Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information for

Confinement induced conformational changes in *n*-alkanes sequestered within a narrow carbon nanotube

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Here we provide optimized coordinates (x, y, and z), partial charges, and Lennard-Jones interaction parameters for the carbon nanotube, alkanes, and bezene simulated in our study of confinement induced conformational changes in the alkanes. Lennard-Jones, bond-streching, bond-bending, and dihedral torsional interactions for the organic molecules were modeled using the Generalized Amber Force Field. [1]Gaussian03 *ab initio* calculations were performed using the B3LYP hybrid-functional and 6-31G* basis set to optimize the *n*-alkanes and benzene geometries.[2] Carbon and hydrogen partial charges were subsequently evaluated from the Gaussian output files using the RED-II implementation of the restrained electrostatic potential method.[3] The Antechamber module from the AMBER 9 simulation package was used to assign atomic partial charges to the carbon nanotube.[4] Water was modeled using the SPC/E potential.[5] Cross interactions between unlike atoms were determined using Lorentz-Berthelot combining rules.[6]

1. Lennard-Jones Interactions by Atom Type.

Table S1. Lennard-Jones intra-molecular interactions for simulated hydrocarbons listed by generalized Amber force field atom type.

atom type	σ (Å)	ε (kcal/mol))
ca	1.9080	0.0860
ha	1.4590	0.0150
c3	1.9080	0.1094
hc	1.4870	0.0157

2. (13,0) Carbon Nanotube

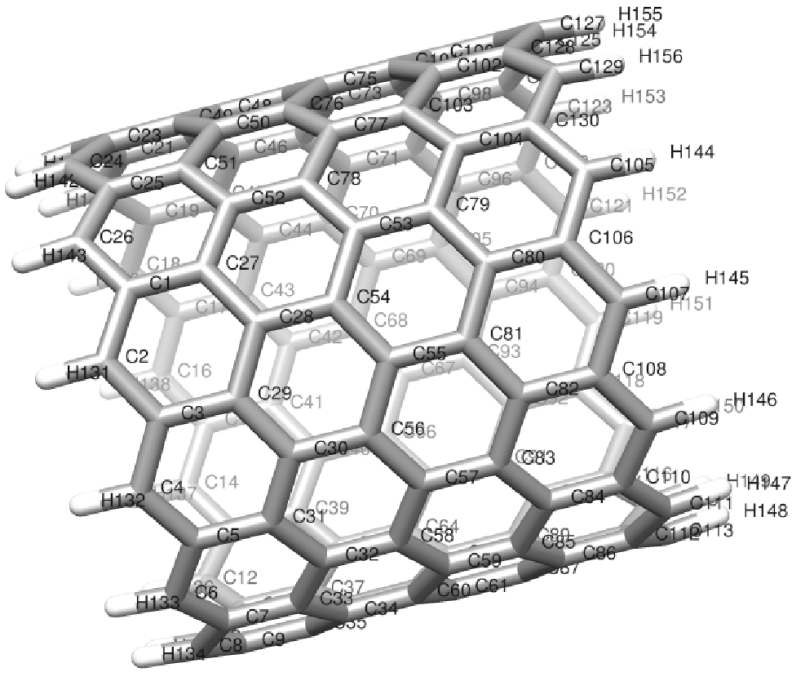

Figure S1. (13,0) Nanotube as simulated

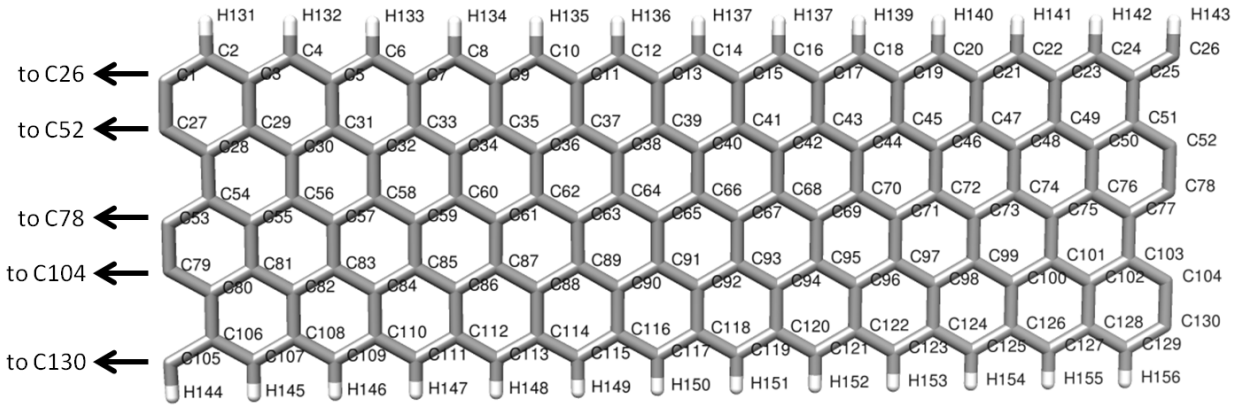

Figure S2. (13,0) nanotube unfurled for clarity.

Table S2. (13,0) nanotube x,y,z coordinates, partial charges, and atom types

atom name	x (Å)	y (Å)	z (Å)	partial charge	atom type
C1	4.971	0.001	0.034	-0.0062	ca
C2	4.830	1.191	-0.663	-0.1095	ca
C3	4.401	2.311	0.034	-0.0333	ca
C4	3.723	3.300	-0.662	-0.0437	ca
C5	2.823	4.092	0.035	-0.0639	ca
C6	1.763	4.652	-0.662	0.0177	ca
C7	0.599	4.936	0.035	-0.0841	ca
C8	-0.601	4.939	-0.661	0.0406	ca
C9	-1.764	4.649	0.035	-0.0823	ca
C10	-2.827	4.094	-0.661	0.0103	ca
C11	-3.722	3.297	0.036	-0.0596	ca
C12	-4.405	2.312	-0.661	-0.0541	ca
C13	-4.827	1.190	0.036	-0.0287	ca
C14	-4.975	0.000	-0.661	-0.1179	ca
C15	-4.827	-1.189	0.035	-0.0029	ca
C16	-4.404	-2.311	-0.662	-0.1595	ca
C17	-3.721	-3.296	0.035	0.0120	ca
C18	-2.825	-4.093	-0.662	-0.1780	ca
C19	-1.762	-4.648	0.034	0.0177	ca
C20	-0.599	-4.938	-0.663	-0.1830	ca
C21	0.600	-4.935	0.034	0.0188	ca
C22	1.764	-4.651	-0.663	-0.1825	ca
C23	2.825	-4.091	0.034	0.0171	ca
C24	3.724	-3.298	-0.663	-0.1760	ca
C25	4.402	-2.310	0.034	0.0102	ca
C26	4.830	-1.190	-0.663	-0.1547	ca
C27	4.987	0.001	1.421	-0.0087	ca
C28	4.842	1.194	2.115	0.0047	ca
C29	4.415	2.318	1.421	-0.0272	ca
C30	3.733	3.307	2.116	0.0195	ca
C31	2.832	4.104	1.422	-0.0471	ca
C32	1.768	4.663	2.116	0.0320	ca
C33	0.601	4.951	1.422	-0.0601	ca
C34	-0.601	4.951	2.116	0.0365	ca
C35	-1.769	4.663	1.422	-0.0589	ca
C36	-2.833	4.105	2.117	0.0306	ca

C37	-3.733	3.307	1.423	-0.0443	ca
C38	-4.416	2.318	2.117	0.0174	ca
C39	-4.842	1.193	1.423	-0.0242	ca
C40	-4.987	0.000	2.117	0.0027	ca
C41	-4.841	-1.193	1.422	-0.0066	ca
C42	-4.415	-2.318	2.116	-0.0099	ca
C43	-3.732	-3.306	1.422	0.0046	ca
C44	-2.832	-4.104	2.116	-0.0189	ca
C45	-1.768	-4.662	1.421	0.0096	ca
C46	-0.600	-4.951	2.115	-0.0234	ca
C47	0.602	-4.950	1.421	0.0107	ca
C48	1.769	-4.663	2.115	-0.0231	ca
C49	2.833	-4.104	1.421	0.0092	ca
C50	3.734	-3.307	2.115	-0.0179	ca
C51	4.416	-2.317	1.421	0.0034	ca
C52	4.843	-1.193	2.115	-0.0083	ca
C53	4.987	0.000	4.196	0.0024	ca
C54	4.842	1.194	3.502	-0.0134	ca
C55	4.415	2.318	4.197	0.0127	ca
C56	3.732	3.307	3.503	-0.0214	ca
C57	2.833	4.104	4.197	0.0192	ca
C58	1.768	4.663	3.503	-0.0261	ca
C59	0.601	4.951	4.197	0.0211	ca
C60	-0.601	4.951	3.504	-0.0273	ca
C61	-1.768	4.663	4.198	0.0210	ca
C62	-2.833	4.104	3.504	-0.0257	ca
C63	-3.732	3.307	4.198	0.0185	ca
C64	-4.415	2.317	3.504	-0.0205	ca
C65	-4.841	1.193	4.198	0.0115	ca
C66	-4.986	0.000	3.504	-0.0121	ca
C67	-4.841	-1.194	4.198	0.0010	ca
C68	-4.414	-2.318	3.503	-0.0024	ca
C69	-3.731	-3.307	4.197	-0.0085	ca
C70	-2.832	-4.104	3.503	0.0065	ca
C71	-1.767	-4.663	4.197	-0.0141	ca
C72	-0.600	-4.950	3.502	0.0116	ca
C73	0.602	-4.951	4.196	-0.0157	ca
C74	1.769	-4.663	3.502	0.0112	ca
C75	2.834	-4.104	4.196	-0.0136	ca
C76	3.733	-3.306	3.502	0.0054	ca
C77	4.416	-2.317	4.196	-0.0075	ca

C78	4.842	-1.193	3.502	-0.0037	ca
C79	4.987	0.000	5.584	-0.0064	ca
C80	4.842	1.194	6.278	-0.0008	ca
C81	4.416	2.318	5.584	-0.0197	ca
C82	3.733	3.307	6.278	0.0145	ca
C83	2.833	4.105	5.584	-0.0322	ca
C84	1.768	4.663	6.279	0.0299	ca
C85	0.601	4.951	5.585	-0.0399	ca
C86	-0.601	4.950	6.279	0.0363	ca
C87	-1.768	4.663	5.585	-0.0393	ca
C88	-2.832	4.104	6.279	0.0283	ca
C89	-3.733	3.307	5.585	-0.0307	ca
C90	-4.415	2.317	6.279	0.0125	ca
C91	-4.841	1.193	5.585	-0.0180	ca
C92	-4.985	-0.001	6.279	-0.0025	ca
C93	-4.841	-1.194	5.585	-0.0048	ca
C94	-4.414	-2.318	6.279	-0.0148	ca
C95	-3.731	-3.308	5.584	0.0061	ca
C96	-2.831	-4.104	6.278	-0.0252	ca
C97	-1.767	-4.664	5.584	0.0129	ca
C98	-0.600	-4.951	6.278	-0.0318	ca
C99	0.603	-4.951	5.583	0.0151	ca
C100	1.770	-4.663	6.277	-0.0313	ca
C101	2.834	-4.104	5.583	0.0123	ca
C102	3.734	-3.307	6.277	-0.0240	ca
C103	4.417	-2.317	5.583	0.0049	ca
C104	4.842	-1.193	6.277	-0.0132	ca
C105	4.975	0.000	8.361	-0.0748	ca
C106	4.827	1.190	7.665	-0.0243	ca
C107	4.405	2.312	8.362	-0.1308	ca
C108	3.722	3.297	7.665	0.0050	ca
C109	2.826	4.094	8.362	-0.1887	ca
C110	1.763	4.649	7.666	0.0291	ca
C111	0.600	4.938	8.362	-0.2256	ca
C112	-0.599	4.935	7.666	0.0378	ca
C113	-1.763	4.651	8.363	-0.2239	ca
C114	-2.823	4.091	7.666	0.0270	ca
C115	-3.722	3.298	8.363	-0.1825	ca
C116	-4.401	2.310	7.666	0.0019	ca
C117	-4.828	1.190	8.363	-0.1238	ca
C118	-4.970	-0.001	7.666	-0.0276	ca

C119	-4.828	-1.191	8.363	-0.0687	ca
C120	-4.400	-2.311	7.666	-0.0528	ca
C121	-3.721	-3.300	8.362	-0.0263	ca
C122	-2.822	-4.092	7.665	-0.0697	ca
C123	-1.762	-4.652	8.362	0.0006	ca
C124	-0.597	-4.936	7.665	-0.0778	ca
C125	0.602	-4.939	8.361	0.0093	ca
C126	1.765	-4.649	7.664	-0.0772	ca
C127	2.828	-4.094	8.361	-0.0019	ca
C128	3.723	-3.297	7.664	-0.0680	ca
C129	4.406	-2.312	8.361	-0.0309	ca
C130	4.828	-1.190	7.664	-0.0501	ca
H131	4.727	1.166	-1.744	0.1383	ha
H132	3.644	3.230	-1.744	0.1396	ha
H133	1.726	4.553	-1.744	0.1409	ha
H134	-0.588	4.834	-1.743	0.1415	ha
H135	-2.767	4.008	-1.743	0.1408	ha
H136	-4.313	2.264	-1.743	0.1393	ha
H137	-4.870	0.001	-1.743	0.1381	ha
H138	-4.312	-2.262	-1.743	0.1377	ha
H139	-2.766	-4.006	-1.744	0.1378	ha
H140	-0.586	-4.833	-1.744	0.1379	ha
H141	1.727	-4.552	-1.745	0.1379	ha
H142	3.645	-3.228	-1.745	0.1378	ha
H143	4.728	-1.164	-1.745	0.1377	ha
H144	4.870	0.000	9.443	0.1400	ha
H145	4.312	2.263	9.443	0.1391	ha
H146	2.767	4.007	9.444	0.1379	ha
H147	0.588	4.834	9.444	0.1373	ha
H148	-1.726	4.553	9.445	0.1374	ha
H149	-3.643	3.228	9.445	0.1381	ha
H150	-4.726	1.164	9.445	0.1392	ha
H151	-4.726	-1.166	9.445	0.1401	ha
H152	-3.642	-3.230	9.444	0.1408	ha
H153	-1.724	-4.554	9.443	0.1413	ha
H154	0.589	-4.835	9.443	0.1414	ha
H155	2.768	-4.008	9.443	0.1412	ha
H156	4.313	-2.263	9.443	0.1408	ha

3. *n*-butane

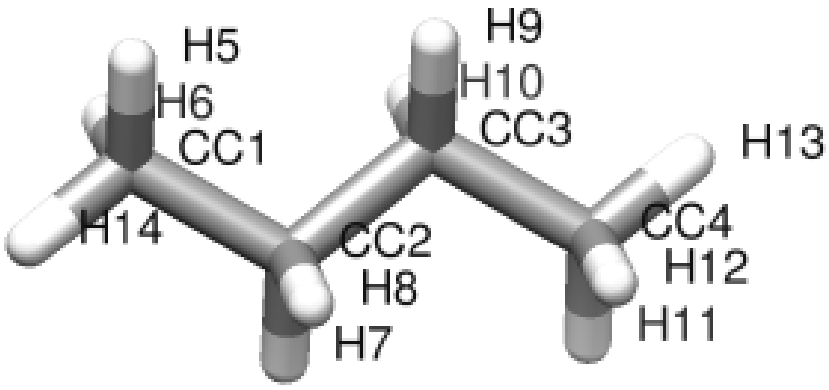

Figure s4. *n*-butane.

Table S3. Butane x,y,z coordinates, partial charges, and atom types.

atom name	x (Å)	y(Å)	z(Å)	partial charge	atom type
CC1	0.453	0.002	2.486	-0.0926	c3
CC2	-0.434	0.003	3.739	-0.0803	c3
CC3	0.434	-0.002	5.004	-0.0803	c3
CC4	-0.453	0.001	6.257	-0.0926	c3
H5	1.095	0.885	2.475	0.0322	hc
H6	1.085	-0.888	2.470	0.0322	hc
H7	-1.080	-0.878	3.733	0.0382	hc
H8	-1.074	0.888	3.736	0.0382	hc
H9	1.081	0.877	5.009	0.0382	hc
H10	1.073	-0.888	5.008	0.0382	hc
H11	-1.097	-0.880	6.269	0.0322	hc
H12	-1.083	0.893	6.273	0.0322	hc
H13	0.164	-0.005	7.159	0.0321	hc
H14	-0.164	0.008	1.584	0.0321	hc

4. *n*-hexane

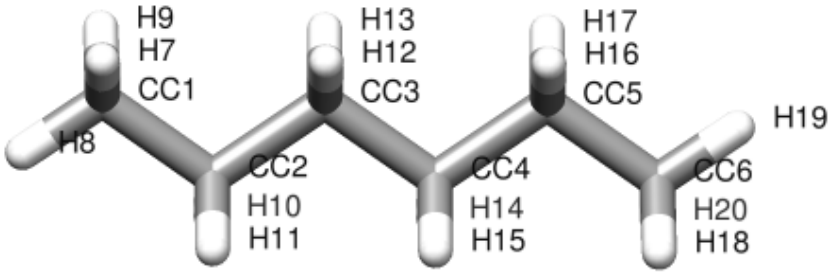

Figure S5. *n*-hexane.

Table S4. Hexane x,y,z coordinates, partial charges, and atom types.

atom name	x (Å)	y (Å)	z (Å)	partial charge	atom type
CC1	-0.437	0.000	1.223	-0.0925	c3
CC2	0.441	-0.001	2.482	-0.0800	c3
CC3	-0.438	0.002	3.741	-0.0793	c3
CC4	0.438	-0.002	5.002	-0.0794	c3
CC5	-0.441	0.004	6.261	-0.0800	c3
CC6	0.438	0.000	7.520	-0.0925	c3
H7	-1.076	-0.885	1.206	0.0324	hc
H8	0.184	-0.001	0.325	0.0323	hc
H9	-1.072	0.889	1.205	0.0323	hc
H10	1.086	0.880	2.481	0.0383	hc
H11	1.081	-0.886	2.482	0.0383	hc
H12	-1.083	-0.879	3.740	0.0392	hc
H13	-1.077	0.887	3.741	0.0391	hc
H14	1.085	0.878	5.002	0.0391	hc
H15	1.076	-0.888	5.003	0.0392	hc
H16	-1.088	-0.876	6.262	0.0383	hc
H17	-1.078	0.891	6.261	0.0383	hc
H18	1.070	-0.891	7.538	0.0324	hc
H19	-0.183	0.004	8.418	0.0322	hc
H20	1.080	0.883	7.536	0.0323	hc

5. *n*-tetracosane

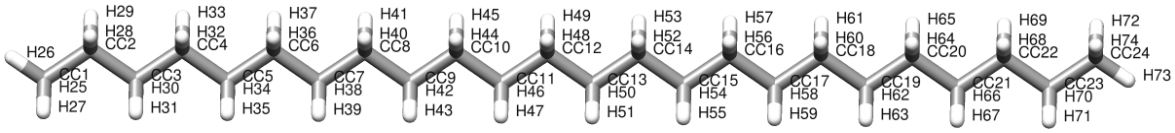

Figure s6. *n*-tetracosane.

Table S5. Tetracosane x,y,z coordinates, partial charges, and atom types

atom name	x (Å)	y(Å)	z(Å)	partial charge	atom type
CC1	0.440	0.000	-5.030	-0.0925	c3
CC2	-0.441	0.000	-3.774	-0.0801	c3
CC3	0.437	-0.001	-2.516	-0.0793	c3
CC4	-0.442	0.001	-1.260	-0.0790	c3
CC5	0.440	-0.001	-0.008	-0.0790	c3
CC6	-0.440	0.001	1.245	-0.0789	c3
CC7	0.441	-0.001	2.495	-0.0790	c3
CC8	-0.441	0.001	3.745	-0.0790	c3
CC9	0.441	-0.001	4.995	-0.0790	c3
CC10	-0.441	0.001	6.244	-0.0790	c3
CC11	0.441	-0.001	7.494	-0.0790	c3
CC12	-0.441	0.001	8.743	-0.0790	c3
CC13	0.441	-0.001	9.992	-0.0790	c3
CC14	-0.441	0.001	11.241	-0.0790	c3
CC15	0.441	-0.001	12.491	-0.0790	c3
CC16	-0.441	0.001	13.740	-0.0790	c3
CC17	0.441	-0.001	14.990	-0.0790	c3
CC18	-0.441	0.001	16.240	-0.0790	c3
CC19	0.440	-0.001	17.490	-0.0790	c3
CC20	-0.440	0.001	18.742	-0.0790	c3
CC21	0.442	-0.001	19.995	-0.0790	c3
CC22	-0.437	0.001	21.251	-0.0793	c3
CC23	0.440	-0.001	22.509	-0.0801	c3
CC24	-0.441	0.000	23.765	-0.0925	c3
H25	1.077	0.887	-5.044	0.0324	hc
H26	-0.180	0.000	-5.928	0.0323	hc

H27	1.077	-0.887	-5.044	0.0324	hc
H28	-1.083	-0.883	-3.773	0.0383	hc
H29	-1.082	0.884	-3.773	0.0383	hc
H30	1.079	0.882	-2.514	0.0394	hc
H31	1.077	-0.885	-2.514	0.0394	hc
H32	-1.085	-0.882	-1.257	0.0393	hc
H33	-1.082	0.886	-1.257	0.0393	hc
H34	1.083	0.881	-0.006	0.0394	hc
H35	1.079	-0.886	-0.006	0.0394	hc
H36	-1.084	-0.881	1.246	0.0395	hc
H37	-1.080	0.886	1.246	0.0394	hc
H38	1.084	0.881	2.496	0.0395	hc
H39	1.080	-0.886	2.496	0.0394	hc
H40	-1.084	-0.881	3.746	0.0395	hc
H41	-1.080	0.887	3.746	0.0395	hc
H42	1.084	0.881	4.995	0.0395	hc
H43	1.080	-0.887	4.995	0.0395	hc
H44	-1.084	-0.881	6.245	0.0395	hc
H45	-1.080	0.887	6.245	0.0395	hc
H46	1.084	0.882	7.494	0.0395	hc
H47	1.080	-0.887	7.494	0.0395	hc
H48	-1.084	-0.881	8.743	0.0395	hc
H49	-1.080	0.887	8.743	0.0395	hc
H50	1.084	0.881	9.992	0.0395	hc
H51	1.080	-0.887	9.992	0.0395	hc
H52	-1.084	-0.881	11.241	0.0395	hc
H53	-1.080	0.887	11.241	0.0395	hc
H54	1.084	0.881	12.491	0.0395	hc
H55	1.080	-0.887	12.491	0.0395	hc
H56	-1.084	-0.881	13.740	0.0395	hc
H57	-1.080	0.887	13.740	0.0395	hc
H58	1.084	0.881	14.989	0.0395	hc
H59	1.080	-0.887	14.989	0.0395	hc
H60	-1.084	-0.881	16.239	0.0394	hc
H61	-1.080	0.887	16.239	0.0395	hc
H62	1.084	0.881	17.489	0.0395	hc
H63	1.080	-0.887	17.489	0.0394	hc
H64	-1.084	-0.881	18.741	0.0394	hc
H65	-1.079	0.887	18.741	0.0394	hc
H66	1.085	0.881	19.991	0.0393	hc
H67	1.081	-0.886	19.991	0.0393	hc

H68	-1.081	-0.881	21.248	0.0394	hc
H69	-1.076	0.886	21.249	0.0394	hc
H70	1.084	0.881	22.508	0.0383	hc
H71	1.080	-0.886	22.508	0.0383	hc
H72	-1.075	0.889	23.780	0.0324	hc
H73	0.180	-0.003	24.663	0.0323	hc
H74	-1.081	-0.885	23.778	0.0324	hc

6. Benzene

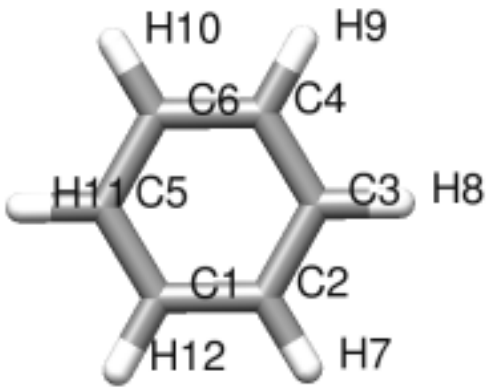

Figure S7. Benzene.

Table S6. Benzene x,y,z coordinates, partial charges, and atom types.

atom name	x (Å)	y (Å)	z (Å)	partial charge	atom type
C1	-0.019	-0.032	0.000	-0.1301	ca
C2	1.369	-0.032	0.000	-0.1301	ca
C3	2.062	1.169	0.000	-0.1301	ca
C4	1.369	2.370	0.000	-0.1301	ca
C5	-0.712	1.169	0.000	-0.1301	ca
C6	-0.019	2.370	0.000	-0.1301	ca
H7	1.912	-0.974	0.000	0.1301	ha
H8	3.149	1.169	0.000	0.1301	ha
H9	1.912	3.312	0.000	0.1301	ha
H10	-0.562	3.312	0.000	0.1301	ha
H11	-1.799	1.169	0.000	0.1301	ha
H12	-0.562	-0.974	0.000	0.1301	ha

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