

Supporting information for

Investigating Inclusion Complexes using Quantum Chemical Methods

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Some illustrative examples:
Binding Energy:

	E(AB)	E(A)	E(B)
2H ₂ @C ₆₀ (PBE/TQZP)	-2286.58955	-1.16670	-2284.28034
C10@2 (BLYP-D3/TZVP)	-8418.55309	-8024.22719	-394.25259
benzene@2 (BLYP-D3/TZVP)	-8256.48911	-8024.22719	-232.24097

Non-Additivity:

C14@2 B97-D/TZVP kcal/mol

E(ABC) = -115.2079

E(AB) = -57.1839

E(AC) = -32.6097

E(BC) = -26.5638

E3 = 0.8707

Deformation energy:

C14@2, A=C14

$E=E(A)_{AB}^{OPT}-E(A)_A^{OPT} = -551.37791 \text{ Eh} - (-551.38225) \text{ Eh} = 2.723 \text{ kcal/mol}$

H2

PBE-D2/def2-TZVPP E(scF)= -1.166697295511 a.u. E(D2)= -0.00000083 a.u.

Cartesian koordinaten (in Å):

H	-0.37520085	0.00000000	0.00000000
H	0.37520085	0.00000000	0.00000000

C60

PBE-D2/def2-TZVPP E(scF)= -2284.280338455 a.u. E(D2)= -0.11483158 a.u.

Cartesian koordinaten (in Å):

C	-3.30431198	-1.28050561	-0.19744092
C	-3.34344190	-0.60454879	1.02619308
C	-3.28120183	0.84512290	1.05671046
C	-3.18209850	1.56604382	-0.13751752
C	-3.14148970	0.86453971	-1.40739786
C	-3.20146311	-0.53233802	-1.43680387
C	-2.48877786	1.23585993	2.20811915
C	-1.62610895	2.33328807	2.12336799
C	-1.52326008	3.08145566	0.88400505
C	-2.28682566	2.70494844	-0.22547179
C	-1.69290781	2.70732610	-1.54971084
C	-0.35705361	3.08612440	-1.71624710
C	0.43537036	3.47686143	-0.56483842
C	-0.13691826	3.47457036	0.71117467
C	0.50107678	2.34180395	-2.61954796
C	1.82385451	2.27252564	-2.02640990
C	1.78324571	2.97402975	-0.75652957
C	-0.00789830	1.24579177	-3.32341626
C	0.78666800	0.03907832	-3.46074869
C	2.06127297	-0.02767701	-2.88921147

C	2.58948440	1.10975813	-2.15874098
C	-1.39424013	0.85267707	-3.15058589
C	-1.45648019	-0.59699462	-3.18110328
C	-0.10860484	-1.09982630	-3.37279443
C	0.30333122	-2.26400977	-2.71650605
C	-0.61703924	-2.96936101	-1.84372258
C	-1.91582783	-2.48484139	-1.65901241
C	-2.34333272	-1.27665847	-2.34010472
C	-2.22111924	1.56989096	-2.28018133
C	-2.50974568	-2.48721905	-0.33477335
C	2.48877786	-1.23585993	-2.20811915
C	1.62610895	-2.33328807	-2.12336799
C	1.52326008	-3.08145566	-0.88400505
C	0.13691826	-3.47457036	-0.71117467
C	-0.43537036	-3.47686143	0.56483842
C	-1.78324571	-2.97402975	0.75652957
C	3.34344190	0.60454879	-1.02619308
C	3.28120183	-0.84512290	-1.05671046
C	3.18209850	-1.56604382	0.13751752
C	2.28682566	-2.70494844	0.22547179
C	3.14148970	-0.86453971	1.40739786
C	3.20146311	0.53233802	1.43680387
C	3.30431198	1.28050561	0.19744092
C	2.50974568	2.48721905	0.33477335
C	0.61703924	2.96936101	1.84372258
C	1.91582783	2.48484139	1.65901241
C	2.34333272	1.27665847	2.34010472
C	2.22111924	-1.56989096	2.28018133
C	1.39424013	-0.85267707	3.15058589
C	1.45648019	0.59699462	3.18110328
C	0.10860484	1.09982630	3.37279443
C	-0.30333122	2.26400977	2.71650605
C	1.69290781	-2.70732610	1.54971084
C	0.35705361	-3.08612440	1.71624710
C	-0.50107678	-2.34180395	2.61954796
C	0.00789830	-1.24579177	3.32341626
C	-0.78666800	-0.03907832	3.46074869
C	-2.06127297	0.02767701	2.88921147
C	-2.58948440	-1.10975813	2.15874098
C	-1.82385451	-2.27252564	2.02640990

H2@C60

PBE-D2/def2-TZVPP E(scf)= -2285.447139215 a.u. E(D2)= -0.12383968 a.u.

Cartesian coordinaten (in Å)

C	-0.35036723	-3.03080351	-1.81213951
C	-1.67808704	-2.59839671	-1.73895310
C	-2.10080292	-1.42453806	-2.47968739
C	-1.18050370	-0.72564084	-3.26690464
C	0.19740163	-1.17426695	-3.34267890
C	0.60483287	-2.30541779	-2.62874865
C	-3.05606913	-0.69889606	-1.66323223
C	-3.05588069	0.69948652	-1.66332980
C	-2.10041918	1.42475765	-2.47988614
C	-1.18030864	0.72550264	-3.26700580
C	-1.67738792	2.59860544	-1.73931584
C	-2.37129244	2.59887356	-0.46494752
C	-3.22320911	1.42518917	-0.41792889
C	-3.38481257	0.72610372	0.78216671
C	-2.70027723	1.17455991	1.98038635
C	-1.87940502	2.30562299	1.93510557
C	-1.71184599	3.03107600	0.68971780
C	-0.33384356	3.47944271	0.61375516
C	0.35036676	3.03080280	1.81213953
C	-0.60483290	2.30541766	2.62874800
C	-2.27746092	0.00049666	2.72102702
C	-1.04925438	0.00037802	3.38970289
C	-0.19740182	1.17426720	3.34267705
C	-0.34955142	3.03064430	-1.81256238
C	0.33477951	3.47926755	-0.61424107
C	1.71266194	3.03051978	-0.69014104
C	2.37199235	2.59830101	0.46458519
C	1.67808843	2.59839698	1.73895352
C	2.10080262	1.42453895	2.47968775

C	1.18050288	0.72564087	3.26690449
C	0.60545336	2.30488780	-2.62907022
C	1.88002559	2.30485031	-1.93542792
C	-3.38500814	-0.72508310	0.78226809
C	-2.70059350	-1.17355630	1.98055041
C	-0.19771786	-1.17374696	3.34284138
C	1.18030736	-0.72550223	3.26700596
C	3.05606949	0.69889602	1.66323368
C	3.22359403	1.42438084	0.41773101
C	2.70059462	1.17355805	-1.98055091
C	3.38501007	0.72508386	-0.78226809
C	0.19771769	1.17374725	-3.34284238
C	3.05588148	-0.69948604	1.66333126
C	2.10041923	-1.42475781	2.47988687
C	-0.60545352	-2.30488763	2.62907024
C	-1.88002585	-2.30484664	1.93542783
C	-3.22359310	-1.42437977	-0.41772995
C	2.27746102	-0.00049619	-2.72102836
C	1.04924660	-0.00037778	-3.38970481
C	-1.71266214	-3.03051910	0.69014120
C	-2.37199231	-2.59830024	-0.46458484
C	0.34955079	-3.03064434	1.81256319
C	1.67738797	-2.59860581	1.73931643
C	3.22321055	-1.42518991	0.41792988
C	3.38481498	-0.72610382	-0.78216689
C	2.70027894	-1.17456187	-1.98038698
C	-0.33477991	-3.47926757	0.61424070
C	2.37129309	-2.59887441	0.46494817
C	1.87940525	-2.30562761	-1.93510626
C	0.33384276	-3.47944378	-0.61375490
C	1.71184627	-3.03107736	-0.68971793
H	0.07660613	-0.00003593	-0.36748834
H	-0.07660612	0.00003601	0.36748847

2H2@C60
PBE-D2/def2-TZVPP E(scf)= -2286.589550234 a.u. E(D2)= -0.14077404 a.u.
Cartesian coordinaten (in Å)

C	0.76749667	-1.57455335	-3.07871444
C	1.94480012	-0.85705015	-2.83935963
C	2.83186859	-1.24484997	-1.75685132
C	2.50042409	-2.33763968	-0.94959965
C	1.27725550	-3.08123339	-1.19768265
C	0.42733037	-2.70884420	-2.24286905
C	3.37775397	-0.03665678	-1.16122460
C	3.57271006	0.03521672	0.22533782
C	3.22413941	-1.10140917	1.06382557
C	2.69824784	-2.26429877	0.48631033
C	2.64772716	-0.59192229	2.29700912
C	2.63701253	0.85672531	2.22258679
C	3.20560293	1.24534204	0.94385430
C	2.66639789	2.33709397	0.25261508
C	1.55265294	3.08116653	0.81527657
C	1.01217965	2.70847779	2.04845764
C	1.56341824	1.57403618	2.76348850
C	0.46288205	0.87492229	3.40063095
C	-0.76746037	1.57459129	3.07865108
C	-0.42706535	2.70892123	2.24266056
C	0.67034786	3.46741546	-0.26969173
C	-0.71685260	3.46771650	-0.08266963
C	-1.27720655	3.08192349	1.19773700
C	1.58260819	-1.26487558	2.90817164
C	0.47212540	-0.51941717	3.47155512
C	-0.74839548	-1.26442281	3.22269878
C	-1.93494554	-0.59063740	2.91274300
C	-1.94497863	0.85707419	2.83983168
C	-2.83354491	1.24553780	1.75797363
C	-2.50109015	2.33847605	0.94981783
C	1.04672156	-2.47319429	2.31177852
C	-0.39260744	-2.47287897	2.50603670
C	2.46988696	2.26294040	-1.18354343
C	1.23662963	2.96117393	-1.50474583

C	-1.59333796	2.96191466	-1.12238957
C	-2.69766406	2.26411946	-0.48642645
C	-3.37767307	0.03637248	1.16122832
C	-2.81589678	-1.09785631	1.87575323
C	-1.23671548	-2.96058436	1.50463404
C	-2.46934283	-2.26228580	1.18330294
C	1.59345083	-2.96204487	1.12240871
C	-3.57271339	-0.03523558	-0.22532754
C	-3.22173105	1.10070799	-1.06318132
C	-1.04694010	2.47324413	-2.31177778
C	0.39234980	2.47297973	-2.50586751
C	2.81766386	1.09842933	-1.87696024
C	-0.67032135	-3.46715543	0.26983745
C	0.71679511	-3.46742484	0.08250709
C	0.74842604	1.26445326	-3.22267938
C	1.93523213	0.59060568	-2.91327568
C	-1.58250869	1.26490633	-2.90778938
C	-2.64687190	0.59195423	-2.29625894
C	-3.20802687	-1.24620564	-0.94442892
C	-2.66709404	-2.33745771	-0.25248375
C	-1.55283396	-3.08138564	-0.81529745
C	-0.47223956	0.51948859	-3.47139510
C	-2.63782845	-0.85678477	-2.22328007
C	-1.01198714	-2.70845885	-2.04847631
C	-0.46272907	-0.87487230	-3.40078522
C	-1.56351210	-1.57406366	-2.76380806
H	-1.04419790	-0.33010710	-0.17997156
H	-1.05199454	0.31475208	0.18731361
H	1.04468957	-0.30155438	0.22085978
H	1.05123466	0.29036687	-0.22676415

3H2@C60
PBE-D2/def2-TZVPP E(scf)= -2287.722572638 a.u. E(D2)= -0.15483641 a.u.

Cartesian coordinates (in Å)			
C	1.06514161	-3.01780276	-1.52724711
C	2.28058660	-2.32101403	-1.45379747
C	2.91566176	-2.08475998	-0.16574976
C	2.28888354	-2.54800111	1.00076159
C	1.02799230	-3.27235171	0.91935490
C	0.42751702	-3.50866125	-0.32024807
C	3.50232327	-0.75027586	-0.19384154
C	3.43955736	0.06599890	0.94563049
C	2.79515839	-0.42098101	2.15283642
C	2.23126334	-1.70125164	2.17938734
C	2.09209461	0.69221889	2.76881650
C	2.29366619	1.86893076	1.94628368
C	3.12165459	1.48183628	0.81934945
C	2.87120141	2.04002921	-0.43708220
C	1.79905721	3.01031058	-0.61110159
C	1.00809274	3.39742106	0.47967331
C	1.26094349	2.80284066	1.78146132
C	-0.01822088	2.58597630	2.42995368
C	-1.06554076	3.04013387	1.53166304
C	-0.43328195	3.54977005	0.32327041
C	1.18081086	2.75903884	-1.90005002
C	-0.20395461	2.89950779	-2.05192011
C	-1.02815054	3.30120557	-0.92327612
C	0.85909901	0.48626940	3.39250659
C	-0.21343063	1.44677056	3.21855234
C	-1.46058239	0.71000923	3.14049746
C	-2.46783559	1.13506771	2.27237411
C	-2.26471605	2.31716518	1.45239692
C	-2.88269102	2.06859666	0.16352745
C	-2.27323183	2.54883610	-1.00047675
C	0.27455753	-0.84111418	3.42021163
C	-1.16058297	-0.70393370	3.26367337
C	2.92029146	1.19544798	-1.61549683
C	1.87335422	1.63931362	-2.51670258
C	-0.94340847	1.91540433	-2.82391189
C	-2.22091430	1.69736771	-2.17508249
C	-3.47015793	0.73626098	0.19137513

C	-3.21515475	0.15904212	1.49747356
C	-1.88089347	-1.64361708	2.51831711
C	-2.93662746	-1.20944073	1.62015253
C	0.94536106	-1.91137816	2.82331632
C	-3.43300191	-0.07844892	-0.94602301
C	-2.78665655	0.41550299	-2.14878687
C	-0.27623284	0.84135915	-3.42010549
C	1.15922515	0.70086522	-3.26445127
C	3.22744066	-0.16816059	-1.49862444
C	-1.18728234	-2.75602930	1.89809071
C	0.20101575	-2.88254124	2.04613488
C	1.46446717	-0.71154314	-3.13894490
C	2.47856425	-1.13991791	-2.27465682
C	-0.86078775	-0.48528927	-3.39236495
C	-2.09460926	-0.69662649	-2.76944971
C	-3.14587550	-1.50177871	-0.82320577
C	-2.90543123	-2.06227138	0.44085678
C	-1.81687910	-3.01619031	0.61417693
C	0.21468710	-1.44334209	-3.21942443
C	-2.30962914	-1.87856810	-1.95209168
C	-1.01458552	-3.37756679	-0.47679015
C	0.01644908	-2.57634615	-2.42796496
C	-1.26741685	-2.79853918	-1.78305588
H	-0.72566843	-0.97772218	0.01298790
H	-1.15627690	-0.37225239	-0.02392891
H	0.90305363	-0.81849617	-0.02540832
H	1.21322109	-0.14682807	0.05311677
H	0.25828336	1.18865317	-0.06812987
H	-0.47301124	1.11764906	0.04956186

resorcinarene monomer

Energy =			
C	4.6284967	0.3398127	-4.1638920
C	4.4419037	0.9093404	-2.7821694
C	3.4186538	1.8520642	-2.8142090
C	2.8006514	1.8404799	-4.1898777
N	3.6360826	0.9955002	-4.9310351
N	5.0548748	0.5404979	-1.6542239
C	4.6535121	1.2037109	-0.5812339
C	3.7564246	2.3126021	-0.6556003
N	3.0793252	2.5999718	-1.7590875
O	5.0422231	0.7570634	0.6575729
C	4.1159299	-0.1844042	1.1694480
C	3.2901562	0.1533449	2.2516925
C	2.4648661	-0.8617059	2.7622322
C	2.4017857	-2.1498481	2.2195392
C	3.1766143	-2.3809961	1.0724428
C	4.0590889	-1.4387442	0.5645269
O	3.0898872	-3.6407110	0.4574932
C	2.3126021	-3.7564246	-0.6556003
C	1.2037109	-4.6535121	-0.5812339
N	0.5404979	-5.0548748	-1.6542239
C	0.9093404	-4.4419037	-2.7821694
C	1.8520642	-3.4186538	-2.8142090
N	2.5999718	-3.0793252	-1.7590875
C	0.3398127	-4.6284967	-4.1638920
N	0.9955002	-3.6360826	-4.9310351
C	1.8404799	-2.8006514	-4.1898777
O	0.7570634	-5.0422231	0.6575729
C	-0.1844042	-4.1159299	1.1694480
C	-1.4387442	-4.0590889	0.5645269
C	-2.3809961	-3.1766143	1.0724428
C	-2.1498481	-2.4017857	2.2195392
C	-0.8617059	-2.4648661	2.7622322
C	0.1533449	-3.2901562	2.2516925
C	-3.2731257	-1.5627520	2.8390695
C	-3.2287208	-1.5678905	4.3786820
O	-3.6407110	-3.0898872	0.4574932
C	-3.7564246	-2.3126021	-0.6556003
C	-4.6535121	-1.2037109	-0.5812339
N	-5.0548748	-0.5404979	-1.6542239
C	-4.4419037	-0.9093404	-2.7821694
C	-3.4186538	-1.8520642	-2.8142090
N	-3.0793252	-2.5999718	-1.7590875
C	-4.6284967	-0.3398127	-4.1638920
N	-3.6360826	-0.9955002	-4.9310351
C	-2.8006514	-1.8404799	-4.1898777
C	1.5627520	-3.2731257	2.8390695
C	1.5678905	-3.2287208	4.3786820
O	-5.0422231	-0.7570634	0.6575729
C	-4.1159299	0.1844042	1.1694480
C	-4.0590889	1.4387442	0.5645269
C	-3.1766143	2.3809961	1.0724428
C	-2.4017857	2.1498481	2.2195392
C	-2.4648661	0.8617059	2.7622322
C	-3.2901562	-0.1533449	2.2516925
O	-3.0898872	3.6407110	0.4574932
C	-2.3126021	3.7564246	-0.6556003
N	-2.5999718	3.0793252	-1.7590875
C	-1.8520642	3.4186538	-2.8142090
C	-0.9093404	4.4419037	-2.7821694
N	-0.5404979	5.0548748	-1.6542239
C	-1.2037109	4.6535121	-0.5812339
C	-0.3398127	4.6284967	-4.1638920
N	-0.9955002	3.6360826	-4.9310351
C	-1.8404799	2.8006514	-4.1898777
O	-2.3933381	1.7982113	-4.5913398
O	0.4690489	5.4259352	-4.5712629
O	-0.7570634	5.0422231	0.6575729
C	0.1844042	4.1159299	1.1694480
C	-0.1533449	3.2901562	2.2516925
C	0.8617059	2.4648661	2.7622322
C	2.1498481	2.4017857	2.2195392

C	2.3809961	3.1766143	1.0724428
C	1.4387442	4.0590889	0.5645269
C	-1.5627520	3.2731257	2.8390695
C	-1.5678905	3.2287208	4.3786820
O	3.6407110	3.0898872	0.4574932
C	3.2731257	1.5627520	2.8390695
C	3.2287208	1.5678905	4.3786820
O	-1.7982113	-2.3933381	-4.5913398
O	-5.4259352	0.4690489	-4.5712629
O	2.3933381	-1.7982113	-4.5913398
O	-0.4690489	-5.4259352	-4.5712629
O	1.7982113	2.3933381	-4.5913398
O	5.4259352	-0.4690489	-4.5712629
H	-4.6769391	1.6651861	-0.2971470
H	-1.8540805	0.6375424	3.6316059
H	-2.0367950	4.2117933	2.5420514
H	-4.2117933	-2.0367950	2.5420514
H	-3.2754521	-2.5991043	4.7481802
H	-2.3156803	-1.1100135	4.7762156
H	-4.0850450	-1.0095472	4.7743118
H	-1.6651861	-4.6769391	-0.2971470
H	-0.6375424	-1.8540805	3.6316059
H	2.0367950	-4.2117933	2.5420514
H	1.0095472	-4.0850450	4.7743118
H	1.1100135	-2.3156803	4.7762156
H	2.5991043	-3.2754521	4.7481802
H	4.6769391	-1.6651861	-0.2971470
H	1.8540805	-0.6375424	3.6316059
H	4.2117933	2.0367950	2.5420514
H	4.0850450	1.0095472	4.7743118
H	3.2754521	2.5991043	4.7481802
H	2.3156803	1.1100135	4.7762156
H	-1.0095472	4.0850450	4.7743118
H	-1.1100135	2.3156803	4.7762156
H	-2.5991043	3.2754521	4.7481802
H	1.6651861	4.6769391	-0.2971470
H	0.6375424	1.8540805	3.6316059
H	3.3827812	0.6638508	-5.8539857
H	0.6638508	-3.3827812	-5.8539857
H	-3.3827812	-0.6638508	-5.8539857
H	-0.6638508	3.3827812	-5.8539857

resorcinarene dimer (2)
B97-D2/TZVP E(DFT-D) = -8020.044164180 a.u.
Cartesian coordinaten (in Å):

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C	-3.3966686	-4.4736611	-1.0599129
C	-1.9900933	-4.6978849	-0.5605882
N	-4.5314978	-5.0370180	-0.6363820
C	-5.6119964	-4.6279199	-1.2860277
C	-5.5442539	-3.7600488	-2.4184932
N	-4.4288159	-3.1307876	-2.7623041
O	-6.8478466	-5.0018986	-0.8225377
C	-7.3623984	-4.0803657	0.1204627
C	-6.7718122	-4.0421925	1.3821319
C	-7.2913981	-3.1727989	2.3311767
C	-8.4271794	-2.3841884	2.0936775
C	-8.9587665	-2.4328046	0.8004344
C	-8.4449943	-3.2534146	-0.2163105
C	-9.0333817	-3.2316706	-1.6255727
C	-8.4074614	-2.1099749	-2.4610840
C	-7.2622672	-2.3477294	-3.2360484
C	-6.7328612	-1.3990743	-4.0998112
C	-7.3232837	-0.1375181	-4.1453019
C	-8.4148724	0.1999247	-3.3305447
C	-8.9381928	-0.8166431	-2.5157578
C	-9.0427433	-1.5409926	3.2153808

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C	-7.3545997	0.1916952	4.0561891
C	-6.7555174	1.4493405	4.0174974
C	-7.2721060	2.4028147	3.1508114
C	-8.4117447	2.1739166	2.3657191
C	-8.9526153	0.8845032	2.4153439
O	-6.7003179	-3.1085203	3.6037343
C	-5.5626334	-2.3711166	3.7350967
C	-5.6149031	-1.2325945	4.5958792
N	-4.5260261	-0.5900583	4.9941884
C	-3.3986218	-1.0276749	4.4270198
C	-3.3798420	-2.0159570	3.4482105
N	-4.4538882	-2.7297145	3.1022063
C	-1.9862835	-0.5402204	4.6395042
N	-1.2298624	-1.2571075	3.6806121
C	-1.9815524	-2.1234026	2.9062439
O	-6.8440881	-0.7560139	4.9750563
O	-6.6741170	3.6719682	3.0863223
C	-5.5369742	3.7982481	2.3475232
C	-5.5846924	4.6658677	1.2140692
N	-4.4940180	5.0602746	0.5723338
C	-3.3701330	4.4817380	1.0043389
C	-3.3578473	3.4957174	1.9854672
N	-4.4329621	3.1536968	2.6992947
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N	-1.2073207	3.7156198	1.2253821
C	-1.9647960	2.9400748	2.0852654
C	-9.0203755	3.3009444	1.5243532
C	-10.5600465	3.2624628	1.5159246
O	-6.8122672	5.0528689	0.7390011
C	-7.3265485	4.1346975	-0.2075936
C	-8.4191413	3.3172733	0.1203396
C	-8.9310833	2.5009064	-0.9007199
C	-8.3884678	2.4464293	-2.1890609
C	-7.2427676	3.2240289	-2.4166202
C	-6.7245503	4.0895905	-1.4636880
O	-6.6407028	3.1530708	-3.6836758
C	-5.5100364	2.4035891	-3.8069090
C	-5.5674649	1.2688723	-4.6725287
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C	-3.3551926	1.0382387	-4.4853426
C	-3.3340381	2.0220505	-3.5021041
N	-4.4029661	2.7468175	-3.1627296
C	-1.9470129	0.5337024	-4.6860287
N	-1.1909232	1.2379837	-3.7173211
C	-1.9395591	2.1103140	-2.9466416
C	-9.0027395	1.6094637	-3.3160862
C	-10.5425530	1.6154766	-3.2794345
O	-6.7986966	0.8054361	-5.0612761
O	-6.6739580	-3.6210612	-3.1664530
O	-1.5444377	2.7873360	-2.0081735
O	-1.5098317	-0.2665676	-5.4760092
O	-1.5773230	1.9972242	2.7606945
O	-1.5118922	5.4774999	-0.2782408
O	-1.5857866	-2.8091587	1.9743062
O	-1.5463903	0.2567960	5.4314032
O	-1.5529108	-2.0191102	-2.8066779
O	-1.5630252	-5.4964208	0.2366884
C	-10.5726209	-3.1794854	-1.6308416
C	-10.5821682	-1.5337001	3.1675314
O	1.5666374	3.3757244	0.5791616
C	1.9727147	3.5637341	-0.5589724
C	3.3729115	3.8883736	-0.9979026
C	3.4080060	3.8947855	-2.3882917
C	2.0040895	3.6882341	-2.9026213
N	1.2347035	3.5009317	-1.7280804
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C	5.5524122	4.3532279	-0.9176067
C	5.6218961	4.1726493	-2.3329005
N	4.5431894	4.0013320	-3.0839296
O	6.6815450	4.7781728	-0.2852664
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C	6.7368965	3.8490182	1.9393868

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C	8.4146237	2.1659621	2.5145198
C	8.9389131	2.3177753	1.2210689
C	8.4107814	3.2018644	0.2739961
C	9.0391283	3.4124738	-1.1077227
C	8.4508058	2.4386453	-2.1265629
C	7.3685256	2.7915114	-2.9469350
C	6.7745030	1.8780622	-3.8159746
C	7.2917413	0.5915577	-3.8804346
C	8.4291855	0.1971657	-3.1598608
C	8.9629193	1.1399483	-2.2745206
C	8.9997254	1.1499577	3.4934305
C	8.3832030	-0.2361211	3.2764329
C	7.2349301	-0.6277738	3.9809745
C	6.7130091	-1.9118840	3.9072295
C	7.3150124	-2.8260105	3.0446812
C	8.4113338	-2.4767245	2.2415290
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O	6.8001645	2.9532820	4.1719051
C	5.5674385	2.3531662	4.2194070
C	5.5064444	0.9371227	4.3964755
N	4.3982402	0.2436395	4.1748908
C	3.3319783	1.0013654	3.9066561
C	3.3560385	2.3920285	3.9192955
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C	1.9498431	2.8957426	3.7030733
O	6.6348770	0.3127890	4.8344897
O	6.7997142	-4.1436816	3.0110779
C	5.5726903	-4.2026246	2.4010029
C	5.5246803	-4.3896313	0.9856976
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C	3.3430010	-3.9281363	1.0301983
C	3.3580176	-3.9256923	2.4211001
N	4.4825311	-4.0275814	3.1344716
C	1.9477767	-3.6097699	0.5689279
N	1.1935253	-3.5410903	1.7276512
C	1.9465946	-3.7191415	2.9140125
C	9.0113922	-3.4530114	1.2319361
C	10.5511268	-3.4216368	1.2113738
O	6.6638578	-4.8158419	0.3721673
C	7.2654752	-3.9556252	-0.5612645
C	8.4043050	-3.2415634	-0.1590150
C	8.9483892	-2.3579878	-1.0974977
C	8.4443590	-2.2048837	-2.3987026
C	7.3582214	-3.0170559	-2.7585776
C	6.7548700	-3.8848715	-1.8501853
O	6.8539552	-2.9875129	-4.0807934
C	5.6224969	-2.3869492	-4.1474068
C	5.5647338	-0.9705801	-4.3241630
N	4.4521006	-0.2775216	-4.1234247
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C	3.4061090	-2.4264962	-3.8875311
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C	1.9965671	-2.9316544	-3.6978822
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O	6.8582838	4.1115751	-2.9237342
O	1.5634527	-4.0575893	-3.7070794
O	1.5799629	0.5518465	-3.3728351
O	1.5058476	-3.7105081	4.0370039
O	1.5562406	-3.4302955	-0.5755172
O	1.5154811	4.0210724	3.7045059
O	1.5442597	-0.5878493	3.3657743
O	1.5793174	3.6853850	-4.0318053
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C	10.5394986	1.1175034	3.4729393
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H	9.8087807	1.7285276	0.9474069

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H	10.9057984	0.4182402	4.2335006
H	10.9427086	0.8005000	2.5040622
H	10.9330415	2.1173118	3.6903401
H	5.8466467	-2.1946341	4.4947318
H	9.8012143	-0.9015896	1.8185692
H	8.7136735	-4.4550159	1.5508954
H	10.9385149	-3.6356164	2.2144015
H	10.9498553	-2.4502525	0.8968057
H	10.9282209	-4.1800747	0.5154870
H	5.8960839	-4.4795157	-2.1412160
H	9.8150024	-1.7704225	-0.8102081
H	8.7584930	-1.5089645	-4.3731621
H	10.9804033	-2.1605434	-3.5377700
H	10.9645134	-0.4603137	-4.0779738
H	10.9744460	-0.8460510	-2.3489805
H	10.9812741	3.5904598	-2.0611054
H	10.9696044	2.4038923	-0.7445845
H	10.9470561	4.1334533	-0.3620829
H	5.9181456	2.1635821	-4.4166665
H	9.8276336	0.8585235	-1.6813855
H	0.2269619	-1.7830034	-3.2975891
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H	0.2295865	3.2790778	-1.7640908
H	-5.9153170	-4.6666531	1.6106527
H	-9.8223944	-1.8149997	0.5739232
H	-8.7413266	-4.1716114	-2.1006208
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H	-5.8604112	4.7062486	-1.6846985
H	-9.8025380	1.8914177	-0.6816765
H	-8.7011311	2.0834570	-4.2534629
H	-10.9105994	2.6465317	-3.3349814
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H	-10.9730855	-4.0306183	-1.0680309
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H	-9.8090203	-0.5898880	-1.9083145
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C1@2

B97-D2/TZVP E(DFT-D) = -8060.561911172 a.u.

Cartesian coordinates (in Å):

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N	1.2150013	3.8055120	0.9911092
N	4.5141093	5.0823644	0.2655732
C	5.5991997	4.7251425	0.9379964
C	5.5407794	3.9361365	2.1271862
N	4.4299319	3.3269493	2.5185615
O	6.8313285	5.0718424	0.4444686
C	7.3438683	4.0912220	-0.4380612
C	8.4314110	3.2923442	-0.0531589
C	8.9424316	2.4077771	-1.0162563

C	8.4030617	2.2703447	-2.2998693
C	7.2622388	3.0366749	-2.5824415
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O	6.6626058	2.8849431	-3.8436638
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C	5.5824875	0.9403729	-4.7003328
N	4.4956333	0.2638699	-5.0440894
C	3.3695828	0.7300402	-4.4975495
C	3.3507973	1.7831993	-3.5890397
N	4.4219813	2.5268506	-3.3015574
C	1.9599792	0.2163682	-4.6615534
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C	7.3325531	-0.4357737	-4.0804887
C	6.7390821	-1.6904823	-3.9548494
C	7.2646107	-2.5824828	-3.0303875
C	8.4083987	-2.2972567	-2.2695030
C	8.9430339	-1.0117130	-2.4076218
C	8.4238647	-0.0488843	-3.2877890
C	9.0281954	-3.3629591	-1.3593369
C	10.5676092	-3.3149526	-1.3610786
O	6.6735380	-3.8477229	-2.8795015
C	5.5411132	-3.9346436	-2.1279731
C	5.6023381	-4.7266799	-0.9408508
N	4.5188816	-5.0865139	-0.2674108
C	3.3876876	-4.5463653	-0.7289703
C	3.3611733	-3.6281389	-1.7733300
N	4.4293611	-3.3241478	-2.5146847
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N	1.2179645	-3.8082174	-0.9812110
C	1.9637740	-3.0895656	-1.8979827
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C	10.5563782	1.3596363	-3.3263443
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C	7.3477228	-4.0903148	0.4321224
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C	7.2661762	-3.0345965	2.5760588
C	8.4061790	-2.2674885	2.2922857
C	8.9444257	-2.4045007	1.0081652
C	8.4337181	-3.2900466	0.0458231
O	6.6678293	-2.8835210	3.8379549
C	5.5331319	-2.1335919	3.9144616
N	4.4247746	-2.5288630	3.3028651
C	3.3534487	-1.7866606	3.5937796
C	3.3739936	-0.7326038	4.5011722
N	4.5011766	-0.2647281	5.0438643
C	5.5877879	-0.9400203	4.6970028
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C	1.9568537	-1.9234519	3.0541021
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C	8.4091746	2.3002762	2.2625548
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O	1.5205595	-0.6358993	-5.3936839
O	1.5670166	2.1993771	2.6474214
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H	8.5964981	-2.9251440	3.6533254
H	10.8034135	-1.8450436	3.7553817
H	10.8256187	-3.2533052	2.6602539
H	10.8278866	-1.6085098	1.9998934
H	10.8051924	-3.7520420	-1.8451697

H	10.8281570	-1.9969892	-1.6046222
H	10.8245814	-2.6535532	-3.2508496
H	5.7491601	-4.9320208	0.5118591
H	9.6820396	-1.9462842	0.2274637
H	0.0745111	-2.7761753	2.4776041
H	0.0762868	2.4765591	2.7724975
H	0.0774859	2.7717112	-2.4702198
H	0.0751511	-2.4767512	-2.7628319
H	6.4418657	0.9173254	0.0183837
H	5.5717725	-0.0650388	-1.1960910
H	6.4830069	-0.8648280	0.1185674
H	4.9675176	0.0151822	0.4889809

c8@2
B97-D2/TZVP E(DFT-D) = -8335.691469976 a.u.
Cartesian coordinates (in Å):

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C	-1.6735496	-0.2755590	-0.1558553
H	-3.8560071	-0.1104976	-0.1321477
H	-3.0224240	1.3617852	-0.6726371
H	-1.6665978	-0.7430468	-1.1481808
C	-0.3994827	0.5684203	-0.0054382
H	-1.6460884	-1.0980055	0.5703758
C	0.8688012	-0.2926913	0.0887732
H	-0.3241739	1.2570047	-0.8567450
H	-0.4751747	1.1938932	0.8932184
C	2.1632408	0.4908043	-0.1560393
H	0.9057660	-0.7558879	1.0826033
H	0.8107331	-1.1147579	-0.6363859
C	3.4370534	-0.3124947	0.1319185
H	2.1775383	0.8178810	-1.2046858
H	2.1666373	1.4045656	0.4541652
C	4.7172173	0.4306246	-0.2755682
H	3.4806288	-0.5513184	1.2060274
H	3.3955624	-1.2767732	-0.3980860
C	5.9943623	-0.3337319	0.0920796
H	4.6918256	0.6095581	-1.3614827
H	4.7276466	1.4218185	0.2022960
H	6.8921054	0.2022229	-0.2374857
H	6.0658427	-0.4741612	1.1786737
H	6.0057218	-1.3276513	-0.3738039
N	-1.4191299	4.1145534	0.0067187
C	-2.1526065	3.7025594	1.1056832
C	-3.5658895	4.1152442	0.8088658
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C	-5.7641312	4.4105631	1.0331757
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C	-7.4495974	2.2179169	-3.2812153
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C	-9.2419570	3.5720858	0.4134102
C	-8.6111997	2.7968108	1.5746692
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C	-8.6020102	0.8941139	3.1465591
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C	-7.4890531	-1.5339664	-3.7917214
C	-6.9047537	-2.7171119	-3.3434458
C	-7.4448146	-3.3410135	-2.2262523
C	-8.5863645	-2.8586699	-1.5686212

C	-9.1142458	-1.6519002	-2.0403464
O	-6.8446346	1.7429379	-4.4569737
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C	-3.5215433	-0.4646065	-4.5099849
C	-3.5121660	0.8081579	-3.9495208
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C	-5.7272201	-4.4446895	-1.0263212
C	-5.7849161	-4.8521067	0.3415920
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N	-1.3834943	-4.0914525	-0.0123287
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O	-6.8404347	-1.7880307	4.4686322
C	-5.7030712	-1.0501636	4.3390681
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N	-4.6637313	1.0581130	4.8957387
C	-3.5391977	0.4525838	4.5049648
C	-3.5221591	-0.8170301	3.9372188
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C	-2.1282746	0.9865928	4.5178555
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O	-1.6814720	2.0016793	4.9920546
O	-1.7237635	-3.0978852	-2.0996275
O	-1.7225192	-5.1558490	2.0392179
O	-1.7298633	2.1073381	-2.8842712
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O	-1.7411256	3.1113126	2.0922450
O	-1.7795761	5.1703863	-2.0452646
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C	3.1834216	-3.4730022	2.2172515
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C	1.7871493	-2.5752935	3.8852609
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C	5.3720908	-3.8789248	2.3331043
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C	7.1893628	-3.7853728	-1.6436116
C	8.2728361	-2.8964752	-1.5769390
C	8.7824176	-2.6132030	-0.3005838
C	8.2506028	-3.1443514	0.8784839
C	8.8615458	-2.8736335	2.2567928

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C	6.5420024	-0.5251858	4.2313359
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C	8.2293845	0.8418831	3.1012369
C	8.7803286	-0.3403180	2.5962982
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C	8.2490304	-0.8705177	-3.0761990
C	7.0961094	-0.7378137	-3.8630190
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C	7.1623091	1.6427530	-3.7040291
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C	8.7914054	0.3126841	-2.5633767
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C	5.4366495	-3.6464459	-3.1393340
C	5.3744391	-2.3603822	-3.7562737
N	4.2635706	-1.6375191	-3.7809630
C	3.1939274	-2.2806646	-3.3069785
C	3.2217756	-3.6036817	-2.8786989
N	4.3534352	-4.3018279	-2.7487773
C	1.7904164	-1.7618482	-3.1669555
N	1.0455979	-2.8539095	-2.7558583
C	1.8110825	-4.0301921	-2.5611396
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C	3.1734255	3.5172521	-2.2345426
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N	4.3332273	2.7376972	-4.1805885
C	1.7617843	3.4648971	-1.7208044
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O	6.5243461	4.4630495	-1.8842578
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C	5.4157599	3.6276757	3.1523391
C	5.3478630	2.3340914	3.7540383
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C	3.1713322	2.2621359	3.2845952
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O	1.3642287	2.1302411	-4.9298342
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O	1.3766060	-5.1072699	-2.2347210
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H	8.5452540	2.8500035	3.6985461
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H	-8.9627369	4.6195825	0.5510944
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H	-11.1317210	0.2516638	-2.5591266
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H	-0.3693616	-3.9421667	0.0924143
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c9@C2

B97-D2/TZVP E(DFT-D) = -8374.996924836 a.u.

Cartesian coordinates (in Å):

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C	-0.0177738	0.5336949	-0.0250332
C	1.2510755	-0.3153581	0.1455322
C	2.5605067	0.4405804	-0.1117669
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H	-6.0354696	-0.3019679	0.0125323
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H	-3.8321734	-0.9076911	-1.0592167
H	-3.8066100	-1.2605404	0.6661494
H	-2.6480386	1.2756323	-0.6125143
H	-2.6028344	0.8892097	1.1041724
H	-1.2272979	-1.1266730	0.6508904
H	-1.3099921	-0.8329991	-1.0776072
H	0.0578320	1.1428131	-0.9340467

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H	1.2635477	-0.7178586	1.1661216
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H	3.7996450	-0.5681674	1.3391280
H	3.7589137	-1.3576630	-0.2355340
H	5.9980368	-0.2529905	0.1796929
H	5.1767692	0.4678152	-1.2197746
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C	-6.7295420	-2.8273356	-3.2524663
C	-7.2720481	-3.4065928	-2.1130221
C	-8.4109559	-2.8942097	-1.4739479
C	-8.9319151	-1.7025999	-1.9889942
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C	-5.5088981	0.8547940	-4.3577220
C	-5.5515557	-0.5230352	-4.7323171
N	-4.4588302	-1.2650871	-4.8448681
C	-3.3383370	-0.6417836	-4.4706792
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N	-4.4071936	1.4299305	-3.8957105
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C	-1.9371321	0.9601707	-3.4745822
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O	-6.7049851	-4.5852475	-1.6012904
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C	-1.9936410	-4.6637905	1.1778829
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C	-10.5801261	-3.5692014	-0.3056403
O	-6.8553798	-4.9859464	1.0873182
C	-7.3554082	-3.7813202	1.6333282
C	-8.4428180	-3.1333101	1.0284427
C	-8.9470999	-1.9962080	1.6784897
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H	0.1806323	-2.6799027	2.6810639
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H	-9.8461591	1.4842262	-1.1923211

H	-8.8144229	4.6148038	0.5444097
H	-8.7300743	0.4876478	-4.6232161
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H	-10.9761164	0.2278659	-2.5417281
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H	-10.9592305	-3.9927533	-1.3515359
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C	3.3622769	-0.3720403	0.1463462
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c11@C2

B97-D2/TZVP E(DFT-D) =

Cartesian coordinates (in Å):

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N	3.6011986	-4.7536970	-3.3532870
C	4.8790900	-4.4080918	-3.3902367
C	5.3045561	-3.0585071	-3.5823293
N	4.4672616	-2.0333816	-3.5111408
O	5.8355995	-5.3682868	-3.1771265

C	6.1747492	-5.4657229	-1.8067085
C	7.4238473	-5.0203828	-1.3489051
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C	6.8228052	-5.8370790	0.9015467
C	5.5607297	-6.1782867	0.3927807
C	5.2345044	-6.0319992	-0.9482046
O	4.6187699	-6.7431115	1.2686266
C	3.6115820	-5.9387408	1.7130536
C	3.6007357	-5.6059815	3.1014273
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C	1.5974317	-4.6583806	2.8420141
C	1.6749024	-4.8609804	1.4683848
N	2.6710578	-5.5230657	0.8755036
C	0.2931745	-3.9668577	3.1511749
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C	0.4745672	-4.2255168	0.8242065
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C	4.5916623	2.5776296	-0.6726909
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O	-0.1937346	-3.6572347	4.2110506
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C	-9.1348800	3.5059238	1.0722271
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H	10.9848960	-3.8804741	-1.2567756
H	5.9358499	-3.0973846	-3.8033178

H	9.8022873	-1.1540076	-1.4040458
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H	10.9778099	-0.4136337	-4.0456395
H	10.9856883	1.3606767	-3.8584181
H	10.9796940	0.3132071	-2.4293380
H	10.9943622	4.2581486	-0.2910998
H	10.9750047	2.6163625	0.3755738
H	10.9353982	4.0059596	1.4741119
H	5.9629112	3.9549933	-3.1046477
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H	0.0963376	-0.0549996	3.8429335
H	0.1935282	4.1655257	-0.2326376
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Cartesian coordinates (in Å):

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C	5.4648175	-1.5411654	4.1818541
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C	8.3117384	0.6200378	3.0545637
C	8.8663966	1.3994648	2.0316586
C	8.3875682	2.6673848	1.6863233
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O	6.8085493	4.4349531	2.0973441
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C	5.6662869	4.9356038	0.0456416
N	4.5718323	5.2113656	-0.6518503
C	3.4386949	5.1117684	0.0482365
C	3.4005617	4.7303109	1.3842389
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C	6.6120148	-2.5091551	-3.4367883
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C	2.0763174	-5.2775803	0.7466550
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O	1.7149371	-5.8297756	1.7587481
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C	7.4125471	-4.1230620	1.2129771
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C	-2.5122303	-0.9039509	0.7246325
C	-3.3310582	-1.4422256	-0.4562382
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benzene@2
B97-D2/TZVP E(DFT-D) = -8252.208404568 a.u.

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C	-1.4612949	0.6879482	0.0391348
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C	-3.2448033	0.5171410	-8.2227679
C	-3.9765014	1.0086061	-7.1322668
C	-3.6651245	2.2205589	-6.5212042
C	-0.8351668	3.5072200	-8.7799673
C	-0.8454380	3.4758854	-10.3199433
O	-5.0824064	0.2781116	-6.6396686
C	-3.5387891	-0.8542142	-8.8271408

C	-3.4797695	-0.8574118	-10.3658823
O	5.3187181	-1.4239390	-1.3615981
O	2.7669388	2.4264446	-1.3356069
O	-1.3936165	-5.2137779	-1.2727252
O	2.3345225	-2.4836320	-1.3302020
O	-5.3187181	1.4239390	-1.3615981
C	0.3377758	0.6094387	-3.0509205
C	-0.3377758	-0.6094387	-3.0509205
C	-0.6771953	-1.2229031	-4.2664718
C	-0.3399875	-0.6103077	-5.4786938
C	0.3399875	0.6103077	-5.4786938
C	0.6771953	1.2229031	-4.2664718
H	-0.6059150	-1.0857981	-6.4189240
H	-1.2163002	-2.1653742	-4.2678950
H	-0.6100573	-1.0907745	-2.1141004
H	0.6100573	1.0907745	-2.1141004
H	1.2163002	2.1653742	-4.2678950
H	0.6059150	1.0857981	-6.4189240
H	1.1510088	-4.7912961	6.0977930
H	0.4903563	-1.9033133	10.0606384
H	-2.4055723	-4.0099854	8.9791383
H	4.0107234	-2.4129710	8.9524278
H	3.9811928	-1.3334555	11.1615367
H	2.2100392	-1.3225317	11.1920006
H	3.0746170	-2.8698678	11.1837866
H	4.8562475	1.1829958	6.1384228
H	1.8983515	0.4783182	10.0387978
H	2.4055723	4.0099854	8.9791383
H	2.8694079	3.0676524	11.2027827
H	1.3343795	2.1820547	11.1988458
H	1.3210443	3.9536217	11.1810697
H	-1.1510088	4.7912961	6.0977930
H	-0.4903563	1.9033133	10.0606384
H	-4.0107234	2.4129710	8.9524278
H	-3.0746170	2.8698678	11.1837866
H	-3.9811928	1.3334555	11.1615367
H	-2.2100392	1.3225317	11.1920006
H	-2.8694079	-3.0676524	11.2027827
H	-1.3343795	-2.1820547	11.1988458
H	-1.3210443	-3.9536217	11.1810697
H	-4.8562475	-1.1829958	6.1384228
H	-1.8983515	-0.4783182	10.0387978
H	-2.8606689	2.3507157	0.4266735
H	2.5366636	2.8957571	0.4416343
H	2.8606689	-2.3507157	0.4266735
H	-2.5366636	-2.8957571	0.4416343
H	2.6267962	4.2164361	-5.6600029
H	1.0246199	1.6816035	-9.5913172
H	-1.1094157	4.5211373	-8.4773906
H	4.5622529	1.1104956	-8.5429076
H	4.1884148	0.1214322	-10.7631071
H	2.4846394	0.6077868	-10.7518662
H	3.7479695	1.8501310	-10.7457989
H	4.2242845	-2.5660071	-5.6590302
H	1.6677986	-0.9943257	-9.5929495
H	1.1094157	-4.5211373	-8.4773906
H	1.8430425	-3.7416062	-10.6884586
H	0.5906330	-2.4893751	-10.7242130
H	0.1182198	-4.1976834	-10.7095948
H	-2.6267962	-4.2164361	-5.6600029
H	-1.0246199	-1.6816035	-9.5913172
H	-4.5622529	-1.1104956	-8.5429076
H	-3.7479695	-1.8501310	-10.7457989
H	-4.1884148	-0.1214322	-10.7631071
H	-2.4846394	-0.6077868	-10.7518662
H	-1.8430425	3.7416062	-10.6884586
H	-0.5906330	2.4893751	-10.7242130
H	-0.1182198	4.1976834	-10.7095948
H	-4.2242845	2.5660071	-5.6590302
H	-1.6677986	0.9943257	-9.5929495
H	-3.8506061	-0.3477089	-0.0021626
H	0.2901643	-3.6200056	0.0347544
H	3.8506061	0.3477089	-0.0021626

H -0.2901643 3.6200056 0.0347544

2benzene@2
B97-D2/TZVP E(DFT-D) = -8484.398611451 a.u.
Cartesian coordinates (in Å):

C	-4.3411870	1.1616847	-0.4798925
C	-5.6077331	0.5981177	-0.2878637
C	-5.7249774	-0.7419080	0.0977760
C	-4.5763538	-1.5146644	0.2969844
C	-3.3103649	-0.9507269	0.1077904
C	-3.1925301	0.3854264	-0.2870320
H	-4.2450379	2.2091901	-0.7495717
H	-6.4997381	1.2031983	-0.4305238
H	-6.7055285	-1.1825746	0.2496631
H	-4.6710533	-2.5554267	0.5911947
H	-2.4165276	-1.5475466	0.2742798
H	-2.2121260	0.8318355	-0.4293386
C	4.4029713	0.7561361	-1.2782465
C	3.1995989	0.2994604	-0.7291666
C	3.2047109	-0.4082568	0.4772621
C	4.4164999	-0.6667028	1.1288701
C	5.6203324	-0.2120335	0.5783364
C	5.6136006	0.5025654	-0.6251703
H	4.3999222	1.3213780	-2.2057838
H	2.2583580	0.5013251	-1.2352351
H	2.2744070	-0.7651052	0.9129821
H	4.4189969	-1.2343050	2.0546925
H	6.5606974	-0.4176483	1.0843818
H	6.5450958	0.8593180	-1.0549415
N	-1.2940058	-2.4992218	-2.3101897
C	-2.1224533	-1.7089581	-3.1140255
C	-3.4771747	-2.3527091	-3.0222828
C	-3.3916875	-3.4321865	-2.1518865
C	-1.9768546	-3.5409521	-1.6672363
N	-4.4441673	-4.1616227	-1.7782744
C	-5.5819906	-3.7999813	-2.3547588
C	-5.6492546	-2.7503691	-3.3235301
N	-4.6038598	-1.9935305	-3.6335679
O	-6.7414759	-4.4321598	-1.9939874
C	-7.3052176	-3.9405375	-0.7943908
C	-6.7623301	-4.3687270	0.4131467
C	-7.2953984	-3.8841938	1.6064781
C	-8.3651925	-2.9746398	1.6193535
C	-8.8915685	-2.6007156	0.3757876
C	-8.4028823	-3.0670477	-0.8500653
C	-9.0608895	-2.6701007	-2.1716148
C	-8.5386017	-1.3387196	-2.7169931
C	-7.4692216	-1.3104303	-3.6224561
C	-7.0286965	-0.1444147	-4.2308974
C	-7.6434715	1.0553239	-3.8831920
C	-8.6831200	1.1131981	-2.9435548
C	-9.1088997	-0.1032720	-2.3883949
C	-8.9385829	-2.4079380	2.9160984
C	-8.3192904	-1.0466195	3.2440135
C	-7.1640044	-0.9676698	4.0345290
C	-6.6209985	0.2390117	4.4474670
C	-7.2132150	1.4202050	4.0063649
C	-8.3266568	1.4191446	3.1532766
C	-8.8587163	0.1666645	2.8051570
O	-6.7461026	-4.3580278	2.8185690
C	-5.5123975	-3.8130731	3.0891536
C	-5.4494854	-2.5734329	3.7921245
N	-4.3469520	-1.8394948	3.8387118
C	-3.2787916	-2.4321611	3.3029517
C	-3.2989283	-3.7328364	2.8082475
N	-4.4274208	-4.4312760	2.6468992
C	-1.8977752	-1.8596418	3.0949706
N	-1.1529000	-2.9329971	2.5970862
C	-1.8917811	-4.1211952	2.4294547
O	-6.5730759	-2.1701283	4.4491823
O	-6.6499693	2.6389625	4.4571044

C	-5.4325982	2.8717519	3.8686771
C	-5.4080364	3.5313347	2.6010437
N	-4.3250369	3.5679685	1.8402270
C	-3.2449626	3.0450401	2.4224401
C	-3.2295189	2.5598340	3.7243243
N	-4.3346827	2.4289832	4.4636554
C	-1.8735862	2.8872537	1.8416772
N	-1.0872962	2.4258477	2.8921595
C	-1.8140878	2.1809149	4.0740055
C	-8.9337075	2.7121001	2.6102622
C	-10.4722613	2.7156011	2.6719900
O	-6.5453665	4.1636591	2.2108709
C	-7.1990572	3.7306505	1.0472852
C	-8.3926775	3.0125793	1.2093250
C	-9.0474277	2.6111745	0.0386080
C	-8.5822296	2.9273519	-1.2452196
C	-7.4035223	3.6859093	-1.3285007
C	-6.7007475	4.0934989	-0.1983526
O	-6.9782561	4.1123721	-2.5943963
C	-5.8298042	3.5939922	-3.1209738
C	-5.9598404	2.6488900	-4.1806074
N	-4.9172029	2.1668579	-4.8415893
C	-3.7389849	2.6212738	-4.4051792
C	-3.6093689	3.5044725	-3.3383899
N	-4.6531707	4.0171642	-2.6792742
C	-2.3632552	2.2877584	-4.9330002
N	-1.4919034	2.9872142	-4.0723173
C	-2.1406027	3.7737615	-3.1029302
C	-9.2935738	2.4466757	-2.5108483
C	-10.8247270	2.3895623	-2.3701665
O	-7.2190181	2.2320059	-4.5290984
O	-6.8411925	-2.5312594	-3.9403736
O	-1.6205052	4.5011254	-2.2885389
O	-2.0503178	1.5998254	-5.8750143
O	-1.3642430	1.7718549	5.1212851
O	-1.5142940	3.0891415	0.6939006
O	-1.4527441	-5.1896671	2.0724359
O	-1.5095497	-0.7226048	3.2629563
O	-1.7817983	-0.7119808	-3.7227414
O	-1.5076175	-4.3220680	-0.8640678
C	-10.5996696	-2.6961534	-2.0818743
C	-10.4785187	-2.3685186	2.9162707
O	1.7290975	2.8777027	2.1239967
C	2.0222862	3.1536640	0.9739494
C	3.3258085	3.6633955	0.4267396
C	3.2166701	3.7541595	-0.9561113
C	1.8326190	3.3201151	-1.3564419
N	1.1940981	3.0236644	-0.1392471
N	4.4361897	3.9664047	1.0952167
C	5.4447635	4.3512090	0.3230914
C	5.3607397	4.3572450	-1.1017240
N	4.2383707	4.0774289	-1.7500402
O	6.6184561	4.7388113	0.8975123
C	7.3134553	3.7076534	1.5607830
C	6.9124104	3.3337538	2.8347416
C	7.5768029	2.2790033	3.4555478
C	8.6280484	1.5931546	2.8311076
C	9.0178662	2.0436604	1.5605664
C	8.3968582	3.1106922	0.9008528
C	8.8804670	3.6509836	-0.4469736
C	8.2474033	2.9293028	-1.6362708
C	7.1184040	3.4362892	-2.2997469
C	6.5905384	2.8237315	-3.4322430
C	7.1771244	1.6508260	-3.9018682
C	8.2837510	1.0706833	-3.2636639
C	8.7892276	1.7424609	-2.1426352
C	9.2880330	0.3804387	3.4862572
C	8.6330795	-0.8932807	2.9502840
C	7.4645634	-1.4037661	3.5396667
C	6.8328605	-2.5500867	3.0649167
C	7.3868040	-3.1969149	1.9647835
C	8.5633156	-2.7556241	1.3402873
C	9.1487733	-1.5909637	1.8507155

O	7.1799855	1.9172784	4.7571716
C	5.9344518	1.3425269	4.8115634
C	5.8327744	-0.0752430	4.6962382
N	4.6675025	-0.7074632	4.6544443
C	3.6072679	0.0977691	4.7792208
C	3.7120358	1.4732315	4.9623777
N	4.8774331	2.1255019	4.9665865
C	2.1430514	-0.2841434	4.7997162
N	1.4766825	0.9361842	5.0023942
C	2.3279010	2.0490554	5.1367562
O	6.9961540	-0.7896363	4.7082640
O	6.8263790	-4.3992732	1.5099372
C	5.6712268	-4.3816807	0.7918188
C	5.7427986	-4.8230502	-0.5647008
N	4.6661700	-5.0572985	-1.2989958
C	3.5187443	-4.7573706	-0.6850890
C	3.4622545	-4.1938001	0.5841832
N	4.5328375	-4.0158352	1.3617271
C	2.1137018	-4.8965636	-1.2120840
N	1.3095028	-4.3296692	-0.1948254
C	2.0320706	-3.8512004	0.8918571
C	9.1620785	-3.5312228	0.1634819
C	10.6998743	-3.4768584	0.1218215
O	6.9791601	-4.9619974	-1.1430792
C	7.4330598	-3.7513367	-1.7113162
C	8.5180873	-3.0695840	-1.1428842
C	8.9708402	-1.9229672	-1.8142471
C	8.3754765	-1.4315581	-2.9804468
C	7.2409974	-2.1156495	-3.4394542
C	6.7787584	-3.2809905	-2.8486997
O	6.6004623	-1.6175780	-4.5868471
C	5.4414398	-0.9263003	-4.4339159
C	5.4396357	0.4419274	-4.8540087
N	4.3212137	1.1343356	-5.0076170
C	3.2201128	0.4792960	-4.6273212
C	3.2541806	-0.7779465	-4.0337918
N	4.3591664	-1.5223177	-3.9539626
C	1.7935278	0.9575399	-4.6683665
N	1.0774985	-0.0438991	-3.9658412
C	1.8718429	-1.1055609	-3.5424481
C	8.9188157	-0.2277263	-3.7533752
C	10.4582199	-0.1709981	-3.7509902
O	6.6405419	1.0655594	-5.0733738
O	6.4989854	4.6122734	-1.8238968
O	1.5033256	-2.0686127	-2.8876829
O	1.3239508	1.9473214	-5.1740292
O	1.6004983	-3.2561167	1.8639693
O	1.7147059	-5.3753581	-2.2458849
O	1.9908326	3.1888695	5.3578945
O	1.6359401	-1.3770487	4.6867179
O	1.3583901	3.1875652	-2.4619912
C	10.4190873	3.6779828	-0.5395644
C	10.8207917	0.3882916	3.3499343
H	6.0818713	3.8283167	3.3253947
H	9.8495565	1.5457850	1.0707508
H	8.5386181	4.6874772	-0.5021237
H	9.0568015	0.4303123	4.5528597
H	11.2451443	-0.4886663	3.8529183
H	11.1541406	0.3726593	2.3055701
H	11.2253325	1.2943794	3.8155407
H	5.9386335	-2.9315138	3.5448694
H	10.0616970	-1.2266528	1.3907766
H	8.8795038	-4.5776927	0.3018215
H	11.1117752	-3.8492490	1.0670805
H	11.0841611	-2.4624302	-0.0364013
H	11.0673886	-4.1054760	-0.6974963
H	5.9214816	-3.8087536	-3.2514444
H	9.8347278	-1.4008138	-1.4140282
H	8.6037261	-0.3565118	-4.7918461
H	10.8632144	-1.1004796	-4.1676810
H	10.7980934	0.6716891	-4.3642177
H	10.8742860	-0.0446330	-2.7448902
H	10.7262184	4.1308267	-1.4894772

H	10.8607110	2.6762969	-0.4848423
H	10.8277201	4.2711503	0.2867615
H	5.7253728	3.2459761	-3.9324089
H	9.6553140	1.3211259	-1.6420874
H	0.0538396	-0.0727768	-3.8970135
H	0.2853643	-4.3241737	-0.2673475
H	0.4612639	1.0235593	5.1063839
H	0.1799054	2.8912447	-0.0329283
H	-5.9251783	-5.0590393	0.4262858
H	-9.7308699	-1.9126059	0.3622779
H	-8.7709811	-3.4335884	-2.8977702
H	-8.6334854	-3.0887054	3.7146520
H	-10.8389364	-2.0168566	3.8899655
H	-10.8836588	-1.7004424	2.1473400
H	-10.8748853	-3.3737903	2.7319996
H	-5.7408421	0.2650476	5.0798220
H	-9.7416645	0.1421745	2.1734721
H	-8.5834627	3.5188382	3.2589592
H	-10.7990094	2.5648006	3.7073387
H	-10.9219955	1.9247746	2.0603910
H	-10.8572248	3.6779510	2.3146273
H	-5.7900468	4.6742289	-0.2900932
H	-9.9710577	2.0485546	0.1292428
H	-9.0665218	3.1701627	-3.2973985
H	-11.2097486	3.3764474	-2.0875291
H	-11.2710266	2.0958316	-3.3273007
H	-11.1553190	1.6694303	-1.6125390
H	-11.0304763	-2.4839160	-3.0672797
H	-10.9925228	-1.9549113	-1.3763617
H	-10.9350865	-3.6861634	-1.7518137
H	-6.2107050	-0.1601410	-4.9420945
H	-9.9304710	-0.0855665	-1.6785371
H	-0.4807134	2.9700431	-4.1884332
H	-0.0713903	2.3370825	2.8016726
H	-0.1388818	-2.9073072	2.4288665
H	-0.2706244	-2.3851759	-2.3218728

p-xylene@2
B97-D2/TZVP E(DFT-D) = -8330.825569724 a.u.
Cartesian coordinates (in Å):

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C	3.2957398	-1.7595952	3.5754102
C	1.9105411	-2.0653973	3.0741649
N	1.1301395	-1.0107813	3.5164865
N	4.3652464	0.0657527	4.7011398
C	5.4789466	-0.6359980	4.5351060
C	5.4834179	-1.9504516	3.9742636
N	4.3971446	-2.5017754	3.4471671
O	6.6729887	-0.0721155	4.8911838
C	7.2371863	0.7571992	3.8956150
C	8.3722522	0.3178008	3.1981970
C	8.9452109	1.2172923	2.2869432
C	8.4373074	2.4993388	2.0502288
C	7.2723069	2.8534450	2.7481686
C	6.6736250	2.0134746	3.6803708
O	6.7617928	4.1444849	2.5449308
C	5.6212287	4.3085932	1.8205763
C	5.7300126	5.0072431	0.5785910
N	4.6717470	5.4221246	-0.1026506
C	3.5031554	5.0539801	0.4315909
C	3.4074824	4.2506855	1.5624801
N	4.4610117	3.8752549	2.2930866
C	2.1081044	5.3498036	-0.0644379
N	1.2705623	4.6270329	0.8168030
C	1.9598297	3.9078915	1.7898597
O	6.9800788	5.2208595	0.0558459
C	7.4288990	4.1467129	-0.7448091
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C	10.8335563	-1.9708900	2.9999633
C	9.2928185	3.0567322	2.0659079
C	10.8321147	3.0099259	2.0562943

O	1.8349615	5.6743931	0.6126924
O	1.8118028	1.6799441	2.9383166
C	9.2748980	2.1095759	-2.9683813
C	8.6973106	0.7115367	-3.1765973
C	7.5954115	0.4891908	-4.0155451
C	7.0159927	-0.7704951	-4.1557637
C	7.5693621	-1.8342828	-3.4554341
C	8.7223531	-1.7022199	-2.6663065
C	9.2406295	-0.4097950	-2.5305845
O	7.0605323	1.5576659	-4.7734431
O	1.7853078	0.4939299	-5.2540882
O	1.7990604	3.2208161	-1.5238693
O	7.0129472	-3.1152814	-3.5925024
C	5.8881122	-3.4220324	-2.8892825
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O	7.2390657	-4.8654823	-1.5144928
O	1.9930740	-5.7870170	-0.6349955
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C	10.8149219	2.1233325	-2.9363262
H	-2.5951339	-2.1768520	-1.4121691
H	-1.6547756	1.2753122	0.9555537
H	-4.0620685	1.7814138	1.1755284
H	-4.9999547	-1.6892986	-1.1762848
H	6.1484185	-0.9134430	-4.7903617
H	10.1196432	-0.2689262	-1.9092481
H	9.1001347	-3.7876751	-2.6352849
H	8.9658754	2.7069425	-3.8295857
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H	11.2253065	1.5516351	-2.0959940
H	11.2077022	1.6890678	-3.8630568
H	6.1638099	4.9724954	-0.9024086
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H	9.0001037	3.9090263	2.6841710
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H	11.2061900	2.8890029	3.0796534
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H	10.1024812	0.4097747	1.9676782
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H	11.2852446	-2.7163509	-3.0169092
H	6.2593544	-4.9119009	0.9251275
H	10.0993669	-1.8421586	0.3837372
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H	0.4631314	3.6252349	1.6078347
H	0.4482780	1.6413129	-3.2616285
H	0.5406997	-3.8409216	-1.6877371
H	-5.6341050	4.1594674	2.7279116
H	-9.6076557	1.6810520	1.1451533
H	-8.4581301	0.9123385	4.6014968
H	-8.5537781	4.6444206	-0.8715810
H	-10.7743581	3.8866492	-1.6151635
H	-10.7576362	2.5409188	-0.4623406
H	-10.7546513	4.2069543	0.1397566
H	-5.6327172	2.7925621	-4.0448183
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H	-8.4978315	-4.5756127	0.9148680
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H	-10.7313698	-3.8325572	1.6205946
H	-10.7091444	-2.4885687	0.4658434
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H	-10.7206626	0.5258898	2.5573722
H	-10.6983222	1.6691858	3.9114246
H	-5.5972917	-2.7052396	4.0679606
H	-9.5971088	-1.0820165	1.6437338
H	0.0838021	-3.9463427	1.2276001
H	0.0799530	-1.2268900	-3.5096874
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H	0.0762126	1.2502128	3.4524616
H	0.0876977	0.0681785	-0.7370661
H	-0.0503977	-1.0206857	0.6509754
H	-0.2765773	-1.6498084	-0.9922496
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2 p-xylene@2
B97-D2/TZVP E(DFT-D) = -8641.632302570 a.u.
Cartesian coordinates (in Å):

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C	-4.7611927	1.2899182	0.3920907
C	-4.9935381	-0.0161407	-0.0587259
C	-3.8821357	-0.8133856	-0.3692904
C	-2.5826823	-0.3187571	-0.2417368
C	-2.3489760	0.9902634	0.2054455
C	3.9587696	0.8950025	-0.2724450
C	2.6360252	0.4519730	-0.2493965
C	2.3215316	-0.8651175	0.1201581
C	3.3741194	-1.7130867	0.4891101
C	4.6992558	-1.2707915	0.4626661
C	5.0133395	0.0370447	0.0770565
N	-1.1708320	-1.3341707	-3.6597017
C	-1.9073636	-0.4980642	-4.5330049
C	-3.3251626	-0.9912300	-4.3999313
C	-3.3321839	-2.0975886	-3.5572503
C	-1.9355315	-2.3050883	-3.0297680
N	-4.4262801	-2.8214435	-3.3048374
C	-5.5226587	-2.3638314	-3.8955063
C	-5.5381491	-1.1442996	-4.6368475
N	-4.4340025	-0.4739117	-4.9331824
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C	-6.8417449	-4.1032414	-1.6709382
C	-7.4598390	-4.1872201	-0.4246169
C	-8.5329429	-3.3542643	-0.0729485
C	-9.0122677	-2.4886766	-1.0684783
C	-8.4514460	-2.3916260	-2.3464601
C	-9.0263185	-1.4785616	-3.4334265
C	-8.4246047	-0.0765518	-3.3514293
C	-7.2923940	0.2801060	-4.0990832
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C	-7.2674364	2.4610249	-3.1281886
C	-8.4323543	2.1954891	-2.3945530
C	-8.9720282	0.9107230	-2.5168608
C	-9.1339055	-3.3544787	1.3333785
C	-8.4985833	-2.2528257	2.1907918
C	-7.3114381	-2.4979259	2.8975610
C	-6.7301514	-1.5623285	3.7443060
C	-7.3342571	-0.3143459	3.8520528
C	-8.4849266	0.0261825	3.1277800
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O	-1.6102376	5.9066868	0.1725858
O	-1.5248926	2.4682869	-2.9108681
O	-1.5373753	-0.4317596	4.9333381
O	-1.5298412	3.6300906	2.7317340
O	-1.7192374	-5.9308684	-0.5191482
O	-1.5491084	-2.4408697	2.5134441
O	-1.4491292	0.3829513	-5.2184398
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H	-6.4023761	-1.6008520	-0.4601868

benzene+p-xylene@2
B97-D2/TZVP E(DFT-D) = -8563.02741675 a.u.
Cartesian coordinates (in Å):
C -4.4909247 -1.3194505 0.4090073

C	-5.6924451	-0.6421444	0.1721637
C	-5.6699380	0.7006860	-0.2215023
C	-4.4461202	1.3615132	-0.3774703
C	-3.2449585	0.6832905	-0.1409553
C	-3.2673740	-0.6577163	0.2551067
C	4.4598607	-0.6319056	1.0682799
C	3.1003749	-0.7538210	1.3682270
C	2.1197537	-0.2273023	0.5159994
C	2.5469389	0.4101871	-0.6561669
C	3.9043733	0.5295189	-0.9596074
C	4.8856467	0.0130001	-0.0996478
N	-1.2072357	3.4791388	1.4633024
C	-1.9733582	2.7478706	2.3591987
C	-3.3625584	3.3114719	2.2290478
C	-3.3529103	4.2822742	1.2330314
C	-1.9372639	4.4622473	0.7528178
N	-4.4616936	4.8712687	0.7798063
C	-5.5650058	4.4993120	1.4124438
C	-5.5450309	3.6327446	2.5468521
N	-4.4513332	2.9878112	2.9287899
O	-6.7766974	4.9349798	0.9410470
C	-7.3199032	4.0901450	-0.0513569
C	-6.7406383	4.1087921	-1.3184243
C	-7.2983089	3.3187907	-2.3157249
C	-8.4515593	2.5467443	-2.1077645
C	-8.9765798	2.5426399	-0.8110576
C	-8.4336574	3.2900725	0.2446596
C	-9.0308232	3.2348063	1.6486209
C	-8.4499441	2.0703910	2.4562922
C	-7.3241108	2.2546493	3.2724999
C	-6.8479149	1.2681367	4.1241507
C	-7.4746607	0.0244105	4.1143526
C	-8.5455761	-0.2603834	3.2558644
C	-9.0154432	0.7906845	2.4538374
C	-9.0875420	1.7592825	-3.2560962
C	-8.4906806	0.3555685	-3.3248564
C	-7.4082775	0.0580834	-4.1653094
C	-6.7979414	-1.1937428	-4.1649959
C	-7.3001508	-2.1739465	-3.3214642
C	-8.4360708	-1.9764711	-2.5228363
C	-8.9862376	-0.6901415	-2.5306167
O	-6.7369215	3.3325040	-3.6025520
C	-5.5984685	2.6114478	-3.8108256
C	-5.6780308	1.4963068	-4.6984646
N	-4.6040147	0.8583622	-5.1419020
C	-3.4595624	1.2798490	-4.5985737
C	-3.4067265	2.2560972	-3.6105429
N	-4.4669298	2.9662647	-3.2199081
C	-2.0575801	0.7829089	-4.8523467
N	-1.2716677	1.4759394	-3.9000055
C	-1.9999371	2.3284339	-3.0880881
O	-6.9179389	1.0366661	-5.0606721
O	-6.6874527	-3.4376525	-3.2971840
C	-5.5504474	-3.5637028	-2.5575194
C	-5.5954747	-4.4388891	-1.4306069
N	-4.5061179	-4.8187928	-0.7790706
C	-3.3882137	-4.2251471	-1.2022527
C	-3.3778868	-3.2403836	-2.1846435
N	-4.4502741	-2.9113167	-2.9061389
C	-1.9836854	-4.4070976	-0.6924429
N	-1.2414178	-3.4122284	-1.3709043
C	-1.9891692	-2.6705586	-2.2718828
C	-9.0412873	-3.1346547	-1.7232550
C	-10.5815308	-3.1110099	-1.7371771
O	-6.8182277	-4.8660384	-0.9803977
C	-7.3649115	-4.0112109	0.0023984
C	-8.4641296	-3.1977549	-0.3109310
C	-9.0123035	-2.4431810	0.7367875
C	-8.5050966	-2.4509756	2.0405060
C	-7.3608598	-3.2324353	2.2654036
C	-6.8007638	-4.0313667	1.2765682
O	-6.8182261	-3.2560189	3.5598884
C	-5.6779070	-2.5470692	3.8005941

C	-5.7729593	-1.4321484	4.6872966
N	-4.7071619	-0.8053745	5.1636334
C	-3.5511507	-1.2411933	4.6589833
C	-3.4740947	-2.2218733	3.6766068
N	-4.5307361	-2.9180869	3.2496261
C	-2.1566509	-0.7578028	4.9640249
N	-1.3409669	-1.4677143	4.0517497
C	-2.0449601	-2.3173987	3.2123749
C	-9.1538904	-1.6582827	3.1776043
C	-10.6909829	-1.6410303	3.0904549
O	-7.0168603	-0.9614950	5.0179909
O	-6.6983358	3.5120791	3.2626191
O	-1.6024810	-2.9653922	2.2769465
O	-1.7705031	0.0376815	5.7855656
O	-1.5929265	-1.7480148	-2.9680412
O	-1.5358031	-5.2024546	0.0979719
O	-1.5897259	2.9683128	-2.1311577
O	-1.6452616	-0.0067506	-5.6662355
O	-1.5936794	1.8378410	3.0795560
O	-1.4746533	5.2501077	-0.0358267
C	-10.5712965	3.2292401	1.6411731
C	-10.6260148	1.7561208	-3.1946629
O	1.4998102	-3.3816601	-0.6977125
C	1.8970723	-3.6414332	0.4269952
C	3.2974879	-3.9800868	0.8509242
C	3.3293168	-4.0648390	2.2383026
C	1.9246880	-3.9124248	2.7593453
N	1.1541220	-3.6611187	1.5981514
N	4.3668435	-4.1750175	0.0774286
C	5.4836817	-4.3899302	0.7576694
C	5.5470993	-4.2817363	2.1800433
N	4.4634870	-4.1741043	2.9341652
O	6.6218731	-4.7708491	0.1151550
C	7.2114433	-3.8811357	-0.7939990
C	6.6829766	-3.7561954	-2.0705216
C	7.2993236	-2.8793351	-2.9604328
C	8.4136889	-2.1088790	-2.5965791
C	8.9321004	-2.3141023	-1.3081155
C	8.3723441	-3.2070832	-0.3874347
C	8.9735877	-3.4708357	0.9953854
C	8.3674337	-2.5384642	2.0428395
C	7.2929321	-2.9250408	2.8580842
C	6.7207225	-2.0542505	3.7849422
C	7.2470755	-0.7738865	3.9157023
C	8.3663787	-0.3485333	3.1824751
C	8.8738653	-1.2464192	2.2381009
C	9.0188287	-1.0772693	-3.5485514
C	8.4097150	0.3081495	-3.3066193
C	7.2665010	0.7255274	-4.0046297
C	6.7351627	2.0012188	-3.8696481
C	7.3251810	2.8802472	-2.9635137
C	8.4244274	2.5046917	-2.1757083
C	8.9461513	1.2193581	-2.3903511
O	6.7880972	-2.8019972	-4.2751465
C	5.5622792	-2.1925839	-4.3316449
C	5.5192675	-0.7813169	-4.5392881
N	4.4038163	-0.0777812	-4.4033052
C	3.3239352	-0.8215023	-4.1520403
C	3.3455323	-2.2098691	-4.0829243
N	4.4718853	-2.9234721	-4.1469897
C	1.9212534	-0.3536803	-3.8876417
N	1.1757469	-1.5108583	-3.7443821
C	1.9353595	-2.7004117	-3.8646069
O	6.6780503	-0.1683413	-4.9139904
O	6.7968226	4.1879852	-2.8804285
C	5.5648332	4.2198387	-2.2749877
C	5.5124523	4.3501635	-0.8555699
N	4.4039338	4.1381896	-0.1612052
C	3.3285192	3.9204727	-0.9201406
C	3.3482385	3.9753449	-2.3100933
N	4.4760728	4.0870797	-3.0181452
C	1.9302267	3.5929667	-0.4741602
N	1.1800464	3.5796735	-1.6409364

C	1.9354379	3.8257495	-2.8128274
C	9.0170767	3.4364608	-1.1183645
C	10.5565282	3.4060428	-1.0941380
O	6.6565600	4.7407442	-0.2292595
C	7.2465312	3.8437200	0.6726367
C	8.4043457	3.1673912	0.2614722
C	8.9552821	2.2634701	1.1777800
C	8.4270604	2.0527811	2.4606874
C	7.3092068	2.8166304	2.8242794
C	6.7043307	3.7071367	1.9435522
O	6.8079141	2.7160411	4.1379867
C	5.5795716	2.1235939	4.2366499
C	5.5214247	0.7290691	4.5386831
N	4.3812305	0.0512186	4.5466758
C	3.3031159	0.8009816	4.3049337
C	3.3537564	2.1743281	4.0931922
N	4.4952688	2.8620716	4.0413614
C	1.8721873	0.3539731	4.1781314
N	1.1510532	1.5142468	3.9487928
C	1.9470886	2.6835258	3.8993786
C	9.0103612	1.0193460	3.4198958
C	10.5486960	0.9617378	3.3828810
O	6.6885719	0.0984298	4.8665245
O	6.7795438	-4.2397964	2.7822685
O	1.5374414	3.8084397	3.7485587
O	1.4332750	-0.7837458	4.2391664
O	1.4934671	3.9074898	-3.9328038
O	1.5379674	3.3666773	0.6589496
O	1.4989494	-3.8237172	-3.8112732
O	1.5177318	0.7965230	-3.8004595
O	1.4993603	-3.9788112	3.8867365
C	10.5132796	-3.4335008	0.9875165
C	10.5579828	-1.0580843	-3.5110494
H	0.1401961	1.5421565	3.7665533
H	0.1657594	3.4161934	-1.6862658
H	0.1680873	-1.5259794	-3.5355214
H	0.1459831	-3.4856671	1.6650443
H	-0.3210857	-1.3269886	4.0370459
H	-0.2236277	-3.3202852	-1.2260971
H	-0.2578999	1.3137825	-3.8167736
H	-0.1928418	3.3743310	1.3235361
C	6.3507593	0.1395364	-0.4227192
C	0.6481300	-0.3188719	0.8391603
H	-4.5081335	-2.3562654	0.7302783
H	-6.6402447	-1.1593823	0.2977158
H	-6.6002158	1.2310586	-0.4088405
H	-4.4280415	2.3981783	-0.6994477
H	-2.2976267	1.1997932	-0.2730974
H	-2.3379217	-1.1866425	0.4493020
H	5.1992386	-1.0409454	1.7550149
H	2.8015540	-1.2607571	2.2796015
H	1.8080541	0.8258910	-1.3354772
H	4.2097124	1.0279969	-1.8779868
H	-5.8675771	4.7204790	-1.5171427
H	-9.8577660	1.9403515	-0.6136920
H	-8.7157461	4.1497523	2.1562945
H	-5.9989933	1.4560295	4.7719596
H	-9.8715602	0.6053058	1.8121672
H	-8.8021083	2.2686520	-4.1796533
H	-5.9397155	-1.3914148	-4.7973556
H	-9.8507687	-0.4942633	-1.9035297
H	-8.7298691	-4.0529672	-2.2271438
H	-10.9947526	-2.2150120	-1.2596126
H	-10.9700193	-3.9866587	-1.2042235
H	-10.9420838	-3.1353869	-2.7720644
H	-9.8843097	-1.8318107	0.5271536
H	-5.9380139	-4.6534595	1.4880691
H	-8.8886086	-2.1704094	4.1056231
H	-11.0583625	-1.1365505	2.1892493
H	-11.0745366	-2.6679640	3.0807957
H	-11.1027496	-1.1161171	3.9601991
H	-10.9884208	2.3381092	1.1579245
H	-10.9459022	3.2580927	2.6709284

H	-10.9419640	4.1092881	1.1027762
H	-11.0128786	1.2590932	-2.2974757
H	-10.9999697	2.7866338	-3.1953957
H	-11.0283655	1.2314736	-4.0689758
H	5.8068835	-4.3214188	-2.3679513
H	9.8158751	-1.7562072	-1.0145808
H	8.6777933	-4.4854162	1.2737524
H	5.8771870	-2.3698083	4.3898688
H	9.7231458	-0.9338670	1.6386614
H	8.7237624	-1.3733683	-4.5582813
H	5.8713683	2.3062014	-4.4501027
H	9.8126822	0.9156070	-1.8113131
H	8.7187494	4.4505498	-1.3962182
H	10.9554651	2.4226247	-0.8192556
H	10.9471166	3.6620777	-2.0858695
H	10.9302070	4.1348753	-0.3655838
H	9.8405716	1.7062973	0.8869452
H	5.8265657	4.2709490	2.2379666
H	8.7236157	1.3271377	4.4282679
H	10.9378713	0.6613084	2.4031809
H	10.9108781	0.2391434	4.1233209
H	10.9601602	1.9499110	3.6197614
H	10.9109753	-2.4491410	0.7145428
H	10.8939448	-3.6851308	1.9841658
H	10.8977811	-4.1631351	0.2653163
H	10.9533263	-0.7658128	-2.5312659
H	10.9458769	-2.0560260	-3.7463629
H	10.9379283	-0.3450956	-4.2519050
H	6.9062925	0.5848819	0.4116164
H	6.5052386	0.7640864	-1.3060191
H	6.7990123	-0.8419396	-0.6218775
H	0.0834142	-0.7110141	-0.0166987
H	0.4679717	-0.9707419	1.6977347
H	0.2384356	0.6723133	1.0758436

2cyclohexane@2
B97-D2/TZVP E(DFT-D) = -8491.699000276 a.u.
Cartesian coordinates (in Å):

N	-1.1944463	2.1034249	3.4078761
C	-1.9555304	1.5225700	4.4511774
C	-3.3669933	1.9706922	4.1656706
C	-3.3425325	2.8300507	3.0731187
C	-1.9411769	2.8749215	2.5314378
N	-4.4213265	3.4655237	2.6119557
C	-5.5412678	3.1605334	3.2531318
C	-5.5875584	2.1645281	4.2757175
N	-4.4961208	1.5990167	4.7729561
O	-6.6940936	3.8278733	2.9673247
C	-7.2776975	3.6232962	1.7047049
C	-6.7519012	4.2744708	0.5959110
C	-7.3480612	4.0602536	-0.6449181
C	-8.4438611	3.1997371	-0.8030919
C	-8.9595835	2.6064639	0.3583750
C	-8.4165695	2.8079646	1.6311887
C	-9.0188911	2.1820750	2.8912653
C	-8.4123623	0.8056831	3.1604690
C	-7.3184247	0.6393196	4.0217078
C	-6.7294110	-0.6047909	4.2386574
C	-7.2657731	-1.7130971	3.5951395
C	-8.4021161	-1.6314656	2.7759695
C	-8.9271198	-0.3525393	2.5600710
C	-9.0330193	2.9005486	-2.1788957
C	-8.3999196	1.6388143	-2.7730486
C	-7.2640598	1.7191359	-3.5930076
C	-6.7288429	0.6100438	-4.2361926
C	-7.3189056	-0.6334414	-4.0185785
C	-8.4128992	-0.7983606	-3.1571178
C	-8.9261470	0.3604830	-2.5566719
O	-6.8480938	4.7667714	-1.7618951
C	-5.6175553	4.3342097	-2.1797925
C	-5.5528395	3.3052674	-3.1687707
N	-4.4227753	2.6796620	-3.4682267

C	-3.3520193	3.1647183	-2.8354555
C	-3.3950247	4.2712346	-1.9946639
N	-4.5341524	4.8613745	-1.6270791
C	-1.9526300	2.6129976	-2.8210371
N	-1.2182690	3.5211373	-2.0736713
C	-1.9910613	4.5788278	-1.5376956
O	-6.7039049	2.9876119	-3.8250722
O	-6.8124853	-1.7454129	-4.7291289
C	-5.5900061	-2.1612760	-4.2729482
C	-5.5448520	-3.1573111	-3.2503139
N	-4.4249937	-3.4645067	-2.6100250
C	-3.3452635	-2.8313720	-3.0722165
C	-3.3689325	-1.9720631	-4.1648236
N	-4.4978236	-1.5980014	-4.7710967
C	-1.9433998	-2.8793724	-2.5319492
N	-1.1958447	-2.1097531	-3.4093520
C	-1.9567931	-1.5271029	-4.4517802
C	-9.0211352	-2.1739003	-2.8877612
C	-10.5608145	-2.1481312	-2.8565557
O	-6.6986384	-3.8227033	-2.9638904
C	-7.2817984	-3.6172377	-1.7012499
C	-8.4195223	-2.8003054	-1.6276703
C	-8.9624022	-2.5981878	-0.3549251
C	-8.4479840	-3.1927310	0.8064466
C	-7.3535948	-4.0549847	0.6481746
C	-6.7572601	-4.2695320	-0.5925471
O	-6.8549234	-4.7627829	1.7649089
C	-5.6234540	-4.3321901	2.1821293
C	-5.5565867	-3.3019139	3.1696211
N	-4.4252798	-2.6779884	3.4677735
C	-3.3555195	-3.1664729	2.8358464
C	-3.4008625	-4.2741470	1.9967380
N	-4.5412684	-4.8623254	1.6299730
C	-1.9549876	-2.6176917	2.8204136
N	-1.2226081	-3.5283146	2.0741741
C	-1.9977650	-4.5848551	1.5393466
C	-9.0367892	-2.8925868	2.1821699
C	-10.5755726	-2.8323055	2.1764400
O	-6.7067672	-2.9821772	3.8263837
O	-6.8105352	1.7505945	4.7323395
O	-1.5789803	-5.5048408	0.8803481
O	-1.5549399	-1.5732892	3.3108597
O	-1.5201122	-0.8468567	-5.3477375
O	-1.5508552	-3.4455775	-1.5240072
O	-1.5701140	5.4977122	-0.8785458
O	-1.5548825	1.5683887	-3.3128585
O	-1.5194341	0.8414530	5.3467597
O	-1.5483700	3.4404388	1.5232181
C	-10.5586003	2.1581795	2.8601293
C	-10.5718829	2.8421039	-2.1731896
O	1.5526759	-4.4475747	-3.2364512
C	1.9793567	-4.2869119	-2.1189881
C	3.3885269	-4.3828794	-1.5908536
C	3.3537954	-4.2098832	-0.2116480
C	1.9455375	-3.8715587	0.1916858
N	1.2072946	-3.9651358	-0.9772776
N	4.5233247	-4.5419655	-2.2753882
C	5.6104138	-4.5755132	-1.5169930
C	5.5550849	-4.5499926	-0.0902260
N	4.4290060	-4.3192285	0.5708266
O	6.8374363	-4.5956434	-2.1253310
C	7.3347939	-3.3023266	-2.4036304
C	6.7404020	-2.5774177	-3.4347012
C	7.2655770	-1.3326231	-3.7578816
C	8.3972268	-0.8039328	-3.1186901
C	8.9274111	-1.5541582	-2.0631186
C	8.4222887	-2.8030293	-1.6726947
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