

Electronic Supporting Information accompanying:

1,1,2,2-tetracyanocyclopropane (TCCP) as supramolecular synthon

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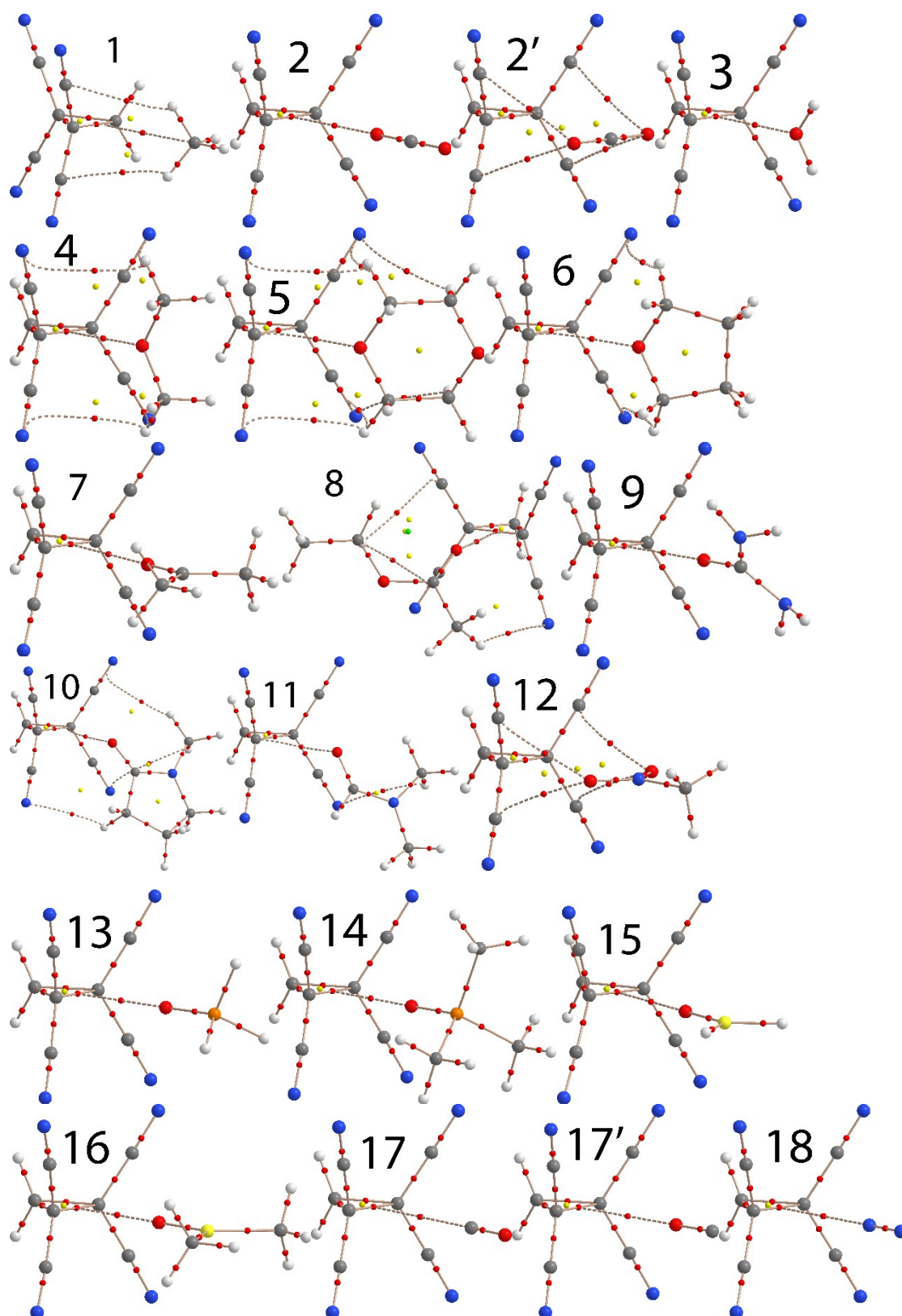
Table S1. Interaction energies (E) and minimum contact distances (D) estimated at the MP2/def2-TZVP level of theory level of theory of complexes involving TCCP and several small molecules.

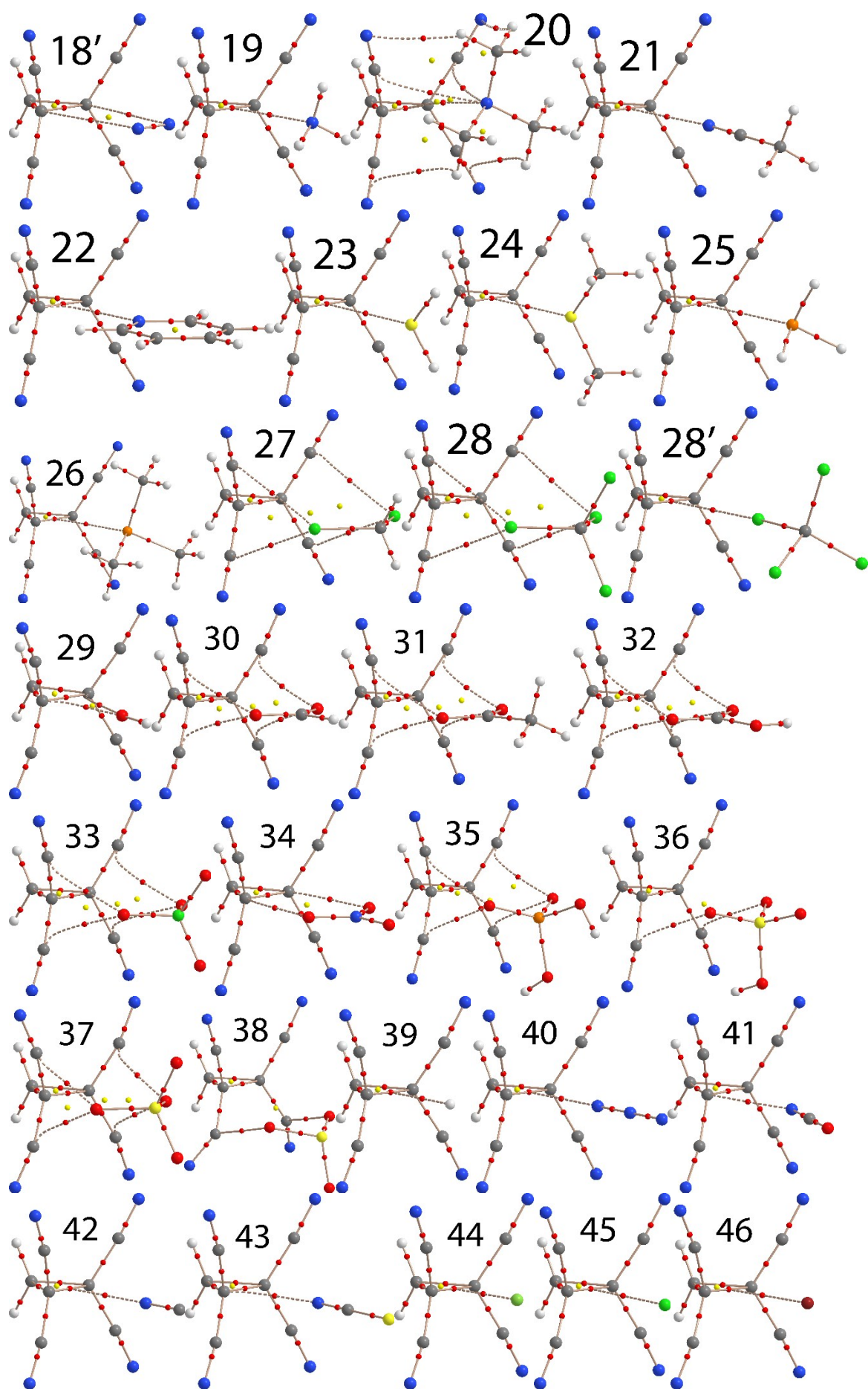
Complex	Guest	E (kcal/mol)	D (Å)
1	CH ₄	-2.36	3.403
2	CO ₂	-3.98	2.883
3	H ₂ O	-7.35	2.798
4	(CH ₃) ₂ O	-9.38	2.803
13	H ₃ PO	-9.97	2.690
14	(CH ₃) ₃ PO	-13.18	2.623
15	H ₂ SO	-9.11	2.637
16	(CH ₃) ₂ SO	-11.67	2.570
17	CO	-3.59	3.195
18	N ₂	-3.11	3.066
19	NH ₃	-8.04	2.985
20	N(CH ₃) ₃	-10.17	3.120
23	H ₂ S	-4.40	3.313
24	S(CH ₃) ₂	-7.41	3.181
25	PH ₃	-5.08	3.478
26	P(CH ₃) ₃	-9.29	3.327

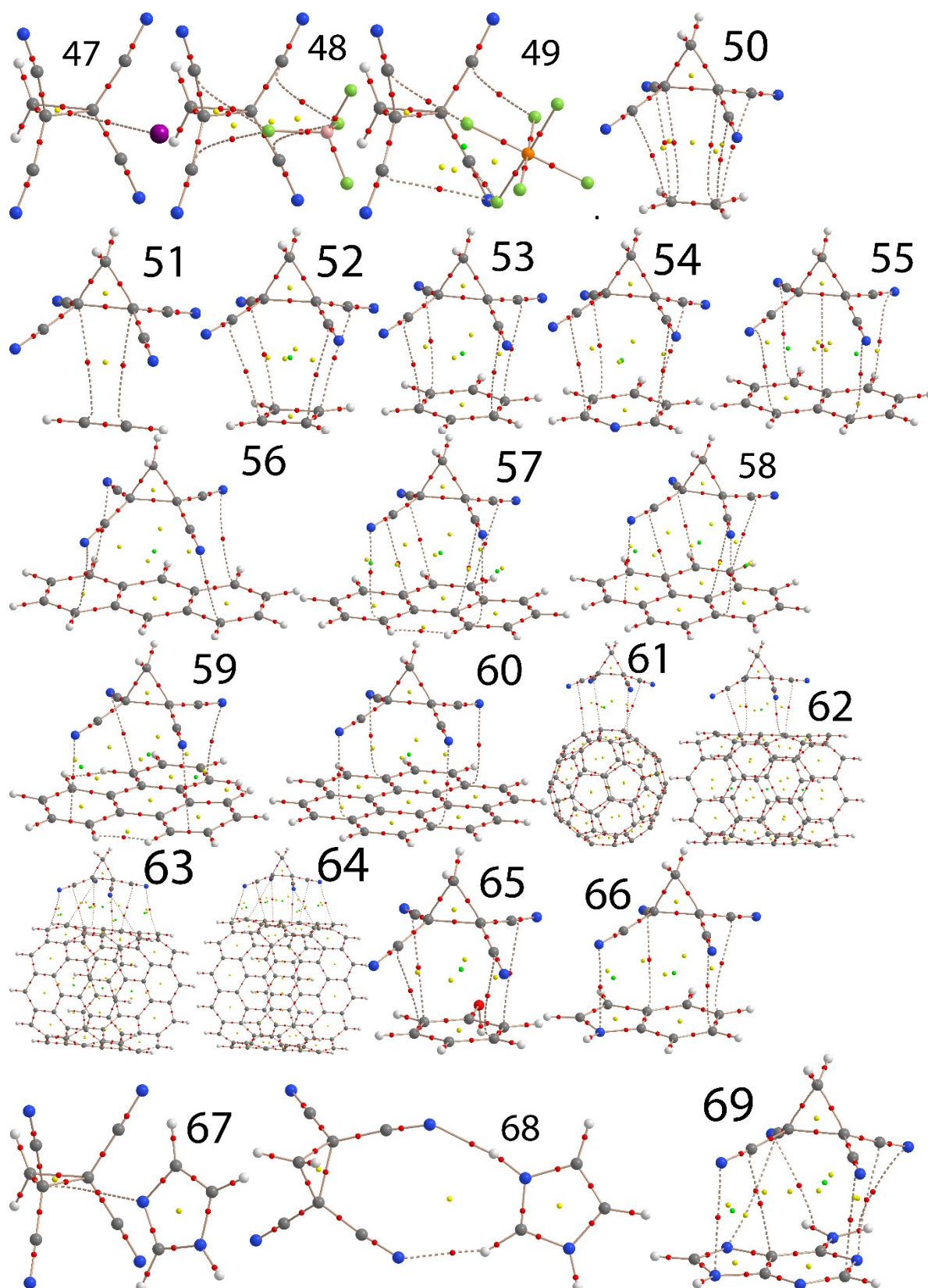
Theoretical methods

The energies of all complexes included in this study were computed using the RI-MP2/BP86-D3 methods and the def2-TZVP basis set. The calculations have been performed by using the program TURBOMOLE version 7.0.¹ For the calculations we have used the DFT-D functional with the latest available correction for dispersion (D3).² The Bader's "Atoms in molecules" theory has been used to study the interactions discussed herein by means of the AIMall calculation package.³ The optimization of the molecular geometries has been performed imposing the C_s and C_{2v} symmetry point groups unless otherwise noticed.

Figure S1. Graphical renderings of perspective views of complexes **1-73** with AIM analysis







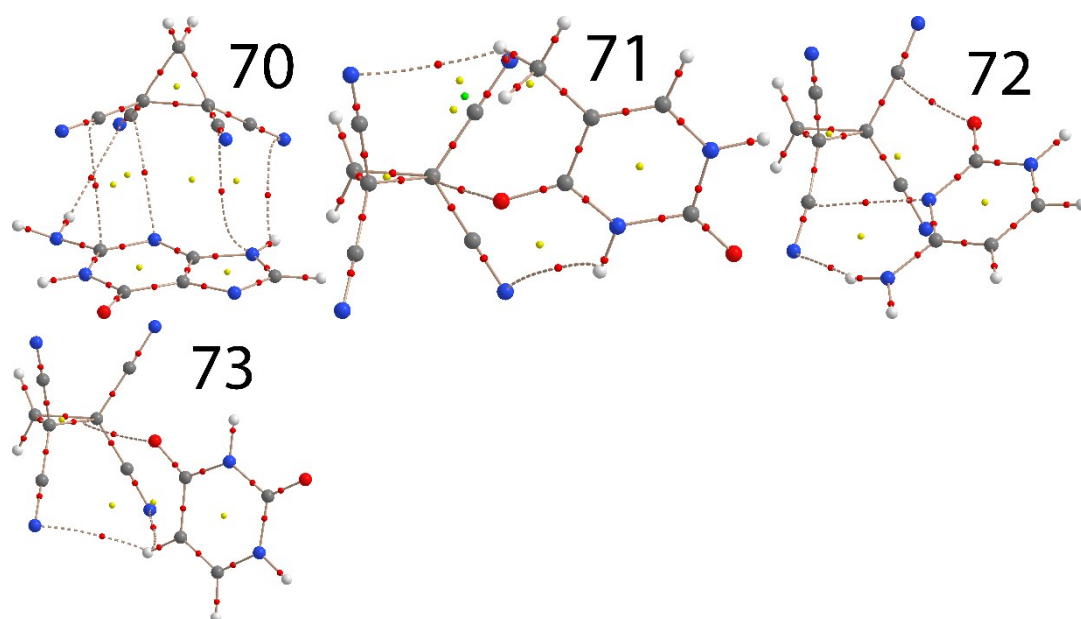


Figure S2. Structures of bipodal (a) and tripodal hosts (b, c), together with perspective views of the geometry of their energy minimum conformer (estimated by MMFF Monte Carlo conformational search, then energy minimized using DFT).

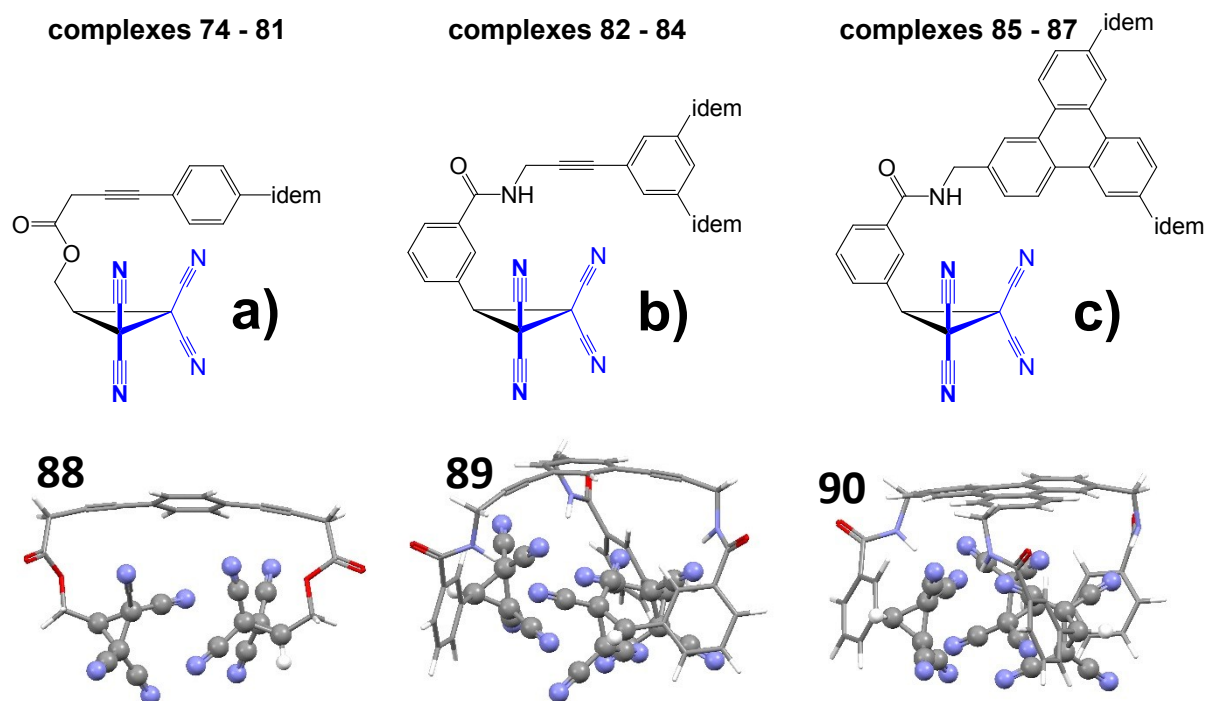
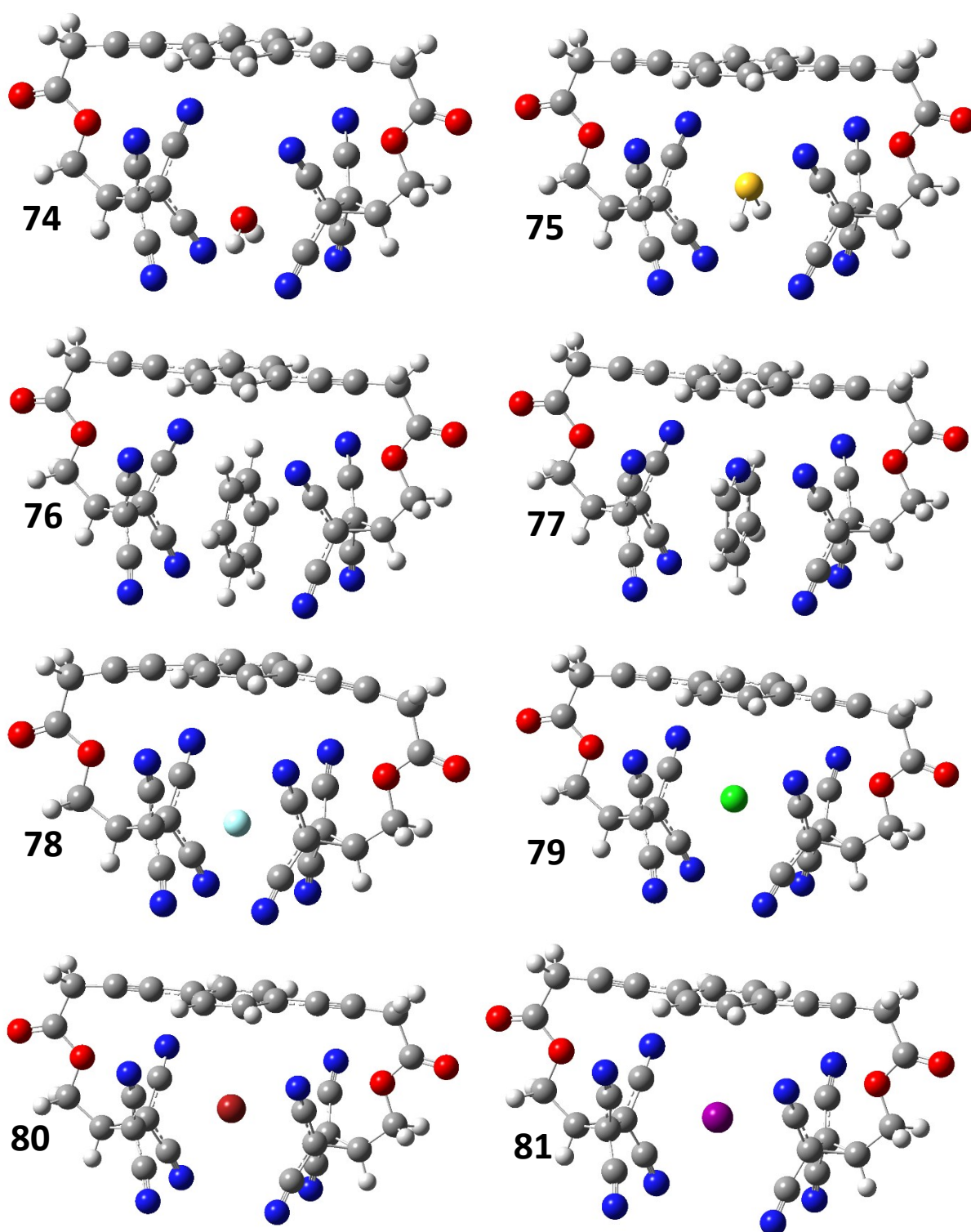
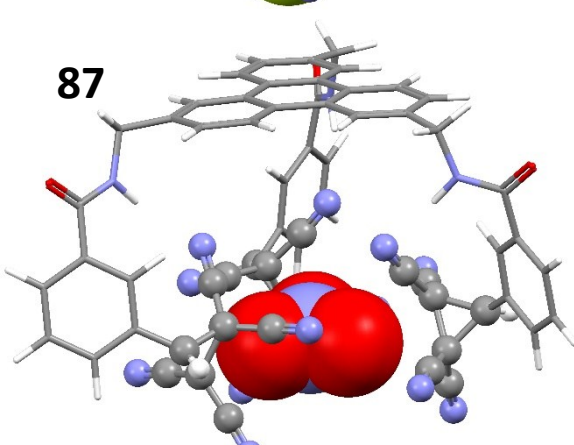
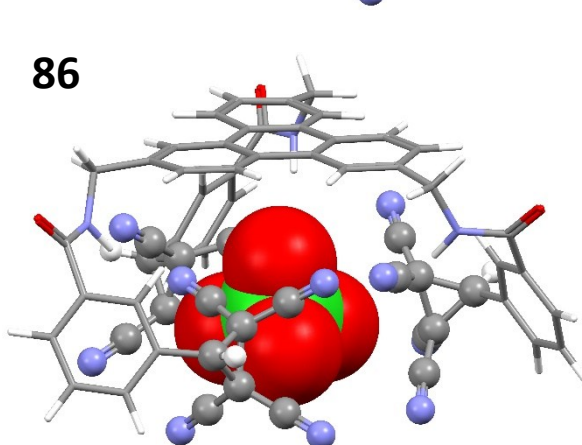
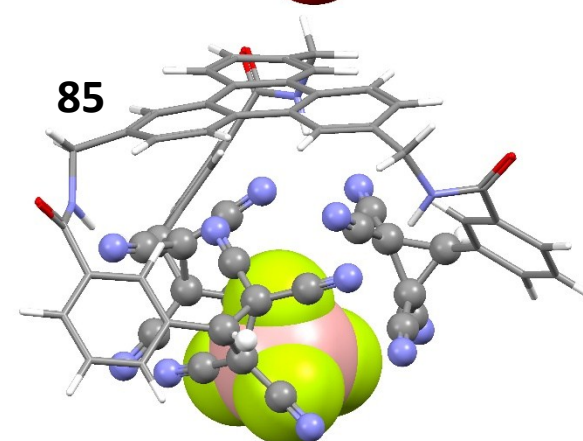
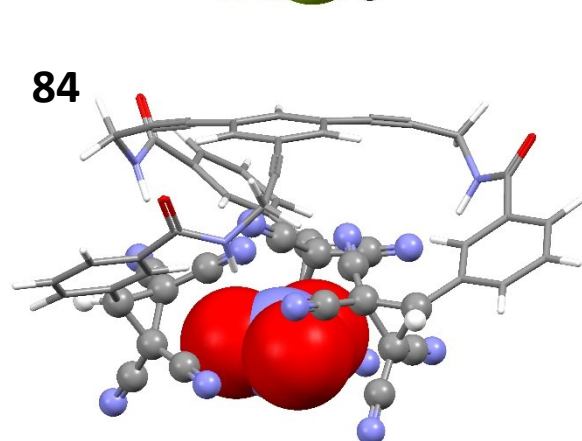
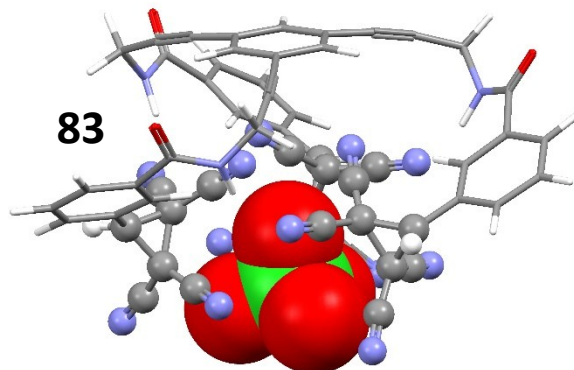
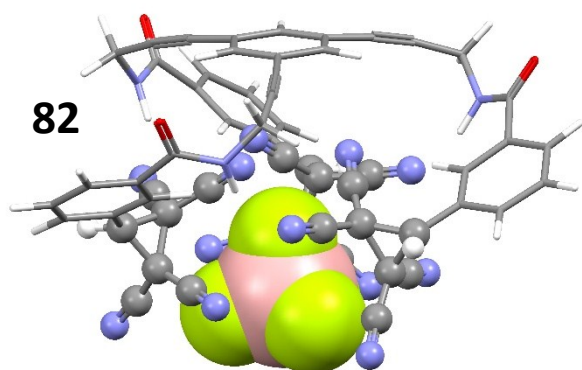


Figure S3. Graphical renderings of perspective views of complexes **74-87**





Cartesian coordinates of complexes **1-87**

1.

C -0.4670731 0.1278309 -1.7719112
C -0.2120269 -0.6170867 -0.3801146
C 0.0359028 0.8708736 -0.5452017
H -0.6714993 1.5359649 -0.0536175
H 1.0766608 1.1884843 -0.5598609
C -1.8414066 0.3029970 -2.1701452
C 0.4616869 -0.1550869 -2.8375406
C -1.3775084 -1.0435563 0.3523410
C 0.9242229 -1.5010005 -0.3149474
N -2.9513339 0.4595299 -2.4778979
N 1.2239022 -0.3704781 -3.6882750
N 1.8537211 -2.1965750 -0.2581137
N -2.3184588 -1.3667395 0.9532824
C 0.8512428 0.5527531 2.7458770
H 1.1316241 0.5729426 3.8049544
H 1.4867688 -0.1711298 2.2214683
H -0.2013708 0.2569651 2.6604854
H 0.9949452 1.5533112 2.3192172

1. MP2

C -0.4672700 0.1206379 -1.7662227
C -0.2259268 -0.5861847 -0.3913420
C 0.0215657 0.8929189 -0.5632174
H -0.6933900 1.5563866 -0.0935597
H 1.0574079 1.2070083 -0.5805143
C -1.8381466 0.2808109 -2.1694310
C 0.4723943 -0.1805337 -2.8121105
C -1.3989659 -1.0021602 0.3280134
C 0.9104361 -1.4632874 -0.3144595

N	-2.9594963	0.4250153	-2.4791959
N	1.2556947	-0.4166308	-3.6516780
N	1.8512395	-2.1602860	-0.2552700
N	-2.3619194	-1.3189816	0.9168818
C	0.8737354	0.5286087	2.7612190
H	1.1700401	0.5520012	3.8074064
H	1.5312858	-0.1515987	2.2226872
H	-0.1567118	0.1841851	2.6932762
H	0.9580274	1.5320902	2.3475170

2.

C	0.000000	-0.797155	-0.749519
C	0.000000	0.797155	-0.749519
C	0.000000	0.000000	-2.042966
C	-1.218705	-1.442748	-0.330256
C	1.218705	-1.442748	-0.330256
C	-1.218705	1.442748	-0.330256
C	1.218705	1.442748	-0.330256
N	-2.207298	-1.962044	-0.008121
N	2.207298	-1.962044	-0.008121
N	2.207298	1.962044	-0.008121
N	-2.207298	1.962044	-0.008121
H	-0.926788	0.000000	-2.613569
H	0.926788	0.000000	-2.613569
C	0.000000	0.000000	3.375906
O	0.000000	0.000000	4.543858
O	0.000000	0.000000	2.202888

2. MP2

C	0.0000000	-0.7797337	-0.7360179
C	0.0000000	0.7797337	-0.7360179

C	0.0000000	0.0000000	-2.0303506
H	-0.9250266	0.0000000	-2.5927315
H	0.9250266	0.0000000	-2.5927315
C	-1.2194617	-1.4162874	-0.3183355
C	1.2194617	-1.4162874	-0.3183355
C	-1.2194617	1.4162874	-0.3183355
C	1.2194617	1.4162874	-0.3183355
N	-2.2234554	-1.9290185	0.0026532
N	2.2234554	-1.9290185	0.0026532
N	2.2234554	1.9290185	0.0026532
N	-2.2234554	1.9290185	0.0026532
C	0.0000000	0.0000000	3.3188929
O	0.0000000	0.0000000	4.4842157
O	0.0000000	0.0000000	2.1474701

2^c.

C	0.000000	-0.801876	-0.621435
C	0.000000	0.801876	-0.621435
C	0.000000	0.000000	-1.911692
C	-1.222186	-1.445466	-0.209563
C	1.222186	-1.445466	-0.209563
C	-1.222186	1.445466	-0.209563
C	1.222186	1.445466	-0.209563
N	-2.219820	-1.953018	0.103586
N	2.219820	-1.953018	0.103586
N	2.219820	1.953018	0.103586
N	-2.219820	1.953018	0.103586
H	-0.927090	0.000000	-2.482045
H	0.927090	0.000000	-2.482045
C	0.000000	0.000000	2.856086
O	0.000000	1.171305	2.843237

O 0.000000 -1.171305 2.843237

3.

C 0.000000 0.793451 0.578801

C 0.000000 -0.793451 0.578801

C 0.000000 0.000000 1.875465

C -1.218557 1.435382 0.154239

C 1.218557 1.435382 0.154239

C -1.218557 -1.435382 0.154239

C 1.218557 -1.435382 0.154239

N -2.211966 1.948631 -0.162466

N 2.211966 1.948631 -0.162466

N 2.211966 -1.948631 -0.162466

N -2.211966 -1.948631 -0.162466

H -0.926716 0.000000 2.446143

H 0.926716 0.000000 2.446143

O 0.000000 0.000000 -2.240023

H 0.774080 0.000000 -2.826211

H -0.774080 0.000000 -2.826211

3. MP2

C 0.0000000 0.7771322 0.5746995

C 0.0000000 -0.7771322 0.5746995

C 0.0000000 0.0000000 1.8712945

H -0.9247564 0.0000000 2.4340206

H 0.9247564 0.0000000 2.4340206

C -1.2192003 1.4102461 0.1526390

C 1.2192003 1.4102461 0.1526390

C -1.2192003 -1.4102461 0.1526390

C 1.2192003 -1.4102461 0.1526390

N -2.2278486 1.9156946 -0.1643734

N	2.2278486	1.9156946	-0.1643734
N	2.2278486	-1.9156946	-0.1643734
N	-2.2278486	-1.9156946	-0.1643734
O	0.0000000	0.0000000	-2.2233142
H	0.7665985	0.0000000	-2.8092415
H	-0.7665985	0.0000000	-2.8092415

4.

C	0.0000000	0.7930316	1.4863609
C	0.0000000	-0.7930316	1.4863609
C	0.0000000	0.0000000	2.7838659
H	-0.9269311	0.0000000	3.3542351
H	0.9269311	0.0000000	3.3542351
C	-1.2186292	1.4351367	1.0630692
C	1.2186292	1.4351367	1.0630692
C	-1.2186292	-1.4351367	1.0630692
C	1.2186292	-1.4351367	1.0630692
N	-2.2146577	1.9456766	0.7501640
N	2.2146577	1.9456766	0.7501640
N	2.2146577	-1.9456766	0.7501640
N	-2.2146577	-1.9456766	0.7501640
O	0.0000000	0.0000000	-1.3493885
C	1.1831352	0.0000000	-2.1470152
H	1.2300293	0.8995782	-2.7872271
H	2.0391543	0.0000000	-1.4628317
H	1.2300293	-0.8995782	-2.7872271
C	-1.1831352	0.0000000	-2.1470152
H	-1.2300293	-0.8995782	-2.7872271
H	-2.0391543	0.0000000	-1.4628317
H	-1.2300293	0.8995782	-2.7872271

4. MP2

C	0.0000000	0.7767927	1.4783171
C	0.0000000	-0.7767927	1.4783171
C	0.0000000	0.0000000	2.7755918
H	-0.9249059	0.0000000	3.3382411
H	0.9249059	0.0000000	3.3382411
C	-1.2188772	1.4100075	1.0560524
C	1.2188772	1.4100075	1.0560524
C	-1.2188772	-1.4100075	1.0560524
C	1.2188772	-1.4100075	1.0560524
N	-2.2293652	1.9151542	0.7432585
N	2.2293652	1.9151542	0.7432585
N	2.2293652	-1.9151542	0.7432585
N	-2.2293652	-1.9151542	0.7432585
O	0.0000000	0.0000000	-1.3247065
C	1.1669675	0.0000000	-2.1332636
H	1.1971260	0.8919584	-2.7682276
H	2.0294952	0.0000000	-1.4709038
H	1.1971260	-0.8919584	-2.7682276
C	-1.1669675	0.0000000	-2.1332636
H	-1.1971260	-0.8919584	-2.7682276
H	-2.0294952	0.0000000	-1.4709038
H	-1.1971260	0.8919584	-2.7682276

5.

C	0.6972853	-2.2640115	0.0000000
C	-0.8464813	-1.9011338	0.0000000
C	-0.3704561	-3.3457542	0.0000000
H	-0.5019167	-3.9010859	0.9269764
H	-0.5019167	-3.9010859	-0.9269764
C	1.4150842	-1.9944949	1.2200221

C	1.4150842	-1.9944949	-1.2200221
C	-1.3748641	-1.3374040	1.2160795
C	-1.3748641	-1.3374040	-1.2160795
N	1.9742780	-1.8014033	2.2202960
N	1.9742780	-1.8014033	-2.2202960
N	-1.8030872	-0.9010597	-2.2045020
N	-1.8030872	-0.9010597	2.2045020
C	0.6644272	1.4738795	-1.1813587
C	0.6644272	1.4738795	1.1813587
C	-0.5085644	2.4425236	1.1738952
C	-0.5085644	2.4425236	-1.1738952
H	0.6148159	0.7924518	2.0409980
H	1.6196614	2.0304896	-1.2160194
H	0.6148159	0.7924518	-2.0409980
H	-1.4573715	1.8728699	1.2243779
H	-0.4579123	3.1226655	2.0358019
H	-1.4573715	1.8728699	-1.2243779
H	-0.4579123	3.1226655	-2.0358019
H	1.6196614	2.0304896	1.2160194
O	0.6359740	0.6504083	0.0000000
O	-0.4854229	3.2616265	0.0000000

6.

C	-2.2671206	0.4318847	0.0000000
C	-1.8915378	-1.1080399	0.0000000
C	-3.3402557	-0.6445264	0.0000000
H	-3.8945914	-0.7802056	-0.9269253
H	-3.8945914	-0.7802056	0.9269253
C	-2.0024742	1.1561433	-1.2175564
C	-2.0024742	1.1561433	1.2175564
C	-1.3236565	-1.6294789	-1.2172698

C	-1.3236565	-1.6294789	1.2172698
N	-1.8143838	1.7310446	-2.2099066
N	-1.8143838	1.7310446	2.2099066
N	-0.8906012	-2.0493496	2.2106919
N	-0.8906012	-2.0493496	-2.2106919
C	1.4506719	0.5867067	1.1455412
O	0.6199308	0.3188472	0.0000000
C	1.4506719	0.5867067	-1.1455412
C	2.8395679	0.0364482	-0.7774724
C	2.8395679	0.0364482	0.7774724
H	1.4817212	1.6773091	1.3272274
H	0.9863007	0.0991295	2.0109695
H	0.9863007	0.0991295	-2.0109695
H	1.4817212	1.6773091	-1.3272274
H	2.9650005	-0.9823955	-1.1655718
H	3.6419365	0.6555655	-1.1989826
H	2.9650005	-0.9823955	1.1655718
H	3.6419365	0.6555655	1.1989826

7.

C	0.0000000	0.7925229	1.9497069
C	0.0000000	-0.7925229	1.9497069
C	-0.0000000	0.0000000	3.2470932
H	-0.9266232	0.0000000	3.8177670
H	0.9266232	0.0000000	3.8177670
C	-1.2169450	1.4415066	1.5297377
C	1.2169450	1.4415066	1.5297377
C	-1.2169450	-1.4415066	1.5297377
C	1.2169450	-1.4415066	1.5297377
N	-2.2043878	1.9736519	1.2259513
N	2.2043878	1.9736519	1.2259513

N	2.2043878	-1.9736519	1.2259513
N	-2.2043878	-1.9736519	1.2259513
C	0.0000000	0.0000000	-2.0042450
O	-0.0000000	0.0000000	-0.7796618
C	0.0000000	-1.3124215	-2.7599920
H	-0.8822419	-1.8918248	-2.4506887
H	0.0000000	-1.1941817	-3.8490757
H	0.8822419	-1.8918248	-2.4506887
C	0.0000000	1.3124215	-2.7599920
H	-0.8822419	1.8918248	-2.4506887
H	0.8822419	1.8918248	-2.4506887
H	0.0000000	1.1941817	-3.8490757

8.

C	1.5413195	-0.2717050	2.1581758
C	0.0093962	0.1325361	2.1696546
C	0.8549119	0.1969138	3.4313977
H	1.1184742	1.1897724	3.7910439
H	0.6596364	-0.5623706	4.1863617
C	2.4341168	0.6343318	1.4792990
C	1.8432799	-1.6736240	2.0131657
C	-0.3367140	1.3614214	1.5000403
C	-0.9530104	-0.9294523	2.0163749
N	3.1543504	1.3893019	0.9676121
N	2.0908759	-2.8067625	1.9443861
N	-1.7482959	-1.7711716	1.9192959
N	-0.6209401	2.3587126	0.9748702
C	0.5354631	0.0612934	-1.6067569
O	0.6457284	-0.5365885	-0.5449608
C	1.6869665	0.6803000	-2.3499418
H	2.2375347	1.3326383	-1.6595156

H	2.3733906	-0.1202505	-2.6582971
H	1.3560400	1.2439165	-3.2277661
O	-0.6421775	0.2313128	-2.2386313
C	-1.8124483	-0.3349328	-1.5699677
H	-1.6027947	-1.3835367	-1.3161981
H	-1.9659020	0.2140864	-0.6293283
C	-2.9875752	-0.1848349	-2.5119077
H	-2.8124205	-0.7308744	-3.4486716
H	-3.8916630	-0.5921957	-2.0386526
H	-3.1675430	0.8717621	-2.7510824

9.

C	0.2311743	0.7560915	1.6565887
C	-0.2311743	-0.7560915	1.6565887
C	0.0000000	0.0000000	2.9557787
H	-0.8878899	0.2661424	3.5266632
H	0.8878899	-0.2661424	3.5266632
C	-0.7398285	1.7313564	1.2258360
C	1.5901210	1.0189837	1.2521580
C	-1.5901210	-1.0189837	1.2521580
C	0.7398285	-1.7313564	1.2258360
N	-1.5244016	2.5296324	0.9132301
N	2.6976659	1.2365010	0.9758635
N	1.5244016	-2.5296324	0.9132301
N	-2.6976659	-1.2365010	0.9758635
C	0.0000000	0.0000000	-2.2642591
O	0.0000000	0.0000000	-1.0300227
N	-0.6082225	0.9983643	-2.9954126
H	-0.9237761	0.8075357	-3.9404353
H	-1.2068891	1.6057440	-2.4452402
N	0.6082225	-0.9983643	-2.9954126
H	0.9237761	-0.8075357	-3.9404353

H 1.2068891 -1.6057440 -2.4452402

10.

C 1.0482485 0.6075270 2.5602264

C -0.3850048 -0.0348912 2.3788236

C 0.3915120 -0.1889622 3.6778938

H 0.0259743 0.3788036 4.5315618

H 0.8075854 -1.1733101 3.8851048

C 1.1111769 2.0423272 2.6778702

C 2.1223574 -0.0143022 1.8260989

C -1.5131123 0.8613221 2.3421737

C -0.4779144 -1.1586382 1.4802292

N 1.1644749 3.1930685 2.8288716

N 2.9924464 -0.5620398 1.2844879

N -0.5573807 -2.0701636 0.7634028

N -2.4444234 1.5563338 2.3511493

C 0.2431204 0.4597059 -1.1524237

O 0.2627091 1.1723122 -0.1422295

N -0.8841226 0.0453994 -1.7982730

C -2.2187493 0.2950492 -1.2987238

H -2.1609633 1.0739900 -0.5292316

H -2.8744249 0.6362489 -2.1130221

H -2.6495416 -0.6180467 -0.8563886

C -0.6231619 -0.9328159 -2.8495692

H -1.2769533 -0.7521776 -3.7160162

H -0.8269275 -1.9518576 -2.4737537

C 1.4433012 -0.1581885 -1.8548413

H 2.2421080 0.5820838 -1.9793477

H 1.8335231 -0.9472816 -1.1932732

C 0.8711802 -0.7186861 -3.1655334

H 0.9751768 0.0217334 -3.9710151

H 1.3577855 -1.6445436 -3.4942518

11.

C 1.4479363 0.5896041 1.9802390

C -0.0684913 0.1391962 2.0622633

C 0.8783347 -0.0478692 3.2379867

H 0.7284680 0.6102787 4.0919562

H 1.1910122 -1.0677906 3.4542146

C 1.7085616 2.0072438 1.9842123

C 2.3017520 -0.2030348 1.1309433

C -1.0643937 1.1790560 2.1210079

C -0.4424301 -1.0136910 1.2817340

N 1.9300258 3.1462336 2.0444110

N 2.9890029 -0.8763074 0.4785842

N -0.7458289 -1.9517951 0.6663051

N -1.8825349 1.9999774 2.2056497

C 0.4440348 0.2769920 -1.5501282

O 0.3755811 1.0979024 -0.6300027

H 1.4172422 -0.1003700 -1.9306469

N -0.6166694 -0.2713435 -2.1888610

C -1.9773004 0.0744135 -1.8046631

H -1.9392509 0.8858325 -1.0695721

H -2.5460919 0.4047625 -2.6867779

H -2.4804631 -0.7979428 -1.3605188

C -0.4475114 -1.3149030 -3.1848933

H -0.9341589 -1.0305818 -4.1308430

H 0.6216109 -1.4761660 -3.3722727

H -0.8884377 -2.2596974 -2.8303277

12.

C -1.5255621 0.1602236 0.7953055

C	-1.5255621	0.1602236	-0.7953055
C	-2.8151311	0.2926280	0.0000000
H	-3.2879857	1.2729908	0.0000000
H	-3.4765866	-0.5717136	0.0000000
C	-1.0035833	1.3370140	1.4442996
C	-1.2541920	-1.0985932	1.4433433
C	-1.0035833	1.3370140	-1.4442996
C	-1.2541920	-1.0985932	-1.4433433
N	-0.6303078	2.3088216	1.9608180
N	-1.0878028	-2.1269275	1.9584200
N	-1.0878028	-2.1269275	-1.9584200
N	-0.6303078	2.3088216	-1.9608180
N	2.1099321	-0.1983395	0.0000000
O	1.5473931	-0.1476689	1.0940287
O	1.5473931	-0.1476689	-1.0940287
C	3.6019448	-0.3723385	0.0000000
H	3.9962162	0.0823369	0.9119580
H	3.7835039	-1.4536402	0.0000000
H	3.9962162	0.0823369	-0.9119580

13.

C	1.1643564	-0.0044423	-0.7908497
C	1.1643564	-0.0044423	0.7908497
C	2.4633312	-0.0051847	0.0000000
H	3.0341252	0.9214006	0.0000000
H	3.0329852	-0.9324414	0.0000000
C	0.7497260	1.2137820	-1.4414956
C	0.7485116	-1.2217632	-1.4424471
C	0.7497260	1.2137820	1.4414956
C	0.7485116	-1.2217632	1.4424471
N	0.4569271	2.2019576	-1.9783140

N	0.4550925	-2.2087950	-1.9809227
N	0.4550925	-2.2087950	1.9809227
N	0.4569271	2.2019576	1.9783140
O	-1.5622306	-0.0103656	0.0000000
P	-3.0568991	0.0104662	0.0000000
H	-3.6951198	-0.6205175	-1.1058556
H	-3.6951198	-0.6205175	1.1058556
H	-3.6702998	1.2956815	0.0000000

13. MP2

C	1.1530684	-0.0043719	-0.7749327
C	1.1530684	-0.0043719	0.7749327
C	2.4519308	-0.0053117	0.0000000
H	3.0155178	0.9189048	0.0000000
H	3.0140807	-0.9303819	0.0000000
C	0.7379879	1.2149775	-1.4134161
C	0.7362878	-1.2227293	-1.4141958
C	0.7379879	1.2149775	1.4134161
C	0.7362878	-1.2227293	1.4141958
N	0.4420066	2.2204796	-1.9371991
N	0.4395765	-2.2271947	-1.9395770
N	0.4395765	-2.2271947	1.9395770
N	0.4420066	2.2204796	1.9371991
O	-1.5371347	-0.0082378	0.0000000
P	-3.0257384	0.0104251	0.0000000
H	-3.6529590	-0.6123955	-1.0903688
H	-3.6529590	-0.6123955	1.0903688
H	-3.6305926	1.2770699	0.0000000

14.

C	2.4307129	0.0014534	-0.7888270
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C	2.4307129	0.0014534	0.7888270
C	3.7314027	0.0080587	0.0000000
H	4.2968759	0.9378890	0.0000000
H	4.3066279	-0.9157549	0.0000000
C	2.0048288	1.2170111	-1.4378215
C	2.0165964	-1.2174730	-1.4390952
C	2.0048288	1.2170111	1.4378215
C	2.0165964	-1.2174730	1.4390952
N	1.7103351	2.2045391	-1.9749677
N	1.7316433	-2.2062404	-1.9790215
N	1.7316433	-2.2062404	1.9790215
N	1.7103351	2.2045391	1.9749677
O	-0.2139503	-0.0157783	0.0000000
P	-1.7170440	-0.0035292	0.0000000
C	-2.4236911	-0.8479963	-1.4463101
H	-3.5219171	-0.8440332	-1.4189832
H	-2.0780660	-0.3380631	-2.3553783
H	-2.0563491	-1.8822715	-1.4637115
C	-2.4236911	-0.8479963	1.4463101
H	-2.0780660	-0.3380631	2.3553783
H	-3.5219171	-0.8440332	1.4189832
H	-2.0563491	-1.8822715	1.4637115
C	-2.4140337	1.6895278	0.0000000
H	-1.5671750	2.3878589	0.0000000
H	-3.0254449	1.8689380	-0.8933799
H	-3.0254449	1.8689380	0.8933799

14. MP2

C	2.4188116	0.0011525	-0.7736122
C	2.4188116	0.0011525	0.7736122

C	3.7190685	0.0061904	0.0000000
H	4.2787239	0.9329618	0.0000000
H	4.2858959	-0.9161615	0.0000000
C	1.9933186	1.2185586	-1.4092466
C	2.0027903	-1.2181042	-1.4119895
C	1.9933186	1.2185586	1.4092466
C	2.0027903	-1.2181042	1.4119895
N	1.6940210	2.2240566	-1.9313934
N	1.7118329	-2.2230232	-1.9398636
N	1.7118329	-2.2230232	1.9398636
N	1.6940210	2.2240566	1.9313934
O	-0.2041312	-0.0126096	0.0000000
P	-1.7008308	-0.0042029	0.0000000
C	-2.4058854	-0.8396102	-1.4329768
H	-3.4968903	-0.8313992	-1.4038557
H	-2.0652970	-0.3336778	-2.3379291
H	-2.0472691	-1.8697742	-1.4563038
C	-2.4058854	-0.8396102	1.4329768
H	-2.0652970	-0.3336778	2.3379291
H	-3.4968903	-0.8313992	1.4038557
H	-2.0472691	-1.8697742	1.4563038
C	-2.4014021	1.6704966	0.0000000
H	-1.5671440	2.3734452	0.0000000
H	-3.0105226	1.8467610	-0.8869920
H	-3.0105226	1.8467610	0.8869920

15.

C	0.0000000	0.7923561	0.9554596
C	0.0000000	-0.7923561	0.9554596

C	0.0000000	0.0000000	2.2529393
H	-0.9271135	0.0000000	2.8228783
H	0.9271135	-0.0000000	2.8228783
C	-1.2180082	1.4454537	0.5429632
C	1.2180082	1.4454537	0.5429632
C	-1.2180082	-1.4454537	0.5429632
C	1.2180082	-1.4454537	0.5429632
N	-2.2034936	1.9895242	0.2541939
N	2.2034936	1.9895242	0.2541939
N	2.2034936	-1.9895242	0.2541939
N	-2.2034936	-1.9895242	0.2541939
S	0.0000000	0.0000000	-3.2522383
H	0.0000000	-1.1128071	-4.0079377
H	0.0000000	1.1128071	-4.0079377
O	0.0000000	0.0000000	-1.7301298

15. MP2

C	-0.000000	0.775621	0.940016
C	-0.000000	-0.775621	0.940016
C	-0.000000	0.000000	2.238052
C	-1.218899	1.418171	0.529103
C	1.218899	1.418171	0.529103
C	-1.218899	-1.418171	0.529103
C	1.218899	-1.418171	0.529103
N	-2.221869	1.951977	0.242219
N	2.221869	1.951977	0.242219
N	2.221869	-1.951977	0.242219
N	-2.221869	-1.951977	0.242219
H	-0.924949	0.000000	2.800282
H	0.924949	0.000000	2.800282
S	-0.000000	0.000000	-3.208951

O 0.000000 0.000000 -1.697354
H -0.000000 -1.101932 -3.948815
H -0.000000 1.101932 -3.948815

16.

C 0.0000000 0.7895657 2.0807654
C 0.0000000 -0.7895657 2.0807654
C 0.0000000 0.0000000 3.3807234
H -0.9269954 -0.0000000 3.9508145
H 0.9269954 0.0000000 3.9508145
C -1.2174224 1.4450871 1.6691291
C 1.2174224 1.4450871 1.6691291
C -1.2174224 -1.4450871 1.6691291
C 1.2174224 -1.4450871 1.6691291
N -2.2016346 1.9992148 1.3952065
N 2.2016346 1.9992148 1.3952065
N 2.2016346 -1.9992148 1.3952065
N -2.2016346 -1.9992148 1.3952065
S 0.0000000 0.0000000 -2.0714022
O 0.0000000 0.0000000 -0.5417087
C 0.0000000 1.5445326 -2.9898469
H 0.9043601 2.1198705 -2.7520594
H 0.0000000 1.2611675 -4.0500916
H -0.9043601 2.1198705 -2.7520594
C 0.0000000 -1.5445326 -2.9898469
H 0.9043601 -2.1198705 -2.7520594
H -0.9043601 -2.1198705 -2.7520594
H 0.0000000 -1.2611675 -4.0500916

16. MP2

C 0.0000000 0.7739662 2.0499456
C 0.0000000 -0.7739662 2.0499456

C	0.0000000	0.0000000	3.3495894
H	-0.9250387	0.0000000	3.9116361
H	0.9250387	0.0000000	3.9116361
C	-1.2180527	1.4174815	1.6373676
C	1.2180527	1.4174815	1.6373676
C	-1.2180527	-1.4174815	1.6373676
C	1.2180527	-1.4174815	1.6373676
N	-2.2191731	1.9583119	1.3573535
N	2.2191731	1.9583119	1.3573535
N	2.2191731	-1.9583119	1.3573535
N	-2.2191731	-1.9583119	1.3573535
S	0.0000000	0.0000000	-2.0415106
O	0.0000000	0.0000000	-0.5198987
C	0.0000000	1.5329885	-2.9417768
H	0.8969269	2.1036115	-2.7029748
H	0.0000000	1.2598998	-3.9973877
H	-0.8969269	2.1036115	-2.7029748
C	0.0000000	-1.5329885	-2.9417768
H	0.8969269	-2.1036115	-2.7029748
H	-0.8969269	-2.1036115	-2.7029748
H	0.0000000	-1.2598998	-3.9973877

17.

C	0.000000	0.797546	0.491991
C	0.000000	-0.797546	0.491991
C	0.000000	0.000000	1.785211
C	-1.218661	1.441991	0.071313
C	1.218661	1.441991	0.071313
C	-1.218661	-1.441991	0.071313
C	1.218661	-1.441991	0.071313
N	-2.207602	1.959475	-0.253096

N	2.207602	1.959475	-0.253096
N	2.207602	-1.959475	-0.253096
N	-2.207602	-1.959475	-0.253096
H	-0.926808	0.000000	2.355849
H	0.926808	0.000000	2.355849
C	0.000000	0.000000	-2.809684
O	0.000000	0.000000	-3.944077

17. MP2

C	0.0000000	0.7797878	0.4758070
C	0.0000000	-0.7797878	0.4758070
C	0.0000000	0.0000000	1.7701910
H	-0.9249953	0.0000000	2.3326426
H	0.9249953	0.0000000	2.3326426
C	-1.2195960	1.4160474	0.0584763
C	1.2195960	1.4160474	0.0584763
C	-1.2195960	-1.4160474	0.0584763
C	1.2195960	-1.4160474	0.0584763
N	-2.2243873	1.9281091	-0.2616741
N	2.2243873	1.9281091	-0.2616741
N	2.2243873	-1.9281091	-0.2616741
N	-2.2243873	-1.9281091	-0.2616741
C	0.0000000	0.0000000	-2.7193321
O	0.0000000	0.0000000	-3.8549669

17^c.

C	0.000000	0.798223	0.458442
C	0.000000	-0.798223	0.458442
C	0.000000	0.000000	1.751142
C	-1.218964	1.443422	0.039641
C	1.218964	1.443422	0.039641

C -1.218964 -1.443422 0.039641
 C 1.218964 -1.443422 0.039641
 N -2.207832 1.961024 -0.284570
 N 2.207832 1.961024 -0.284570
 N 2.207832 -1.961024 -0.284570
 N -2.207832 -1.961024 -0.284570
 H -0.926998 0.000000 2.321484
 H 0.926998 0.000000 2.321484
 O 0.000000 0.000000 -2.596898
 C 0.000000 0.000000 -3.734381

18.

C 0.00000000 0.79802900 0.47136800
 C 0.00000000 -0.79802900 0.47136800
 C 0.00000000 0.00000000 1.76417800
 C -1.21888000 1.44289300 0.05193500
 C 1.21888000 1.44289300 0.05193500
 C -1.21888000 -1.44289300 0.05193500
 C 1.21888000 -1.44289300 0.05193500
 N -2.20781500 1.96044100 -0.27227600
 N 2.20781500 1.96044100 -0.27227600
 N 2.20781500 -1.96044100 -0.27227600
 N -2.20781500 -1.96044100 -0.27227600
 H -0.92687900 0.00000000 2.33470300
 H 0.92687900 0.00000000 2.33470300
 N 0.00000000 0.00000000 -2.69656000
 N 0.00000000 0.00000000 -3.79839700

18. MP2

C 0.00000000 0.7803023 0.4595262
 C 0.00000000 -0.7803023 0.4595262

C	0.0000000	0.0000000	1.7533501
H	-0.9250216	0.0000000	2.3157777
H	0.9250216	0.0000000	2.3157777
C	-1.2195363	1.4156582	0.0404935
C	1.2195363	1.4156582	0.0404935
C	-1.2195363	-1.4156582	0.0404935
C	1.2195363	-1.4156582	0.0404935
N	-2.2237489	1.9256418	-0.2847678
N	2.2237489	1.9256418	-0.2847678
N	2.2237489	-1.9256418	-0.2847678
N	-2.2237489	-1.9256418	-0.2847678
N	0.0000000	0.0000000	-2.6067766
N	0.0000000	0.0000000	-3.7200838

18^c

C	0.0000000	0.799932	0.424389
C	0.0000000	-0.799932	0.424389
C	0.0000000	0.0000000	1.716107
C	-1.220903	1.445316	0.011523
C	1.220903	1.445316	0.011523
C	-1.220903	-1.445316	0.011523
C	1.220903	-1.445316	0.011523
N	-2.214954	1.959564	-0.302150
N	2.214954	1.959564	-0.302150
N	2.214954	-1.959564	-0.302150
N	-2.214954	-1.959564	-0.302150
H	-0.927047	0.0000000	2.286384
H	0.927047	0.0000000	2.286384
N	0.0000000	0.551339	-2.987573
N	0.0000000	-0.551339	-2.987573

19.

C	-0.7579386	0.0041086	0.7900506
C	-0.7579386	0.0041086	-0.7900506
C	-2.0574818	-0.0031591	0.0000000
H	-2.6330320	0.9205579	0.0000000
H	-2.6229711	-0.9330666	0.0000000
C	-0.3327758	1.2216699	1.4340452
C	-0.3184720	-1.2100695	1.4309788
C	-0.3327758	1.2216699	-1.4340452
C	-0.3184720	-1.2100695	-1.4309788
N	-0.0115157	2.2063513	1.9612569
N	0.0124435	-2.1946445	1.9524381
N	0.0124435	-2.1946445	-1.9524381
N	-0.0115157	2.2063513	-1.9612569
N	2.2450635	-0.0044994	0.0000000
H	2.6055834	-0.9609053	0.0000000
H	2.6396776	0.4631203	0.8188062
H	2.6396776	0.4631203	-0.8188062

19 MP2

C	-0.7527006	0.0032788	0.7752076
C	-0.7527006	0.0032788	-0.7752076
C	-2.0507904	-0.0038084	0.0000000
H	-2.6185969	0.9178578	0.0000000
H	-2.6088094	-0.9314277	0.0000000
C	-0.3325153	1.2221080	1.4103194
C	-0.3185923	-1.2120908	1.4077272
C	-0.3325153	1.2221080	-1.4103194
C	-0.3185923	-1.2120908	-1.4077272
N	-0.0142278	2.2232851	1.9298716
N	0.0116743	-2.2125204	1.9212732

N	0.0116743	-2.2125204	-1.9212732
N	-0.0142278	2.2232851	-1.9298716
N	2.2327337	-0.0005101	0.0000000
H	2.5908252	-0.9512677	0.0000000
H	2.6336806	0.4605173	0.8116181
H	2.6336806	0.4605173	-0.8116181

20.

C	-1.8180917	0.0697739	0.7898643
C	-1.8180917	0.0697739	-0.7898643
C	-3.1099122	-0.0815701	0.0000000
H	-3.7856879	0.7718679	0.0000000
H	-3.5658498	-1.0700507	0.0000000
C	-1.5496034	1.3306869	1.4343217
C	-1.2665178	-1.0897460	1.4446357
C	-1.5496034	1.3306869	-1.4343217
C	-1.2665178	-1.0897460	-1.4446357
N	-1.3563093	2.3541318	1.9498644
N	-0.8760408	-2.0355694	1.9959122
N	-0.8760408	-2.0355694	-1.9959122
N	-1.3563093	2.3541318	-1.9498644
N	1.3545559	-0.0972844	0.0000000
C	1.7737428	0.6232257	1.2035654
H	1.3481161	1.6353455	1.2038016
H	1.4142244	0.0941920	2.0974958
H	2.8796385	0.7115414	1.2785090
C	1.7737428	0.6232257	-1.2035654
H	1.4142244	0.0941920	-2.0974958
H	1.3481161	1.6353455	-1.2038016
H	2.8796385	0.7115414	-1.2785090
C	1.8989038	-1.4563434	0.0000000

H	1.5495712	-1.9972846	0.8892199
H	1.5495712	-1.9972846	-0.8892199
H	3.0105305	-1.4592138	0.0000000

20. MP2

C	-1.8087086	0.0651459	0.7752166
C	-1.8087086	0.0651459	-0.7752166
C	-3.0996904	-0.0812362	0.0000000
H	-3.7648866	0.7729985	0.0000000
H	-3.5515839	-1.0650663	0.0000000
C	-1.5366178	1.3265058	1.4081680
C	-1.2624348	-1.0975724	1.4190773
C	-1.5366178	1.3265058	-1.4081680
C	-1.2624348	-1.0975724	-1.4190773
N	-1.3461165	2.3672144	1.9133958
N	-0.8695609	-2.0613127	1.9590486
N	-0.8695609	-2.0613127	-1.9590486
N	-1.3461165	2.3672144	-1.9133958
N	1.3073089	-0.0923771	0.0000000
C	1.7618039	0.6186888	1.1891555
H	1.3575082	1.6318873	1.1976031
H	1.4216138	0.0963583	2.0856781
H	2.8618753	0.6840376	1.2278633
C	1.7618039	0.6186888	-1.1891555
H	1.4216138	0.0963583	-2.0856781
H	1.3575082	1.6318873	-1.1976031
H	2.8618753	0.6840376	-1.2278633
C	1.8777535	-1.4353982	0.0000000
H	1.5463527	-1.9795647	0.8849412
H	1.5463527	-1.9795647	-0.8849412
H	2.9796679	-1.4016972	0.0000000

21.

C	-1.5748328	-0.0482091	0.7920540
C	-1.5748328	-0.0482091	-0.7920540
C	-2.8692187	-0.1482788	0.0000000
H	-3.5090194	0.7321673	0.0000000
H	-3.3664055	-1.1164106	0.0000000
C	-1.2581469	1.1995597	1.4411273
C	-1.0705208	-1.2312232	1.4438263
C	-1.2581469	1.1995597	-1.4411273
C	-1.0705208	-1.2312232	-1.4438263
N	-1.0404397	2.2105962	1.9709452
N	-0.7014731	-2.1950748	1.9779428
N	-0.7014731	-2.1950748	-1.9779428
N	-1.0404397	2.2105962	-1.9709452
C	2.5422250	0.1125923	0.0000000
N	1.3821494	0.1184338	0.0000000
C	3.9953004	0.1083528	0.0000000
H	4.3705888	-0.4086637	0.8934720
H	4.3705888	-0.4086637	-0.8934720
H	4.3746177	1.1391730	0.0000000

22.

C	0.8844573	-2.0588456	0.0000000
C	-0.6916508	-2.1407253	0.0000000
C	0.1636991	-3.3983603	0.0000000
H	0.1930138	-3.9675717	0.9271657
H	0.1930138	-3.9675717	-0.9271657
C	1.5110386	-1.6019588	1.2154248
C	1.5110386	-1.6019588	-1.2154248
C	-1.3627977	-1.7511346	1.2149645

C	-1.3627977	-1.7511346	-1.2149645
N	2.0346678	-1.2574884	2.1940665
N	2.0346678	-1.2574884	-2.1940665
N	-1.9206325	-1.4617187	-2.1925258
N	-1.9206325	-1.4617187	2.1925258
C	-1.2159124	1.5481007	0.0000000
C	1.0755890	1.6614032	0.0000000
C	1.0594350	3.0573509	0.0000000
C	-0.1741384	3.7096635	0.0000000
C	-1.3373973	2.9388533	0.0000000
H	-2.1081689	0.9168915	0.0000000
H	2.0257947	1.1210000	0.0000000
H	1.9957297	3.6156596	0.0000000
H	-0.2280594	4.7991313	0.0000000
H	-2.3242305	3.4021439	0.0000000
N	-0.0357271	0.9074778	0.0000000

22^c (Equal to complex **54**)

C	1.6391156	0.0422926	-0.7964046
C	1.6391156	0.0422926	0.7964046
C	2.9338919	0.0122109	0.0000000
H	3.5263362	0.9251629	0.0000000
H	3.4804459	-0.9289870	0.0000000
C	1.2674697	1.2757848	-1.4442275
C	1.2164145	-1.1651710	-1.4608405
C	1.2674697	1.2757848	1.4442275
C	1.2164145	-1.1651710	1.4608405
N	1.0024769	2.2805697	-1.9648245
N	0.9186767	-2.1449960	-2.0101548
N	0.9186767	-2.1449960	2.0101548
N	1.0024769	2.2805697	1.9648245

C	-2.1719050	-0.9518550	-1.1450604
C	-1.9201601	0.4230809	-1.2000234
C	-1.7899382	1.1254620	0.0000000
C	-1.9201601	0.4230809	1.2000234
C	-2.1719050	-0.9518550	1.1450604
H	-2.2666139	-1.5331815	-2.0659780
H	-1.8224658	0.9292629	-2.1608525
H	-1.5802220	2.1955080	0.0000000
H	-1.8224658	0.9292629	2.1608525
H	-2.2666139	-1.5331815	2.0659780
N	-2.2965310	-1.6409317	0.0000000

23.

C	0.0000000	0.7985878	0.7223890
C	0.0000000	-0.7985878	0.7223890
C	0.0000000	0.0000000	2.0153046
H	-0.9270015	0.0000000	2.5856085
H	0.9270015	0.0000000	2.5856085
C	-1.2213264	1.4428545	0.3086094
C	1.2213264	1.4428545	0.3086094
C	-1.2213264	-1.4428545	0.3086094
C	1.2213264	-1.4428545	0.3086094
N	-2.2193248	1.9550172	0.0042475
N	2.2193248	1.9550172	0.0042475
N	2.2193248	-1.9550172	0.0042475
N	-2.2193248	-1.9550172	0.0042475
S	0.0000000	0.0000000	-2.6773854
H	0.9833431	0.0000000	-3.6026709
H	-0.9833431	0.0000000	-3.6026709

23. MP2

C	0.0000000	0.7812039	0.7042744
C	0.0000000	-0.7812039	0.7042744
C	0.0000000	0.0000000	1.9980486
H	-0.9251935	0.0000000	2.5602070
H	0.9251935	0.0000000	2.5602070
C	-1.2221538	1.4160301	0.2921070
C	1.2221538	1.4160301	0.2921070
C	-1.2221538	-1.4160301	0.2921070
C	1.2221538	-1.4160301	0.2921070
N	-2.2364337	1.9191581	-0.0118993
N	2.2364337	1.9191581	-0.0118993
N	2.2364337	-1.9191581	-0.0118993
N	-2.2364337	-1.9191581	-0.0118993
S	0.0000000	0.0000000	-2.6085577
H	0.9772121	0.0000000	-3.5196424
H	-0.9772121	0.0000000	-3.5196424

24.

C	0.0000000	0.7970543	1.7895930
C	0.0000000	-0.7970543	1.7895930
C	0.0000000	0.0000000	3.0841308
H	-0.9268981	0.0000000	3.6545438
H	0.9268981	0.0000000	3.6545438
C	-1.2217847	1.4383956	1.3721135
C	1.2217847	1.4383956	1.3721135
C	-1.2217847	-1.4383956	1.3721135
C	1.2217847	-1.4383956	1.3721135
N	-2.2247590	1.9454816	1.0753708
N	2.2247590	1.9454816	1.0753708
N	2.2247590	-1.9454816	1.0753708
N	-2.2247590	-1.9454816	1.0753708

S	0.0000000	0.0000000	-1.4764032
C	1.4017835	0.0000000	-2.6247083
H	1.3936707	0.9003297	-3.2539324
H	2.3106914	0.0000000	-2.0103960
H	1.3936707	-0.9003297	-3.2539324
C	-1.4017835	0.0000000	-2.6247083
H	-1.3936707	-0.9003297	-3.2539324
H	-2.3106914	0.0000000	-2.0103960
H	-1.3936707	0.9003297	-3.2539324

24. MP2

C	0.0000000	0.7801163	1.7581186
C	0.0000000	-0.7801163	1.7581186
C	0.0000000	0.0000000	3.0531041
H	-0.9250686	0.0000000	3.6155176
H	0.9250686	0.0000000	3.6155176
C	-1.2224222	1.4105790	1.3403850
C	1.2224222	1.4105790	1.3403850
C	-1.2224222	-1.4105790	1.3403850
C	1.2224222	-1.4105790	1.3403850
N	-2.2414705	1.9061756	1.0394251
N	2.2414705	1.9061756	1.0394251
N	2.2414705	-1.9061756	1.0394251
N	-2.2414705	-1.9061756	1.0394251
S	0.0000000	0.0000000	-1.4228105
C	1.3816918	0.0000000	-2.5740879
H	1.3643790	0.8935587	-3.1985726
H	2.2937572	0.0000000	-1.9771703
H	1.3643790	-0.8935587	-3.1985726
C	-1.3816918	0.0000000	-2.5740879
H	-1.3643790	-0.8935587	-3.1985726

H	-2.2937572	0.0000000	-1.9771703
H	-1.3643790	0.8935587	-3.1985726

25.

C	-0.9494180	-0.0085170	0.7956024
C	-0.9494180	-0.0085170	-0.7956024
C	-2.2445228	-0.0197405	0.0000000
H	-2.8228945	0.9022047	0.0000000
H	-2.8068177	-0.9515964	0.0000000
C	-0.5400867	1.2137529	1.4413964
C	-0.5192450	-1.2231308	1.4422451
C	-0.5400867	1.2137529	-1.4413964
C	-0.5192450	-1.2231308	-1.4422451
N	-0.2352140	2.2058046	1.9648144
N	-0.1984568	-2.2093336	1.9672431
N	-0.1984568	-2.2093336	-1.9672431
N	-0.2352140	2.2058046	-1.9648144
P	2.6176869	0.0091616	0.0000000
H	3.4173288	-1.1718288	0.0000000
H	3.3620302	0.6373235	1.0427541
H	3.3620302	0.6373235	-1.0427541

25. MP2

C	-0.9246627	-0.0021930	0.7789810
C	-0.9246627	-0.0021930	-0.7789810
C	-2.2198403	-0.0268501	0.0000000
H	-2.7999228	0.8871975	0.0000000
H	-2.7644653	-0.9624615	0.0000000
C	-0.5296740	1.2251184	1.4147556
C	-0.4836193	-1.2131388	1.4158283
C	-0.5296740	1.2251184	-1.4147556

C	-0.4836193	-1.2131388	-1.4158283
N	-0.2348985	2.2367161	1.9286985
N	-0.1509936	-2.2118547	1.9319117
N	-0.1509936	-2.2118547	-1.9319117
N	-0.2348985	2.2367161	-1.9286985
P	2.5534789	0.0093070	0.0000000
H	3.2878144	-1.1936372	0.0000000
H	3.2953157	0.6085741	1.0382654
H	3.2953157	0.6085741	-1.0382654

26.

C	-2.1317859	-0.0047288	0.7905059
C	-2.1317859	-0.0047288	-0.7905059
C	-3.4296669	-0.0767269	0.0000000
H	-4.0504139	0.8173635	0.0000000
H	-3.9483215	-1.0337431	0.0000000
C	-1.7644590	1.2330582	1.4332633
C	-1.6294377	-1.1954116	1.4315278
C	-1.7644590	1.2330582	-1.4332633
C	-1.6294377	-1.1954116	-1.4315278
N	-1.5011980	2.2356634	1.9592389
N	-1.2597242	-2.1646736	1.9565762
N	-1.2597242	-2.1646736	-1.9565762
N	-1.5011980	2.2356634	-1.9592389
P	1.2714590	0.0460142	0.0000000
C	2.1481896	0.8315704	-1.4243071
H	1.8352266	0.3415399	-2.3566206
H	1.8626601	1.8902233	-1.4884906
H	3.2421170	0.7552985	-1.3289101
C	2.1481896	0.8315704	1.4243071
H	1.8626601	1.8902233	1.4884906

H	1.8352266	0.3415399	2.3566206
H	3.2421170	0.7552985	1.3289101
C	2.0346930	-1.6349428	0.0000000
H	1.6922258	-2.1850115	0.8872876
H	1.6922258	-2.1850115	-0.8872876
H	3.1346212	-1.5930216	0.0000000

26. MP2

C	-2.097692	-0.005761	0.776109
C	-2.097692	-0.005761	-0.776109
C	-3.393877	-0.076388	0.000000
C	-1.730794	1.232779	1.406893
C	-1.599317	-1.197225	1.407692
C	-1.730794	1.232779	-1.406893
C	-1.599317	-1.197225	-1.407692
N	-1.462373	2.252277	1.920274
N	-1.224626	-2.180939	1.924673
N	-1.224626	-2.180939	-1.924673
N	-1.462373	2.252277	-1.920274
H	-4.006360	0.816348	0.000000
H	-3.905447	-1.030591	0.000000
P	1.228663	0.045757	0.000000
C	2.108361	0.823724	-1.410935
C	2.108361	0.823724	1.410935
C	1.999860	-1.618678	0.000000
H	1.800060	0.342726	-2.341683
H	1.836354	1.879149	-1.474700
H	3.193704	0.737429	-1.310361
H	1.836354	1.879149	1.474700
H	1.800060	0.342726	2.341683
H	3.193704	0.737429	1.310361

H 1.669039 -2.171687 0.881640
H 1.669039 -2.171687 -0.881640
H 3.091729 -1.561395 0.000000

27.

C 0.0000000 0.7969471 1.1918539
C 0.0000000 -0.7969471 1.1918539
C 0.0000000 0.0000000 2.4867525
H -0.9272937 0.0000000 3.0564779
H 0.9272937 0.0000000 3.0564779
C -1.2232172 1.4498095 0.7963235
C 1.2232172 1.4498095 0.7963235
C -1.2232172 -1.4498095 0.7963235
C 1.2232172 -1.4498095 0.7963235
N -2.2219198 1.9763096 0.5204666
N 2.2219198 1.9763096 0.5204666
N 2.2219198 -1.9763096 0.5204666
N -2.2219198 -1.9763096 0.5204666
C 0.0000000 0.0000000 -3.3999725
Cl 0.0000000 -1.4920159 -2.4151718
Cl 0.0000000 1.4920159 -2.4151718
H -0.9072314 0.0000000 -4.0101302
H 0.9072314 0.0000000 -4.0101302

28.

C 0.0000000 0.7973665 1.2578953
C 0.0000000 -0.7973665 1.2578953
C 0.0000000 0.0000000 2.5520558
H -0.9272615 0.0000000 3.1218600
H 0.9272615 0.0000000 3.1218600
C -1.2214711 1.4495059 0.8563743

C	1.2214711	1.4495059	0.8563743
C	-1.2214711	-1.4495059	0.8563743
C	1.2214711	-1.4495059	0.8563743
N	-2.2151803	1.9775107	0.5654033
N	2.2151803	1.9775107	0.5654033
N	2.2151803	-1.9775107	0.5654033
N	-2.2151803	-1.9775107	0.5654033
C	0.0000000	0.0000000	-3.4052004
Cl	0.0000000	-1.4620733	-2.3672900
Cl	0.0000000	1.4620733	-2.3672900
Cl	-1.4608222	0.0000000	-4.4294483
Cl	1.4608222	0.0000000	-4.4294483

28°.

C	-1.4013376	-0.0193323	0.8007648
C	-1.4013376	-0.0193323	-0.8007648
C	-2.6921245	-0.0365224	0.0000000
H	-3.2736300	0.8836365	0.0000000
H	-3.2506185	-0.9706744	0.0000000
C	-1.0080554	1.2079036	1.4469869
C	-0.9730663	-1.2328462	1.4506826
C	-1.0080554	1.2079036	-1.4469869
C	-0.9730663	-1.2328462	-1.4506826
N	-0.7131964	2.2062466	1.9639766
N	-0.6488673	-2.2179148	1.9755445
N	-0.6488673	-2.2179148	-1.9755445
N	-0.7131964	2.2062466	-1.9639766
C	3.7534580	0.0471445	0.0000000
Cl	1.9503756	0.0602278	0.0000000
Cl	4.3458858	1.7292235	0.0000000
Cl	4.3278498	-0.8005747	1.4607473

Cl 4.3278498 -0.8005747 -1.4607473

29.

C 0.0000000 -0.7779227 -0.2857785

C 0.0000000 0.7779227 -0.2857785

C 0.0000000 0.0000000 -1.6047650

H -0.9279669 0.0000000 -2.1743697

H 0.9279669 0.0000000 -2.1743697

C -1.2164554 -1.4334411 0.1308891

C 1.2164554 -1.4334411 0.1308891

C -1.2164554 1.4334411 0.1308891

C 1.2164554 1.4334411 0.1308891

N -2.2114887 -2.0281721 0.2568199

N 2.2114887 -2.0281721 0.2568199

N 2.2114887 2.0281721 0.2568199

N -2.2114887 2.0281721 0.2568199

O 0.0000000 0.0000000 2.0006454

H 0.0000000 0.0000000 2.9735801

30.

C -0.5304307 0.8779475 0.0000000

C 0.9471954 0.3663159 0.0000000

C 0.6389343 1.8654371 0.0000000

H 0.8238112 2.4015359 0.9289242

H 0.8238112 2.4015359 -0.9289242

C -1.2820815 0.7579740 1.2274025

C -1.2820815 0.7579740 -1.2274025

C 1.4580634 -0.1937262 1.2294454

C 1.4580634 -0.1937262 -1.2294454

N -1.8260981 0.8516889 2.2519604

N -1.8260981 0.8516889 -2.2519604

N	1.9328525	-0.4453235	-2.2620362
N	1.9328525	-0.4453235	2.2620362
C	-0.8137433	-2.4515988	0.0000000
H	-1.1763125	-3.5240987	0.0000000
O	0.4415823	-2.3059085	0.0000000
O	-1.7203206	-1.5723928	0.0000000

31.

C	1.3497393	0.0124531	-0.7824772
C	1.3497393	0.0124531	0.7824772
C	2.6651636	-0.0115613	0.0000000
H	3.2485835	0.9069429	0.0000000
H	3.2160420	-0.9500163	0.0000000
C	1.0088126	1.2457956	-1.4518327
C	0.9647370	-1.2085583	-1.4503272
C	1.0088126	1.2457956	1.4518327
C	0.9647370	-1.2085583	1.4503272
N	0.9408036	2.2739043	-1.9934855
N	0.8551436	-2.2350876	-1.9880890
N	0.8551436	-2.2350876	1.9880890
N	0.9408036	2.2739043	1.9934855
C	-1.8873644	0.0465650	0.0000000
C	-3.4275610	-0.0407726	0.0000000
H	-3.8441989	0.4245343	-0.9034672
H	-3.7124554	-1.1044598	0.0000000
H	-3.8441989	0.4245343	0.9034672
O	-1.3262414	0.0636096	-1.1367887
O	-1.3262414	0.0636096	1.1367887

32.

C	0.8996806	-0.0051534	-0.7358245
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C	0.8994675	-0.0027601	0.8337863
C	2.2121180	-0.0141525	0.0487822
H	2.7863890	0.9099964	0.0477135
H	2.7726249	-0.9467363	0.0503184
C	0.5541020	1.2245906	-1.4089627
C	0.5352972	-1.2307882	-1.4064660
C	0.5567414	1.2299836	1.5024124
C	0.5371153	-1.2284748	1.5050882
N	0.4711183	2.2480960	-1.9563973
N	0.4359557	-2.2543922	-1.9509579
N	0.4406330	-2.2554091	2.0435907
N	0.4790057	2.2591274	2.0398115
C	-2.3182620	0.0161415	0.0704956
O	-1.7853413	0.0147423	-1.0782718
O	-1.7949845	0.0225640	1.2062022
O	-3.7337644	0.0087857	0.0703159
H	-3.9478964	0.0038389	-0.8816365

33.

C	-0.9014371	-0.0165607	0.7869890
C	-0.9014371	-0.0165607	-0.7869890
C	-2.2087602	-0.0477701	0.0000000
H	-2.7978638	0.8668882	0.0000000
H	-2.7536116	-0.9894877	0.0000000
C	-0.5925302	1.2224164	1.4610777
C	-0.5334681	-1.2395419	1.4605496
C	-0.5925302	1.2224164	-1.4610777
C	-0.5334681	-1.2395419	-1.4605496
N	-0.5121007	2.2442421	2.0095578
N	-0.4045928	-2.2571806	2.0075737
N	-0.4045928	-2.2571806	-2.0075737

N	-0.5121007	2.2442421	-2.0095578
Cl	2.7444621	0.0525396	0.0000000
O	1.8762034	0.0543560	-1.2045455
O	3.5738566	-1.1515613	0.0000000
O	3.5777676	1.2539289	0.0000000
O	1.8762034	0.0543560	1.2045455

34.

C	0.0000000	0.7866199	0.6865023
C	0.0000000	-0.7866199	0.6865023
C	0.0000000	0.0000000	1.9978128
H	-0.9282044	0.0000000	2.5654048
H	0.9282044	0.0000000	2.5654048
C	-1.2276985	1.4563466	0.3321409
C	1.2276985	1.4563466	0.3321409
C	-1.2276985	-1.4563466	0.3321409
C	1.2276985	-1.4563466	0.3321409
N	-2.2492301	2.0017948	0.2199446
N	2.2492301	2.0017948	0.2199446
N	2.2492301	-2.0017948	0.2199446
N	-2.2492301	-2.0017948	0.2199446
O	0.0000000	1.1021131	-2.0437146
O	0.0000000	-1.1021131	-2.0437146
O	0.0000000	0.0000000	-3.9349189
N	0.0000000	0.0000000	-2.6876209

35.

C	-1.2259187	0.0875545	0.7875066
C	-1.2259187	0.0875545	-0.7875066

C	-2.5191557	-0.1135380	0.0000000
H	-3.2204456	0.7186352	0.0000000
H	-2.9399020	-1.1172331	0.0000000
C	-1.0721861	1.3532161	1.4644473
C	-0.6845988	-1.0856352	1.4346196
C	-1.0721861	1.3532161	-1.4644473
C	-0.6845988	-1.0856352	-1.4346196
N	-1.1636201	2.3792734	2.0046866
N	-0.4460615	-2.1201976	1.9122369
N	-0.4460615	-2.1201976	-1.9122369
N	-1.1636201	2.3792734	-2.0046866
P	2.1706221	0.2221944	0.0000000
O	2.8156223	-1.3129012	0.0000000
H	2.0789063	-1.9486772	0.0000000
O	3.6060332	1.0220469	0.0000000
H	4.3210456	0.3648645	0.0000000
O	1.4360222	0.4680931	-1.2959587
O	1.4360222	0.4680931	1.2959587

36.

C	-0.9951674	0.1129201	0.7886045
C	-0.9951674	0.1129201	-0.7886045
C	-2.2879859	-0.0798201	0.0000000
H	-2.9839143	0.7568817	0.0000000
H	-2.7157120	-1.0804757	0.0000000
C	-0.8327993	1.3755123	1.4670376
C	-0.4572538	-1.0637315	1.4295338
C	-0.8327993	1.3755123	-1.4670376
C	-0.4572538	-1.0637315	-1.4295338
N	-0.8819541	2.3993312	2.0157342
N	-0.1936632	-2.0933514	1.9034077

N	-0.1936632	-2.0933514	-1.9034077
N	-0.8819541	2.3993312	-2.0157342
S	2.5139069	0.2729158	0.0000000
O	1.7098135	0.4714221	1.2290874
O	1.7098135	0.4714221	-1.2290874
O	3.8224705	0.9053136	0.0000000
O	2.9022561	-1.3492209	0.0000000
H	2.0510275	-1.8298000	0.0000000

37.

C	-0.7617251	-0.0435010	0.7977732
C	-0.7981254	-0.0465127	-0.7617253
C	-2.0979685	-0.1583648	0.0491588
H	-2.7429653	0.7189099	0.0627652
H	-2.5806103	-1.1344533	0.0619111
C	-0.5039676	1.2109128	1.4704376
C	-0.2913897	-1.2320696	1.4764692
C	-0.5724213	1.2052550	-1.4503695
C	-0.3603003	-1.2377809	-1.4572061
N	-0.6218478	2.2317732	2.0259032
N	-0.2548148	-2.2556859	2.0394150
N	-0.3515451	-2.2634872	-2.0174653
N	-0.7147469	2.2244635	-2.0030016
S	2.5688336	0.1560927	-0.0599499
O	3.4138259	-1.0627526	-0.0725855
O	3.3610463	1.4105169	-0.0807889
O	1.6280220	0.1337001	-1.2779641
O	1.6807002	0.1429839	1.1972230

38.

C	-0.5638322	0.1660503	0.7882588
C	-0.5942543	0.1642134	-0.7584824

C	-1.8463423	-0.1762575	0.0393636
H	-2.6681651	0.5408192	0.0552971
H	-2.1084221	-1.2348212	0.0443350
C	-0.5361935	1.4411767	1.4577775
C	0.1509567	-0.9294725	1.4936989
C	-0.5930498	1.4388134	-1.4297661
C	0.0985654	-0.9336785	-1.4864185
N	-0.6350648	2.4620431	2.0135991
N	-0.0092614	-1.9149791	2.1311425
N	-0.1014451	-1.9301057	-2.0975494
N	-0.7149443	2.4586855	-1.9829497
S	2.8359592	-0.0952648	-0.0742003
O	3.5232369	-1.4330510	-0.0884193
O	1.8485859	-0.0163039	-1.3185793
O	1.9136707	-0.0078671	1.2128925

39.

C	0.0000000	0.7596520	0.0914332
C	0.0000000	-0.7596520	0.0914332
C	0.0000000	0.0000000	1.4379170
H	-0.9292016	0.0000000	2.0067762
H	0.9292016	0.0000000	2.0067762
C	-1.2143718	1.4103298	-0.3609179
C	1.2143718	1.4103298	-0.3609179
C	-1.2143718	-1.4103298	-0.3609179
C	1.2143718	-1.4103298	-0.3609179
N	-2.2217959	1.9897808	-0.4683688
N	2.2217959	1.9897808	-0.4683688
N	2.2217959	-1.9897808	-0.4683688
N	-2.2217959	-1.9897808	-0.4683688
H	0.0000000	0.0000000	-2.3171892

40.

C	0.0000000	0.7839955	0.6129290
C	0.0000000	-0.7839955	0.6129290
C	0.0000000	0.0000000	1.9259292
H	-0.9278395	0.0000000	2.4946696
H	0.9278395	0.0000000	2.4946696
C	-1.2205117	1.4498429	0.2286934
C	1.2205117	1.4498429	0.2286934
C	-1.2205117	-1.4498429	0.2286934
C	1.2205117	-1.4498429	0.2286934
N	-2.2214570	2.0277140	0.0878762
N	2.2214570	2.0277140	0.0878762
N	2.2214570	-2.0277140	0.0878762
N	-2.2214570	-2.0277140	0.0878762
N	0.0000000	0.0000000	-1.9448131
N	0.0000000	0.0000000	-3.1428196
N	0.0000000	0.0000000	-4.3197723

41.

C	0.5289265	-0.6822727	0.0000000
C	0.7004451	0.8644281	0.0000000
C	1.9228128	-0.0596860	0.0000000
H	2.4883114	-0.1140831	-0.9283501
H	2.4883114	-0.1140831	0.9283501
C	0.0731450	-1.2969513	-1.2258434
C	0.0731450	-1.2969513	1.2258434
C	0.3924780	1.5725664	-1.2183615
C	0.3924780	1.5725664	1.2183615
N	-0.0714287	-1.8464096	-2.2423198
N	-0.0714287	-1.8464096	2.2423198

N	0.2636324	2.1687482	2.2082918
N	0.2636324	2.1687482	-2.2082918
C	-3.1441125	-0.3661247	0.0000000
N	-2.0030480	0.0245930	0.0000000
O	-4.2973003	-0.7486788	0.0000000

42.

C	0.0000000	-0.7754186	-0.3418221
C	0.0000000	0.7754186	-0.3418221
C	0.0000000	0.0000000	-1.6602105
H	-0.9283450	0.0000000	-2.2282699
H	0.9283450	0.0000000	-2.2282699
C	-1.2233118	-1.4425332	0.0378573
C	1.2233118	-1.4425332	0.0378573
C	-1.2233118	1.4425332	0.0378573
C	1.2233118	1.4425332	0.0378573
N	-2.2253450	-2.0121287	0.1894334
N	2.2253450	-2.0121287	0.1894334
N	2.2253450	2.0121287	0.1894334
N	-2.2253450	2.0121287	0.1894334
C	0.0000000	0.0000000	3.5369017
N	0.0000000	0.0000000	2.3543297

43.

C	0.4125195	-0.9047618	0.0000000
C	0.8807287	0.5845332	0.0000000
C	1.8996802	-0.5546506	0.0000000
H	2.4424451	-0.7239175	-0.9281420
H	2.4424451	-0.7239175	0.9281420
C	-0.1484759	-1.4267732	-1.2231298
C	-0.1484759	-1.4267732	1.2231298

C	0.7188255	1.3362138	-1.2209510
C	0.7188255	1.3362138	1.2209510
N	-0.4649858	-1.9221238	-2.2266463
N	-0.4649858	-1.9221238	2.2266463
N	0.7267782	1.9350721	2.2176027
N	0.7267782	1.9350721	-2.2176027
C	-3.1014967	0.7974407	0.0000000
N	-1.9309021	0.5759696	0.0000000
S	-4.7097036	1.1045261	0.0000000

44.

C	0.0000000	0.7704524	0.0809809
C	0.0000000	-0.7704524	0.0809809
C	0.0000000	0.0000000	1.4077132
H	-0.9287901	0.0000000	1.9764005
H	0.9287901	0.0000000	1.9764005
C	-1.2183231	1.4252147	-0.3323612
C	1.2183231	1.4252147	-0.3323612
C	-1.2183231	-1.4252147	-0.3323612
C	1.2183231	-1.4252147	-0.3323612
N	-2.2136142	2.0080609	-0.4908090
N	2.2136142	2.0080609	-0.4908090
N	2.2136142	-2.0080609	-0.4908090
N	-2.2136142	-2.0080609	-0.4908090
F	0.0000000	0.0000000	-2.2297950

45.

C	0.0000000	0.7740343	0.0872401
C	0.0000000	-0.7740343	0.0872401

C	0.0000000	0.0000000	1.4100001
H	-0.9288651	0.0000000	1.9776053
H	0.9288651	0.0000000	1.9776053
C	-1.2233080	1.4462238	-0.2901212
C	1.2233080	1.4462238	-0.2901212
C	-1.2233080	-1.4462238	-0.2901212
C	1.2233080	-1.4462238	-0.2901212
N	-2.2239483	2.0323011	-0.3897935
N	2.2239483	2.0323011	-0.3897935
N	2.2239483	-2.0323011	-0.3897935
N	-2.2239483	-2.0323011	-0.3897935
Cl	0.0000000	0.0000000	-2.8200322

46.

C	0.0000000	0.7758640	0.0956246
C	0.0000000	-0.7758640	0.0956246
C	0.0000000	0.0000000	1.4165996
H	-0.9289870	0.0000000	1.9838048
H	0.9289870	0.0000000	1.9838048
C	-1.2241719	1.4510930	-0.2745260
C	1.2241719	1.4510930	-0.2745260
C	-1.2241719	-1.4510930	-0.2745260
C	1.2241719	-1.4510930	-0.2745260
N	-2.2256026	2.0368980	-0.3671513
N	2.2256026	2.0368980	-0.3671513
N	2.2256026	-2.0368980	-0.3671513
N	-2.2256026	-2.0368980	-0.3671513
Br	0.0000000	0.0000000	-3.0087491

47.

C	0.0000000	0.7779161	0.1084021
C	0.0000000	-0.7779161	0.1084021

C	0.0000000	0.0000000	1.4276933
H	-0.9291104	0.0000000	1.9944825
H	0.9291104	0.0000000	1.9944825
C	-1.2255007	1.4551436	-0.2546545
C	1.2255007	1.4551436	-0.2546545
C	-1.2255007	-1.4551436	-0.2546545
C	1.2255007	-1.4551436	-0.2546545
N	-2.2300136	2.0370927	-0.3384479
N	2.2300136	2.0370927	-0.3384479
N	2.2300136	-2.0370927	-0.3384479
N	-2.2300136	-2.0370927	-0.3384479
I	0.0000000	0.0000000	-3.2610529

48.

C	-0.8829166	-0.0165582	0.7861267
C	-0.8829166	-0.0165582	-0.7861267
C	-2.1900836	-0.0471996	0.0000000
H	-2.7789997	0.8676220	0.0000000
H	-2.7353631	-0.9887189	0.0000000
C	-0.5733156	1.2220216	1.4609377
C	-0.5159980	-1.2393699	1.4609699
C	-0.5733156	1.2220216	-1.4609377
C	-0.5159980	-1.2393699	-1.4609699
N	-0.4822527	2.2418231	2.0106344
N	-0.3788749	-2.2540924	2.0105532
N	-0.3788749	-2.2540924	-2.0105532
N	-0.4822527	2.2418231	-2.0106344
B	2.7005192	0.0522836	0.0000000
F	1.8459794	0.0508898	-1.1595979
F	3.4908677	-1.1052015	0.0000000
F	3.4878163	1.2117866	0.0000000

F 1.8459794 0.0508898 1.1595979

49.

C -1.2291606 -0.0016914 0.7870113

C -1.2291606 -0.0016914 -0.7870113

C -2.5241393 -0.1750422 0.0000000

H -3.2125544 0.6676385 0.0000000

H -2.9601946 -1.1719991 0.0000000

C -1.0639306 1.2695130 1.4529022

C -0.7514152 -1.1653151 1.4958105

C -1.0639306 1.2695130 -1.4529022

C -0.7514152 -1.1653151 -1.4958105

N -1.0731485 2.2954312 1.9983396

N -0.5248823 -2.1266281 2.1074890

N -0.5248823 -2.1266281 -2.1074890

N -1.0731485 2.2954312 -1.9983396

P 2.5932631 0.0153235 0.0000000

F 3.3473827 1.4603115 0.0000000

F 3.5886006 -0.5379560 -1.1643230

F 1.5441092 0.5750487 1.1630733

F 3.5886006 -0.5379560 1.1643230

F 1.7758972 -1.4130367 0.0000000

F 1.5441092 0.5750487 -1.1630733

50.

C 0.0000000 -0.7959129 1.0677115

C 0.0000000 0.7959129 1.0677115

C 0.0000000 0.0000000 2.3628207

H -0.9270650 0.0000000 2.9330058

H 0.9270650 0.0000000 2.9330058

C -1.2195480 -1.4430474 0.6531327

C	1.2195480	-1.4430474	0.6531327
C	-1.2195480	1.4430474	0.6531327
C	1.2195480	1.4430474	0.6531327
N	-2.2110404	-1.9653288	0.3448293
N	2.2110404	-1.9653288	0.3448293
N	2.2110404	1.9653288	0.3448293
N	-2.2110404	1.9653288	0.3448293
C	0.0000000	0.6676550	-2.3904948
C	0.0000000	-0.6676550	-2.3904948
H	-0.9294849	1.2400508	-2.3937785
H	0.9294849	1.2400508	-2.3937785
H	-0.9294849	-1.2400508	-2.3937785
H	0.9294849	-1.2400508	-2.3937785

51.

C	0.0000000	-0.7948981	-0.7805970
C	0.0000000	0.0000000	-2.0762241
C	0.0000000	0.7948981	-0.7805970
H	-0.9270861	0.0000000	-2.6463234
H	0.9270861	0.0000000	-2.6463234
C	1.2173532	1.4477761	-0.3672812
C	-1.2173532	1.4477761	-0.3672812
C	1.2173532	-1.4477761	-0.3672812
C	-1.2173532	-1.4477761	-0.3672812
N	-2.2000621	1.9860441	-0.0582973
N	2.2000621	1.9860441	-0.0582973
N	2.2000621	-1.9860441	-0.0582973
N	-2.2000621	-1.9860441	-0.0582973
C	0.0000000	-0.6039646	2.6507086
H	0.0000000	-1.6748506	2.6654810
C	0.0000000	0.6039646	2.6507086

H 0.0000000 1.6748506 2.6654810

52.

C 0.0000000 0.7940793 1.2915522

C 0.0000000 -0.7940793 1.2915522

C 0.0000000 0.0000000 2.5886925

H 0.9274665 0.0000000 3.1581984

H -0.9274665 0.0000000 3.1581984

C 1.2211158 1.4579658 0.9054245

C -1.2211158 1.4579658 0.9054245

C 1.2211158 -1.4579658 0.9054245

C -1.2211158 -1.4579658 0.9054245

N 2.2111478 2.0132139 0.6552138

N -2.2111478 2.0132139 0.6552138

N -2.2111478 -2.0132139 0.6552138

N 2.2111478 -2.0132139 0.6552138

C -0.7923381 -0.6703309 -2.2100918

C 0.7923381 -0.6703309 -2.2100918

C 0.7923381 0.6703309 -2.2100918

C -0.7923381 0.6703309 -2.2100918

H 1.5617559 1.4390579 -2.2225949

H 1.5617559 -1.4390579 -2.2225949

H -1.5617559 1.4390579 -2.2225949

H -1.5617559 -1.4390579 -2.2225949

53.

C -0.0000000 -0.7954487 -1.6847827

C -0.0000000 0.7954487 -1.6847827

C	-0.0000000	0.0000000	-2.9815561
H	-0.9275818	0.0000000	-3.5508215
H	0.9275818	0.0000000	-3.5508215
C	-1.2242532	-1.4561765	-1.3046317
C	1.2242532	-1.4561765	-1.3046317
C	-1.2242532	1.4561765	-1.3046317
C	1.2242532	1.4561765	-1.3046317
N	-2.2251534	-1.9940131	-1.0608995
N	2.2251534	-1.9940131	-1.0608995
N	2.2251534	1.9940131	-1.0608995
N	-2.2251534	1.9940131	-1.0608995
C	1.3985657	0.0000000	1.9111534
C	0.6992608	-1.2108178	1.9188442
C	-0.6992608	-1.2108178	1.9188442
C	-1.3985657	0.0000000	1.9111534
C	-0.6992608	1.2108178	1.9188442
C	0.6992608	1.2108178	1.9188442
H	2.4886699	0.0000000	1.8886878
H	1.2465133	-2.1539926	1.9099575
H	-1.2465133	-2.1539926	1.9099575
H	-2.4886699	-0.0000000	1.8886878
H	-1.2465133	2.1539926	1.9099575
H	1.2465133	2.1539926	1.9099575

54.

C	1.6391156	0.0422926	-0.7964046
C	1.6391156	0.0422926	0.7964046
C	2.9338919	0.0122109	0.0000000
H	3.5263362	0.9251629	0.0000000
H	3.4804459	-0.9289870	0.0000000
C	1.2674697	1.2757848	-1.4442275

C	1.2164145	-1.1651710	-1.4608405
C	1.2674697	1.2757848	1.4442275
C	1.2164145	-1.1651710	1.4608405
N	1.0024769	2.2805697	-1.9648245
N	0.9186767	-2.1449960	-2.0101548
N	0.9186767	-2.1449960	2.0101548
N	1.0024769	2.2805697	1.9648245
C	-2.1719050	-0.9518550	-1.1450604
C	-1.9201601	0.4230809	-1.2000234
C	-1.7899382	1.1254620	0.0000000
C	-1.9201601	0.4230809	1.2000234
C	-2.1719050	-0.9518550	1.1450604
H	-2.2666139	-1.5331815	-2.0659780
H	-1.8224658	0.9292629	-2.1608525
H	-1.5802220	2.1955080	0.0000000
H	-1.8224658	0.9292629	2.1608525
H	-2.2666139	-1.5331815	2.0659780
N	-2.2965310	-1.6409317	0.0000000

55.

C	0.0000000	0.7969971	2.1691523
C	0.0000000	-0.7969971	2.1691523
C	0.0000000	0.0000000	3.4650255
H	0.9276523	0.0000000	4.0341565
H	-0.9276523	0.0000000	4.0341565
C	1.2265508	1.4519279	1.7891059
C	-1.2265508	1.4519279	1.7891059
C	1.2265508	-1.4519279	1.7891059
C	-1.2265508	-1.4519279	1.7891059
N	2.2339051	1.9739087	1.5386407
N	-2.2339051	1.9739087	1.5386407

N	-2.2339051	-1.9739087	1.5386407
N	2.2339051	-1.9739087	1.5386407
C	0.7079696	-2.4350370	-1.6278516
C	1.4045520	-1.2442589	-1.6283995
C	0.7194202	0.0000000	-1.6309713
C	-0.7194202	0.0000000	-1.6309713
C	-1.4045520	-1.2442589	-1.6283995
C	-0.7079696	-2.4350370	-1.6278516
H	2.4956977	1.2436516	-1.6096401
H	1.2491107	-3.3818279	-1.6142806
H	2.4956977	-1.2436516	-1.6096401
C	1.4045520	1.2442589	-1.6283995
C	-1.4045520	1.2442589	-1.6283995
H	-2.4956977	-1.2436516	-1.6096401
H	-1.2491107	-3.3818279	-1.6142806
C	-0.7079696	2.4350370	-1.6278516
C	0.7079696	2.4350370	-1.6278516
H	-2.4956977	1.2436516	-1.6096401
H	-1.2491107	3.3818279	-1.6142806
H	1.2491107	3.3818279	-1.6142806

56.

C	0.0000000	-0.7965863	-2.3912532
C	0.0000000	0.7965863	-2.3912532
C	0.0000000	0.0000000	-3.6876736
H	-0.9276717	0.0000000	-4.2566598
H	0.9276717	0.0000000	-4.2566598
C	-1.2281025	-1.4500439	-2.0138206
C	1.2281025	-1.4500439	-2.0138206
C	-1.2281025	1.4500439	-2.0138206
C	1.2281025	1.4500439	-2.0138206

N	-2.2383431	-1.9707489	-1.7724357
N	2.2383431	-1.9707489	-1.7724357
N	2.2383431	1.9707489	-1.7724357
N	-2.2383431	1.9707489	-1.7724357
C	1.4059522	0.0000000	1.3262997
C	0.7239783	-1.2254377	1.3402455
C	-0.7239783	-1.2254377	1.3402455
C	-1.4059522	0.0000000	1.3262997
C	-0.7239783	1.2254377	1.3402455
C	0.7239783	1.2254377	1.3402455
H	2.4983289	0.0000000	1.3074888
H	-2.4983289	0.0000000	1.3074888
C	1.4088521	2.4787833	1.3456228
C	0.7124320	3.6619802	1.3518157
H	2.4997275	2.4768042	1.3271172
H	1.2495505	4.6113767	1.3504357
C	-1.4088521	2.4787833	1.3456228
C	-0.7124320	3.6619802	1.3518157
H	-2.4997275	2.4768042	1.3271172
H	-1.2495505	4.6113767	1.3504357
C	1.4088521	-2.4787833	1.3456228
C	0.7124320	-3.6619802	1.3518157
H	2.4997275	-2.4768042	1.3271172
H	1.2495505	-4.6113767	1.3504357
C	-1.4088521	-2.4787833	1.3456228
C	-0.7124320	-3.6619802	1.3518157
H	-2.4997275	-2.4768042	1.3271172
H	-1.2495505	-4.6113767	1.3504357

57.

C	2.2777920	0.7710887	0.7961375
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C	2.2777920	0.7710887	-0.7961375
C	3.3717950	1.4673615	0.0000000
H	4.3503021	0.9905341	0.0000000
H	3.3535684	2.5555242	0.0000000
C	2.6226090	-0.4563004	1.4689238
C	1.3018722	1.6069987	1.4504891
C	2.6226090	-0.4563004	-1.4689238
C	1.3018722	1.6069987	-1.4504891
N	2.9610093	-1.4187406	2.0252661
N	0.5738765	2.3494756	1.9697529
N	0.5738765	2.3494756	-1.9697529
N	2.9610093	-1.4187406	-2.0252661
C	-0.7379215	-1.1648859	-1.4231330
C	-1.5261744	-0.1935484	-0.7276860
C	-1.5261744	-0.1935484	0.7276860
C	-0.7379215	-1.1648859	1.4231330
C	-0.0019162	-2.1465215	0.6816972
C	-0.0019162	-2.1465215	-0.6816972
C	-2.2541133	0.7417635	1.4983569
C	-2.1975212	0.7378800	2.8816842
H	-2.8584932	1.4998638	1.0026148
H	-2.7576443	1.4836204	3.4464899
C	-0.6896739	-1.1438616	2.8382882
C	-1.4055830	-0.2073024	3.5607686
H	-0.0687125	-1.8824179	3.3490523
H	-1.3552402	-0.1971259	4.6501389
C	-2.2541133	0.7417635	-1.4983569
C	-2.1975212	0.7378800	-2.8816842
H	-2.8584932	1.4998638	-1.0026148
H	-2.7576443	1.4836204	-3.4464899
C	-0.6896739	-1.1438616	-2.8382882

C	-1.4055830	-0.2073024	-3.5607686
H	-0.0687125	-1.8824179	-3.3490523
H	-1.3552402	-0.1971259	-4.6501389
H	0.5780021	-2.8866960	1.2347323
H	0.5780021	-2.8866960	-1.2347323

58.

C	0.5248955	-0.7943385	2.4799392
C	0.5454694	0.7979501	2.4812231
C	0.3859747	0.0026466	3.7687587
H	1.2423065	-0.0090390	4.4406178
H	-0.6009089	0.0150605	4.2276223
C	1.7725028	-1.4804482	2.2546951
C	-0.6611302	-1.4334704	1.9661514
C	1.8105352	1.4514621	2.2567116
C	-0.6230711	1.4697728	1.9689829
N	2.7828135	-2.0430976	2.1406283
N	-1.6537188	-1.9398418	1.6352708
N	-1.6004241	2.0062087	1.6400852
N	2.8354238	1.9872238	2.1432534
C	0.9208855	2.8366653	-1.0334039
C	0.9554183	1.4301832	-1.0671060
C	-0.2552680	0.7109551	-1.3232967
C	-1.4713038	1.4250331	-1.5601826
C	-1.4521309	2.8306458	-1.5264067
C	-0.2712317	3.5240459	-1.2614593
C	-0.2532571	-0.7134382	-1.3195355
C	-2.6715097	0.6771180	-1.7964493
C	-2.6693096	-0.6890792	-1.7940334
C	-1.4669337	-1.4322555	-1.5542983
H	1.8416431	3.3833370	-0.8222345

H	-0.2814230	4.6141152	-1.2260711
C	2.1628860	0.6863783	-0.8460154
C	2.1643490	-0.6795544	-0.8398917
C	0.9588483	-1.4277808	-1.0569543
H	3.0853885	1.2382310	-0.6601529
H	3.0879179	-1.2278674	-0.6489091
C	0.9277845	-2.8341147	-1.0138127
C	-0.2617415	-3.5261660	-1.2414967
C	-1.4438240	-2.8376139	-1.5137565
H	1.8493349	-3.3767600	-0.7960335
H	-0.2687069	-4.6160811	-1.2005112
H	-3.5989480	1.2266792	-1.9685616
H	-3.5949317	-1.2423023	-1.9640523
H	-2.3721438	-3.3871480	-1.6781800
H	-2.3824608	3.3766854	-1.6911347

59.

C	2.5158467	-0.1768872	0.7973988
C	2.5158467	-0.1768872	-0.7973988
C	3.8047233	-0.3147645	0.0000000
H	4.2709897	-1.2983731	0.0000000
H	4.4699835	0.5465645	0.0000000
C	2.0264909	-1.3484324	1.4785265
C	2.2759134	1.0872888	1.4476095
C	2.0264909	-1.3484324	-1.4785265
C	2.2759134	1.0872888	-1.4476095
N	1.7020632	-2.3095857	2.0456510
N	2.1702953	2.1240114	1.9622589
N	2.1702953	2.1240114	-1.9622589
N	1.7020632	-2.3095857	-2.0456510
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C	-1.0935203	1.3212709	-0.7316419
C	-1.0935203	1.3212709	0.7316419
C	-1.0856629	0.0842880	1.4394395
C	-1.2425983	-1.1743377	0.7111553
C	-1.2425983	-1.1743377	-0.7111553
C	-1.4152191	-2.4036077	-1.3868891
C	-1.5690892	-3.5961334	-0.7012189
H	-1.4317748	-2.4252370	-2.4743538
H	-1.6955135	-4.5279496	-1.2533586
C	-1.4152191	-2.4036077	1.3868891
C	-1.5690892	-3.5961334	0.7012189
H	-1.4317748	-2.4252370	2.4743538
H	-1.6955135	-4.5279496	1.2533586
C	-1.0484578	2.5217206	1.4752399
C	-0.9527741	2.5221146	2.8564774
H	-1.0601394	3.4793756	0.9587416
H	-0.9026177	3.4673601	3.3973588
C	-0.9450568	0.1127166	2.8468831
C	-0.8796998	1.3048071	3.5484635
H	-0.8752808	-0.8226315	3.3990550
H	-0.7660532	1.2931352	4.6329398
C	-1.0484578	2.5217206	-1.4752399
C	-0.9527741	2.5221146	-2.8564774
H	-1.0601394	3.4793756	-0.9587416
H	-0.9026177	3.4673601	-3.3973588
C	-0.9450568	0.1127166	-2.8468831
C	-0.8796998	1.3048071	-3.5484635
H	-0.8752808	-0.8226315	-3.3990550
H	-0.7660532	1.2931352	-4.6329398

60.

C	0.0000000	-0.7963437	2.6916251
C	0.0000000	0.7963437	2.6916251
C	0.0000000	0.0000000	3.9887680
H	0.9279971	0.0000000	4.5572262
H	-0.9279971	0.0000000	4.5572262
C	1.2266418	-1.4578237	2.3240881
C	-1.2266418	-1.4578237	2.3240881
C	1.2266418	1.4578237	2.3240881
C	-1.2266418	1.4578237	2.3240881
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N	-2.2385430	-1.9884204	2.1110429
N	-2.2385430	1.9884204	2.1110429
N	2.2385430	1.9884204	2.1110429
C	2.4387441	2.8477949	-1.0110791
C	2.4699519	1.4255982	-1.0241659
C	1.2364358	0.7131705	-1.0117775
C	0.0000000	1.4263857	-0.9964875
C	0.0000000	2.8523259	-0.9863869
C	1.2483234	3.5356947	-0.9895534
C	1.2364358	-0.7131705	-1.0117775
C	-1.2364358	0.7131705	-1.0117775
C	-1.2364358	-0.7131705	-1.0117775
C	0.0000000	-1.4263857	-0.9964875
C	-2.4699519	-1.4255982	-1.0241659
C	-3.6857779	-0.6877615	-1.0274463
C	-3.6857779	0.6877615	-1.0274463
C	-2.4699519	1.4255982	-1.0241659
C	-2.4387441	2.8477949	-1.0110791
C	-1.2483234	3.5356947	-0.9895534
H	-1.2463290	4.6273552	-0.9749880
H	-3.3856724	3.3902615	-1.0043772

H	3.3856724	3.3902615	-1.0043772
H	1.2463290	4.6273552	-0.9749880
H	-4.6295952	-1.2364045	-1.0219242
H	-4.6295952	1.2364045	-1.0219242
C	3.6857779	0.6877615	-1.0274463
C	3.6857779	-0.6877615	-1.0274463
C	2.4699519	-1.4255982	-1.0241659
H	4.6295952	1.2364045	-1.0219242
H	4.6295952	-1.2364045	-1.0219242
C	2.4387441	-2.8477949	-1.0110791
C	1.2483234	-3.5356947	-0.9895534
C	0.0000000	-2.8523259	-0.9863869
H	3.3856724	-3.3902615	-1.0043772
H	1.2463290	-4.6273552	-0.9749880
C	-2.4387441	-2.8477949	-1.0110791
H	-3.3856724	-3.3902615	-1.0043772
C	-1.2483234	-3.5356947	-0.9895534
H	-1.2463290	-4.6273552	-0.9749880

61.

C	5.6351102	-0.5194039	0.7977895
C	5.6351102	-0.5194039	-0.7977895
C	6.9237281	-0.6371100	0.0000000
H	7.4068197	-1.6125833	0.0000000
H	7.5757986	0.2344466	0.0000000
C	5.1231055	-1.7001101	1.4477091
C	5.3467573	0.7342861	1.4481786
C	5.1231055	-1.7001101	-1.4477091
C	5.3467573	0.7342861	-1.4481786
N	4.7479989	-2.6697658	1.9674513
N	5.1474278	1.7542394	1.9684150

N	5.1474278	1.7542394	-1.9684150
N	4.7479989	-2.6697658	-1.9674513
C	-0.9151577	-0.5101888	3.4837606
C	0.4623578	-0.6266359	3.0346051
C	1.1552989	0.5095844	2.6046226
C	0.4980947	1.8063146	2.6033962
C	-0.8275467	1.9179288	3.0348885
C	-1.5474736	0.7373138	3.4833385
C	-1.6350707	-1.6903198	3.0340981
C	-0.7027686	-2.5368511	2.3079679
C	0.5938349	-1.8799005	2.3082499
C	1.4113162	-1.9492876	1.1762601
C	2.0026384	0.4377435	1.4256147
C	0.9432287	2.5360231	1.4270913
C	0.0455808	3.3488664	0.7269773
C	-1.3315848	3.4652206	1.1760864
C	-1.7597736	2.7634938	2.3078276
C	-3.0564828	2.1061425	2.3078735
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C	-2.9603790	-1.5781316	2.6019066
C	-1.1309714	-3.2386441	1.1760878
C	-2.5081162	-3.1212968	0.7268274
C	-3.4056661	-2.3075913	1.4261170
C	-4.3385621	-1.4620587	0.6993830
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C	-3.8760743	2.1752209	1.1761427
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C	-2.1830991	3.5375020	0.0000000
C	1.8730722	1.6897732	0.6987907

C -0.8275467 1.9179288 -3.0348885
C 0.4980947 1.8063146 -2.6033962
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C 2.1280891 -0.7673145 0.7272354
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62.

C 3.5597208 -1.2206629 -3.8632480
C 2.8769245 -2.2429848 -3.1599217
C 3.5603025 -2.9517325 -2.1420462
C 2.8770178 -3.1783006 -0.9223831
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C 1.4282382 0.0000000 2.2210862
C 0.7177257 1.2112951 1.9802264
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C 0.7183893 2.9340955 0.2867283
C 1.4299002 3.1779300 -0.9231046
C 0.7185454 2.9287854 -2.1320516
C 1.4295311 2.2413523 -3.1577693

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C	-1.4299002	-3.1779300	-0.9231046
C	-0.7183893	-2.9340955	0.2867283
C	-1.4296186	-2.2463275	1.3119219
C	-0.7177257	-1.2112951	1.9802264
C	-1.4282382	0.0000000	2.2210862
C	-0.7177257	1.2112951	1.9802264
C	-1.4296186	2.2463275	1.3119219
C	-0.7183893	2.9340955	0.2867283
C	-1.4299002	3.1779300	-0.9231046
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C	-0.7185300	1.2101834	-3.8365037
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C	-0.7185300	-1.2101834	-3.8365037
C	-1.4295311	-2.2413523	-3.1577693
C	-2.8770178	-3.1783006	-0.9223831
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C	-2.8760172	-2.2465163	1.3158671
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C	-3.5597208	1.2206629	-3.8632480

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C	-3.5597208	-1.2206629	-3.8632480
C	-2.8769245	-2.2429848	-3.1599217
C	-3.5603025	-2.9517325	-2.1420462
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C	0.7978234	0.0000000	5.6055941
C	0.0000000	0.0000000	6.9008855
H	0.0000000	-0.9276077	7.4699368
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H	4.6515720	-1.2117051	-3.8419422
H	4.6515720	1.2117051	-3.8419422
H	4.6521306	2.9295693	-2.1327885
H	4.6519773	2.9333270	0.2897929
H	4.6491249	1.2161181	2.0045148
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H	4.6519773	-2.9333270	0.2897929
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H	-4.6519773	-2.9333270	0.2897929
H	-4.6491249	-1.2161181	2.0045148

H -4.6491249 1.2161181 2.0045148
H -4.6519773 2.9333270 0.2897929

63.

C 3.5594552 -3.9751081 -0.8501394
C 2.8769223 -3.7660282 0.3698683
C 3.5591381 -3.2157124 1.4794543
C 2.8756414 -2.3249845 2.3374388
C 3.5564272 -1.2270899 2.9108746
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C 3.5594552 3.9751081 -0.8501394
C 2.8767777 3.7623480 -2.0695706
C 3.5591437 3.2120702 -3.1786703
C 2.8765707 2.3217199 -4.0385131
C 3.5586647 1.2258705 -4.6151093
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C 2.8767777 -3.7623480 -2.0695706
C 1.4291872 -3.7622794 0.3675310
C 0.7183828 -3.1962943 1.4614781
C 1.4290668 -2.3222612 2.3291048
C 0.7178779 -1.2172462 2.8684782
C 1.4277507 0.0000000 3.0622211
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C 1.4290668 2.3222612 2.3291048

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C	1.4289905	3.7569943	-2.0676126
C	0.7185399	3.1891645	-3.1610594
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C	1.4287911	0.0000000	-4.7807740
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C	-3.5591437	-3.2120702	-3.1786703
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64.

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C	3.5476918	-4.6027181	2.0310086
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C	3.5476094	3.3692226	-2.5544283
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C	3.5476094	-3.3692226	-2.5544283
C	2.8661969	-4.1160431	-1.5652254
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C	2.8657154	-2.3693052	4.8935990
C	2.8658400	0.0000000	5.5231491
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C	2.8655128	4.1102842	3.1673817
C	2.8657745	4.7520333	0.8016943
C	2.8661969	4.1160431	-1.5652254
C	2.8651205	2.3715343	-3.2866775
C	2.8649441	0.0000000	-3.9089231
C	2.8651205	-2.3715343	-3.2866775
C	1.4239406	-4.1129148	-1.5615328
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C	1.4234742	-4.1055384	3.1646465
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C	1.4234791	0.0000000	5.5171580
C	1.4235105	2.3664077	4.8883656
C	1.4234742	4.1055384	3.1646465
C	1.4235760	4.7474775	0.8021883
C	1.4239406	4.1129148	-1.5615328
C	1.4236188	2.3688474	-3.2767468
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C	-0.7147723	-3.3529670	-2.5333143
C	-1.4239406	-4.1129148	-1.5615328
C	-1.4235760	-4.7474775	0.8021883
C	-1.4234742	-4.1055384	3.1646465
C	-1.4235105	-2.3664077	4.8883656
C	-1.4234791	0.0000000	5.5171580
C	-1.4235105	2.3664077	4.8883656
C	-1.4234742	4.1055384	3.1646465

C	-1.4235760	4.7474775	0.8021883
C	-1.4239406	4.1129148	-1.5615328
C	-1.4236188	2.3688474	-3.2767468
C	-1.4227820	0.0000000	-3.8949517
C	-1.4236188	-2.3688474	-3.2767468
C	-2.8661969	-4.1160431	-1.5652254
C	-2.8657745	-4.7520333	0.8016943
C	-2.8655128	-4.1102842	3.1673817
C	-2.8657154	-2.3693052	4.8935990
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C	-3.5476918	-4.6027181	2.0310086
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C	-3.5476385	3.3640629	4.1557525
C	-3.5476918	4.6027181	2.0310086
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C	-3.5476094	3.3692226	-2.5544283
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C	-3.5456039	-1.2313355	-3.7717821
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65.

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67.

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68.

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H	-1.2664806	-5.1660982	-2.1788995
N	-0.2993921	-2.5022330	-0.5404729
H	0.2230256	-1.9188896	0.1448658

69.

C	0.654955	2.122697	-0.010672
C	0.334836	1.346614	1.344821
C	0.966037	2.731116	1.348168
C	-0.471499	2.646221	-0.741975
C	1.764809	1.644258	-0.795799
C	-1.051284	1.245541	1.727192
C	1.168645	0.217142	1.670784
N	-1.387156	3.109230	-1.287095
N	2.701932	1.301373	-1.391154

N 1.874181 -0.656026 1.971396
 N -2.167708 1.219152 2.047842
 H 0.329591 3.552873 1.672157
 H 2.017581 2.784709 1.624431
 N 0.698074 -3.118646 0.391663
 C -0.335177 -2.991049 1.299190
 N -1.240548 -2.104421 0.935883
 C -0.763040 -1.610992 -0.269893
 C -1.253226 -0.638349 -1.172039
 N -2.448918 -0.023017 -1.003249
 N -0.499612 -0.319729 -2.247418
 C 0.649323 -0.993896 -2.452717
 N 1.198312 -1.964453 -1.708831
 C 0.453498 -2.222100 -0.625653
 H 1.540202 -3.674569 0.495412
 H -0.364028 -3.576307 2.214048
 H -2.652745 0.785576 -1.581158
 H -2.929378 -0.117636 -0.115352
 H 1.212342 -0.695311 -3.339979

70.

C 0.8818641 2.0306363 0.3059129
 C 0.6395367 1.2944134 1.6890287
 C 0.9288581 2.7863674 1.6243648
 H 0.0921806 3.4491990 1.8382094
 H 1.9114046 3.1100655 1.9631729
 C -0.2578808 2.1988021 -0.5605456
 C 2.1236791 1.7697930 -0.3789364
 C -0.7081255 0.8739236 1.9828313
 C 1.6799852 0.4040203 2.1371565
 N -1.1596125 2.3565559 -1.2767373

N	3.1289452	1.6168723	-0.9420134
N	2.5148810	-0.3128007	2.5113334
N	-1.8012033	0.5793979	2.2464412
N	0.1202389	-2.2231095	1.1589932
C	-1.0244492	-2.8271186	1.6590966
H	-1.0251609	-3.3386291	2.6173535
N	-2.0578734	-2.6963514	0.8581420
C	-1.5780525	-1.9789747	-0.2206749
C	-2.2421373	-1.5492678	-1.4260843
O	-3.3928186	-1.6892252	-1.8076317
N	-1.2936113	-0.8618666	-2.2744761
H	-1.6905126	-0.5723408	-3.1668028
C	0.0208891	-0.6019037	-1.9965682
N	0.7592699	0.0336054	-2.9667463
H	0.2909799	0.7263467	-3.5422696
H	1.6996922	0.2856242	-2.6748649
N	0.6087547	-0.9667665	-0.8691218
C	-0.2205766	-1.6738388	-0.0550924
H	1.0508551	-2.2234296	1.5665294

71.

C	1.2221758	2.5779112	-0.1597396
C	1.2252189	1.6593091	1.1303593
C	1.5954079	3.1313337	1.2069829
H	0.8716186	3.7911729	1.6821032
H	2.6472019	3.3609168	1.3673338
C	-0.0722536	2.9046692	-0.7040160
C	2.2726148	2.3533882	-1.1207268
C	-0.0624380	1.2323037	1.6189129
C	2.2598625	0.6597483	1.2213466
N	-1.1202978	3.2033375	-1.1072611

N	3.1451911	2.2118995	-1.8747109
N	3.0889713	-0.1482994	1.3239008
N	-1.0975504	0.8864192	2.0186292
N	0.6405138	-2.1862973	-0.0935924
C	-0.1000615	-1.1304331	-0.6434822
C	-1.5386532	-1.3515135	-0.7344093
C	-2.0263739	-2.5369843	-0.2841779
N	-1.2188957	-3.5204012	0.2398479
C	0.1643208	-3.4067742	0.3753086
O	0.8665920	-4.2838858	0.8511112
H	1.6460748	-2.0382389	0.0004650
O	0.4744401	-0.0950449	-0.9968967
C	-2.3871757	-0.2494899	-1.2874016
H	-2.3267344	0.6433476	-0.6491996
H	-2.0307521	0.0548390	-2.2815045
H	-3.4384806	-0.5552450	-1.3631492
H	-3.0906270	-2.7721580	-0.3091346
H	-1.6099104	-4.3958305	0.5731009

72.

C	1.4109647	2.0788779	0.5785727
C	0.8054159	1.2243623	1.7611777
C	1.3651529	2.6242657	1.9971389
H	0.6317471	3.3992433	2.2116017
H	2.3189902	2.6915545	2.5165626
C	0.4769523	2.5730062	-0.4017349
C	2.7261086	1.7141862	0.1043033
C	-0.6290303	1.1073714	1.8636850
C	1.5453969	0.0622522	2.1807307
N	-0.2948136	3.0174160	-1.1480568
N	3.8378299	1.5310165	-0.1796258

N	2.1464407	-0.8645204	2.5415816
N	-1.7728991	1.0800113	2.0682322
N	0.2291747	-1.8100216	-2.3557741
C	-0.8596101	-2.6129819	-2.4569179
H	-0.8726099	-3.3259578	-3.2809720
C	-1.8728797	-2.5015632	-1.5536973
H	-2.7557214	-3.1328549	-1.6182151
C	-1.7105324	-1.5142402	-0.5190082
N	-2.6797357	-1.3571708	0.4125316
H	-2.6084632	-0.5791412	1.0673780
H	-3.5607179	-1.8452983	0.3265566
N	-0.6299609	-0.7398047	-0.4161984
C	0.3729717	-0.8305268	-1.3350872
O	1.3848567	-0.1267961	-1.3429324
H	0.9949718	-1.8626856	-3.0218325

73.

C	0.7278957	2.4485134	-0.3399057
C	0.8990561	2.1741888	1.2102290
C	0.8146697	3.5901632	0.6609016
H	-0.1057722	4.1365104	0.8593913
H	1.7371812	4.1674110	0.6610058
C	-0.5586830	2.1221631	-0.9029564
C	1.8636391	2.1762772	-1.1845244
C	-0.2515553	1.6302247	1.8877836
C	2.1770120	1.6750684	1.6512563
N	-1.6110060	1.8934935	-1.3402407
N	2.7850129	1.9987787	-1.8699149
N	3.2171149	1.3125280	2.0212868
N	-1.1979465	1.2338209	2.4336543
N	0.4219056	-2.6031636	-0.6988093

C	-0.0783639	-1.3748814	-0.2263917
C	-1.5099090	-1.3643951	0.0039074
C	-2.2359791	-2.4823354	-0.2443124
N	-1.6548108	-3.6358546	-0.7086567
C	-0.2858335	-3.7695483	-0.9651844
O	0.2155519	-4.8020972	-1.3767754
H	1.4256266	-2.6480424	-0.8711321
O	0.6945014	-0.4305892	-0.0481656
H	-3.3136360	-2.5274495	-0.0908697
H	-2.2065201	-4.4681203	-0.8923813
H	-1.9691516	-0.4526643	0.3708046

74.

C	-1.2157997	-0.6939552	2.8742111
C	-1.2157997	0.6939552	2.8742111
H	-2.1551451	-1.2443009	2.8478229
H	-2.1551451	1.2443009	2.8478229
C	0.0000000	-2.8299511	2.8394655
C	0.0000000	-4.0434859	2.7778623
C	0.0000000	-5.6048610	-1.0593292
H	0.8883059	-6.2328224	-1.2312436
H	-0.8883059	-6.2328224	-1.2312436
C	0.0000000	-4.4597532	-2.0364475
C	-0.7953612	-3.1665007	-1.8624623
C	0.7953612	-3.1665007	-1.8624623
H	0.0000000	-4.8046843	-3.0729234
C	1.4870189	-2.8535837	-0.6367708
N	2.1163652	-2.5824983	0.3012066
C	-1.4870189	-2.8535837	-0.6367708
N	-2.1163652	-2.5824983	0.3012066
C	-1.4366694	-2.6324942	-3.0402151

N	-1.9557729	-2.2344711	-4.0015480
C	1.4366694	-2.6324942	-3.0402151
N	1.9557729	-2.2344711	-4.0015480
O	0.0000000	-5.0986556	0.2803101
C	0.0000000	-5.4881993	2.6600869
H	0.8771697	-5.9339076	3.1593122
H	-0.8771697	-5.9339076	3.1593122
C	0.0000000	-6.0661079	1.2482524
O	0.0000000	-7.2495203	0.9949130
C	1.2157997	0.6939552	2.8742111
C	0.0000000	1.4101928	2.8735483
C	0.0000000	-1.4101928	2.8735483
C	1.2157997	-0.6939552	2.8742111
H	2.1551451	1.2443009	2.8478229
H	2.1551451	-1.2443009	2.8478229
C	0.0000000	2.8299511	2.8394655
C	0.0000000	4.0434859	2.7778623
C	0.0000000	5.6048610	-1.0593292
H	-0.8883059	6.2328224	-1.2312436
H	0.8883059	6.2328224	-1.2312436
C	0.0000000	4.4597532	-2.0364475
C	0.7953612	3.1665007	-1.8624623
C	-0.7953612	3.1665007	-1.8624623
H	0.0000000	4.8046843	-3.0729234
C	-1.4870189	2.8535837	-0.6367708
N	-2.1163652	2.5824983	0.3012066
C	1.4870189	2.8535837	-0.6367708
N	2.1163652	2.5824983	0.3012066
C	1.4366694	2.6324942	-3.0402151
N	1.9557729	2.2344711	-4.0015480
C	-1.4366694	2.6324942	-3.0402151

N	-1.9557729	2.2344711	-4.0015480
O	0.0000000	5.0986556	0.2803101
C	0.0000000	5.4881993	2.6600869
H	-0.8771697	5.9339076	3.1593122
H	0.8771697	5.9339076	3.1593122
C	0.0000000	6.0661079	1.2482524
O	0.0000000	7.2495203	0.9949130
O	0.0000000	0.0000000	-2.4805493
H	0.7637320	0.0000000	-3.0860897
H	-0.7637320	0.0000000	-3.0860897

75.

C	-1.2152495	-0.6943210	2.5983665
C	-1.2152495	0.6943210	2.5983665
H	-2.1546635	-1.2451355	2.5767252
H	-2.1546635	1.2451355	2.5767252
C	0.0000000	-2.8322340	2.6540285
C	0.0000000	-4.0472661	2.6767903
C	0.0000000	-5.8219478	-1.0514410
H	0.8895422	-6.4537980	-1.1998554
H	-0.8895422	-6.4537980	-1.1998554
C	0.0000000	-4.6981676	-2.0548948
C	-0.7954311	-3.4064674	-1.8704321
C	0.7954311	-3.4064674	-1.8704321
H	0.0000000	-5.0507429	-3.0883776
C	1.5144137	-3.1108202	-0.6559950
N	2.1870924	-2.8531925	0.2555099
C	-1.5144137	-3.1108202	-0.6559950
N	-2.1870924	-2.8531925	0.2555099
C	-1.4178451	-2.8342496	-3.0412145
N	-1.9193578	-2.3851253	-3.9891653

C	1.4178451	-2.8342496	-3.0412145
N	1.9193578	-2.3851253	-3.9891653
O	0.0000000	-5.2606828	0.2660988
C	0.0000000	-5.4974431	2.6588600
H	0.8775868	-5.9069820	3.1874444
H	-0.8775868	-5.9069820	3.1874444
C	0.0000000	-6.1688374	1.2878817
O	0.0000000	-7.3649118	1.1070450
C	1.2152495	0.6943210	2.5983665
C	0.0000000	1.4119877	2.6170927
C	0.0000000	-1.4119877	2.6170927
C	1.2152495	-0.6943210	2.5983665
H	2.1546635	1.2451355	2.5767252
H	2.1546635	-1.2451355	2.5767252
C	0.0000000	2.8322340	2.6540285
C	0.0000000	4.0472661	2.6767903
C	0.0000000	5.8219478	-1.0514410
H	-0.8895422	6.4537980	-1.1998554
H	0.8895422	6.4537980	-1.1998554
C	0.0000000	4.6981676	-2.0548948
C	0.7954311	3.4064674	-1.8704321
C	-0.7954311	3.4064674	-1.8704321
H	0.0000000	5.0507429	-3.0883776
C	-1.5144137	3.1108202	-0.6559950
N	-2.1870924	2.8531925	0.2555099
C	1.5144137	3.1108202	-0.6559950
N	2.1870924	2.8531925	0.2555099
C	1.4178451	2.8342496	-3.0412145
N	1.9193578	2.3851253	-3.9891653
C	-1.4178451	2.8342496	-3.0412145
N	-1.9193578	2.3851253	-3.9891653

O	0.0000000	5.2606828	0.2660988
C	0.0000000	5.4974431	2.6588600
H	-0.8775868	5.9069820	3.1874444
H	0.8775868	5.9069820	3.1874444
C	0.0000000	6.1688374	1.2878817
O	0.0000000	7.3649118	1.1070450
H	0.9665005	0.0000000	-2.1806280
H	-0.9665005	0.0000000	-2.1806280
S	0.0000000	0.0000000	-1.2304459

76.

C	-1.2154848	0.6943705	-2.9583081
C	-1.2154848	-0.6943705	-2.9583081
H	-2.1547188	1.2457666	-2.9340362
H	-2.1547188	-1.2457666	-2.9340362
C	0.0000000	2.8315528	-2.9956676
C	0.0000000	4.0460423	-3.0257760
C	0.0000000	5.9684990	0.6425085
H	0.8884522	6.6096419	0.7544249
H	-0.8884522	6.6096419	0.7544249
C	0.0000000	4.9209278	1.7229401
C	-0.7965068	3.6165266	1.6799084
C	0.7965068	3.6165266	1.6799084
H	0.0000000	5.3643986	2.7210842
C	1.4905258	3.2027452	0.4846242
N	2.1166944	2.8757983	-0.4375490
C	-1.4905258	3.2027452	0.4846242
N	-2.1166944	2.8757983	-0.4375490
C	-1.4551359	3.2366877	2.9079057
N	-1.9944578	3.0048873	3.9110302
C	1.4551359	3.2366877	2.9079057

N	1.9944578	3.0048873	3.9110302
O	0.0000000	5.3396530	-0.6442470
C	0.0000000	5.4954001	-3.0467155
H	0.8775921	5.8883888	-3.5877012
H	-0.8775921	5.8883888	-3.5877012
C	0.0000000	6.2089460	-1.6984171
O	0.0000000	7.4116540	-1.5635880
C	1.2154848	-0.6943705	-2.9583081
C	0.0000000	-1.4121492	-2.9687296
C	0.0000000	1.4121492	-2.9687296
C	1.2154848	0.6943705	-2.9583081
H	2.1547188	-1.2457666	-2.9340362
H	2.1547188	1.2457666	-2.9340362
C	0.0000000	-2.8315528	-2.9956676
C	0.0000000	-4.0460423	-3.0257760
C	0.0000000	-5.9684990	0.6425085
H	-0.8884522	-6.6096419	0.7544249
H	0.8884522	-6.6096419	0.7544249
C	0.0000000	-4.9209278	1.7229401
C	0.7965068	-3.6165266	1.6799084
C	-0.7965068	-3.6165266	1.6799084
H	0.0000000	-5.3643986	2.7210842
C	-1.4905258	-3.2027452	0.4846242
N	-2.1166944	-2.8757983	-0.4375490
C	1.4905258	-3.2027452	0.4846242
N	2.1166944	-2.8757983	-0.4375490
C	1.4551359	-3.2366877	2.9079057
N	1.9944578	-3.0048873	3.9110302
C	-1.4551359	-3.2366877	2.9079057
N	-1.9944578	-3.0048873	3.9110302
O	0.0000000	-5.3396530	-0.6442470

C	0.0000000	-5.4954001	-3.0467155
H	-0.8775921	-5.8883888	-3.5877012
H	0.8775921	-5.8883888	-3.5877012
C	0.0000000	-6.2089460	-1.6984171
O	0.0000000	-7.4116540	-1.5635880
C	-0.6985183	0.0000000	3.0819954
C	0.6985183	0.0000000	3.0819954
C	1.3968170	0.0000000	1.8695454
C	0.6990105	0.0000000	0.6579238
C	-0.6990105	0.0000000	0.6579238
C	-1.3968170	0.0000000	1.8695454
H	-1.2446710	0.0000000	4.0246702
H	1.2446710	0.0000000	4.0246702
H	2.4876162	0.0000000	1.8696110
H	1.2381155	0.0000000	-0.2877360
H	-1.2381155	0.0000000	-0.2877360
H	-2.4876162	0.0000000	1.8696110

77.

C	-1.2152223	-0.6937557	2.8639985
C	-1.2152223	0.6937557	2.8639985
H	-2.1541392	-1.2460074	2.8418829
H	-2.1541392	1.2460074	2.8418829
C	0.0000000	-2.8296331	2.9105305
C	0.0000000	-4.0444971	2.9467342
C	0.0000000	-5.9876895	-0.7095789
H	0.8887919	-6.6281003	-0.8232052
H	-0.8887919	-6.6281003	-0.8232052
C	0.0000000	-4.9317629	-1.7828384
C	-0.7973954	-3.6296570	-1.7087644
C	0.7973954	-3.6296570	-1.7087644

H	0.0000000	-5.3595173	-2.7876920
C	1.5053648	-3.2453264	-0.5123562
N	2.1538604	-2.9295905	0.3983214
C	-1.5053648	-3.2453264	-0.5123562
N	-2.1538604	-2.9295905	0.3983214
C	-1.4388798	-3.2002523	-2.9295190
N	-1.9572454	-2.9040100	-3.9268757
C	1.4388798	-3.2002523	-2.9295190
N	1.9572454	-2.9040100	-3.9268757
O	0.0000000	-5.3566635	0.5749898
C	0.0000000	-5.4940134	2.9781242
H	0.8772426	-5.8843365	3.5220396
H	-0.8772426	-5.8843365	3.5220396
C	0.0000000	-6.2193591	1.6365224
O	0.0000000	-7.4224786	1.5062608
C	1.2152223	0.6937557	2.8639985
C	0.0000000	1.4096747	2.8774346
C	0.0000000	-1.4096747	2.8774346
C	1.2152223	-0.6937557	2.8639985
H	2.1541392	1.2460074	2.8418829
H	2.1541392	-1.2460074	2.8418829
C	0.0000000	2.8296331	2.9105305
C	0.0000000	4.0444971	2.9467342
C	0.0000000	5.9876895	-0.7095789
H	-0.8887919	6.6281003	-0.8232052
H	0.8887919	6.6281003	-0.8232052
C	0.0000000	4.9317629	-1.7828384
C	0.7973954	3.6296570	-1.7087644
C	-0.7973954	3.6296570	-1.7087644
H	0.0000000	5.3595173	-2.7876920
C	-1.5053648	3.2453264	-0.5123562

N	-2.1538604	2.9295905	0.3983214
C	1.5053648	3.2453264	-0.5123562
N	2.1538604	2.9295905	0.3983214
C	1.4388798	3.2002523	-2.9295190
N	1.9572454	2.9040100	-3.9268757
C	-1.4388798	3.2002523	-2.9295190
N	-1.9572454	2.9040100	-3.9268757
O	0.0000000	5.3566635	0.5749898
C	0.0000000	5.4940134	2.9781242
H	-0.8772426	5.8843365	3.5220396
H	0.8772426	5.8843365	3.5220396
C	0.0000000	6.2193591	1.6365224
O	0.0000000	7.4224786	1.5062608
C	-1.2011895	0.0000000	-2.2296721
C	0.0000000	0.0000000	-2.9426231
C	1.2011895	0.0000000	-2.2296721
C	1.1466396	0.0000000	-0.8319420
C	-1.1466396	0.0000000	-0.8319420
H	-2.1593789	0.0000000	-2.7484618
H	0.0000000	0.0000000	-4.0323204
H	2.1593789	0.0000000	-2.7484618
H	2.0618186	0.0000000	-0.2352580
H	-2.0618186	0.0000000	-0.2352580
N	0.0000000	0.0000000	-0.1374507

78.

C	-1.2160009	-0.6934226	2.9808196
C	-1.2160009	0.6934226	2.9808196
H	-2.1537072	-1.2436139	2.9257119
H	-2.1537072	1.2436139	2.9257119
C	0.0000000	-2.8218957	2.8484890

C	0.0000000	-4.0245220	2.6746592
C	0.0000000	-5.0267460	-1.3524070
H	0.8884843	-5.6313607	-1.5949211
H	-0.8884843	-5.6313607	-1.5949211
C	0.0000000	-3.7774897	-2.1886768
C	-0.7770433	-2.4823008	-1.9153290
C	0.7770433	-2.4823008	-1.9153290
H	0.0000000	-4.0232575	-3.2530838
C	1.4734867	-2.2898521	-0.6671906
N	2.1207917	-2.2160444	0.2946529
C	-1.4734867	-2.2898521	-0.6671906
N	-2.1207917	-2.2160444	0.2946529
C	-1.4459445	-1.9033428	-3.0588205
N	-2.0363487	-1.6262299	-4.0216975
C	1.4459445	-1.9033428	-3.0588205
N	2.0363487	-1.6262299	-4.0216975
O	0.0000000	-4.7186759	0.0532570
C	0.0000000	-5.4365259	2.3505124
H	0.8778661	-5.9515128	2.7766117
H	-0.8778661	-5.9515128	2.7766117
C	0.0000000	-5.8022182	0.8645541
O	0.0000000	-6.9498681	0.4635280
C	1.2160009	0.6934226	2.9808196
C	0.0000000	1.4076138	2.9664542
C	0.0000000	-1.4076138	2.9664542
C	1.2160009	-0.6934226	2.9808196
H	2.1537072	1.2436139	2.9257119
H	2.1537072	-1.2436139	2.9257119
C	0.0000000	2.8218957	2.8484890
C	0.0000000	4.0245220	2.6746592
C	0.0000000	5.0267460	-1.3524070

H	-0.8884843	5.6313607	-1.5949211
H	0.8884843	5.6313607	-1.5949211
C	0.0000000	3.7774897	-2.1886768
C	0.7770433	2.4823008	-1.9153290
C	-0.7770433	2.4823008	-1.9153290
H	0.0000000	4.0232575	-3.2530838
C	-1.4734867	2.2898521	-0.6671906
N	-2.1207917	2.2160444	0.2946529
C	1.4734867	2.2898521	-0.6671906
N	2.1207917	2.2160444	0.2946529
C	1.4459445	1.9033428	-3.0588205
N	2.0363487	1.6262299	-4.0216975
C	-1.4459445	1.9033428	-3.0588205
N	-2.0363487	1.6262299	-4.0216975
O	0.0000000	4.7186759	0.0532570
C	0.0000000	5.4365259	2.3505124
H	-0.8778661	5.9515128	2.7766117
H	0.8778661	5.9515128	2.7766117
C	0.0000000	5.8022182	0.8645541
O	0.0000000	6.9498681	0.4635280
F	0.0000000	0.0000000	-1.7339222

79.

C	-1.2151957	-0.6935854	2.6565362
C	-1.2151957	0.6935854	2.6565362
H	-2.1526086	-1.2456822	2.6049721
H	-2.1526086	1.2456822	2.6049721
C	0.0000000	-2.8294678	2.6573020
C	0.0000000	-4.0442162	2.6099510
C	0.0000000	-5.3906270	-1.2883780
H	0.8900881	-6.0039582	-1.5008483

H	-0.8900881	-6.0039582	-1.5008483
C	0.0000000	-4.1662759	-2.1644633
C	-0.7813157	-2.8797844	-1.8610250
C	0.7813157	-2.8797844	-1.8610250
H	0.0000000	-4.4180596	-3.2268681
C	1.5307917	-2.7454532	-0.6326597
N	2.2560117	-2.7593160	0.2755645
C	-1.5307917	-2.7454532	-0.6326597
N	-2.2560117	-2.7593160	0.2755645
C	-1.4292926	-2.2555867	-2.9943631
N	-1.9805238	-1.8911052	-3.9509852
C	1.4292926	-2.2555867	-2.9943631
N	1.9805238	-1.8911052	-3.9509852
O	0.0000000	-4.9952935	0.0909541
C	0.0000000	-5.4838990	2.4361023
H	0.8781651	-5.9513729	2.9134941
H	-0.8781651	-5.9513729	2.9134941
C	0.0000000	-6.0007440	0.9958338
O	0.0000000	-7.1786937	0.6977757
C	1.2151957	0.6935854	2.6565362
C	0.0000000	1.4089730	2.6713983
C	0.0000000	-1.4089730	2.6713983
C	1.2151957	-0.6935854	2.6565362
H	2.1526086	1.2456822	2.6049721
H	2.1526086	-1.2456822	2.6049721
C	0.0000000	2.8294678	2.6573020
C	0.0000000	4.0442162	2.6099510
C	0.0000000	5.3906270	-1.2883780
H	-0.8900881	6.0039582	-1.5008483
H	0.8900881	6.0039582	-1.5008483
C	0.0000000	4.1662759	-2.1644633

C	0.7813157	2.8797844	-1.8610250
C	-0.7813157	2.8797844	-1.8610250
H	0.0000000	4.4180596	-3.2268681
C	-1.5307917	2.7454532	-0.6326597
N	-2.2560117	2.7593160	0.2755645
C	1.5307917	2.7454532	-0.6326597
N	2.2560117	2.7593160	0.2755645
C	1.4292926	2.2555867	-2.9943631
N	1.9805238	1.8911052	-3.9509852
C	-1.4292926	2.2555867	-2.9943631
N	-1.9805238	1.8911052	-3.9509852
O	0.0000000	4.9952935	0.0909541
C	0.0000000	5.4838990	2.4361023
H	-0.8781651	5.9513729	2.9134941
H	0.8781651	5.9513729	2.9134941
C	0.0000000	6.0007440	0.9958338
O	0.0000000	7.1786937	0.6977757
Cl	0.0000000	0.0000000	-1.0019580

80.

C	-1.2150885	-0.6936646	2.5721582
C	-1.2150885	0.6936646	2.5721582
H	-2.1523154	-1.2463277	2.5215533
H	-2.1523154	1.2463277	2.5215533
C	0.0000000	-2.8294603	2.6180998
C	0.0000000	-4.0451717	2.6211539
C	0.0000000	-5.5682716	-1.2095859
H	0.8900881	-6.1901011	-1.3953793
H	-0.8900881	-6.1901011	-1.3953793
C	0.0000000	-4.3829554	-2.1375088
C	-0.7823771	-3.0850735	-1.8896814

C	0.7823771	-3.0850735	-1.8896814
H	0.0000000	-4.6794709	-3.1883370
C	1.5319318	-2.8993778	-0.6676207
N	2.2548222	-2.8774742	0.2424881
C	-1.5319318	-2.8993778	-0.6676207
N	-2.2548222	-2.8774742	0.2424881
C	-1.4317806	-2.5131032	-3.0499018
N	-1.9837291	-2.1979232	-4.0235665
C	1.4317806	-2.5131032	-3.0499018
N	1.9837291	-2.1979232	-4.0235665
O	0.0000000	-5.1117458	0.1500097
C	0.0000000	-5.4913974	2.5141511
H	0.8781753	-5.9358997	3.0131398
H	-0.8781753	-5.9358997	3.0131398
C	0.0000000	-6.0750162	1.1000345
O	0.0000000	-7.2651171	0.8554768
C	1.2150885	0.6936646	2.5721582
C	0.0000000	1.4090443	2.5964630
C	0.0000000	-1.4090443	2.5964630
C	1.2150885	-0.6936646	2.5721582
H	2.1523154	1.2463277	2.5215533
H	2.1523154	-1.2463277	2.5215533
C	0.0000000	2.8294603	2.6180998
C	0.0000000	4.0451717	2.6211539
C	0.0000000	5.5682716	-1.2095859
H	-0.8900881	6.1901011	-1.3953793
H	0.8900881	6.1901011	-1.3953793
C	0.0000000	4.3829554	-2.1375088
C	0.7823771	3.0850735	-1.8896814
C	-0.7823771	3.0850735	-1.8896814
H	0.0000000	4.6794709	-3.1883370

C	-1.5319318	2.8993778	-0.6676207
N	-2.2548222	2.8774742	0.2424881
C	1.5319318	2.8993778	-0.6676207
N	2.2548222	2.8774742	0.2424881
C	1.4317806	2.5131032	-3.0499018
N	1.9837291	2.1979232	-4.0235665
C	-1.4317806	2.5131032	-3.0499018
N	-1.9837291	2.1979232	-4.0235665
O	0.0000000	5.1117458	0.1500097
C	0.0000000	5.4913974	2.5141511
H	-0.8781753	5.9358997	3.0131398
H	0.8781753	5.9358997	3.0131398
C	0.0000000	6.0750162	1.1000345
O	0.0000000	7.2651171	0.8554768
Br	0.0000000	0.0000000	-1.1326731

81.

C	-1.2150165	-0.6938367	2.4713621
C	-1.2150165	0.6938367	2.4713621
H	-2.1520661	-1.2470863	2.4217379
H	-2.1520661	1.2470863	2.4217379
C	0.0000000	-2.8283020	2.5702454
C	0.0000000	-4.0424304	2.6309216
C	0.0000000	-5.8016997	-1.0964998
H	0.8900506	-6.4337120	-1.2440725
H	-0.8900506	-6.4337120	-1.2440725
C	0.0000000	-4.6762493	-2.0957324
C	-0.7836425	-3.3653940	-1.9319854
C	0.7836425	-3.3653940	-1.9319854
H	0.0000000	-5.0375151	-3.1261479
C	1.5304889	-3.1008988	-0.7223922

N	2.2465780	-3.0219314	0.1902108
C	-1.5304889	-3.1008988	-0.7223922
N	-2.2465780	-3.0219314	0.1902108
C	-1.4344097	-2.8736955	-3.1282949
N	-1.9849466	-2.6350515	-4.1245403
C	1.4344097	-2.8736955	-3.1282949
N	1.9849466	-2.6350515	-4.1245403
O	0.0000000	-5.2615090	0.2314177
C	0.0000000	-5.4923598	2.6135548
H	0.8782413	-5.9041551	3.1399247
H	-0.8782413	-5.9041551	3.1399247
C	0.0000000	-6.1641037	1.2397495
O	0.0000000	-7.3669260	1.0695352
C	1.2150165	0.6938367	2.4713621
C	0.0000000	1.4091798	2.5068582
C	0.0000000	-1.4091798	2.5068582
C	1.2150165	-0.6938367	2.4713621
H	2.1520661	1.2470863	2.4217379
H	2.1520661	-1.2470863	2.4217379
C	0.0000000	2.8283020	2.5702454
C	0.0000000	4.0424304	2.6309216
C	0.0000000	5.8016997	-1.0964998
H	-0.8900506	6.4337120	-1.2440725
H	0.8900506	6.4337120	-1.2440725
C	0.0000000	4.6762493	-2.0957324
C	0.7836425	3.3653940	-1.9319854
C	-0.7836425	3.3653940	-1.9319854
H	0.0000000	5.0375151	-3.1261479
C	-1.5304889	3.1008988	-0.7223922
N	-2.2465780	3.0219314	0.1902108
C	1.5304889	3.1008988	-0.7223922

N	2.2465780	3.0219314	0.1902108
C	1.4344097	2.8736955	-3.1282949
N	1.9849466	2.6350515	-4.1245403
C	-1.4344097	2.8736955	-3.1282949
N	-1.9849466	2.6350515	-4.1245403
O	0.0000000	5.2615090	0.2314177
C	0.0000000	5.4923598	2.6135548
H	-0.8782413	5.9041551	3.1399247
H	0.8782413	5.9041551	3.1399247
C	0.0000000	6.1641037	1.2397495
O	0.0000000	7.3669260	1.0695352
I	0.0000000	0.0000000	-1.3756056

82.

C	1.3936028	-0.2140765	-3.2297187
C	-1.3856701	0.2099357	-3.2407171
C	0.5110255	-1.3049934	-3.2407171
C	0.8746447	1.0950577	-3.2407171
C	-0.5114057	1.3139336	-3.2297187
C	-0.8821971	-1.0998572	-3.2297187
H	1.5573536	1.9415250	-3.1855814
H	-2.4600868	0.3779453	-3.1855814
C	2.7954682	-0.4026653	-3.0579356
C	-1.7464524	-2.2196138	-3.0579356
C	-1.0490157	2.6222791	-3.0579356
C	-2.4231236	-3.1987615	-2.8026402
C	-1.5586469	3.6978674	-2.8026402
C	3.9817705	-0.4991059	-2.8026402
C	-3.0767682	-4.4166023	-2.3160013
H	-3.2053563	-5.1528719	-3.1228916
H	-4.0706979	-4.1877246	-1.9025583

N	-2.2547158	-5.0434592	-1.2785917
H	-2.1665015	-4.5047288	-0.4147900
C	-1.3478186	-6.0138019	-1.5969236
O	-1.4296427	-6.7067663	-2.6163219
C	-0.1629691	-6.1629962	-0.6736620
C	2.2959998	-6.3549999	0.6400180
C	0.5579794	-7.3635777	-0.7040574
C	0.3352522	-5.0739125	0.0501602
C	1.5872372	-5.1418759	0.6773951
C	1.7695686	-7.4648795	-0.0231256
H	0.1666889	-8.1903317	-1.2971300
H	-0.2269392	-4.1461202	0.0641547
H	2.3295763	-8.4007385	-0.0370313
H	3.2714707	-6.4255370	1.1258176
C	2.2569923	-4.0000272	1.3579677
C	1.9501656	-2.4926453	1.1907586
C	1.6997098	-3.2133463	2.5657122
H	3.3315323	-4.1507585	1.4791181
C	0.3277537	-3.4499422	2.9314233
N	-0.7694746	-3.7480634	3.1699944
C	0.8009980	-2.0761151	0.4315120
N	-0.1197325	-1.8252550	-0.2287661
C	2.6418161	-2.9964791	3.6362134
N	3.4784228	-2.9441294	4.4412637
C	3.0957823	-1.6287441	1.0522918
N	4.0425202	-0.9829410	0.8708187
C	-2.2865057	4.8728605	-2.3160013
H	-2.8598398	5.3523559	-3.1228916
H	-1.5913269	5.6191901	-1.9025583
N	-3.2404059	4.4743708	-1.2785917
H	-2.8179588	4.1286097	-0.4147900

C	-4.5341959	4.1741461	-1.5969236
O	-5.0934086	4.5914900	-2.6163219
C	-5.2558268	3.2226335	-0.6736620
C	-6.6515912	1.1891057	0.6400180
C	-6.6560351	3.1985646	-0.7040574
C	-4.5617632	2.2466193	0.0501602
C	-5.2466138	1.1963502	0.6773951
C	-7.3495596	2.1999484	-0.0231256
H	-7.1763798	3.9508090	-1.2971300
H	-3.4771758	2.2695953	0.0641547
H	-8.4400411	2.1828970	-0.0370313
H	-7.2004136	0.3795917	1.1258176
C	-4.5926213	0.0454010	1.3579677
C	-3.1337770	-0.4425703	1.1907586
C	-3.6326944	0.1346813	2.5657122
H	-5.2604284	-0.8098124	1.4791181
C	-3.1516144	1.4411281	2.9314233
N	-2.8611809	2.5404162	3.1699944
C	-2.1984674	0.3443730	0.4315120
N	-1.5208509	1.0163189	-0.2287661
C	-3.9159351	-0.7896403	3.6362134
N	-4.2889023	-1.5403378	4.4412637
C	-2.9584249	-1.8666540	1.0522918
N	-2.8725120	-3.0094546	0.8708187
C	5.3632739	-0.4562583	-2.3160013
H	6.0651961	-0.1994840	-3.1228916
H	5.6620248	-1.4314655	-1.9025583
N	5.4951217	0.5690884	-1.2785917
H	4.9844603	0.3761190	-0.4147900
C	5.8820145	1.8396558	-1.5969236
O	6.5230513	2.1152763	-2.6163219

C	5.4187958	2.9403628	-0.6736620
C	4.3555914	5.1658941	0.6400180
C	6.0980557	4.1650132	-0.7040574
C	4.2265110	2.8272931	0.0501602
C	3.6593765	3.9455257	0.6773951
C	5.5799910	5.2649311	-0.0231256
H	7.0096908	4.2395227	-1.2971300
H	3.7041151	1.8765250	0.0641547
H	6.1104648	6.2178415	-0.0370313
H	3.9289429	6.0459452	1.1258176
C	2.3356291	3.9546263	1.3579677
C	1.1836113	2.9352156	1.1907586
C	1.9329846	3.0786650	2.5657122
H	1.9288961	4.9605709	1.4791181
C	2.8238608	2.0088141	2.9314233
N	3.6306554	1.2076472	3.1699944
C	1.3974694	1.7317422	0.4315120
N	1.6405834	0.8089361	-0.2287661
C	1.2741190	3.7861195	3.6362134
N	0.8104795	4.4844672	4.4412637
C	-0.1373573	3.4953981	1.0522918
N	-1.1700082	3.9923957	0.8708187
H	0.9027332	-2.3194703	-3.1855814
B	-0.0000000	-0.0000000	3.6423885
F	0.3319960	1.2974013	4.0926283
F	0.9575845	-0.9362176	4.0926283
F	-1.2895805	-0.3611837	4.0926283
F	0.0000000	0.0000000	2.2112007

83.

C	1.3928933	-0.2186157	-3.2315840
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C	-1.3849663	0.2143826	-3.2427238
C	0.5068224	-1.3066073	-3.2427238
C	0.8781439	1.0922247	-3.2427238
C	-0.5071199	1.3155888	-3.2315840
C	-0.8857734	-1.0969731	-3.2315840
H	1.5636430	1.9363443	-3.1865952
H	-2.4587448	0.3859824	-3.1865952
C	2.7939465	-0.4113622	-3.0575058
C	-1.7532234	-2.2139475	-3.0575058
C	-1.0407231	2.6253097	-3.0575058
C	-2.4317104	-3.1912231	-2.7997134
C	-1.5478250	3.7015346	-2.7997134
C	3.9795355	-0.5103115	-2.7997134
C	-3.0864920	-4.4075583	-2.3105360
H	-3.2197235	-5.1434137	-3.1170239
H	-4.0784429	-4.1764037	-1.8936042
N	-2.2627812	-5.0364989	-1.2755858
H	-2.1729660	-4.4992679	-0.4108602
C	-1.3549086	-6.0044519	-1.5980023
O	-1.4373018	-6.6946499	-2.6192229
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C	-5.1010282	-1.1354793	1.5380042
C	-4.1821975	-0.5668511	2.6328888
C	-3.7320418	-0.5588193	1.1256660
C	-2.7000926	-1.4990838	0.7660893
N	-1.9819443	-2.3540083	0.4482860
C	-3.5199607	-1.4904797	3.5211557
N	-3.0762033	-2.2693102	4.2602992
C	-3.7540598	0.6919878	0.4096437
N	-3.9018579	1.6701591	-0.1995851
C	-4.5571360	0.6957160	3.2205101
N	-4.9277500	1.6974770	3.6787888
C	-0.3855252	3.7417911	-2.9208806
C	0.6162422	2.7891317	-2.9202168
C	-2.0360301	2.0010697	-2.8293824

C	0.3280959	1.4030361	-2.8746414
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C	-1.3791128	-0.4173786	-2.8746414
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C	2.7509922	0.7627189	-2.8293824
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C	2.1073379	-1.9282472	-2.9202168
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H	-6.5011770	-5.3716568	2.9973761
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H	-0.1313165	4.8036051	-2.9575379
H	1.6511326	3.1244300	-2.9603050
H	-3.0816127	1.7149301	-2.7375804
H	0.0556333	-3.5262199	-2.7375804
H	-4.0943858	-2.5155260	-2.9575379
H	-3.5314020	-0.1322922	-2.9603050
H	4.2257023	-2.2880792	-2.9575379
H	3.0259793	1.8112898	-2.7375804
H	1.8802694	-2.9921377	-2.9603050
Cl	0.0000000	0.0000000	1.9434627
O	0.9548137	1.0072918	2.4411043
O	0.3949334	-1.3305388	2.4411043
O	-1.3497471	0.3232471	2.4411043
O	-0.0000000	-0.0000000	0.4775255

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C	0.3727305	5.2002890	-3.4192814
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H	1.0056307	5.8221477	-4.0687853
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H	1.3235118	8.8151920	-0.0189729
H	2.3164049	4.6432692	-0.1601953
H	1.7391054	8.8198155	2.4534450
H	2.3274601	6.7054698	3.6180920
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C	1.4450878	-3.5218660	4.6834033
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H	-4.3831266	-3.3131722	-3.6412027
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N	-5.1588390	-2.1617831	-2.0427932
H	-4.4430557	-2.0675107	-1.3218984
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O	-7.4061140	-2.3573875	-2.4739461
C	-6.6924245	-1.8456451	-0.2290016
C	-6.9182682	-1.4508656	2.5345329
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O	0.9240652	-0.8609017	3.3308224
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H	2.7765430	3.9238805	-3.6206608
C	1.9367597	3.2272774	-3.6529055
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C	2.1645997	1.8652559	-3.7001033
C	-0.4317736	2.8219111	-3.6525739
C	1.1029519	0.9289681	-3.7096265
C	0.6194400	3.7241093	-3.6190218
C	-0.2314719	1.4230627	-3.7034245
H	-2.9104376	2.0089935	-3.7191980

H	-1.4438257	3.2208628	-3.6020383
C	-1.1166725	-0.9119919	-3.7034245
C	-2.2279599	-1.7848825	-3.6525739
C	-1.3559859	0.4907003	-3.7096265
C	-3.5348933	-1.3256038	-3.6190218
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H	-4.7864517	0.4426166	-3.6206608
C	-2.6976588	0.9419704	-3.7001033
C	2.9154532	-2.3985054	-3.6190218
C	0.2530341	-1.4196684	-3.7096265
C	1.8265243	-3.2909218	-3.6529055
C	2.6597335	-1.0370286	-3.6525739
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C	-0.5853198	-4.0620875	2.5746799
C	0.3842101	-4.8390801	-1.2836771
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C	-0.1668806	-3.5584068	-1.8535665
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C	2.0199890	-3.0303166	-3.0800167
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C	1.4171648	-2.2133636	-0.3667990
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C	-0.6090951	-1.1373988	-1.1479057
N	-1.3523060	-0.2533196	-1.0227701
C	-0.0700480	-2.0426768	-3.8722143
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C	-0.4221484	-5.4775185	2.2763422
H	0.1441211	-6.0017255	3.0581681
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O	1.4034145	-6.2175529	0.8230350
C	0.5379688	0.6349570	3.2452181
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H	1.4468011	1.1567879	3.5403033
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C	-0.4958832	2.8006489	2.7223692
C	-0.3839922	3.9956058	2.5316285
C	0.5774171	4.8912440	-1.3881705
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H	1.6332278	5.1912224	-1.4810878
C	0.3314021	3.6340693	-2.1856181
C	0.6767329	2.2390632	-1.6647914
C	-0.8322002	2.6840246	-1.9077967
H	0.5334651	3.7582269	-3.2513469

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C	1.2040150	1.2522328	-2.5770402
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C	-1.4787436	2.1068460	-3.0639159
N	-1.9879837	1.6863055	-4.0203275
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H	0.4832436	5.9037430	2.8683793
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O	0.3845266	6.8699344	0.3871019

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C	1.2780402	-0.3672126	-3.9821768
C	-1.2413457	0.8839227	-3.9922161
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C	-1.1593823	-0.5150060	-3.8872121
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C	2.5393866	-1.0176449	-3.8709970
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C	-0.1656749	3.0839227	-3.9893099
C	-3.2426736	-2.0500380	-3.3763243
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H	-5.2250311	-2.3929370	-2.7298865
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C	-3.4048767	-4.9064061	0.3125984
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C	-0.0177018	-4.4037166	1.9328536
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H	0.7129734	-5.1893480	1.7215046
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C	-0.4619295	-2.0181700	1.1521610
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C	1.7108136	-3.7768500	3.6900519
N	2.7159534	-4.0826403	4.1866797
C	1.8045478	-2.9244588	0.9117965
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H	-0.2439216	4.9666889	-1.3016736
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H	-2.4769247	6.3063329	3.2744161
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C	-3.7325460	2.3512111	1.1484348
C	-3.1296032	1.2407287	0.2839194
C	-3.0332248	1.1886935	1.8683405
H	-4.8210977	2.2738447	1.2178334
C	-1.7115099	1.4019915	2.3918181
N	-0.6326961	1.5891269	2.7740648
C	-1.8889968	1.4745370	-0.4082418
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C	-3.8285786	0.1925918	2.5371803
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C	4.7889760	-2.2971665	-3.2265315
H	5.6946370	-1.9534404	-3.7497006
H	4.7082975	-3.3840885	-3.3934606
N	4.9767382	-1.9973689	-1.8074297
H	4.1729115	-2.1111539	-1.1887058

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C	5.4246705	0.4994292	2.4918343
C	6.6891449	-1.0484770	1.1244647
C	4.8455318	0.1916982	0.1627735
C	4.6258645	0.8273501	1.3859750
C	6.4524998	-0.4343663	2.3563164
H	7.5004245	-1.7668184	1.0045180
H	4.2325804	0.4288731	-0.7071547
H	7.0697224	-0.6854698	3.2190572
H	5.2433157	0.9770407	3.4563784
C	3.6008648	1.9015845	1.5386993
C	2.2205602	1.8588864	0.8740017
C	2.3828918	1.7067756	2.4495027
H	3.9864385	2.9230194	1.6028885
C	2.1014375	0.3847325	2.9457544
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C	1.9918995	2.8175971	3.2786466
N	1.7620511	3.7513934	3.9313373
C	1.6318942	3.0841908	0.3968984
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H	0.1728871	-2.2154987	-3.7960814

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C	-0.8065008	5.0100311	-2.7247499
H	-1.8964132	5.0239534	-2.8608254
H	-0.3609021	5.7881770	-3.3586738
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C	1.1523840	5.8648373	0.3480236
C	2.3719530	5.1754328	2.7707099
C	1.2081299	6.7939343	1.3895168
C	1.7308302	4.6012705	0.5102783
C	2.3486553	4.2550131	1.7134839
C	1.8033595	6.4393803	2.6031813
H	0.7752277	7.7847813	1.2499835
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C	4.5685439	-3.4539600	0.2863062
C	3.4016147	-3.2174486	2.8258248
C	5.2940391	-2.8921232	1.3421228
C	3.2700817	-3.9098394	0.5118581
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C	4.7207031	-2.8088971	2.6143603
H	6.2980643	-2.5044347	1.1668679
H	2.7089545	-4.3179105	-0.3310734
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H	2.9431930	-3.0860735	3.8062301
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C	0.2845149	-3.3169961	0.8636600
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C	-3.0564391	-2.2494826	-2.7388263
C	-3.6081164	-0.9524019	-2.7427254
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C	-2.7907926	0.1531801	-2.8807733
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C	2.8630628	-0.5108191	-3.2696909
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H	0.5752090	-3.6073474	-3.4516127
H	-1.2737658	-3.3925605	-2.9061614

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