

Theoretical Study of the UV Absorption of 4-MethylBenzylidene Camphor: From the UVB to the UVA Region

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Figure S1. HOMO(-1) (a, b), HOMO (c, d) and LUMO (e, f) orbitals of MBC₁₃ (a, c, and e), and MBC₁₇ (b, d, and f).

Table S1. Cartesian coordinates of 4-MBC.

Table S2. Cartesian coordinates of BC.

Table S3. Cartesian coordinates of MBC₁₁.

Table S4. Cartesian coordinates of MBC₁₅-COH.

Table S5. Cartesian coordinates of MBC₁₁-NH₂.

Table S6. Cartesian coordinates of MBC₁₁-OH.

Table S7. Cartesian coordinates of DSBC1.

Table S8. Cartesian coordinates of DSBC2.

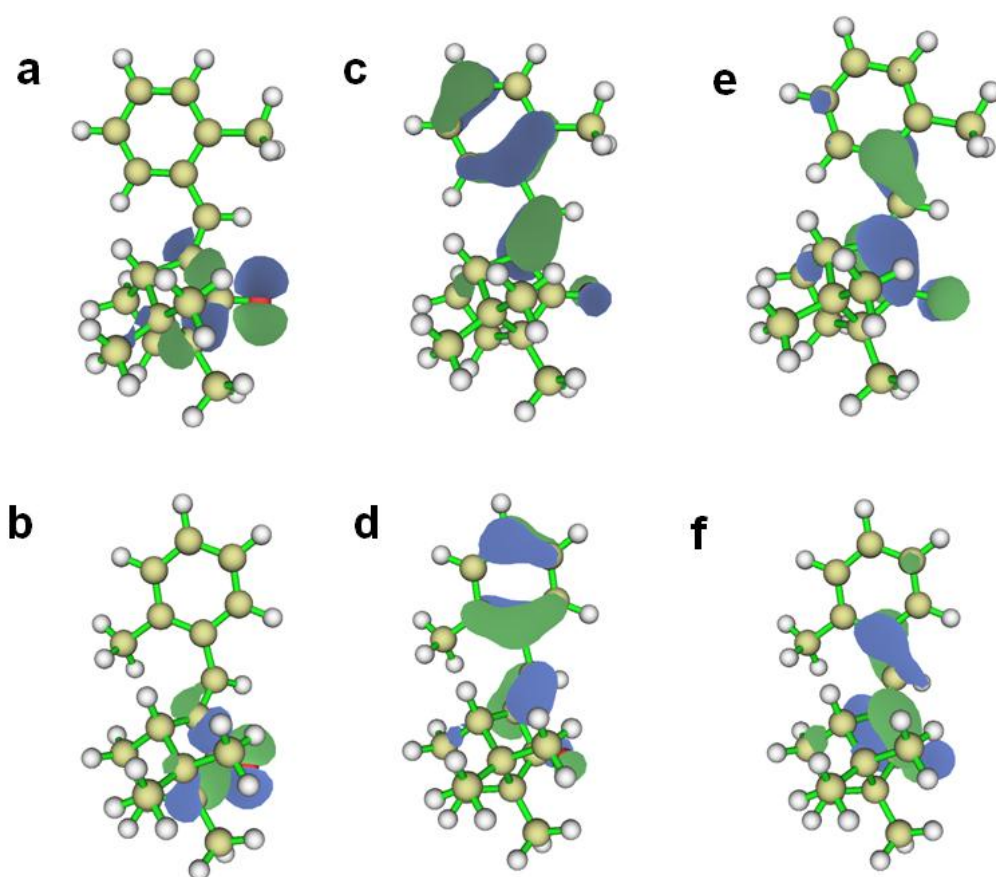


Figure S1. HOMO(-1) (**a**, **b**), HOMO (**c**, **d**) and LUMO (**e**, **f**) orbitals of MBC_{13} (**a**, **c**, and **e**), and MBC_{17} (**b**, **d**, and **f**).

Table S1. Cartesian coordinates of 4-MBC.			
C	-6.08282	-0.79682	0.14794
C	-4.66549	-0.29799	0.04663
C	-3.62018	-1.15438	-0.34903
C	-2.29826	-0.70800	-0.41366
C	-1.96449	0.62518	-0.08465
C	-3.02023	1.48857	0.28498
C	-4.33887	1.03512	0.35621
C	-0.60678	1.16632	-0.13406
C	0.59192	0.53728	-0.13338
C	1.01869	-0.91464	-0.05517
C	1.51351	-1.29092	-1.48328
C	2.82296	-0.45968	-1.61996
C	2.98320	0.25377	-0.23357
C	1.86821	1.29894	-0.23012
O	2.00347	2.52933	-0.31145
C	4.36188	0.80992	0.04975
C	2.36242	-0.80598	0.74843
C	2.16475	-0.26980	2.17268
C	3.14446	-2.12133	0.82827
H	-6.29038	-1.58264	-0.59958
H	-6.81055	0.01978	-0.00131
H	-3.85011	-2.18951	-0.62187
H	-1.52213	-1.39510	-0.75649
H	-2.79265	2.53248	0.52253
H	-5.13298	1.72903	0.64988
H	-0.53839	2.26423	-0.15657
H	0.28035	-1.60426	0.38033
H	0.76406	-1.02898	-2.24932
H	1.70183	-2.37547	-1.56716
H	2.78028	0.27847	-2.44010
H	3.70412	-1.09843	-1.80943
H	4.40647	1.28009	1.04861
H	4.61566	1.59354	-0.68697
H	5.13204	0.01878	-0.00227

H	1.60904	0.68488	2.19579
H	3.14093	-0.10516	2.66540
H	1.60045	-1.00052	2.78213
H	3.38285	-2.55484	-0.15707
H	2.56353	-2.87300	1.39612
H	4.09927	-1.96676	1.36436
H	-6.28087	-1.23452	1.14657

Table S2. Cartesian coordinates of BC.

C	-4.99739	-0.62094	0.11213
C	-3.92747	-1.43357	-0.28945
C	-2.63419	-0.90873	-0.37687
C	-2.38015	0.44608	-0.06301
C	-3.47509	1.25578	0.31700
C	-4.76626	0.72874	0.41211
C	-1.05391	1.06172	-0.13801
C	0.17536	0.49596	-0.13207
C	0.67646	-0.92935	-0.02213
C	1.17108	-1.31625	-1.44753
C	2.43621	-0.42529	-1.62294
C	2.57761	0.33134	-0.25776
C	1.41124	1.31897	-0.26500
O	1.48160	2.55175	-0.37899
C	3.92954	0.96361	-0.00708
C	2.02319	-0.73206	0.75935
C	1.81644	-0.16852	2.17165
C	2.87093	-2.00414	0.86198
H	-4.10375	-2.48248	-0.54441
H	-1.81998	-1.54874	-0.72207
H	-3.29873	2.31163	0.54471
H	-5.59599	1.37332	0.71551
H	-1.04582	2.16066	-0.18934
H	-0.02032	-1.64365	0.44121
H	0.40020	-1.11074	-2.20953

H	1.41160	-2.39195	-1.50728
H	2.34751	0.28738	-2.46168
H	3.34557	-1.02493	-1.80689
H	3.96460	1.45355	0.98259
H	4.13081	1.74554	-0.76158
H	4.73911	0.21281	-0.05757
H	1.21589	0.75897	2.17761
H	2.78934	0.05563	2.64709
H	1.29523	-0.90894	2.80714
H	3.11674	-2.45126	-0.11532
H	2.33657	-2.76809	1.45832
H	3.82424	-1.78777	1.37910
H	-6.00727	-1.03497	0.18005

Table S3. Cartesian coordinates of MBC₁₁.

C	-4.68303	-1.04213	0.11135
C	-3.69359	-1.45745	-0.78927
C	-2.48659	-0.75445	-0.88434
C	-2.24320	0.38241	-0.08555
C	-3.25870	0.79991	0.80149
C	-4.45979	0.08994	0.90671
C	-0.97524	1.15592	-0.19264
C	0.24257	0.54625	-0.20808
C	0.57605	-0.93133	-0.06493
C	1.12044	-1.40508	-1.44481
C	2.49315	-0.68116	-1.54106
C	2.61707	0.08738	-0.18344
C	1.57759	1.20640	-0.30179
O	1.85208	2.40890	-0.45938
C	4.01010	0.57346	0.15434
C	1.87697	-0.88012	0.80763
C	1.64694	-0.26727	2.19561
C	2.56109	-2.23978	0.98808
H	-3.86342	-2.32989	-1.42677

H	-1.73193	-1.07260	-1.60756
H	-3.10074	1.68137	1.42857
H	-5.22617	0.42405	1.61199
C	-1.11893	2.65731	-0.24985
H	-0.23657	-1.54845	0.34604
H	0.44073	-1.12341	-2.26680
H	1.22820	-2.50343	-1.47404
H	2.55554	0.01550	-2.39556
H	3.33459	-1.38968	-1.64308
H	4.03027	1.08512	1.13346
H	4.35121	1.30593	-0.59925
H	4.72996	-0.26493	0.17965
H	1.16718	0.72674	2.14975
H	2.60574	-0.15563	2.73516
H	0.99584	-0.92553	2.80111
H	2.80704	-2.74179	0.03776
H	1.90616	-2.91817	1.56743
H	3.50240	-2.12240	1.55683
H	-5.62464	-1.59291	0.18852
H	-0.15791	3.13901	-0.48342
H	-1.47171	3.05569	0.72196
H	-1.87580	2.94303	-1.00348

Table S4. Cartesian coordinates of MBC₁₅-COH.

C	-4.37384	0.03797	0.08508
C	-3.39710	-0.88648	-0.33325
C	-2.06070	-0.50660	-0.42715
C	-1.65674	0.81223	-0.10258
C	-2.65159	1.73776	0.29016
C	-3.98902	1.35511	0.39126
C	-0.27099	1.27532	-0.17498
C	0.88455	0.57183	-0.15946
C	1.22584	-0.89829	-0.04106
C	1.70748	-1.33739	-1.45657

C	3.06513	-0.59082	-1.60450
C	3.25902	0.14899	-0.23629
C	2.20853	1.25577	-0.26992
O	2.40807	2.47355	-0.38173
C	4.66656	0.62959	0.04346
C	2.56943	-0.84478	0.76936
C	2.39431	-0.25767	2.17645
C	3.27203	-2.20067	0.89161
H	-3.71809	-1.90060	-0.58752
H	-1.32352	-1.22727	-0.78522
H	-2.35767	2.76513	0.52406
H	-4.74598	2.08148	0.70587
H	-0.13713	2.36607	-0.22347
H	0.44783	-1.53507	0.40515
H	0.98053	-1.05297	-2.23626
H	1.82982	-2.43302	-1.50901
H	3.07266	0.12553	-2.44475
H	3.90753	-1.28576	-1.76931
H	4.73223	1.12653	1.02804
H	4.97432	1.37257	-0.71440
H	5.38687	-0.20838	0.02298
H	1.89431	0.72781	2.17006
H	3.37529	-0.13487	2.67137
H	1.78611	-0.93750	2.80213
H	3.48984	-2.67596	-0.07907
H	2.64564	-2.90030	1.47711
H	4.23135	-2.08627	1.42948
C	-5.78522	-0.36650	0.18807
O	-6.20677	-1.50235	-0.06661
H	-6.48845	0.43109	0.52116

Table S5. Cartesian coordinates of $\text{MBC}_{11}\text{-NH}_2$.

C	-4.75999	-0.98453	0.13866
C	-3.74847	-1.50795	-0.67814

C	-2.51962	-0.84742	-0.79059
C	-2.28398	0.35045	-0.08859
C	-3.31053	0.87158	0.72546
C	-4.53692	0.20773	0.84047
C	-0.99358	1.07473	-0.20486
C	0.24153	0.45642	-0.18829
C	0.64759	-0.99808	-0.02856
C	1.19188	-1.46134	-1.41400
C	2.49799	-0.62760	-1.56016
C	2.61057	0.16162	-0.21083
C	1.48452	1.19419	-0.29148
O	1.63420	2.44007	-0.42158
C	3.97609	0.74374	0.08396
C	1.97028	-0.85582	0.80759
C	1.74002	-0.25862	2.20206
C	2.75742	-2.16149	0.96975
H	-3.91899	-2.43272	-1.23641
H	-1.74308	-1.24757	-1.44653
H	-3.13268	1.78943	1.29383
H	-5.31831	0.61907	1.48569
N	-1.06331	2.43645	-0.28152
H	-0.11368	-1.65918	0.41465
H	0.46901	-1.25050	-2.22040
H	1.39182	-2.54759	-1.42901
H	2.47151	0.06731	-2.41781
H	3.38870	-1.26780	-1.69330
H	3.98833	1.26090	1.06030
H	4.24322	1.49470	-0.68144
H	4.75396	-0.04183	0.09086
H	1.18265	0.69385	2.16791
H	2.70512	-0.07099	2.70889
H	1.16413	-0.96473	2.82992
H	3.02459	-2.64057	0.01366
H	2.16526	-2.88890	1.55765
H	3.69697	-1.97603	1.52327

H	-5.71860	-1.50331	0.22699
H	-0.17000	2.94257	-0.35116
H	-1.94908	2.90240	-0.42910

Table S6. Cartesian coordinates of MBC₁₁-OH.

C	-4.86818	-0.92960	0.12072
C	-3.77734	-1.65451	-0.37821
C	-2.51497	-1.05758	-0.46367
C	-2.32690	0.27657	-0.04990
C	-3.43527	1.00505	0.42880
C	-4.69337	0.40311	0.52000
C	-1.01872	0.94626	-0.12675
C	0.22848	0.36134	-0.12429
C	0.74501	-1.06148	-0.02564
C	1.25922	-1.43215	-1.44927
C	2.49612	-0.50011	-1.61487
C	2.61192	0.25357	-0.24161
C	1.41286	1.18610	-0.23996
O	1.42936	2.45008	-0.33172
C	3.94326	0.92427	0.01991
C	2.08692	-0.84326	0.76286
C	1.86937	-0.31265	2.18594
C	2.97395	-2.09038	0.84415
H	-3.91169	-2.68733	-0.71139
H	-1.68235	-1.62244	-0.88703
H	-3.28666	2.04565	0.72395
H	-5.54299	0.97676	0.90054
O	-1.09849	2.30206	-0.17210
H	0.06104	-1.79151	0.43242
H	0.48662	-1.24557	-2.21418
H	1.53563	-2.49907	-1.51496
H	2.38802	0.21592	-2.44814
H	3.42516	-1.06881	-1.79835
H	3.95834	1.41060	1.01174

H	4.12939	1.71341	-0.73086
H	4.77269	0.19553	-0.02786
H	1.23986	0.59429	2.21183
H	2.83724	-0.06872	2.66209
H	1.37516	-1.08184	2.80872
H	3.23554	-2.51410	-0.13910
H	2.46201	-2.87999	1.42642
H	3.91895	-1.85438	1.36789
H	-5.85359	-1.39917	0.18888
H	-0.14958	2.69643	-0.24125

Table S7. Cartesian coordinates of DSBC1.

C	-4.24311	-0.14516	0.15303
C	-3.31921	-0.82556	-0.66219
C	-2.01254	-0.35611	-0.78700
C	-1.59966	0.80723	-0.10246
C	-2.53174	1.48890	0.70727
C	-3.83873	1.01388	0.83677
C	-0.21775	1.33014	-0.23672
C	0.90697	0.53083	-0.20965
C	1.09092	-0.96332	-0.01600
C	1.56595	-1.53259	-1.38693
C	2.98625	-0.91302	-1.53844
C	3.20757	-0.11454	-0.20787
C	2.24986	1.07180	-0.32125
O	2.58076	2.27815	-0.47484
C	4.64290	0.26473	0.08620
C	2.41601	-0.99987	0.82764
C	2.27070	-0.34287	2.20655
C	2.99656	-2.40496	1.02524
H	-3.65510	-1.71972	-1.19472
H	-1.30617	-0.87420	-1.43928
H	-2.21629	2.37942	1.25813
H	-4.55270	1.54148	1.47831

N	-0.08423	2.68662	-0.33374
H	0.23924	-1.49506	0.43656
H	0.88882	-1.23093	-2.20419
H	1.59638	-2.63643	-1.37729
H	3.07570	-0.24749	-2.41486
H	3.76859	-1.68648	-1.64110
H	4.72586	0.80407	1.04692
H	5.02634	0.94270	-0.69763
H	5.29378	-0.62783	0.12536
H	1.86371	0.68187	2.14774
H	3.24996	-0.29159	2.71787
H	1.59183	-0.93979	2.84467
H	3.18997	-2.94321	0.08275
H	2.30081	-3.01999	1.62742
H	3.95265	-2.34981	1.57857
C	-5.62367	-0.64231	0.28726
O	-6.05926	-1.65108	-0.28144
H	-6.28625	-0.04272	0.95280
H	0.87483	3.05106	-0.41274
H	-0.88817	3.27859	-0.49760

Table S8. Cartesian coordinates of DSBC2.

C	-4.33897	-0.12179	0.10225
C	-3.35531	-1.00054	-0.38829
C	-2.02683	-0.58884	-0.47568
C	-1.65261	0.71168	-0.07178
C	-2.64565	1.59705	0.39570
C	-3.97382	1.17988	0.48802
C	-0.26243	1.19063	-0.14719
C	0.88834	0.43634	-0.14093
C	1.20685	-1.04340	-0.03769
C	1.68654	-1.48122	-1.45482
C	3.03811	-0.72381	-1.60440
C	3.23877	0.00707	-0.22852

C	2.17939	1.09264	-0.24122
O	2.36594	2.34172	-0.32865
C	4.64625	0.48894	0.04973
C	2.55549	-1.00625	0.76934
C	2.39229	-0.44660	2.18879
C	3.26443	-2.36150	0.86425
H	-3.66164	-2.00150	-0.70435
H	-1.28149	-1.26784	-0.89283
H	-2.35076	2.60854	0.68036
H	-4.73950	1.86896	0.85998
H	0.42688	-1.67664	0.41031
H	0.95623	-1.19733	-2.23131
H	1.81840	-2.57561	-1.51387
H	3.03639	0.00067	-2.43740
H	3.88483	-1.41093	-1.77914
H	4.71389	0.98135	1.03629
H	4.95379	1.23378	-0.70628
H	5.36554	-0.34957	0.02456
H	1.88712	0.53538	2.20589
H	3.37784	-0.32982	2.67630
H	1.79439	-1.14221	2.80699
H	3.48261	-2.81926	-0.11439
H	2.64147	-3.07343	1.43842
H	4.22386	-2.25360	1.40322
C	-5.74299	-0.55828	0.19982
O	-6.14672	-1.68358	-0.11964
H	-6.45513	0.20341	0.59190
O	-0.15659	2.54517	-0.19007
H	0.83711	2.80714	-0.25213