Electronic Supplementary Material (ESI) for RSC Advances

Importance of the CH/π hydrogen bond in the enhancement of CD amplitude of exomethylene steroids

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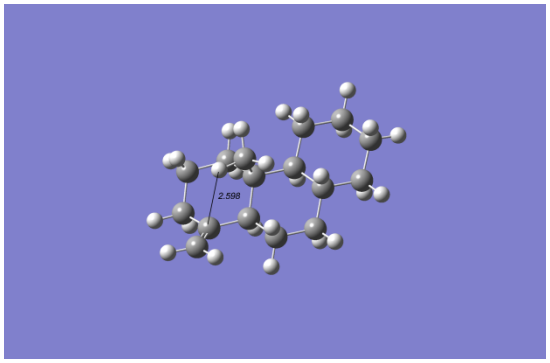
Supplementary materials

Optimized Cartesian coordinates of model molecules.

(a) **1”**

C	0.1201	0.822466	−0.23057
C	−0.34016	−0.64792	0.003042
C	0.005141	−1.09693	1.401987
C	−0.61544	−0.25043	2.479389
C	−0.21392	1.214137	2.289007
C	−0.52214	1.68975	0.869597
H	−1.44074	−0.61942	−0.04937
H	−1.70691	−0.3265	2.413134
H	−0.32407	−0.60922	3.468992
H	−0.73954	1.845743	3.009692
H	0.852963	1.324038	2.496943
H	−1.60886	1.682433	0.722112
H	−0.19684	2.726662	0.762927
C	−0.39614	1.284502	−1.62024
C	0.126594	−1.58274	−1.1071
H	1.218951	−1.62179	−1.13623
H	−0.21825	−2.59806	−0.89553
C	−0.01287	0.32693	−2.76271
H	1.078258	0.360391	−2.88212
C	−0.41241	−1.11279	−2.45223
H	−1.50661	−1.17815	−2.44107

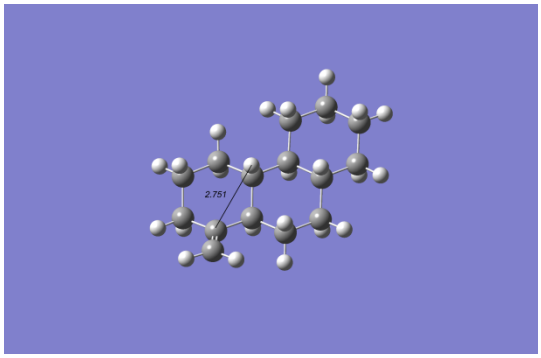
H	−0.06825	−1.77012	−3.25626
H	−1.49619	1.266899	−1.55655
C	1.647583	0.929736	−0.14162
H	2.138315	0.52026	−1.02366
H	1.955053	1.971835	−0.04645
H	2.027244	0.386642	0.722754
C	0.823033	−2.12237	1.686335
H	1.288168	−2.72297	0.918123
H	1.036566	−2.39074	2.712947
C	−0.63134	0.787009	−4.08559
H	−0.33367	0.099986	−4.88309
H	−1.72204	0.717842	−4.00218
C	−0.2437	2.218818	−4.44037
H	−0.72769	2.525296	−5.37077
H	0.835953	2.267885	−4.61408
C	0.017266	2.716089	−1.9877
H	1.106439	2.761805	−2.08509
H	−0.25943	3.413778	−1.19566
C	−0.61216	3.168006	−3.30496
H	−1.70097	3.191686	−3.1935
H	−0.2968	4.187444	−3.54018



(b) **2”**

C	−0.02577	0.799879	−0.23578
C	−0.4232	−0.67334	0.022258
C	0.016822	−1.09859	1.40377
C	−0.52397	−0.23766	2.511662
C	−0.10252	1.213925	2.278904

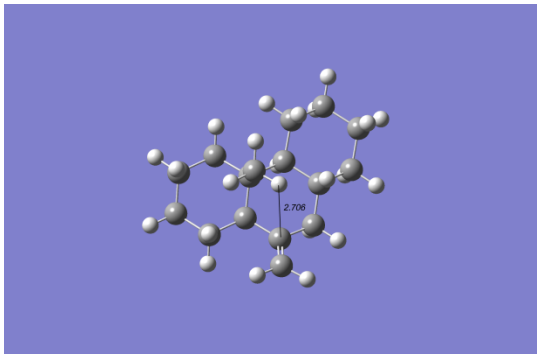
C	−0.53765	1.696808	0.897428
H	−1.52479	−0.69883	0.014548
H	−1.61849	−0.29229	2.5192
H	−0.17326	−0.59495	3.482142
H	−0.52056	1.863179	3.052249
H	0.986393	1.280124	2.358033
H	−1.63305	1.722977	0.850728
H	−0.19228	2.721393	0.754206
C	−0.51427	1.270621	−1.61897
C	0.067337	−1.58293	−1.09893
H	1.161954	−1.58249	−1.10725
H	−0.2494	−2.6109	−0.90571
C	−0.03038	0.330613	−2.73411
H	1.0691	0.372528	−2.73662
C	−0.44284	−1.11067	−2.45386
H	−1.53639	−1.178	−2.47891
H	−0.06981	−1.76276	−3.2491
H	−1.61499	1.22573	−1.60932
C	0.864288	−2.10994	1.64806
H	1.283691	−2.72224	0.863589
H	1.151833	−2.3536	2.66258
C	−0.51803	0.794065	−4.10716
H	−0.14276	0.112185	−4.87563
H	−1.61163	0.725748	−4.13249
C	−0.09455	2.227902	−4.40858
H	−0.47657	2.54344	−5.38232
H	0.997484	2.276531	−4.46562
C	−0.10504	2.714625	−1.93273
H	0.988174	2.784798	−1.88582
H	−0.49737	3.397433	−1.17813
C	−0.5841	3.167226	−3.31164
H	−1.67872	3.185565	−3.31903
H	−0.2514	4.189944	−3.50465
H	1.073907	0.840876	−0.23563



(c) **3”**

C	0.25997	0.921333	0.268385
C	−0.36612	−0.49991	0.142003
C	−0.07922	−1.39248	1.348726
C	−0.57167	−0.74181	2.638009
C	0.048849	0.639468	2.819126
C	−0.21043	1.530101	1.603507
H	−1.4557	−0.3344	0.13071
H	−1.66127	−0.64352	2.594587
H	−0.34629	−1.37879	3.496697
H	−0.35373	1.122378	3.713052
H	1.124377	0.535702	2.984401
H	−1.28816	1.720437	1.531928
H	0.270534	2.498237	1.759646
C	−0.2746	1.782792	−0.90982
C	−0.01156	−1.10071	−1.19243
C	−0.017	1.152794	−2.28986
H	1.066552	1.144028	−2.46316
C	−0.51742	−0.29437	−2.35296
H	−1.6145	−0.27629	−2.32792
H	−0.22418	−0.74949	−3.30322
H	−1.36882	1.818501	−0.7823
C	1.789784	0.841682	0.243265
H	2.156738	0.441101	−0.70012
H	2.228426	1.828431	0.393761
H	2.168855	0.196611	1.034245
H	0.991777	−1.59582	1.42753

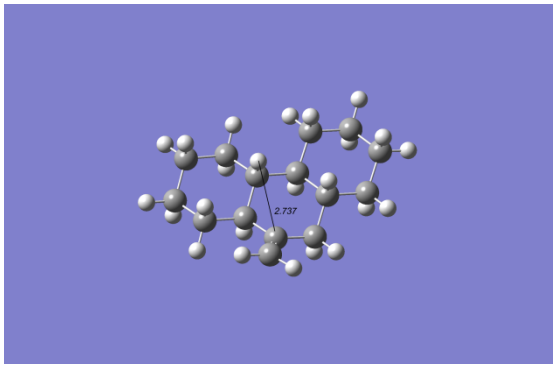
H	−0.56874	−2.35784	1.197975
C	0.71705	−2.21545	−1.35728
H	0.945979	−2.58474	−2.34863
H	1.091895	−2.79068	−0.52306
C	−0.65599	1.9897	−3.40089
H	−0.44476	1.528425	−4.37006
H	−1.74418	1.96625	−3.27155
C	−0.17829	3.43796	−3.38087
H	−0.67746	4.014303	−4.1635
H	0.893682	3.468013	−3.60024
C	0.225713	3.233865	−0.90534
H	1.309537	3.244806	−1.0552
H	0.033871	3.704064	0.060377
C	−0.42766	4.061719	−2.01169
H	−0.0508	5.087001	−1.98347
H	−1.50605	4.116245	−1.83112



(d) **4”**

C	0.08325	0.919971	0.274592
C	−0.44271	−0.53129	0.164779
C	0.011665	−1.38223	1.349381
C	−0.41381	−0.76884	2.67901
C	0.130834	0.648823	2.807126
C	−0.30765	1.518742	1.630979
H	−1.5416	−0.46261	0.207956
H	−1.50676	−0.74456	2.734821
H	−0.06856	−1.38912	3.509457
H	−0.19211	1.102685	3.747119

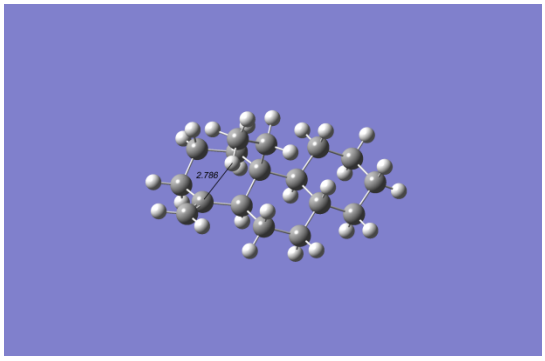
H	1.224516	0.610282	2.834667
H	−1.39733	1.639359	1.655065
H	0.122264	2.514817	1.743545
C	−0.40036	1.782141	−0.9065
C	−0.08746	−1.1068	−1.18319
C	−0.04737	1.139388	−2.25627
H	1.049011	1.082305	−2.31366
C	−0.58839	−0.29001	−2.33868
H	−1.68456	−0.24681	−2.31825
H	−0.29958	−0.74698	−3.28915
H	−1.4994	1.831872	−0.8465
H	1.102832	−1.46879	1.327675
H	−0.39005	−2.3932	1.247068
C	0.66133	−2.20508	−1.36747
H	0.892545	−2.55168	−2.36633
H	1.052531	−2.78848	−0.54716
C	−0.53861	1.988926	−3.42838
H	−0.25848	1.507806	−4.36984
H	−1.63392	2.020755	−3.40396
C	0.010727	3.41053	−3.36737
H	−0.37433	4.00567	−4.19877
H	1.099406	3.380529	−3.47637
C	0.137743	3.217096	−0.85427
H	1.233424	3.178267	−0.85774
H	−0.1577	3.704313	0.075686
C	−0.34452	4.06032	−2.03427
H	0.079486	5.065412	−1.97208
H	−1.43161	4.172694	−1.96975
H	1.181296	0.868669	0.223596



(e) C^{10}-alkyl-substituted model (R=Et1)

C	0.062936	−0.04315	−0.00883
C	0.029952	−0.02821	1.547022
C	1.394423	0.137192	2.175976
C	2.130726	1.360379	1.700398
C	2.234882	1.376035	0.174706
C	0.86462	1.190474	−0.47723
H	−0.49754	0.909821	1.792034
H	1.57519	2.251224	2.017468
H	3.119981	1.417565	2.159904
H	2.662978	2.325613	−0.15779
H	2.923844	0.597646	−0.15313
H	0.2627	2.080645	−0.2558
H	0.986765	1.15994	−1.5622
C	−1.41452	0.132912	−0.48654
C	−0.83502	−1.15083	2.111438
H	−0.44993	−2.12791	1.807354
H	−0.80419	−1.12417	3.203379
C	−2.38678	−0.89895	0.115203
H	−2.13955	−1.88551	−0.2974
C	−2.27331	−0.97809	1.635451
H	−2.67396	−0.05195	2.063737
H	−2.9043	−1.79122	2.00659
H	−1.73501	1.115407	−0.10495
C	0.621852	−1.34946	−0.6285
H	−0.17422	−2.09671	−0.63671
H	0.829354	−1.13722	−1.68122

C	1.901868	−0.67189	3.118159
H	1.379911	−1.54999	3.470973
H	2.872878	−0.47359	3.553192
C	−3.82749	−0.58551	−0.29989
H	−4.49868	−1.33637	0.127212
H	−4.1143	0.377545	0.137848
C	−3.9935	−0.51909	−1.81457
H	−5.02325	−0.26182	−2.07396
H	−3.79661	−1.50701	−2.24297
C	−1.58114	0.167883	−2.01198
H	−1.31181	−0.8065	−2.43031
H	−0.90691	0.901638	−2.4569
C	−3.02005	0.490117	−2.41443
H	−3.27661	1.49373	−2.06017
H	−3.10908	0.507456	−3.50341
C	1.853283	−2.03194	−0.03056
H	1.679532	−2.36614	0.987736
H	2.093062	−2.90797	−0.63555
H	2.731419	−1.39316	−0.01647

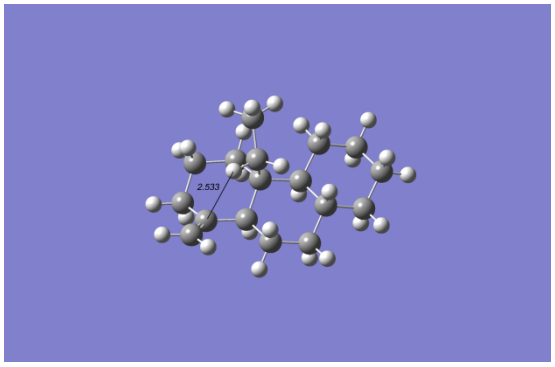


(f) C^{10}-alkyl-substituted model (R=Et2)

C	−0.00997	−0.00905	−0.05493
C	−0.00801	−0.00869	1.509292
C	1.39752	0.051202	2.052266
C	2.159734	1.268781	1.611807
C	2.197333	1.315985	0.08313
C	0.790176	1.227372	−0.50919
H	−0.48648	0.941376	1.797935

H	1.655066	2.168114	1.982854
H	3.170191	1.266354	2.026418
H	2.680063	2.236301	−0.2562
H	2.812237	0.487155	−0.27419
H	0.229324	2.119105	−0.20426
H	0.853511	1.261757	−1.59781
C	−1.49128	0.145163	−0.51021
C	−0.87164	−1.12479	2.085911
H	−0.49291	−2.1017	1.773609
H	−0.81454	−1.10026	3.177109
C	−2.44599	−0.88995	0.114225
H	−2.1899	−1.87726	−0.2929
C	−2.31476	−0.95128	1.633441
H	−2.70722	−0.01854	2.054941
H	−2.94324	−1.758	2.022356
H	−1.81331	1.128001	−0.12907
C	0.634352	−1.32227	−0.56436
H	−0.11886	−2.11294	−0.55408
C	1.95628	−0.90223	2.814464
H	1.421521	−1.79227	3.113343
H	2.97385	−0.8006	3.169246
C	−3.89737	−0.59298	−0.27758
H	−4.5516	−1.35261	0.160177
H	−4.18585	0.364813	0.170485
C	−4.09876	−0.51942	−1.78728
H	−5.13529	−0.26422	−2.02039
H	−3.90872	−1.50381	−2.22673
C	−1.69636	0.164725	−2.03071
H	−1.45708	−0.82249	−2.43595
H	−1.02188	0.879239	−2.50568
C	−3.14111	0.495224	−2.40248
H	−3.38887	1.497242	−2.03764
H	−3.25262	0.517571	−3.48928
C	1.291712	−1.30705	−1.94665
H	1.655851	−2.30748	−2.18353
H	0.606527	−1.01129	−2.73657

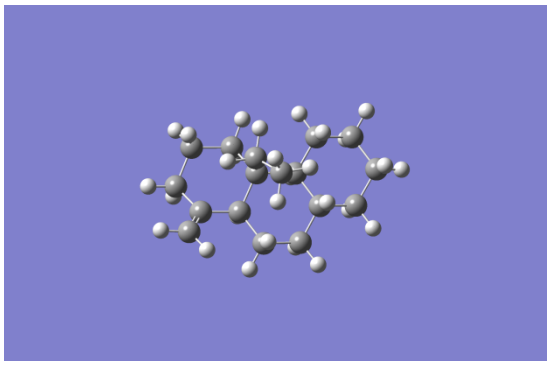
H	2.147335	−0.63562	−1.98258
H	1.39339	−1.63144	0.158955



(g) C^{10}-alkyl-substituted model (R=Et3)

C	−0.03258	−0.04774	0.004598
C	−0.03753	−0.02106	1.564647
C	1.375155	−0.07268	2.088261
C	2.209214	1.105421	1.661042
C	2.192808	1.261128	0.13638
C	0.768996	1.208575	−0.42233
H	−0.41253	0.985078	1.815167
H	1.785992	2.012235	2.10849
H	3.23329	1.011211	2.029356
H	2.656496	2.210473	−0.14395
H	2.803377	0.47674	−0.31464
H	0.222564	2.093237	−0.07593
H	0.812104	1.273139	−1.51199
C	−1.49253	0.114194	−0.49961
C	−1.0221	−0.98461	2.219078
H	−0.75545	−2.02282	2.021499
H	−0.97557	−0.85181	3.303458
C	−2.52677	−0.79481	0.193122
H	−2.3336	−1.83259	−0.09488
C	−2.43156	−0.70418	1.713583
H	−2.72749	0.304783	2.024573
H	−3.1493	−1.39425	2.167064
H	−1.78074	1.141706	−0.22184
C	0.713855	−1.26619	−0.59151

C	1.866927	−1.07095	2.83785
H	1.263851	−1.91517	3.140755
H	2.89451	−1.05605	3.177555
C	−3.93955	−0.44324	−0.28151
H	−4.66124	−1.10375	0.207959
H	−4.17396	0.576416	0.045844
C	−4.07979	−0.52896	−1.79826
H	−5.09155	−0.25143	−2.10357
H	−3.92657	−1.56522	−2.11648
C	−1.63395	0.01393	−2.02491
H	−1.40179	−1.00468	−2.34812
H	−0.91745	0.671704	−2.5205
C	−3.0493	0.363116	−2.4832
H	−3.25863	1.40933	−2.23786
H	−3.12527	0.272123	−3.56952
H	1.682739	−1.32978	−0.0949
H	0.931098	−1.02451	−1.63684
C	0.107942	−2.67029	−0.56326
H	−0.81709	−2.74068	−1.13031
H	0.817339	−3.36412	−1.01708
H	−0.08563	−3.02415	0.44577

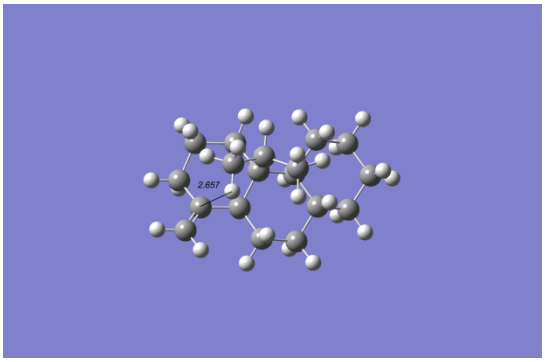


(h) C^{10}-alkyl-substituted model (R=ipr1)

C	0.056513	−0.16816	−0.01579
C	0.008922	−0.05812	1.539877
C	1.357588	0.148948	2.188495
C	2.086193	1.362285	1.673136
C	2.19298	1.355057	0.146005

C	0.841054	1.07781	−0.51405
H	−0.50376	0.905741	1.703577
H	1.520187	2.253574	1.970064
H	3.074039	1.443918	2.132314
H	2.553706	2.3286	−0.19746
H	2.939362	0.630555	−0.17677
H	0.205173	1.952605	−0.33392
H	0.982613	1.016605	−1.59521
C	−1.42169	0.034865	−0.49159
C	−0.89781	−1.10144	2.183874
H	−0.55455	−2.11323	1.960061
H	−0.86267	−0.99103	3.270632
C	−2.46968	−0.8766	0.181043
H	−2.34725	−1.89915	−0.17693
C	−2.33077	−0.88752	1.703456
H	−2.67688	0.078427	2.089986
H	−2.99917	−1.64561	2.122729
H	−1.67571	1.047836	−0.13944
C	0.729309	−1.46222	−0.60913
C	1.840823	−0.59634	3.193571
H	1.313958	−1.45713	3.580312
H	2.797271	−0.36547	3.644587
C	−3.88047	−0.43369	−0.21938
H	−4.61413	−1.09395	0.252541
H	−4.06038	0.572059	0.178169
C	−4.0699	−0.4163	−1.73293
H	−5.08165	−0.09106	−1.98696
H	−3.95735	−1.433	−2.12327
C	−1.61332	0.074317	−2.01557
H	−1.40816	−0.90335	−2.45639
H	−0.90608	0.772712	−2.46573
C	−3.03586	0.49292	−2.38885
H	−3.20444	1.522856	−2.05769
H	−3.15333	0.487938	−3.47531
H	1.043918	−1.16004	−1.61562
C	−0.13286	−2.71816	−0.81825

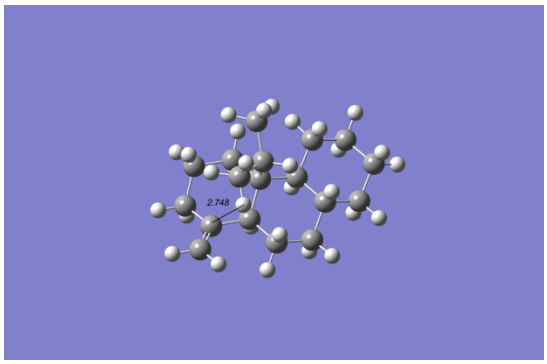
H	−0.98187	−2.56172	−1.47458
H	0.493426	−3.48213	−1.28258
H	−0.49608	−3.13043	0.121395
C	1.987944	−1.96007	0.11785
H	1.725616	−2.43465	1.061862
H	2.475107	−2.71125	−0.50665
H	2.714501	−1.18868	0.337415



(i) C^{10}-alkyl-substituted model (R=ipr2)

C	0.066171	−0.04938	−0.06819
C	0.046679	−0.0485	1.496851
C	1.408622	0.125621	2.132762
C	2.157542	1.336833	1.645365
C	2.229769	1.356286	0.118809
C	0.836577	1.219464	−0.49321
H	−0.4773	0.892198	1.739473
H	1.626	2.237796	1.975039
H	3.15604	1.373164	2.086736
H	2.684606	2.291128	−0.21996
H	2.880484	0.551271	−0.22623
H	0.242568	2.085128	−0.17531
H	0.907494	1.282656	−1.57874
C	−1.43149	0.130064	−0.50328
C	−0.82558	−1.15375	2.088324
H	−0.46963	−2.1436	1.796538
H	−0.77717	−1.10835	3.17899
C	−2.3954	−0.90162	0.114922
H	−2.15162	−1.89002	−0.29725

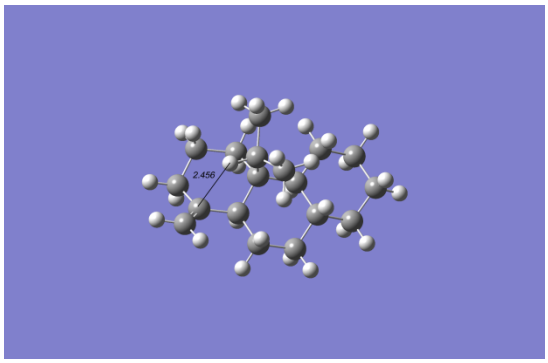
C	−2.26556	−0.96961	1.633234
H	−2.65283	−0.03556	2.056531
H	−2.89962	−1.77338	2.019342
H	−1.73203	1.107272	−0.09253
C	0.663946	−1.35401	−0.70873
C	1.901344	−0.65747	3.104367
H	1.376481	−1.52729	3.472664
H	2.866515	−0.4473	3.54678
C	−3.84905	−0.58965	−0.26018
H	−4.50094	−1.35698	0.1675
H	−4.12936	0.358152	0.213696
C	−4.06869	−0.47542	−1.76367
H	−5.10758	−0.21273	−1.97698
H	−3.88384	−1.4461	−2.23467
C	−1.66846	0.201204	−2.01808
H	−1.44834	−0.77191	−2.46542
H	−0.99923	0.929161	−2.47985
C	−3.11585	0.556645	−2.35427
H	−3.3523	1.545466	−1.94815
H	−3.24103	0.620953	−3.43789
C	1.724646	−2.12038	0.093499
H	1.392766	−2.41351	1.0826
H	1.97819	−3.02863	−0.45714
H	2.639721	−1.54449	0.214684
C	1.256975	−1.15027	−2.11262
H	2.201622	−0.60868	−2.058
H	1.470173	−2.12565	−2.55299
H	0.604301	−0.61688	−2.79538
H	−0.17655	−2.04663	−0.82036



(j) C^{10}-alkyl-substituted model (R=ipr3)

C	−0.02934	−0.08668	−0.05851
C	−0.03595	−0.036	1.511075
C	1.36812	−0.0109	2.058929
C	2.153919	1.194079	1.621946
C	2.153774	1.295682	0.094094
C	0.736598	1.195497	−0.4756
H	−0.45504	0.958774	1.735156
H	1.682755	2.093144	2.035579
H	3.175061	1.155479	2.007961
H	2.603758	2.242281	−0.21718
H	2.786212	0.5028	−0.30886
H	0.161591	2.054631	−0.11157
H	0.769947	1.292604	−1.56107
C	−1.5095	0.07347	−0.52213
C	−0.98049	−1.01927	2.193397
H	−0.67231	−2.05149	2.031449
H	−0.93252	−0.85246	3.273115
C	−2.53255	−0.84463	0.178917
H	−2.36883	−1.87395	−0.15049
C	−2.40397	−0.79365	1.700419
H	−2.73409	0.195782	2.038702
H	−3.0896	−1.51881	2.149017
H	−1.78291	1.093306	−0.20325
C	0.742465	−1.341	−0.59564
C	1.893421	−0.96843	2.839012
H	1.328446	−1.83714	3.146005

H	2.911048	−0.8933	3.200128
C	−3.95788	−0.45589	−0.23011
H	−4.66866	−1.1272	0.26078
H	−4.16473	0.551644	0.149328
C	−4.1634	−0.47137	−1.74097
H	−5.18214	−0.16406	−1.98926
H	−4.04152	−1.49358	−2.11346
C	−1.72212	0.031156	−2.04221
H	−1.54372	−0.98236	−2.40959
H	−1.00825	0.683366	−2.54826
C	−3.14532	0.435058	−2.42408
H	−3.32109	1.471882	−2.11942
H	−3.26602	0.399271	−3.50959
C	1.349308	−1.18668	−2.0002
H	1.923024	−2.08548	−2.23251
H	0.583917	−1.08374	−2.76651
H	2.028262	−0.34274	−2.08686
H	1.587946	−1.4614	0.088661
C	0.003363	−2.68645	−0.58802
H	−0.77889	−2.71881	−1.34564
H	0.716851	−3.47596	−0.83085
H	−0.44213	−2.937	0.3684

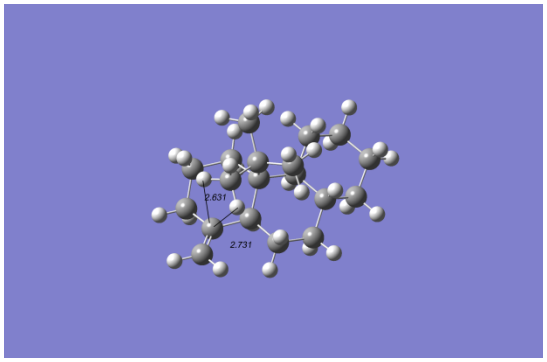


(k) C^{10}-alkyl-substituted model (R=tbu)

C	0.060039	−0.18998	−0.08134
C	0.019985	−0.09841	1.485286
C	1.358122	0.145672	2.147956
C	2.082098	1.358075	1.623567

C	2.173092	1.346289	0.096743
C	0.80204	1.099842	−0.53166
H	−0.51238	0.854305	1.650473
H	1.520316	2.251756	1.921726
H	3.073311	1.438732	2.075568
H	2.552251	2.310558	−0.25327
H	2.89616	0.599436	−0.23039
H	0.163687	1.944077	−0.24581
H	0.884658	1.14433	−1.61628
C	−1.44006	0.015532	−0.51806
C	−0.86907	−1.15024	2.141569
H	−0.52129	−2.16133	1.927148
H	−0.8239	−1.02999	3.226829
C	−2.48766	−0.89002	0.166439
H	−2.41025	−1.90177	−0.23233
C	−2.31056	−0.94698	1.684804
H	−2.66106	0.003695	2.103728
H	−2.96305	−1.72289	2.096586
H	−1.67139	1.023301	−0.13747
C	0.760767	−1.497	−0.67406
C	1.832948	−0.55977	3.185572
H	1.317786	−1.42098	3.586547
H	2.775077	−0.29593	3.648456
C	−3.90124	−0.39358	−0.16115
H	−4.6321	−1.05151	0.318455
H	−4.03467	0.60005	0.282479
C	−4.15916	−0.30856	−1.66128
H	−5.16887	0.06205	−1.85385
H	−4.10124	−1.3109	−2.09775
C	−1.70434	0.096334	−2.03039
H	−1.58024	−0.88308	−2.49645
H	−0.98681	0.7667	−2.50622
C	−3.12128	0.589405	−2.32482
H	−3.23365	1.610867	−1.94688
H	−3.2829	0.632413	−3.40477
C	−0.17303	−2.71062	−0.84181

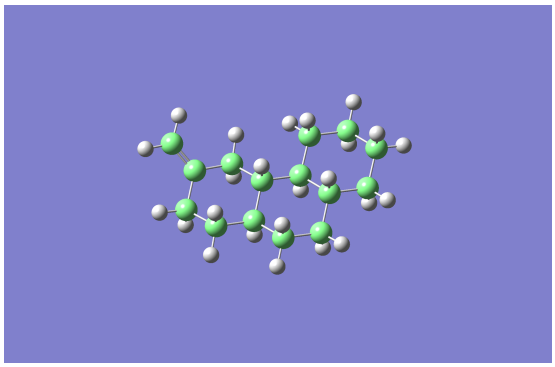
H	−0.96156	−2.53924	−1.56926
H	0.424712	−3.54763	−1.20833
H	−0.62686	−3.02633	0.093773
C	1.919949	−2.02075	0.192142
H	1.57471	−2.39026	1.154192
H	2.386473	−2.85504	−0.33681
H	2.689246	−1.28006	0.382224
C	1.355248	−1.23198	−2.07098
H	2.19113	−0.5353	−2.03451
H	1.737467	−2.1731	−2.4708
H	0.619826	−0.85041	−2.77546



(l) **5'**

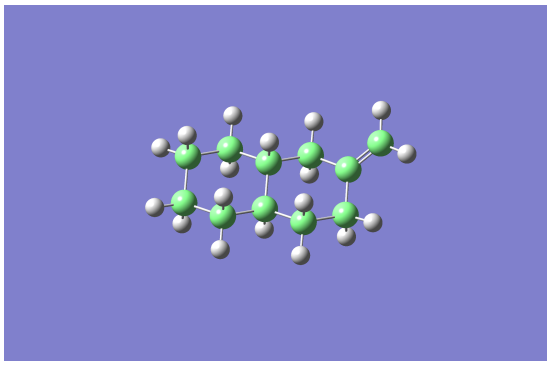
C	0.167315	0.145659	0.548834
C	−0.35131	−1.2354	1.023065
C	−0.10985	−1.48978	2.511752
C	−0.72625	−0.38537	3.375794
C	−0.26805	0.963689	2.898308
C	−0.50284	1.22087	1.435315
H	−1.44318	−1.20711	0.881933
H	−1.81719	−0.44547	3.286927
H	−0.47866	−0.52806	4.429978
H	−1.58145	1.207493	1.230849
H	−0.13455	2.215298	1.175726
C	−0.26342	0.339188	−0.93041
C	0.174505	−2.37519	0.154559
H	1.262846	−2.44115	0.242128
H	−0.22283	−3.32506	0.524589

C	0.201092	−0.81033	−1.84352
H	1.298	−0.78502	−1.88702
C	−0.22778	−2.17246	−1.30127
H	−1.31864	−2.24706	−1.37909
H	0.184996	−2.96504	−1.93253
H	−1.36523	0.311512	−0.92995
C	1.686776	0.269515	0.708102
H	2.230427	−0.42972	0.074771
H	2.013014	1.276888	0.448069
H	1.989208	0.09755	1.739566
C	−0.32018	−0.61722	−3.2705
H	0.042986	−1.43313	−3.9022
H	−1.41328	−0.69631	−3.25342
C	0.074641	0.732928	−3.85948
H	−0.34258	0.846889	−4.86284
H	1.163489	0.778886	−3.96217
C	0.153657	1.686476	−1.53488
H	1.245534	1.745174	−1.57298
H	−0.18659	2.511845	−0.90703
C	−0.39116	1.865902	−2.95124
H	−1.48538	1.876076	−2.91862
H	−0.07822	2.832776	−3.35275
C	0.340255	1.851191	3.698798
H	0.674096	2.810675	3.325899
H	0.510272	1.641872	4.746929
H	0.962271	−1.56072	2.71276
H	−0.54132	−2.45826	2.780942



(m) **6'**

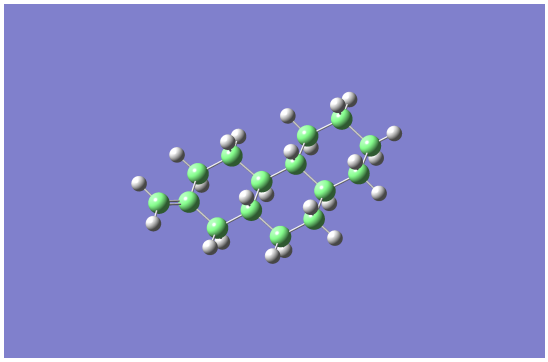
C	−0.17773	−0.66239	−0.14368
C	−0.38514	0.80276	0.260582
C	−1.69304	1.344761	−0.31688
C	−2.89169	0.487457	0.084911
C	−2.68271	−0.96988	−0.32135
C	−1.37956	−1.51685	0.25798
H	−0.46444	0.828008	1.357995
H	−3.02344	0.541996	1.170237
H	−3.80676	0.880968	−0.36377
H	−3.52808	−1.58127	0.002831
H	−2.64502	−1.03643	−1.41326
H	−1.44754	−1.53349	1.351751
H	−1.22167	−2.55031	−0.06331
C	1.131522	−1.208	0.441069
H	1.296457	−2.23457	0.103284
C	0.814599	1.658649	−0.14439
H	0.888654	1.668524	−1.23682
H	0.657978	2.692974	0.175088
C	2.294717	−0.33223	0.066275
C	2.123246	1.114636	0.43961
H	2.084124	1.205622	1.531116
H	2.975847	1.70405	0.095717
H	1.03128	−1.23818	1.533439
H	−1.61128	1.364073	−1.4095
H	−1.83786	2.379564	0.006039
C	3.364008	−0.79102	−0.59914
H	3.452675	−1.83381	−0.87411
H	4.179002	−0.13585	−0.8775
H	−0.08932	−0.68924	−1.23915



(n) **7'**

C	0.195324	1.082614	0.272509
C	0.065329	−0.38977	−0.19444
C	−0.19012	−1.35272	0.98098
C	−1.43931	−0.91986	1.767554
C	−1.34644	0.534097	2.223112
C	−1.06754	1.468642	1.051117
H	−0.83855	−0.4286	−0.8245
H	−2.28975	−0.99738	1.073024
H	−2.28063	0.821157	2.715201
H	−0.56084	0.625056	2.979195
H	−1.9217	1.43746	0.364875
H	−0.97833	2.504379	1.395318
C	0.303638	1.986712	−0.97269
H	0.40405	3.030867	−0.66043
C	1.242815	−0.80011	−1.08586
H	2.166416	−0.81275	−0.49996
H	1.096371	−1.81373	−1.46098
C	1.451787	1.57954	−1.85009
C	1.400273	0.142966	−2.2863
H	0.534164	0.002987	−2.94393
H	2.28929	−0.11762	−2.86514
H	−0.63352	1.904027	−1.53745
C	1.435915	1.312909	1.142385
H	2.354486	1.162727	0.577782
H	1.439253	2.345349	1.499472
H	1.463406	0.661966	2.01418

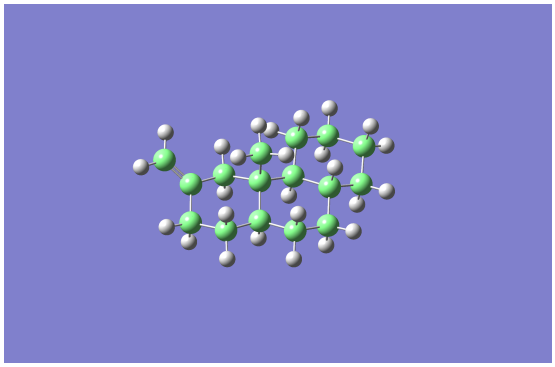
H	0.669038	−1.30723	1.664706
C	2.451636	2.409676	−2.17999
H	2.465829	3.437244	−1.841
H	3.273598	2.083197	−2.80377
C	−1.71429	−1.85864	2.94238
H	−2.61321	−1.52823	3.470818
C	−0.33828	−2.8123	0.53474
H	−1.15547	−2.87591	−0.19385
C	−0.62728	−3.74804	1.708311
H	0.236959	−3.7502	2.380469
H	−0.74684	−4.77253	1.347625
C	−1.86195	−3.30693	2.487203
H	−2.0286	−3.96338	3.344548
H	−2.74448	−3.39371	1.845501
H	−0.88471	−1.78358	3.654749
H	0.565416	−3.15081	0.026195



(o) 8’

C	−0.08246	0.150767	0.078008
C	−0.02794	0.08608	1.612951
C	1.40934	−0.03109	2.120522
C	2.286357	1.117255	1.61527
C	2.20946	1.184765	0.116727
C	0.814349	1.290843	−0.435
H	−0.4416	1.033627	1.990132
H	1.918274	2.056429	2.043653
H	3.320261	0.992782	1.944131
H	0.365532	2.242982	−0.12254

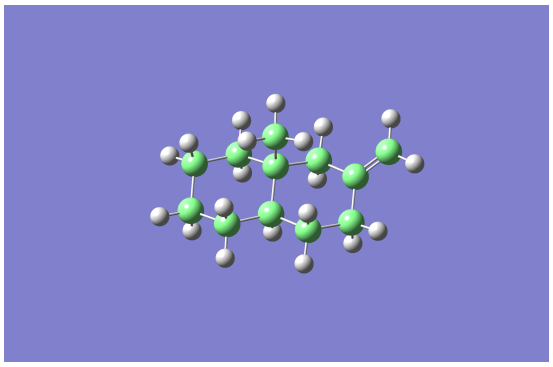
H	0.854461	1.294352	−1.52468
C	−1.53306	0.267113	−0.4228
C	−0.89747	−1.04969	2.146244
H	−0.47306	−2.00369	1.813878
H	−0.86651	−1.05561	3.239716
C	−2.399	−0.87765	0.127812
H	−1.97803	−1.81575	−0.26377
C	−2.33385	−0.93442	1.65149
H	−2.78714	−0.02319	2.057887
H	−2.93412	−1.77331	2.015791
H	−1.94383	1.208883	−0.02537
C	−3.84269	−0.77304	−0.36502
H	−4.42387	−1.61114	0.030136
H	−4.28814	0.140293	0.04565
C	−3.92435	−0.73391	−1.88761
H	−4.96259	−0.63346	−2.21262
H	−3.55582	−1.6817	−2.29263
C	−1.63252	0.318563	−1.95148
H	−1.1678	−0.58586	−2.36174
H	−1.07	1.167301	−2.34317
C	−3.07896	0.410848	−2.43587
H	−3.5057	1.362112	−2.10184
H	−3.10693	0.420215	−3.52811
C	3.289781	1.093521	−0.67188
H	3.20516	1.119111	−1.75041
H	4.284583	0.998748	−0.25672
H	1.830582	−0.98076	1.774515
H	1.411076	−0.05954	3.214038
H	0.329085	−0.79453	−0.30718



(p) **9'**

C	0.169256	−0.616	−0.004
C	0.381566	0.899123	−0.22465
C	1.711824	1.385296	0.352032
C	2.889007	0.601851	−0.22834
C	2.708029	−0.90421	−0.04386
C	1.364639	−1.36684	−0.60807
H	0.442711	1.03638	−1.31559
H	2.962368	0.820963	−1.29861
H	3.826938	0.931512	0.224843
H	3.520422	−1.44253	−0.53812
H	2.774267	−1.15444	1.017907
H	1.363665	−1.20301	−1.69197
H	1.233288	−2.44248	−0.45225
C	−1.12104	−1.03049	−0.73968
H	−1.31111	−2.09704	−0.58442
C	−0.80973	1.725646	0.258218
H	−0.9119	1.635381	1.343021
H	−0.627	2.783494	0.048108
C	−2.29796	−0.21032	−0.28828
C	−2.1077	1.27629	−0.42453
H	−2.04067	1.530709	−1.48878
H	−2.96825	1.812375	−0.01827
H	−0.96426	−0.88068	−1.81529
C	0.018983	−0.97794	1.477326
H	−0.89603	−0.56524	1.898674
H	−0.03635	−2.06398	1.580284

H	0.856042	−0.63182	2.080867
H	1.702065	1.292564	1.441989
H	1.828613	2.451044	0.135151
C	−3.4074	−0.75599	0.230911
H	−3.51517	−1.82825	0.329117
H	−4.23646	−0.14355	0.560884



(q) **10’**

C	−0.05477	0.11373	0.061814
C	−0.05278	0.091136	1.599176
C	1.385825	0.049886	2.148528
C	2.225952	1.209671	1.588642
C	2.20902	1.218798	0.062741
C	0.786119	1.266385	−0.4789
H	−0.50875	1.033813	1.941747
H	1.757883	2.142564	1.937077
H	2.790064	2.06837	−0.30793
H	2.707561	0.313421	−0.30135
H	0.31633	2.212657	−0.18747
H	0.78861	1.239941	−1.57257
C	−1.48425	0.163584	−0.49454
H	−1.45959	0.134657	−1.58718
C	−0.91726	−1.06508	2.114229
H	−0.44725	−2.0113	1.824415
H	−0.96783	−1.05283	3.203782
C	−2.31448	−0.96233	0.0498
C	−2.3425	−1.01998	1.54992
H	−2.84144	−0.12406	1.937086

H	−2.91636	−1.88352	1.893293
H	−1.93052	1.123532	−0.20535
H	1.845252	−0.88696	1.795836
C	−2.9211	−1.86727	−0.73078
H	−2.8648	−1.80958	−1.80986
H	−3.49445	−2.68218	−0.30871
C	3.656108	1.176108	2.128759
H	4.217874	2.022746	1.723844
C	1.438893	0.052208	3.680639
H	0.928462	0.951432	4.045696
C	2.871392	0.030853	4.21249
H	3.343708	−0.91356	3.923416
H	2.864221	0.057163	5.30479
C	3.690929	1.188934	3.653452
H	4.721302	1.138487	4.013236
H	3.274775	2.134425	4.015474
H	4.148036	0.267828	1.762346
H	0.896358	−0.80373	4.084067
H	0.398434	−0.82887	−0.27683