

ELECTRONIC SUPPLEMENTARY INFORMATION FOR #####
FUNCTIONALIZED DIAMOND NANOTHEADS FROM BENZENE DERIVATIVES
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Porto Alegre, Brazil
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This file contains the coordinates and supercell dimensions for seven different functionalized DNT configurations (with -OH functional groups attached; extension to other functional groups should be trivial). See Fig.1 of the manuscript for reference.

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OH[1,2] primitive CIF file created by Jmol 14.6.4_2016.11.05 2016-11-05 10:17

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_cell_length_a 19.299992

_cell_length_b 19.999983

_cell_length_c 4.3115025

_cell_angle_alpha 90.0

_cell_angle_beta 90.0

_cell_angle_gamma 90.0

_symmetry_space_group_name_H-M 'P 1'

loop_

_space_group_symop_operation_xyz

'x,y,z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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C	0.06425	-0.03564	0.43796
C	-0.06345	-0.03533	0.07256
C	0.00068	-0.07118	-0.06284
C	-0.06373	-0.03514	0.43723
C	0.00015	-0.07138	-0.42746
C	0.06342	0.03565	-0.42399
C	0.06615	0.03487	-0.06250
C	-0.06383	0.03657	-0.42656
C	0.00014	0.07194	0.43789
C	-0.06275	0.03623	-0.06210
C	0.00230	0.06983	0.07683
H	-0.11072	0.06316	-0.50277
H	0.10992	0.06184	-0.50210
O	0.13052	0.06643	0.02723
H	-0.10889	0.06336	0.01797
H	0.11263	-0.06221	-0.00174
H	0.11156	-0.06079	0.51750
H	-0.11112	-0.06078	0.51328
H	-0.11055	-0.06128	-0.00493
O	-0.00017	0.14356	0.49736
H	0.00559	0.12295	0.01827
H	0.00070	-0.12353	0.01424
H	-0.00043	-0.12379	-0.50398
H	-0.02391	0.15232	0.69213
H	0.13179	0.10979	-0.07630

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OH[1,3] primitive CIF file created by Jmol 14.6.4_2016.11.05 2016-11-05 10:17

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_cell_length_c 4.3098426

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_cell_angle_beta 90.0

_cell_angle_gamma 90.0

_symmetry_space_group_name_H-M 'P 1'

loop_

_space_group_symop_operation_xyz

'x,y,z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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C	0.06084	-0.03831	0.43118
C	-0.06569	-0.03681	0.06857
C	-0.00232	-0.07422	-0.06793
C	-0.06640	-0.03605	0.43314
C	-0.00323	-0.07334	-0.43229
C	0.06361	0.03302	-0.43110
C	0.06491	0.03080	-0.06754
C	-0.06445	0.03566	-0.43074
C	0.00032	0.07003	0.43261
C	-0.06393	0.03469	-0.06640
C	0.00156	0.06677	0.07111
H	-0.11031	0.06374	-0.50697
H	0.11063	0.05892	-0.50948
H	0.11260	0.05552	0.01151
H	-0.10961	0.06244	0.01383
O	0.12232	-0.08041	-0.02151
H	0.10669	-0.06543	0.51133
H	-0.11447	-0.06052	0.50922
H	-0.11299	-0.06239	-0.00897
O	0.00077	0.14163	0.48266
H	0.00489	0.12007	0.01591
H	-0.00279	-0.12660	0.00835
H	-0.00391	-0.12551	-0.51126
H	-0.00663	0.15106	0.70166
H	0.16057	-0.06773	0.11389

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OH[1,4] primitive CIF file created by Jmol 14.6.4_2016.11.05 2016-11-05 10:17

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_cell_length_c 4.310035

_cell_angle_alpha 90.0

_cell_angle_beta 90.0

_cell_angle_gamma 90.0

_symmetry_space_group_name_H-M 'P 1'

loop_

_space_group_symop_operation_xyz

'x,y,z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z			
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C	0.06464	-0.03572	0.43917
C	-0.06369	-0.03670	0.07488
C	-0.00001	-0.07271	-0.06183
C	-0.06369	-0.03480	0.43914
C	0.00016	-0.07014	-0.42425
C	0.06535	0.03601	-0.42533
C	0.06543	0.03400	-0.06132
C	-0.06316	0.03692	-0.42528
C	0.00134	0.07189	0.43778
C	-0.06306	0.03497	-0.06126
C	0.00147	0.06862	0.07622
H	-0.10929	0.06461	-0.50134
H	0.11187	0.06303	-0.50181
H	0.11242	0.05968	0.01838
H	-0.10960	0.06133	0.01895
H	0.11099	-0.06516	-0.00126
H	0.11150	-0.06188	0.51792
H	-0.11073	-0.06054	0.51783
H	-0.11023	-0.06364	-0.00142
O	0.00183	0.14349	0.48671
H	0.00217	0.12204	0.02153
O	-0.00370	-0.14255	0.02905
H	-0.00087	-0.12204	-0.50442
H	0.00025	0.15300	0.70800
H	0.02547	-0.16768	-0.11394

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OH[1,2,3,4] primitive CIF file created by Jmol 14.6.4_2016.11.05 2016-11-05 10:17

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_cell_length_b 19.999983

_cell_length_c 8.624973

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_cell_angle_beta 90.0

_cell_angle_gamma 90.0

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loop_

_space_group_symop_operation_xyz

'x,y,z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

C	0.06106	-0.03749	-0.21468
C	0.06345	-0.03949	-0.03255
C	-0.06565	-0.03682	-0.21390
C	-0.00262	-0.07273	-0.28396
C	-0.06441	-0.03757	-0.03071
C	-0.00147	-0.06940	-0.46496
C	0.06367	0.03700	-0.46084
C	0.06245	0.03474	-0.27976
C	-0.06415	0.03821	-0.46425
C	0.00001	0.06847	-0.02949
C	-0.06491	0.03561	-0.28105
C	-0.00094	0.06994	-0.20979
H	-0.11039	0.06578	-0.50210
H	0.11094	0.06258	-0.49702
H	0.10997	0.05929	-0.23894
H	-0.11216	0.06121	-0.24246

H	0.10792	-0.06419	-0.25242
O	0.12460	-0.07747	0.00923
H	-0.11113	-0.06419	0.00729
H	-0.11283	-0.06277	-0.25198
H	0.00164	0.12054	0.01093
H	-0.00085	0.12343	-0.23880
O	-0.00684	-0.14257	-0.24118
H	-0.00215	-0.12181	-0.50277
C	0.06499	-0.03601	0.28978
C	0.06330	-0.03436	0.47059
C	-0.06425	-0.03578	0.28678
C	0.00038	-0.07154	0.22118
C	-0.06496	-0.03358	0.46791
C	-0.00025	-0.07374	0.03919
C	0.06383	0.03162	0.03562
C	0.06571	0.03414	0.21757
C	-0.06444	0.03388	0.03686
C	0.00075	0.07317	0.46638
C	-0.06360	0.03493	0.21795
C	0.00145	0.06968	0.28405
H	-0.11106	0.06060	-0.00202
H	0.11137	0.05742	-0.00141
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H	-0.10944	0.06270	0.25731
H	0.11142	-0.06282	0.25302
H	0.10996	-0.06054	0.51095
H	-0.11226	-0.05889	0.50765
H	-0.11106	-0.06231	0.24838
O	0.00175	0.14495	0.49034
H	0.00192	0.12228	0.24688
H	0.00079	-0.12368	0.26068
H	-0.00088	-0.12598	0.00285
H	0.00309	0.15386	0.60120
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H	0.16431	-0.04755	-0.00006
H	0.03854	-0.16232	-0.26068

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OH[1,4,2,5] primitive CIF file created by Jmol 14.6.4_2016.11.05 2016-11-05
10:17

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_cell_angle_beta 90.0

_cell_angle_gamma 90.0

_symmetry_space_group_name_H-M 'P 1'

loop_

_space_group_symop_operation_xyz

'x,y,z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

C	0.06345	-0.03485	-0.21653
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C	0.06598	-0.03449	-0.03450
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C	-0.06547	-0.03538	-0.21413
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C	-0.00141	-0.07086	-0.28250
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C	-0.06256	-0.03469	-0.03266
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C	-0.00111	-0.07126	-0.46376
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C	0.06318	0.03616	-0.46731
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C	0.06320	0.03646	-0.28546
C	-0.06451	0.03680	-0.46658
C	0.00126	0.07133	-0.03121
C	-0.06543	0.03579	-0.28315
C	-0.00083	0.07089	-0.21322
H	-0.11109	0.06368	-0.50467
H	0.11006	0.06256	-0.50599
H	0.10992	0.06225	-0.24668
H	-0.11289	0.06119	-0.24496
H	0.10981	-0.06151	-0.25662
H	0.11355	-0.06010	0.00276
H	-0.10925	-0.06136	0.00585
O	-0.13007	-0.06723	-0.25712
H	0.00200	0.12380	0.00714
H	-0.00358	0.12403	-0.24371
H	-0.00175	-0.12325	-0.24301
H	-0.00154	-0.12330	-0.50189
C	0.06364	-0.03834	0.28572
C	0.06315	-0.03621	0.46773
C	-0.06401	-0.03798	0.28351
C	-0.00006	-0.07359	0.21514
C	-0.06434	-0.03539	0.46531
C	0.00167	-0.06985	0.03305
C	0.06578	0.03589	0.03639
C	0.06308	0.03308	0.21802
C	-0.06335	0.03592	0.03559
C	-0.00029	0.07224	0.46363
C	-0.06458	0.03354	0.21618
C	-0.00089	0.06873	0.28307
H	-0.10984	0.06257	-0.00405
O	0.12972	0.06900	-0.00663
H	0.11016	0.05885	0.25743
H	-0.11180	0.05891	0.25585
H	0.11082	-0.06458	0.24744
H	0.11052	-0.06139	0.50739
H	-0.11156	-0.06020	0.50413
H	-0.11040	-0.06544	0.24609
O	0.00149	0.14390	0.48969
H	-0.00069	0.12116	0.24568
O	-0.00437	-0.14368	0.25673
H	0.00180	-0.12219	-0.00569
H	0.13009	0.11223	0.04571
H	0.01625	0.15235	0.59573
H	0.03735	-0.16519	0.21685
H	-0.12872	-0.11265	-0.21600

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OH[1,2,3,4,5,6] primitive CIF file created by Jmol 14.6.4_2016.11.05 2016-11-05 10:17

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_cell_length_b 20.000008

_cell_length_c 12.9294405

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_cell_angle_gamma 90.0

_symmetry_space_group_name_H-M 'P 1'

loop_

_space_group_symop_operation_xyz

'x,y,z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y	_atom_site_fract_z		
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C	0.05980	-0.03565	-0.18674
C	-0.06634	-0.03251	-0.31014
C	-0.00192	-0.06888	-0.35344
C	-0.06889	-0.03529	-0.18812
C	0.00053	-0.06930	-0.47382
C	0.06396	0.03887	-0.47156
C	0.06129	0.03829	-0.35035
C	-0.06270	0.03802	-0.47678
C	-0.00425	0.07104	-0.18367
C	-0.06632	0.03859	-0.35478
C	-0.00345	0.07356	-0.30488
H	-0.10961	0.06425	-0.50276
H	0.11113	0.06486	-0.49579
H	0.10773	0.06473	-0.32326
O	-0.13153	0.06979	-0.32698
H	0.10893	-0.05937	-0.33261
H	0.10597	-0.06301	-0.16055
O	-0.13014	-0.07295	-0.16070
H	-0.11333	-0.05856	-0.33612
H	-0.00460	0.12307	-0.15658
H	-0.00338	0.12596	-0.32906
H	-0.00360	-0.12103	-0.32700
H	0.00129	-0.12167	-0.49931
C	0.06068	-0.03873	0.02333
C	0.06439	-0.03978	0.14531
C	-0.06596	-0.03981	0.02825
C	-0.00347	-0.07473	-0.02135
C	-0.06303	-0.03923	0.14950
C	-0.00512	-0.07132	-0.14336
C	0.06036	0.03512	-0.14055
C	0.06115	0.03319	-0.02013
C	-0.06830	0.03465	-0.13827
C	-0.00015	0.06811	0.14654
C	-0.06660	0.03205	-0.01709
C	-0.00236	0.06852	0.02615
H	-0.11516	0.06120	-0.16231
H	0.10722	0.06155	-0.16613
H	0.10868	0.05844	0.00585
H	-0.11363	0.05739	0.01014
H	0.10759	-0.06539	-0.00209
O	0.12633	-0.07655	0.17295
H	-0.10923	-0.06595	0.17660
H	-0.11278	-0.06616	0.00397
H	0.00095	0.12038	0.17276
H	-0.00310	0.12091	0.00067
O	-0.00489	-0.14464	0.00695
H	-0.00633	-0.12372	-0.16864
C	0.06692	-0.03501	0.36180
C	0.06488	-0.03288	0.48299
C	-0.06208	-0.03615	0.35950
C	0.00285	-0.07153	0.31631
C	-0.06294	-0.03399	0.47988
C	0.00173	-0.07442	0.19511
C	0.06425	0.03174	0.19008
C	0.06681	0.03463	0.31193
C	-0.06364	0.03271	0.19275
C	0.00106	0.07367	0.47852
C	-0.06228	0.03455	0.31314
C	0.00253	0.07026	0.35657
H	-0.11089	0.05841	0.16710
H	0.11162	0.05734	0.16342
O	0.13065	0.06870	0.34015
H	-0.10845	0.06182	0.33936

H	0.11377	-0.06141	0.33786
H	0.11196	-0.05814	0.51011
H	-0.11048	-0.05887	0.50623
H	-0.10865	-0.06303	0.33393
O	-0.00418	0.14385	0.50620
H	0.00238	0.12273	0.33082
H	0.00389	-0.12346	0.34354
H	0.00150	-0.12678	0.17121
H	0.03935	0.16464	0.48530
H	0.13155	0.11073	0.30189
H	0.16554	-0.04612	0.16587
H	0.04153	-0.16245	-0.00441
H	-0.16931	-0.04800	-0.18883
H	-0.12992	0.11514	-0.35471

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OH[1,4,2,5,3,6] primitive CIF file created by Jmol 14.6.4_2016.11.05 2016-11-05 10:17

data_primitive

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_cell_length_b 20.000008

_cell_length_c 12.928799

_cell_angle_alpha 90.0

_cell_angle_beta 90.0

_cell_angle_gamma 90.0

_symmetry_space_group_name_H-M 'P 1'

loop_

_space_group_symop_operation_xyz

'x,y,z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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C	0.06301	-0.03705	-0.18791
C	-0.06727	-0.03358	-0.30811
C	-0.00338	-0.06965	-0.35314
C	-0.06529	-0.03548	-0.18692
C	-0.00160	-0.07097	-0.47322
C	0.06270	0.03691	-0.47437
C	0.06134	0.03710	-0.35291
C	-0.06427	0.03642	-0.47613
C	-0.00097	0.07043	-0.18502
C	-0.06678	0.03755	-0.35378
C	-0.00273	0.07255	-0.30617
H	-0.11115	0.06298	-0.50137
H	0.10990	0.06317	-0.49984
H	0.10823	0.06325	-0.32674
O	-0.13088	0.07043	-0.32586
H	0.10714	-0.06146	-0.33432
O	0.12405	-0.07557	-0.16014
H	-0.11158	-0.06190	-0.16110
H	-0.11491	-0.05881	-0.33345
H	0.00064	0.12258	-0.15843
H	-0.00321	0.12489	-0.33045
H	-0.00409	-0.12171	-0.32617
H	-0.00135	-0.12304	-0.49845
C	0.06356	-0.03688	0.02588
C	0.06575	-0.03548	0.14701
C	-0.06504	-0.03685	0.02687
C	-0.00125	-0.07263	-0.01966
C	-0.06222	-0.03536	0.14781

C	-0.00092	-0.07235	-0.14198
C	0.06353	0.03388	-0.14154
C	0.06386	0.03405	-0.02073
C	-0.06493	0.03504	-0.13913
C	0.00205	0.07114	0.14713
C	-0.06478	0.03423	-0.01821
C	0.00022	0.06993	0.02568
H	-0.11151	0.06134	-0.16432
H	0.11088	0.05956	-0.16788
H	0.11077	0.05971	0.00468
H	-0.11199	0.05976	0.00814
H	0.10938	-0.06383	-0.00051
H	0.11329	-0.06101	0.17225
H	-0.10924	-0.06141	0.17370
O	-0.13006	-0.06835	-0.00115
H	0.00277	0.12376	0.17233
H	-0.00089	0.12216	-0.00049
H	-0.00178	-0.12525	0.00546
H	-0.00041	-0.12467	-0.16773
C	0.06334	-0.03836	0.36041
C	0.06273	-0.03561	0.48170
C	-0.06452	-0.03781	0.35837
C	-0.00048	-0.07380	0.31354
C	-0.06482	-0.03555	0.47975
C	0.00156	-0.07052	0.19230
C	0.06604	0.03525	0.19320
C	0.06332	0.03281	0.31451
C	-0.06267	0.03571	0.19229
C	-0.00098	0.07212	0.47857
C	-0.06424	0.03382	0.31290
C	-0.00038	0.06886	0.35783
H	-0.10918	0.06224	0.16581
O	0.13064	0.06744	0.16517
H	0.11082	0.05820	0.34012
H	-0.11136	0.05964	0.33876
H	0.11037	-0.06494	0.33527
H	0.10989	-0.06088	0.50862
H	-0.11241	-0.06032	0.50597
H	-0.11104	-0.06477	0.33285
O	-0.00568	0.14221	0.50714
H	-0.00033	0.12121	0.33184
O	-0.00507	-0.14371	0.34196
H	0.00165	-0.12288	0.16642
H	0.03564	0.16427	0.48027
H	0.12792	0.11349	0.18965
H	-0.12782	0.11574	-0.35354
H	-0.12885	-0.11366	0.02673
H	0.03549	-0.16593	0.31289
H	0.16412	-0.05075	-0.18545

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