.629014	29	-1.076390
C	41	1.457945	36	108.391488	28	-142.185669
C	45	1.394725	32	120.821392	25	-155.887027
C	54	1.457702	44	108.308828	32	-142.181464
C	41	1.394513	36	120.497570	28	1.440819
C	47	1.460592	35	119.892577	28	139.186610
C	61	1.389418	47	120.006224	35	0.686522
C	50	1.384572	39	122.226646	34	0.058205
N	49	1.465308	40	119.201896	34	179.631678
N	50	1.467017	39	118.980354	34	179.859287
N	53	1.394573	42	120.453937	33	-1.003297
C	55	1.461164	43	119.942150	33	-139.428845
C	67	1.389460	55	120.080623	43	-0.676237
C	54	1.395285	44	120.550390	32	1.387803
C	59	1.389927	54	120.190688	44	143.765745
C	56	1.457902	46	119.951150	37	138.686645
C	57	1.390307	41	120.139975	36	143.559633
C	60	1.457955	41	120.002065	36	-138.669471
C	61	1.458697	47	107.745197	35	-141.692157
C	62	1.458524	61	120.080225	47	-137.885260
H	63	1.077484	50	121.233788	39	179.946249
C	66	1.458046	53	119.997890	42	138.652189
O	65	1.282266	50	116.852059	39	-0.284934
O	65	1.280781	50	116.944591	39	179.981097
O	64	1.278334	49	117.163562	40	179.010054
O	64	1.287031	49	117.230791	40	-0.130829
C	67	1.458762	55	107.751156	43	141.760104
C	71	1.391197	56	120.095844	46	1.008257
C	77	1.391417	66	120.031594	53	0.669761
C	74	1.391144	61	119.944502	47	142.296814
C	75	1.391175	62	119.939521	61	0.193972
C	73	1.391417	60	120.027348	41	-0.696283
C	69	1.458155	54	119.956862	44	-138.646103
C	88	1.391039	69	120.046857	54	-0.768572
C	68	1.458667	67	120.099135	55	137.867556
C	82	1.391106	67	119.950351	55	-142.320797
C	86	1.458491	75	120.007411	62	138.037614
C	92	1.391376	86	119.937164	75	-0.137760
C	87	1.456236	73	120.089754	60	138.150958
C	84	1.456318	77	120.098168	66	-138.166106
C	94	1.391315	87	120.045596	73	-0.220124
C	90	1.391122	68	119.932046	67	-0.125371
C	89	1.456474	88	120.070409	69	138.184178
C	95	1.391189	84	120.044874	77	0.224314
C	92	1.459220	86	108.008000	75	-142.614392
C	98	1.391426	89	120.076792	88	-0.126535
C	100	1.390747	92	120.065088	86	142.807642
H	27	1.099199	22	113.148232	21	-87.505684
H	27	1.096537	22	107.491143	21	31.269625

Compound 5: N(4-nitrobenzoyl)-2-Ferrocenyl-fulleropyrrolidine

```
%mem=120MB
%chk=ferg-3bg
#P B3LYP/3-21G* scf=conver=7 int(ultrafine) opt optcyc=5
```

```
[5] ferrocenyl-nitrobenzoyl-fulleropyrrolidine
RMS FORCE = .000507
E(RB+HF-LYP) = -4594.107713 au
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C	1	1.440127				
C	1	1.440254	2	108.164084		
Fe	3	2.042131	1	69.385201	2	58.876098
H	1	1.075659	2	125.855487	4	124.969018
C	2	1.438499	1	107.813290	3	-0.046017
C	3	1.439942	1	107.893705	2	0.074035
C	4	2.030642	3	120.319050	1	80.565496
C	8	1.442170	4	68.952258	3	-160.763544
C	9	1.445712	8	107.743419	4	-58.319556
C	10	1.439228	9	107.995810	8	-0.667069
C	11	1.438371	10	108.049995	9	0.632416
H	2	1.075506	1	126.086385	3	178.872175
H	3	1.075739	1	126.036681	2	-176.158371
H	6	1.075603	2	125.793778	1	176.357892
H	11	1.075561	10	125.813039	9	-176.629718
H	12	1.075674	11	126.023029	10	-177.606517
H	8	1.075236	4	129.659528	3	-40.531610

H	10	1.075947	9	125.925306	8	-175.871699
H	7	1.075711	3	125.910462	1	-176.234754
C	9	1.491697	8	127.235363	4	127.557718
N	21	1.478056	9	112.359932	8	-25.816274
C	21	1.592383	9	113.163548	8	92.459483
H	21	1.091803	9	110.077881	8	-144.679687
C	23	1.601624	21	105.553263	9	-108.848748
C	22	1.473801	21	111.064230	9	95.638825
C	22	1.383099	21	117.720542	9	-110.301991
C	23	1.537105	21	109.722819	9	128.069785
C	23	1.535900	21	113.525955	9	16.753499
H	26	1.093360	22	111.362148	21	-88.432485
H	26	1.088114	22	110.735340	21	150.060662
C	25	1.534591	23	114.753431	21	125.153125
C	25	1.537587	23	114.440534	21	-119.467715
C	27	1.495947	22	117.118270	21	179.437357
C	28	1.441218	23	109.872362	21	-101.843109
C	28	1.370001	23	124.697677	21	104.673531
C	29	1.370860	23	124.347735	21	-108.828096
C	29	1.442469	23	109.824435	21	99.385849
C	34	1.400612	27	116.912827	22	147.205702
C	34	1.401149	27	122.694417	22	-39.114774
C	36	1.451458	28	120.069123	23	151.141295
C	33	1.370277	25	124.424107	23	11.619398
C	33	1.442410	25	109.739152	23	-140.752090
C	32	1.370537	25	124.036818	23	-11.987376
C	32	1.440593	25	109.961255	23	140.584477
C	37	1.451663	29	120.163163	23	-150.302500
C	35	1.393750	28	120.795427	23	-156.397767
C	38	1.393275	29	121.071009	23	155.829243
C	40	1.392400	34	119.878705	27	-175.603513
C	39	1.390234	34	120.138245	27	176.932584
H	39	1.081091	34	118.859964	27	-2.978565
H	40	1.081479	34	120.014626	27	2.866360
C	42	1.451864	33	120.107585	25	-150.368547
C	44	1.451647	32	119.887905	25	150.604216
C	43	1.393539	33	120.853548	25	155.681313
C	46	1.393337	37	120.562811	29	-1.012205
C	53	1.456608	42	108.373155	33	142.546935
C	45	1.393636	32	120.825756	25	-155.753343
C	54	1.456141	44	108.334160	32	-142.567321
C	41	1.393543	36	120.453932	28	1.332587
C	47	1.458944	35	119.911462	28	139.230893
C	61	1.388703	47	119.999880	35	0.636416
C	49	1.387683	40	118.861462	34	-0.018607
C	53	1.393538	42	120.446168	33	-1.030413
C	55	1.459593	43	119.956333	33	-139.375996
C	65	1.388715	55	120.065397	43	-0.682138
C	54	1.393928	44	120.504931	32	1.033661
C	59	1.389338	54	120.148118	44	143.678179
C	56	1.456612	46	120.011175	37	138.792033
C	57	1.389415	53	120.129143	42	-143.537202
C	60	1.456627	41	119.996318	36	-138.653571
C	61	1.457397	47	107.743080	35	-141.755386
C	62	1.457367	61	120.071202	47	-137.879121
C	64	1.456750	53	119.999960	42	138.668075
C	65	1.457347	55	107.733075	43	141.783423
C	69	1.390473	56	120.047314	46	0.836560
C	74	1.390449	64	119.996594	53	0.623633
C	72	1.390315	61	119.932866	47	142.265875
C	73	1.390347	62	119.931580	61	0.195551
C	71	1.390525	60	120.018999	41	-0.691515
C	67	1.456936	54	119.997377	44	-138.715930
C	81	1.390402	67	119.978370	54	-0.625276
C	66	1.457473	65	120.083349	55	137.844243
C	75	1.390344	65	119.917155	55	-142.278310
C	79	1.457071	73	119.990886	62	138.001829
C	85	1.390606	79	119.975921	73	-0.065649
C	80	1.455109	71	120.066425	60	138.122922
C	77	1.455188	74	120.078123	64	-138.117433
C	87	1.390639	80	120.049919	71	-0.166339
C	83	1.390374	66	119.909179	65	-0.119884
C	82	1.455123	81	120.071496	67	138.094378
C	88	1.390536	77	120.042370	74	0.203717
C	85	1.457958	79	108.012896	73	-142.619947
C	91	1.390555	82	120.046434	81	-0.213885
C	93	1.389932	85	120.056785	79	142.833651
O	27	1.243494	22	121.951505	21	0.345202
H	49	1.077889	40	122.505092	34	179.395413
H	50	1.077813	39	122.565536	34	178.743229
N	63	1.470844	49	118.773839	40	-179.597941
O	99	1.279956	63	116.993262	49	176.897038
O	99	1.280533	63	117.050253	49	-3.182626