

Supporting Information for “Magnetically Induced Current Density using London Atomic Orbitals of Dihydroindeno-[1,2-*b*]-Fluorenes”

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Table S1. Selected molecular structural parameters obtained at B3LYP/6-311++G(d,p) level for dihydroindeno-[1,2-*b*]-fluorene. Parameters refer to annotation in Figure 1.

Substituent	r ₁	r ₂	r ₃	α	r ₁	r ₂	r ₃	α
	<i>cis</i>				<i>trans</i>			
H	1.08	1.40	1.39	120	1.08	1.40	1.39	120
NH₂	1.40	1.41	1.39	120	1.38	1.41	1.39	120
O-<i>t</i>Bu	1.38	1.40	1.39	120	1.37	1.40	1.40	127
CH₃	1.51	1.40	1.39	121	1.51	1.40	1.40	121
Si(CH₃)₃	1.90	1.41	1.39	121	1.90	1.41	1.39	122
OH	1.37	1.40	1.39	122	1.37	1.40	1.39	117
OCH₃	1.34	1.41	1.39	120	1.37	1.40	1.40	115
F	1.36	1.41	1.40	120	1.36	1.39	1.39	118
Cl	2.13	1.40	1.39	119	2.13	1.40	1.39	119
Br	1.76	1.39	1.39	119	1.76	1.40	1.39	119
CN	1.43	1.41	1.39	120	1.43	1.41	1.39	119
NO₂	1.47	1.40	1.39	119	1.48	1.40	1.39	118

Table S2. Molecular Structures optimized at B3LYP/6-311++G(d,p) level.

R	<i>cis</i>				<i>trans</i>			
H	C	2.589615	0.500472	-0.000041	C	2.810371	-0.403606	-0.000014
	C	3.439029	-0.622787	0.000011	C	3.316014	0.911441	0.000078
	C	3.125372	1.788965	-0.000027	C	3.682572	-1.493513	-0.000076
	C	4.818513	-0.463667	0.000112	C	4.685459	1.140254	0.000096
	C	4.511204	1.943479	0.000085	C	5.056833	-1.258008	-0.000045
	H	2.479820	2.660550	-0.000085	H	3.303924	-2.509914	-0.000160
	C	5.352785	0.827832	0.000157	C	5.556596	0.047120	0.000040
	H	5.477522	-1.325997	0.000168	H	5.079973	2.151319	0.000158
	H	4.941031	2.939009	0.000111	H	5.745661	-2.095488	-0.000092
	C	1.195449	0.036947	-0.000108	H	6.628165	0.212307	0.000051
	C	-0.000004	0.755973	-0.000053	C	1.344227	-0.343958	-0.000072
	C	1.194063	-1.374815	-0.000163	C	0.391679	-1.367868	-0.000104
	H	-0.000077	1.840705	0.000030	C	0.949921	1.012041	-0.000039
	C	0.000015	-2.089364	-0.000163	H	0.692875	-2.410657	-0.000081
	C	-1.195445	0.036917	-0.000126	C	-0.391704	1.367798	-0.000088
	H	0.000041	-3.175505	-0.000154	C	-0.949913	-1.012092	-0.000150
	C	-1.194137	-1.374862	-0.000219	H	-0.692865	2.410603	-0.000036
	C	2.616409	-1.893685	-0.000077	C	-1.344262	0.343921	-0.000151
	H	2.825106	-2.513818	-0.879813	C	2.173633	1.904568	0.000152
	H	2.824991	-2.513961	0.879581	H	2.201879	2.557707	0.880044
	C	-2.589601	0.500490	0.000126	H	2.201997	2.558117	-0.879410
	C	-3.439040	-0.622784	0.000355	C	-2.810301	0.403598	-0.000010
	C	-2.616223	-1.893690	0.000141	C	-3.316074	-0.911399	0.000143
	H	-2.825528	-2.513885	-0.879466	C	-2.173630	-1.904662	0.000071
	H	-2.824681	-2.514234	0.879705	H	-2.201796	-2.557903	0.879942
	C	-4.818514	-0.463673	0.000184	H	-2.202203	-2.558053	-0.879691
	C	-4.511237	1.943463	-0.000097	C	-4.685494	-1.140191	0.000177
	C	-5.352809	0.827819	-0.000012	C	-5.056783	1.258065	-0.000072
	C	-3.125396	1.788959	-0.000075	C	-5.556621	-0.047036	0.000091
	H	-5.477527	-1.326002	0.000251	C	-3.682518	1.493510	-0.000137
	H	-4.941089	2.938982	-0.000266	H	-5.080013	-2.151255	0.000267
	H	-2.479858	2.660555	-0.000270	H	-6.628189	-0.212199	0.000139
	H	6.428207	0.965842	0.000246	H	-5.745538	2.095605	-0.000172
	H	-6.428234	0.965821	-0.000099	H	-3.303898	2.509927	-0.000302
NH₂	C	-2.590230	-0.397139	-0.004684	C	-2.803933	0.452680	0.004599
	C	-3.441441	0.723966	-0.005714	C	-3.334629	-0.851934	0.005630
	C	-3.144483	-1.677110	-0.004721	C	-3.673308	1.544032	0.004520
	C	-4.819325	0.578937	-0.006347	C	-4.702386	-1.070650	0.006390
	C	-4.527620	-1.827886	-0.005348	C	-5.047954	1.328899	0.005279
	H	-2.511713	-2.558217	-0.003398	H	-3.292688	2.559890	0.002996
	C	-5.379699	-0.709866	-0.004340	C	-5.579454	0.027694	0.004531
	H	-5.470716	1.448469	-0.013175	H	-5.104724	-2.079886	0.013091
	H	-4.961093	-2.823091	-0.011298	H	-5.725740	2.176841	0.011001
	C	-1.197079	0.063586	-0.002309	C	-1.341005	0.369651	0.002165
	C	-0.000005	-0.654453	0.000005	C	-0.366412	1.373894	-0.000050
	C	-1.194572	1.475564	-0.002487	C	-0.968036	-0.992614	0.002240
	H	0.000066	-1.739412	0.000182	H	-0.646304	2.422905	0.000065
	C	0.000033	2.189056	-0.000178	C	0.366412	-1.373894	0.000054
	C	1.197083	0.063619	0.002112	C	0.968036	0.992614	-0.002235
	H	0.000024	3.275533	-0.000217	H	0.646304	-2.422905	-0.000061
	C	1.194754	1.475619	0.002074	C	1.341005	-0.369650	-0.002159
	C	-2.617894	1.995184	-0.005252	C	-2.208192	-1.864489	0.004956

	H	-2.827238	2.613270	-0.886366	H	-2.247809	-2.515455	0.886038
	H	-2.829868	2.615724	0.873487	H	-2.249848	-2.518210	-0.873979
	C	2.590199	-0.397170	0.004985	C	2.803934	-0.452680	-0.004598
	C	3.441439	0.723951	0.006198	C	3.334629	0.851934	-0.005633
	C	2.617715	1.995140	0.005332	C	2.208192	1.864489	-0.004957
	H	2.830613	2.615707	-0.873236	H	2.249853	2.518212	0.873975
	H	2.826760	2.613626	0.886312	H	2.247804	2.515454	-0.886040
	C	4.819307	0.578934	0.006494	C	4.702386	1.070650	-0.006396
	C	4.527606	-1.827896	0.005295	C	5.047954	-1.328900	-0.005276
	C	5.379691	-0.709862	0.004387	C	5.579453	-0.027694	-0.004534
	C	3.144485	-1.677133	0.004720	C	3.673308	-1.544032	-0.004515
	H	5.470685	1.448481	0.013237	H	5.104724	2.079885	-0.013101
	H	4.961110	-2.823087	0.011057	H	5.725740	-2.176841	-0.010995
	H	2.511729	-2.558256	0.003155	H	3.292687	-2.559889	-0.002986
	N	-6.768021	-0.878649	-0.063121	N	-6.963945	-0.171366	0.063649
	H	-7.315117	-0.103954	0.282736	H	-7.289853	-1.061576	-0.283558
	H	-7.112353	-1.764971	0.275849	H	-7.527178	0.594473	-0.276120
	N	6.767995	-0.878698	0.062982	N	6.963945	0.171365	-0.063656
	H	7.315138	-0.103789	-0.282303	H	7.527178	-0.594474	0.276113
	H	7.112368	-1.764847	-0.276382	H	7.289854	1.061575	0.283549
O- <i>t</i> Bu	C	-2.590240	0.252703	0.015625	C	-2.825321	0.287256	-0.001874
	C	-3.441772	1.376161	0.020165	C	-3.278430	-1.048389	-0.002078
	C	-3.145831	-1.021777	0.018993	C	-3.756250	1.320519	-0.002752
	C	-4.815451	1.228185	0.026769	C	-4.628120	-1.342383	-0.002988
	C	-4.534239	-1.180984	0.026949	C	-5.123673	1.031978	-0.003863
	H	-2.515393	-1.904638	0.016415	H	-3.438039	2.357677	-0.002716
	C	-5.378222	-0.061153	0.030011	C	-5.570166	-0.297229	-0.003893
	H	-5.485835	2.080377	0.029590	H	-4.994505	-2.362895	-0.003070
	H	-4.936733	-2.181369	0.031796	H	-5.821918	1.853697	-0.004846
	C	-1.196787	0.713712	0.007570	C	-1.359581	0.289906	-0.000655
	C	-0.000017	-0.004292	0.000933	C	-0.446480	1.349923	0.000008
	C	-1.194743	2.125687	0.007006	C	-0.908356	-1.048483	-0.000113
	H	-0.000014	-1.089278	0.001435	H	-0.788049	2.380455	-0.000404
	C	-0.000026	2.839168	-0.000430	C	0.446497	-1.349934	0.001103
	C	1.196751	0.713712	-0.006391	C	0.908372	1.048472	0.001230
	H	-0.000026	3.925528	-0.000954	H	0.788065	-2.380466	0.001519
	C	1.194700	2.125688	-0.007173	C	1.359598	-0.289917	0.001789
	C	-2.617487	2.646943	0.015252	C	-2.094278	-1.992847	-0.001020
	H	-2.832490	3.266525	-0.863216	H	-2.097111	-2.646403	0.878863
	H	-2.822235	3.266396	0.896268	H	-2.095667	-2.646487	-0.880847
	C	2.590204	0.252705	-0.014105	C	2.825338	-0.287264	0.003113
	C	3.441736	1.376161	-0.019788	C	3.278444	1.048379	0.003360
	C	2.617437	2.646957	-0.015849	C	2.094293	1.992838	0.002207
	H	2.822202	3.265871	-0.897231	H	2.095630	2.646474	0.882037
	H	2.832408	3.267058	0.862268	H	2.097177	2.646398	-0.877673
	C	4.815407	1.228188	-0.026529	C	4.628134	1.342373	0.004376
	C	4.534228	-1.180982	-0.024316	C	5.123694	-1.031986	0.005514
	C	5.378213	-0.061149	-0.028648	C	5.570184	0.297224	0.005447
	C	3.145817	-1.021764	-0.016340	C	3.756272	-1.320524	0.004162
	H	5.485788	2.080380	-0.030285	H	4.994518	2.362887	0.004453
	H	4.936672	-2.181394	-0.028110	H	5.821933	-1.853714	0.006868
	H	2.515399	-1.904637	-0.012807	H	3.438063	-2.357683	0.004174
	8	-6.745531	-0.061263	0.043584	O	6.867243	0.729943	0.008023
	C	-7.617586	-1.228113	-0.013482	C	8.063880	-0.102518	-0.002974
	8	6.745504	-0.061194	-0.042034	O	-6.867231	-0.729948	-0.005643
	C	7.617657	-1.228087	0.012037	C	-8.063885	0.102538	0.000985
	C	-9.010533	-0.587691	-0.017500	C	8.147534	-0.939346	-1.286943
	H	-9.124683	0.066453	-0.884390	H	8.032901	-0.294108	-2.161050

	H	-9.784588	-1.357999	-0.055471	H	9.127164	-1.421369	-1.344870
	H	-9.155557	0.009882	0.884939	H	7.389109	-1.719675	-1.339709
	C	-7.461798	-2.099232	1.240909	C	8.162142	-0.951437	1.272083
	H	-8.242177	-2.864942	1.252939	H	7.405341	-1.733295	1.325547
	H	-6.498614	-2.605540	1.294091	H	9.142900	-1.432740	1.315205
	H	-7.573022	-1.484965	2.137456	H	8.055895	-0.314565	2.153347
	C	-7.412898	-2.013058	-1.316216	C	9.183245	0.945088	-0.004228
	H	-6.443964	-2.508222	-1.369613	H	9.112852	1.576120	0.884207
	H	-8.186046	-2.781078	-1.404174	H	10.161503	0.458338	-0.011449
	H	-7.499736	-1.342196	-2.174101	H	9.103618	1.583925	-0.886278
	C	7.459573	-2.097861	-1.242975	C	-8.150500	0.941775	1.283188
	H	7.568997	-1.482672	-2.139113	H	-7.392407	1.722412	1.336118
	H	8.240027	-2.863449	-1.257292	H	-9.130368	1.423677	1.338102
	H	6.496335	-2.604209	-1.294853	H	-8.037586	0.298207	2.158745
	C	7.415282	-2.014438	1.314299	C	-8.159276	0.949044	-1.275883
	H	6.446305	-2.509389	1.368960	H	-9.139926	1.430289	-1.322055
	H	8.188387	-2.782744	1.400039	H	-7.402327	1.730773	-1.329151
	H	7.503811	-1.344513	2.172747	H	-8.051142	0.310513	-2.155714
	C	9.010608	-0.587695	0.014271	C	-9.183263	-0.945065	0.001700
	H	9.126212	0.065710	0.881527	H	-9.105377	-1.582449	0.884956
	H	9.784705	-1.358058	0.050360	H	-10.161539	-0.458324	0.006175
	H	9.154184	0.010614	-0.887907	H	-9.111083	-1.577569	-0.885546
CH ₃	C	-2.589919	-0.392859	0.001934	C	2.802754	-0.453297	-0.001366
	C	-3.439755	0.728808	0.002745	C	3.332872	0.851167	-0.003761
	C	-3.136088	-1.675593	0.008023	C	3.663932	-1.550179	-0.006035
	C	-4.818391	0.572445	0.007978	C	4.704487	1.057992	-0.009008
	C	-4.522362	-1.821864	0.012823	C	5.040660	-1.331145	-0.010829
	H	-2.499023	-2.553561	0.013229	H	3.277223	-2.563708	-0.010007
	C	-5.379966	-0.712751	0.009854	C	5.580785	-0.037482	-0.009262
	H	-5.469963	1.441930	0.012722	H	5.107889	2.066837	-0.014891
	H	-4.950900	-2.819111	0.021326	H	5.713545	-2.182802	-0.018197
	C	-1.195827	0.069301	0.001319	C	1.338553	-0.368498	-0.000930
	C	-0.000002	-0.649516	0.000022	C	0.366802	-1.374498	0.001707
	C	-1.194264	1.481168	0.001588	C	0.968102	0.994382	-0.002850
	H	-0.000016	-1.734320	-0.000014	H	0.648835	-2.422734	0.003207
	C	0.000007	2.195426	0.000023	C	-0.366799	1.374489	-0.001733
	C	1.195844	0.069297	-0.001274	C	-0.968101	-0.994389	0.002822
	H	0.000027	3.281670	0.000030	H	-0.648836	2.422725	-0.003228
	C	1.194298	1.481163	-0.001511	C	-1.338552	0.368487	0.000908
	C	-2.617047	2.000224	0.003659	C	2.208106	1.865094	-0.006185
	H	-2.826772	2.621971	-0.874720	H	2.248495	2.521034	0.871156
	H	-2.825102	2.618747	0.884719	H	2.247757	2.514475	-0.888471
	C	2.589905	-0.392850	-0.001959	C	-2.802752	0.453288	0.001352
	C	3.439757	0.728801	-0.002841	C	-3.332870	-0.851174	0.003747
	C	2.617032	2.000233	-0.003647	C	-2.208104	-1.865101	0.006139
	H	2.824952	2.618834	-0.884676	H	-2.247756	-2.514536	0.888382
	H	2.826835	2.621858	0.874813	H	-2.248493	-2.520987	-0.871244
	C	4.818393	0.572448	-0.008056	C	-4.704489	-1.057996	0.009020
	C	4.522350	-1.821857	-0.012804	C	-5.040657	1.331141	0.010854
	C	5.379965	-0.712745	-0.009883	C	-5.580785	0.037475	0.009300
	C	3.136086	-1.675595	-0.007993	C	-3.663932	1.550172	0.006033
	H	5.469953	1.441939	-0.012828	H	-5.107901	-2.066835	0.014901
	H	4.950907	-2.819098	-0.021271	H	-5.713533	2.182806	0.018232
	H	2.499023	-2.553564	-0.013137	H	-3.277228	2.563703	0.009999
	C	-6.878752	-0.896808	-0.019019	C	7.075689	0.174844	0.018875
	H	-7.258191	-0.884482	-1.047083	H	7.435158	0.315868	1.044511
	H	-7.172213	-1.850594	0.425508	H	7.608316	-0.682576	-0.398731
	H	-7.389663	-0.098714	0.525502	H	7.363876	1.061925	-0.550962

	C	6.878749	-0.896821	0.018998	C	-7.075696	-0.174805	-0.018808
	H	7.258217	-0.884248	1.047048	H	-7.435477	-0.313812	-1.044610
	H	7.172182	-1.850720	-0.425304	H	-7.363701	-1.062988	0.549390
	H	7.389666	-0.098870	-0.525730	H	-7.608208	0.681801	0.400626
Si(CH ₃) ₃	C	-2.586491	-0.093126	0.000060	C	2.788448	-0.527840	-0.000184
	C	-3.441669	1.025522	0.000077	C	3.353768	0.762506	-0.000163
	C	-3.124012	-1.378920	0.000054	C	3.616819	-1.649247	-0.000112
	C	-4.818450	0.859606	0.000092	C	4.730332	0.928297	-0.000074
	C	-4.510729	-1.532194	0.000059	C	5.000013	-1.468288	-0.000002
	H	-2.480772	-2.252705	0.000040	H	3.199984	-2.651031	-0.000123
	C	-5.385720	-0.430529	0.000078	C	5.588155	-0.190127	0.000019
	H	-5.460000	1.737626	0.000116	H	5.144834	1.933625	-0.000050
	H	-4.917008	-2.538276	0.000047	H	5.634046	-2.348799	0.000081
	C	-1.194928	0.375383	0.000044	C	1.327453	-0.403420	-0.000235
	C	0.003520	-0.338882	0.000041	C	0.330252	-1.384196	-0.000256
	C	-1.199511	1.787454	0.000036	C	0.994116	0.969302	-0.000223
	H	0.007924	-1.423606	0.000050	H	0.585314	-2.439218	-0.000274
	C	-0.008307	2.507001	0.000016	C	-0.330247	1.384160	-0.000206
	C	1.195875	0.385281	0.000018	C	-0.994111	-0.969338	-0.000248
	H	-0.012849	3.593136	0.000008	H	-0.585308	2.439182	-0.000188
	C	1.188751	1.797483	0.000003	C	-1.327447	0.403385	-0.000211
	C	-2.624069	2.300664	0.000065	C	2.256534	1.806579	-0.000195
	H	-2.834512	2.920239	-0.879646	H	2.313311	2.457952	0.879640
	H	-2.834474	2.920242	0.879785	H	2.313354	2.457964	-0.880018
	C	2.591496	-0.070884	0.000003	C	-2.788441	0.527806	-0.000159
	C	3.436686	1.053009	-0.000032	C	-3.353764	-0.762538	-0.000160
	C	2.609198	2.321660	-0.000024	C	-2.256531	-1.806613	-0.000231
	H	2.814812	2.943026	-0.879646	H	-2.313298	-2.458018	0.879581
	H	2.814835	2.943009	0.879607	H	-2.313362	-2.457966	-0.880076
	C	4.817137	0.899777	-0.000069	C	-4.730328	-0.928331	-0.000090
	C	4.525749	-1.494074	-0.000007	C	-5.000006	1.468253	-0.000017
	C	5.393514	-0.383863	-0.000053	C	-5.588152	0.190092	-0.000016
	C	3.139874	-1.353994	0.000015	C	-3.616812	1.649212	-0.000090
	H	5.451895	1.781060	-0.000104	H	-5.144818	-1.933665	-0.000112
	H	4.939662	-2.498537	0.000001	H	-5.634035	2.348765	0.000026
	H	2.503622	-2.232847	0.000038	H	-3.199978	2.650997	-0.000094
	Si	-7.268964	-0.643704	-0.000040	Si	-7.468020	-0.050354	0.000194
	Si	7.270891	-0.643798	-0.000015	Si	7.468007	0.050385	0.000171
	C	-7.715624	-2.478920	0.000121	C	8.338048	-1.626114	0.000217
	H	-7.328707	-2.993097	-0.884650	H	8.084437	-2.217512	0.885007
	H	-7.328739	-2.992960	0.884987	H	8.084668	-2.217524	-0.884630
	H	-8.803433	-2.600644	0.000111	H	9.423598	-1.485674	0.000359
	C	-7.994124	0.179514	1.540386	C	7.976366	1.022201	-1.540442
	H	-9.084878	0.086725	1.558452	H	9.057847	1.191715	-1.558719
	H	-7.603070	-0.278759	2.453501	H	7.705447	0.483864	-2.453414
	H	-7.752980	1.246165	1.577334	H	7.488230	2.000764	-1.577515
	C	-7.993740	0.179215	-1.540810	C	7.976192	1.022034	1.540949
	H	-7.602834	-0.279528	-2.453750	H	7.706451	0.482970	2.453838
	H	-9.084536	0.086918	-1.558898	H	9.057499	1.192738	1.558607
	H	-7.752112	1.245746	-1.578095	H	7.487016	2.000046	1.578783
	C	8.154520	1.026094	-0.000398	C	-8.337963	1.626194	0.000936
	H	7.906647	1.619544	0.884714	H	-8.084766	2.217786	-0.883843
	H	9.238914	0.877042	-0.001008	H	-9.423521	1.485839	0.001332
	H	7.905671	1.619623	-0.885183	H	-8.084072	2.217371	0.885793
	C	7.771128	-1.618260	1.541265	C	-7.976585	-1.021481	-1.540789
	H	7.506143	-1.076267	2.453822	H	-7.705932	-0.482670	-2.453557
	H	7.273198	-2.591741	1.579911	H	-7.488359	-1.999976	-1.578434
	H	8.850919	-1.798302	1.558803	H	-9.058050	-1.191126	-1.558892

	C	7.771337	-1.618890	-1.540823	C	-7.976086	-1.022635	1.540608
	H	8.851123	-1.799029	-1.557918	H	-9.057410	-1.193196	1.558426
	H	7.273353	-2.592348	-1.579285	H	-7.487012	-2.000718	1.577911
	H	7.506730	-1.077199	-2.453668	H	-7.706079	-0.484017	2.453686
OH	C	-2.589915	-0.399470	-0.000077	C	-2.803977	0.451535	0.000001
	C	-3.438693	0.721594	-0.000037	C	-3.331509	-0.853041	0.000010
	C	-3.138266	-1.683518	-0.000067	C	-3.668603	1.547852	-0.000017
	C	-4.819080	0.571848	0.000048	C	-4.702788	-1.068109	-0.000000
	C	-4.520234	-1.841086	0.000033	C	-5.044356	1.339427	-0.000027
	H	-2.500880	-2.560926	-0.000104	H	-3.282622	2.561393	-0.000024
	C	-5.356003	-0.719587	0.000092	C	-5.558109	0.039029	-0.000020
	H	-5.477185	1.437157	0.000096	H	-5.112808	-2.074879	0.000005
	H	-4.972825	-2.825197	0.000066	H	-5.737633	2.171553	-0.000043
	C	-1.196171	0.062424	-0.000104	C	-1.339884	0.368420	0.000003
	C	0.000006	-0.656278	-0.000026	C	-0.367660	1.374133	0.000000
	C	-1.194060	1.474016	-0.000175	C	-0.967012	-0.993404	0.000011
	H	0.000083	-1.741081	0.000075	H	-0.648807	2.422631	-0.000004
	C	-0.000019	2.188321	-0.000171	C	0.367660	-1.374136	0.000010
	C	1.196163	0.062466	-0.000091	C	0.967012	0.993403	-0.000002
	H	-0.000049	3.274618	-0.000171	H	0.648806	-2.422634	0.000014
	C	1.194113	1.474072	-0.000208	C	1.339883	-0.368423	-0.000001
	C	-2.617240	1.993266	-0.000108	C	-2.206344	-1.865738	0.000034
	H	-2.827787	2.612346	-0.880158	H	-2.246635	-2.517996	0.880103
	H	-2.827708	2.612483	0.879859	H	-2.246643	-2.518083	-0.879967
	C	2.589907	-0.399476	0.000174	C	2.803977	-0.451537	0.000008
	C	3.438709	0.721590	0.000392	C	3.331508	0.853039	0.000017
	C	2.617067	1.993291	0.000166	C	2.206343	1.865736	0.000012
	H	2.828257	2.612446	-0.879726	H	2.246624	2.518030	0.880053
	H	2.827387	2.612748	0.880052	H	2.246652	2.518041	-0.880018
	C	4.819089	0.571847	0.000156	C	4.702786	1.068110	0.000015
	C	4.520251	-1.841083	-0.000102	C	5.044358	-1.339424	-0.000013
	C	5.356022	-0.719587	0.000017	C	5.558110	-0.039027	0.000001
	C	3.138278	-1.683509	-0.000086	C	3.668606	-1.547853	-0.000010
	H	5.477196	1.437155	0.000169	H	5.112803	2.074881	0.000026
	H	4.972860	-2.825184	-0.000240	H	5.737635	-2.171550	-0.000028
	H	2.500890	-2.560919	-0.000273	H	3.282627	-2.561395	-0.000022
	O	-6.707788	-0.950530	0.000198	O	-6.923351	-0.090900	-0.000031
	H	-7.180693	-0.112005	0.000124	H	-7.161488	-1.023617	-0.000046
	O	6.707813	-0.950529	-0.000140	O	6.923351	0.090906	0.000003
	H	7.180719	-0.112006	0.000823	H	7.161487	1.023622	-0.000027
OCH ₃	C	-2.590221	-0.417948	0.000068	C	-2.773564	0.609466	0.000085
	C	-3.438657	0.699627	-0.000010	C	-3.375193	-0.658976	0.000315
	C	-3.141029	-1.703150	0.000080	C	-3.577214	1.754199	0.000052
	C	-4.823262	0.559146	-0.000053	C	-4.758865	-0.805528	0.000477
	C	-4.520237	-1.854918	0.000037	C	-4.958210	1.619258	0.000168
	H	-2.505625	-2.582094	0.000131	H	-3.136321	2.745154	-0.000092
	C	-5.363382	-0.732436	-0.000023	C	-5.552921	0.347667	0.000343
	H	-5.460578	1.434228	-0.000119	H	-5.202897	-1.792843	0.000813
	H	-4.976878	-2.837299	0.000046	H	-5.606861	2.486936	0.000133
	C	-1.196277	0.042715	0.000114	C	-1.316774	0.444258	-0.000014
	C	-0.000014	-0.676117	0.000176	C	-0.288624	1.392953	-0.000192
	C	-1.194163	1.454405	0.000064	C	-1.022200	-0.936799	0.000171
	H	-0.000042	-1.760961	0.000156	H	-0.509627	2.455813	-0.000336
	C	0.000003	2.168654	0.000107	C	0.288624	-1.392952	0.000193
	C	1.196250	0.042688	0.000238	C	1.022199	0.936801	-0.000169
	H	0.000005	3.255011	0.000046	H	0.509627	-2.455812	0.000340
	C	1.194124	1.454381	0.000247	C	1.316774	-0.444257	0.000015

	C	-2.617742	1.972146	-0.000047	C	-2.310208	-1.735447	0.000345
	H	-2.828512	2.591330	-0.880098	H	-2.388013	-2.384454	0.880396
	H	-2.828604	2.591494	0.879859	H	-2.388151	-2.384508	-0.879664
	C	2.590214	-0.417955	0.000049	C	2.773564	-0.609464	-0.000068
	C	3.438605	0.699654	-0.000145	C	3.375193	0.658975	-0.000290
	C	2.617805	1.972097	0.000168	C	2.310209	1.735447	-0.000343
	H	2.828403	2.591690	-0.879614	H	2.388146	2.384520	0.879658
	H	2.828680	2.590994	0.880393	H	2.388021	2.384442	-0.880402
	C	4.823224	0.559165	-0.000202	C	4.758867	0.805525	-0.000432
	C	4.520243	-1.854900	0.000065	C	4.958208	-1.619261	-0.000119
	C	5.363373	-0.732405	-0.000140	C	5.552923	-0.347669	-0.000300
	C	3.141031	-1.703146	0.000190	C	3.577215	-1.754200	0.000001
	H	5.460526	1.434254	-0.000329	H	5.202899	1.792839	-0.000737
	H	4.976885	-2.837279	0.000146	H	5.606861	-2.486939	-0.000069
	H	2.505632	-2.582092	0.000376	H	3.136318	-2.745153	0.000155
	O	-6.703061	-1.005840	-0.000097	O	-6.920279	0.340281	0.000634
	O	6.703065	-1.005817	-0.000197	O	6.920286	-0.340284	-0.000552
	C	-7.619040	0.078876	-0.000271	C	-7.594518	-0.909201	-0.001139
	H	-7.503389	0.701512	-0.894492	H	-7.354143	-1.496097	0.892406
	H	-8.611472	-0.369229	-0.000461	H	-8.657713	-0.673914	-0.001131
	H	-7.503672	0.701523	0.893980	H	-7.353753	-1.493742	-0.896092
	C	7.619115	0.078841	-0.000214	C	7.594513	0.909205	0.000915
	H	7.503692	0.701508	0.894015	H	7.354023	1.495906	-0.892727
	H	8.611525	-0.369316	-0.000221	H	7.353844	1.493937	0.895773
	H	7.503603	0.701477	-0.894454	H	8.657709	0.673929	0.000822
F	C	-2.589179	-0.395950	-0.000072	C	-2.804380	0.441367	0.000003
	C	-3.437751	0.728130	-0.000032	C	-3.326494	-0.867411	0.000012
	C	-3.128203	-1.682873	-0.000054	C	-3.664869	1.540251	-0.000011
	C	-4.818368	0.579685	0.000062	C	-4.697143	-1.088807	0.000004
	C	-4.512997	-1.844000	0.000042	C	-5.043000	1.329575	-0.000017
	H	-2.487302	-2.557251	-0.000111	H	-3.278194	2.553101	-0.000017
	C	-5.321972	-0.714941	0.000095	C	-5.524995	0.026888	-0.000010
	H	-5.498486	1.423356	0.000112	H	-5.129876	-2.082271	0.000008
	H	-4.970811	-2.825256	0.000070	H	-5.743607	2.155117	-0.000029
	C	-1.195203	0.067168	-0.000151	C	-1.339524	0.362469	0.000004
	C	0.000004	-0.652143	-0.000087	C	-0.373160	1.373119	-0.000000
	C	-1.193671	1.478628	-0.000162	C	-0.963109	-0.998311	0.000012
	H	0.000083	-1.736874	-0.000014	H	-0.658940	2.420188	-0.000005
	C	-0.000020	2.193438	-0.000125	C	0.373160	-1.373120	0.000010
	C	1.195199	0.067204	-0.000149	C	0.963108	0.998311	-0.000002
	H	-0.000049	3.279456	-0.000113	H	0.658939	-2.420190	0.000014
	C	1.193752	1.478683	-0.000208	C	1.339524	-0.362472	0.000001
	C	-2.615860	1.998540	-0.000130	C	-2.198214	-1.875441	0.000032
	H	-2.826524	2.617495	-0.879966	H	-2.237151	-2.527708	0.879935
	H	-2.826445	2.617672	0.879592	H	-2.237157	-2.527778	-0.879816
	C	2.589158	-0.395964	0.000137	C	2.804379	-0.441369	0.000003
	C	3.437759	0.728115	0.000366	C	3.326494	0.867409	0.000006
	C	2.615640	1.998536	0.000159	C	2.198213	1.875441	0.000004
	H	2.826938	2.617614	-0.879494	H	2.237147	2.527737	0.879883
	H	2.826105	2.617905	0.879816	H	2.237162	2.527743	-0.879870
	C	4.818375	0.579695	0.000225	C	4.697142	1.088808	0.000002
	C	4.513023	-1.843980	-0.000088	C	5.043001	-1.329573	-0.000011
	C	5.322004	-0.714921	0.000082	C	5.524996	-0.026886	-0.000005
	C	3.128227	-1.682874	-0.000081	C	3.664870	-1.540251	-0.000007
	H	5.498469	1.423383	0.000305	H	5.129872	2.082273	0.000005
	H	4.970888	-2.825213	-0.000278	H	5.743607	-2.155115	-0.000018
	H	2.487339	-2.557262	-0.000314	H	3.278199	-2.553103	-0.000012
	F	-6.669446	-0.884233	0.000213	F	-6.869244	-0.165835	-0.000019

	F	6.669478	-0.884222	-0.000055	F	6.869244	0.165838	-0.000009
Cl	C	-2.588255	-0.300817	-0.000095	C	-2.797789	0.472694	0.000004
	C	-3.436984	0.822328	-0.000039	C	-3.335740	-0.828978	0.000019
	C	-3.129306	-1.586313	-0.000106	C	-3.646884	1.579918	-0.000017
	C	-4.816813	0.674012	0.000041	C	-4.708198	-1.033565	0.000009
	C	-4.513802	-1.745543	-0.000022	C	-5.026483	1.383752	-0.000024
	H	-2.491068	-2.462800	-0.000170	H	-3.251015	2.589236	-0.000030
	C	-5.336878	-0.620030	0.000049	C	-5.538852	0.086837	-0.000013
	H	-5.482461	1.528725	0.000104	H	-5.135798	-2.029020	0.000017
	H	-4.956003	-2.733522	-0.000016	H	-5.703756	2.228176	-0.000041
	C	-1.194837	0.161627	-0.000146	C	-1.334637	0.377499	0.000000
	C	0.000001	-0.558131	-0.000098	C	-0.357481	1.377825	-0.000006
	C	-1.193533	1.573449	-0.000158	C	-0.974363	-0.988036	0.000011
	H	0.000075	-1.642796	-0.000044	H	-0.632107	2.427798	-0.000011
	C	-0.000017	2.288465	-0.000129	C	0.357482	-1.377829	0.000004
	C	1.194830	0.161657	-0.000152	C	0.974361	0.988033	-0.000011
	H	-0.000043	3.374404	-0.000103	H	0.632103	-2.427804	0.000010
	C	1.193608	1.573497	-0.000203	C	1.334638	-0.377507	-0.000011
	C	-2.615480	2.093469	-0.000099	C	-2.219478	-1.850661	0.000050
	H	-2.825521	2.712527	-0.879950	H	-2.265531	-2.502372	0.879959
	H	-2.825445	2.712663	0.879667	H	-2.265550	-2.502495	-0.879762
	C	2.588234	-0.300837	0.000097	C	2.797784	-0.472700	0.000005
	C	3.436993	0.822317	0.000329	C	3.335741	0.828970	0.000022
	C	2.615281	2.093471	0.000140	C	2.219473	1.850660	0.000015
	H	2.825923	2.712612	-0.879565	H	2.265516	2.502413	0.879888
	H	2.825137	2.712919	0.879821	H	2.265568	2.502433	-0.879839
	C	4.816812	0.674008	0.000222	C	4.708194	1.033566	0.000021
	C	4.513824	-1.745538	-0.000070	C	5.026486	-1.383748	-0.000022
	C	5.336900	-0.620031	0.000063	C	5.538856	-0.086833	0.000001
	C	3.129321	-1.586314	-0.000087	C	3.646889	-1.579919	-0.000022
	H	5.482463	1.528718	0.000307	H	5.135787	2.029025	0.000037
	H	4.956048	-2.733507	-0.000223	H	5.703757	-2.228173	-0.000043
	H	2.491092	-2.462809	-0.000300	H	3.251031	-2.589242	-0.000044
	Cl	-7.084426	-0.838114	0.000176	Cl	-7.283822	-0.143699	-0.000026
	Cl	7.084450	-0.838098	0.000015	Cl	7.283822	0.143708	0.000005
Br	C	-2.588092	-0.144600	-0.000130	C	-2.792939	0.499004	0.000005
	C	-3.436831	0.978443	-0.000148	C	-3.343180	-0.797459	0.000026
	C	-3.129034	-1.430064	-0.000059	C	-3.631023	1.614537	-0.000021
	C	-4.817127	0.830496	-0.000087	C	-4.717872	-0.988953	0.000015
	C	-4.513989	-1.589733	0.000007	C	-5.012847	1.431937	-0.000029
	H	-2.490970	-2.306765	-0.000048	H	-3.225267	2.619939	-0.000039
	C	-5.337042	-0.463908	-0.000002	C	-5.537855	0.139739	-0.000012
	H	-5.478772	1.688129	-0.000099	H	-5.150635	-1.982091	0.000025
	H	-4.951417	-2.579665	0.000067	H	-5.677912	2.285896	-0.000050
	C	-1.194764	0.317913	-0.000197	C	-1.330809	0.390004	-0.000000
	C	0.000050	-0.401862	-0.000067	C	-0.344416	1.381249	-0.000007
	C	-1.193541	1.729782	-0.000288	C	-0.983656	-0.978974	0.000013
	H	0.000153	-1.486520	0.000079	H	-0.609224	2.433729	-0.000011
	C	-0.000056	2.444925	-0.000221	C	0.344417	-1.381254	0.000004
	C	1.194795	0.318057	-0.000089	C	0.983652	0.978970	-0.000017
	H	-0.000134	3.530834	-0.000271	H	0.609219	-2.433736	0.000013
	C	1.193507	1.729929	-0.000224	C	1.330810	-0.390014	-0.000017
	C	-2.615424	2.249812	-0.000280	C	-2.236769	-1.829851	0.000062
	H	-2.825356	2.868779	-0.880197	H	-2.288990	-2.481059	0.879993
	H	-2.825297	2.869031	0.879476	H	-2.289017	-2.481207	-0.879753
	C	2.588107	-0.144458	0.000318	C	2.792931	-0.499011	0.000005
	C	3.436961	0.978483	0.000601	C	3.343182	0.797448	0.000034

	C 2.615211 2.250179 0.000420 H 2.825943 2.869427 -0.879138 H 2.824707 2.869313 0.880325 C 4.817217 0.830550 0.000358 C 4.513949 -1.589678 -0.000085 C 5.337071 -0.463899 0.000095 C 3.129003 -1.429942 -0.000026 H 5.478896 1.688155 0.000433 H 4.951322 -2.579632 -0.000314 H 2.490892 -2.306618 -0.000307 Br -7.242278 -0.701781 0.000114 Br 7.242284 -0.701849 -0.000097	C 2.236763 1.829849 0.000022 H 2.288970 2.481105 0.879912 H 2.289044 2.481134 -0.879842 C 4.717869 0.988953 0.000033 C 5.012850 -1.431933 -0.000029 C 5.537859 -0.139736 0.000006 C 3.631026 -1.614539 -0.000032 H 5.150623 1.982095 0.000055 H 5.677911 -2.285896 -0.000058 H 3.225284 -2.619947 -0.000066 Br -7.443043 -0.093026 -0.000030 Br 7.443044 0.093033 0.000015
CN	C -2.585395 -0.333357 -0.000187 C -3.435175 0.791282 -0.000087 C -3.120061 -1.623062 -0.000179 C -4.810300 0.637989 0.000062 C -4.500331 -1.783710 -0.000027 H -2.476589 -2.495289 -0.000287 C -5.347544 -0.661902 0.000104 H -5.475451 1.493700 0.000142 H -4.936111 -2.775092 -0.000009 C -1.193744 0.129174 -0.000290 C 0.000018 -0.591827 -0.000186 C -1.192815 1.541879 -0.000311 H 0.000102 -1.676294 -0.000074 C 0.000013 2.257650 -0.000251 C 1.193789 0.129273 -0.000228 H -0.000005 3.343278 -0.000181 C 1.193049 1.542004 -0.000296 C -2.613765 2.061801 -0.000233 H -2.822688 2.681117 -0.879968 H -2.822561 2.681377 0.879340 C 2.585351 -0.333303 0.000322 C 3.435277 0.791278 0.000750 C 2.613466 2.061931 0.000278 H 2.823290 2.681340 -0.879228 H 2.822053 2.681764 0.879808 C 4.810345 0.638013 0.000391 C 4.500276 -1.783684 -0.000096 C 5.347541 -0.661911 0.000130 C 3.120025 -1.623028 -0.000056 H 5.475512 1.493709 0.000496 H 4.936052 -2.775071 -0.000386 H 2.476572 -2.495274 -0.000412 C -6.765930 -0.843684 0.000278 N -7.913019 -0.988056 0.000425 C 6.765905 -0.843789 -0.000043 N 7.912998 -0.988140 -0.000183	C -2.794292 0.469646 0.000001 C -3.332014 -0.833992 0.000016 C -3.638019 1.582649 -0.000021 C -4.701241 -1.033114 0.000003 C -5.013871 1.388864 -0.000031 H -3.235788 2.589148 -0.000031 C -5.549713 0.088928 -0.000020 H -5.128191 -2.029196 0.000009 H -5.686113 2.237779 -0.000048 C -1.332904 0.374852 0.000002 C -0.359216 1.378868 -0.000002 C -0.972663 -0.991591 0.000013 H -0.636403 2.427899 -0.000007 C 0.359216 -1.378870 0.000010 C 0.972661 0.991589 -0.000007 H 0.636401 -2.427902 0.000014 C 1.332904 -0.374856 -0.000006 C -2.216016 -1.855123 0.000044 H -2.261547 -2.506733 0.879890 H -2.261560 -2.506840 -0.879718 C 2.794291 -0.469649 0.000006 C 3.332014 0.833989 0.000023 C 2.216014 1.855122 0.000015 H 2.261531 2.506771 0.879830 H 2.261576 2.506791 -0.879782 C 4.701239 1.033115 0.000023 C 5.013873 -1.388861 -0.000015 C 5.549715 -0.088925 0.000006 C 3.638021 -1.582649 -0.000017 H 5.128186 2.029199 0.000037 H 5.686115 -2.237777 -0.000032 H 3.235795 -2.589150 -0.000035 C -6.967856 -0.093720 -0.000035 N -8.114206 -0.243829 -0.000047 C 6.967857 0.093725 0.000010 N 8.114207 0.243835 0.000013
NO ₂	C -2.584042 -0.236525 -0.000093 C -3.433977 0.889179 0.000018 C -3.116933 -1.527940 -0.000160 C -4.809570 0.737326 0.000078 C -4.497278 -1.690977 -0.000110 H -2.472923 -2.399465 -0.000253 C -5.317888 -0.562757 0.000004 H -5.490615 1.578014 0.000168 H -4.950627 -2.672412 -0.000161	C -2.791368 0.476638 -0.000005 C -3.332665 -0.826607 -0.000003 C -3.631179 1.593878 -0.000013 C -4.702363 -1.023744 -0.000010 C -5.008033 1.405892 -0.000020 H -3.225798 2.598877 -0.000014 C -5.520083 0.107835 -0.000019 H -5.151617 -2.007995 -0.000011 H -5.693132 2.242199 -0.000026

C	-1.193389	0.226217	-0.000120	C	-1.331310	0.377578	0.000001
C	0.000007	-0.495212	-0.000144	C	-0.356058	1.380285	-0.000000
C	-1.192614	1.639481	-0.000009	C	-0.974770	-0.990476	0.000007
H	0.000061	-1.579595	-0.000146	H	-0.631681	2.429616	-0.000005
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C	-2.613082	2.159496	0.000038	C	-2.219896	-1.850761	0.000010
H	-2.821969	2.779025	-0.879471	H	-2.267474	-2.502266	0.879722
H	-2.821931	2.779044	0.879531	H	-2.267468	-2.502290	-0.879683
C	2.584058	-0.236546	0.000039	C	2.791368	-0.476638	0.000010
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C	4.809574	0.737305	0.000124	C	4.702363	1.023744	0.000003
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C	5.317886	-0.562780	-0.000012	C	5.520083	-0.107835	0.000009
C	3.116938	-1.527942	-0.000127	C	3.631178	-1.593877	0.000016
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H	4.950607	-2.672445	-0.000228	H	5.693132	-2.242200	0.000021
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N	-6.781219	-0.749414	0.000055	N	-6.983374	-0.077767	-0.000028
O	-7.211906	-1.897008	-0.000007	O	-7.687801	0.925538	-0.000012
O	-7.483928	0.255621	0.000165	O	-7.412155	-1.226792	-0.000033
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O	7.211893	-1.897013	0.000874	O	7.412155	1.226792	-0.000007
O	7.483876	0.255632	-0.000763	O	7.687801	-0.925539	0.000041