

Supporting Information
Conformation-Dependent Antioxidant Properties of β -Carotene

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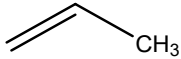
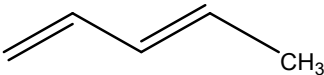
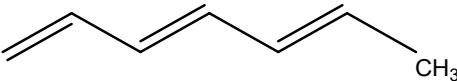
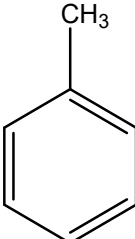
#Present Address: CSIR-National Institute of Science Communication and Policy Research, New Delhi, India

Computational Details.

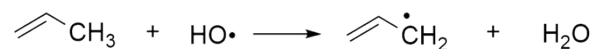
The geometries of all the reactive species studied are optimized at (U)B3LYP/6-31G(d) level of theory in the gas phase and further single point calculations are performed with these optimized geometries at higher level of theories. Throughout the manuscript the small basis (SB) refers to the 6-31G(d) basis set and the medium basis (MB) refers to the 6-311++G(d,p) basis set for B3LYP calculations and 6-311+G(d,p) basis set for ROB2-PLYP calculations.

H-atom abstraction reactions

Reference Systems

		
propene	penta-1,3-diene	hepta-1,3,5-triene
		
	toluene	

H-atom abstraction from propene by OH radical



Scheme S1. H-atom abstraction from propene by OH radical

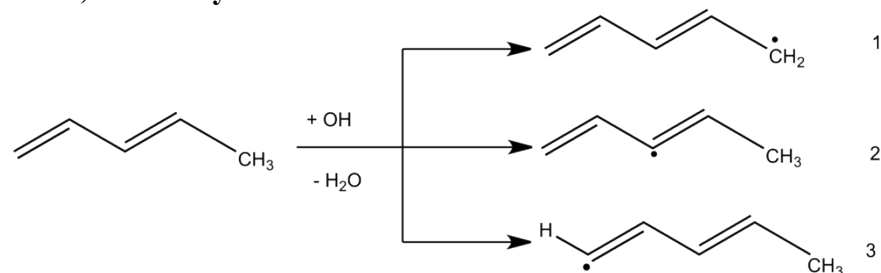
Table S1: Energetics of reaction in Scheme 1.

Reactive Species	E _{Tot} (B3LYP/6-31G(d))	H ₂₉₈ (1.00) (B3LYP/6-31G(d))	G ₂₉₈ (1.00) (B3LYP/6-31G(d))	H ₂₉₈ (0.9806) (B3LYP/6-31G(d))	G ₂₉₈ (0.9806) (B3LYP/6-31G(d))	E _{Tot} URCCSD(T)/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2(FC)/G3MP2large// B3LYP/6-31G(d)	E ₀ (G3(MP2)-RAD)	H ₂₉₈ (G3(MP2)-RAD)
pro_001	-117.907556	-117.822453	-117.852475	-117.823722	-117.853776	-117.50787812	-117.4554608	-117.6127572	-117.74989152	-117.66605752
OH	-75.7234548	-75.711846	-75.732093	-75.711979	-75.732207	-75.53697775	-75.5210509	-75.6146059	-75.64391475	-75.63243895
proh_001	-117.2603538	-117.189242	-117.219158	-117.190290	-117.220237	-116.87040768	-116.8211896	-116.9699539	-117.09844498	-117.02838118
H ₂ O	-76.408953	-76.384023	-76.405470	-76.384359	-76.405782	-76.20783765	-76.1968428	-76.3147407	-76.34456155	-76.31996755

Reactive Species	E _{Tot} (G3B3)	H ₂₉₈ (G3B3)	G ₂₉₈ (G3B3)	E _{Tot} (B3LYP/6-311++G(d,p)//B3LYP/6-31G(d))	E _{Tot} (B3LYP/6-311++G(3df,2p)//B3LYP/6-31G(d))	E _{Tot} (MPW1K/6-31G(d))	H ₂₉₈ (1.00) (MPW1K/6-31G(d))	G ₂₉₈ (1.00) (MPW1K/6-31G(d))	E _{Tot} (ROB2PLYP/6-31G(d)//B3LYP/6-31G(d))	E _{Tot} (ROB2PLYP/6-311++G(3df,2p)//B3LYP/6-31G(d))
pro_001	-117.780674	-117.779730	-117.809892	-117.9455864	-117.9535794	-117.873827	-117.786445	-117.816394	-117.746213687	-117.827138145
OH	-75.6963668	-75.693062	-75.713309	-75.7623691	-75.7655697	-75.6996746	-75.687631	-75.707852	-75.654958988	-75.71256850178
proh_001	-117.142603	-117.141659	-117.171710	-117.2982428	-117.306367	-117.2270004	-117.154228	-117.184064	-117.100603781	-117.17922870
H ₂ O	-76.3837261	-76.379947	-76.401395	-76.4584074	-76.4632079	-76.3821166	-76.356234	-76.377640	-76.3350369298	-76.409257653

Reactive Species	E _{Tot} (CBS-QB3)	H ₂₉₈ (CBS-QB3)	G ₂₉₈ (CBS-QB3)	E _{Tot} (ROB2PLYP/6- 311++G(d,p)//B3LY P/6-31G(d))	H ₂₉₈ (ROB2PLYP/6- 311++G(d,p)//B3LY P/6-31G(d))	G ₂₉₈ (ROB2PLYP/6- 311++G(d,p)//B3LY P/6-31G(d))
pro_001	-117.642120	-117.641176	-117.671257	-117.8001344	-117.7150314	-117.7450534
OH	-75.647359	-75.646415	-75.666647	-75.6992103	-75.6876015	-75.7078485
proh_001	-117.005667	-117.004723	-117.034661	-117.1525635	-117.0814517	-117.1113677
H ₂ O	-76.334655	-76.333711	-76.355138	-76.3928182	-76.3678882	-76.3893352

H-atom abstraction from penta-1,3-diene by OH radical



Scheme S2. H-atom abstraction from penta-1,3-diene by OH radical

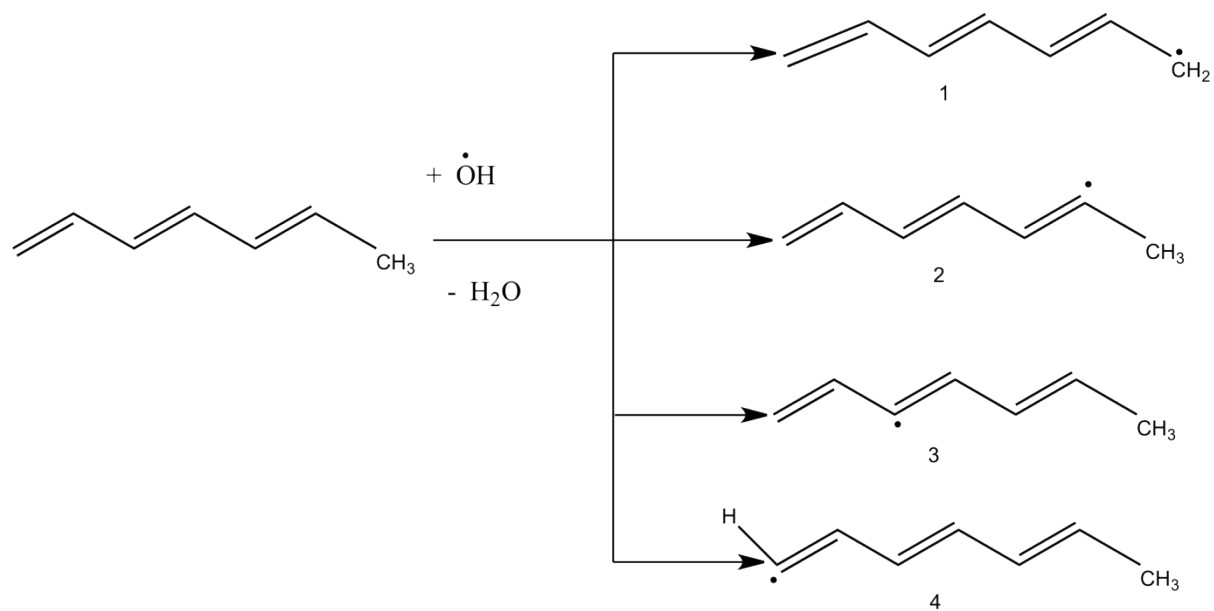
Table S2: Energetics of reaction in Scheme S2.

Reactive Species	E _{Tot} (B3LYP/6-31G(d))	H ₂₉₈ (1.00) (B3LYP/6-31G(d))	G ₂₉₈ (1.00) (B3LYP/6-31G(d))	H ₂₉₈ (0.9806) (B3LYP/6-31G(d))	G ₂₉₈ (0.9806) (B3LYP/6-31G(d))	E _{Tot} URCCSD(T)/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2(FC)/G3MP2 large// B3LYP/6-31G(d)	E ₀ (G3(MP2)-RAD)	H ₂₉₈ (G3(MP2)-RAD)
pen_001	-195.3122523	-195.191398	-195.227223	-195.193205	-195.229127	-194.67342059	-194.5937496	-194.8363339	-195.04778689	-194.92873959
pen H abs 001	-194.6748639	-194.567731	-194.603302	-194.569323	-194.604988	-194.04408019	-193.9646485	-194.1991347	-194.40490439	-194.29936349
pen H abs 002	-194.6298179	-194.522634	-194.562064	-194.524220	-194.563747	-194.00246625	-193.9219007	-194.1527975	-194.35970105	-194.25410315
pen H abs 003	-194.6242003	-194.517315	-194.553669	-194.518899	-194.555351	-193.99928714	-193.9185807	-194.1497454	-194.35678984	-194.25148854

Reactive Species	E _{Tot} (B3LYP/6-311++G(d,p)//B3LYP/6-31G(d))	E _{Tot} (B3LYP/6-311++G(3df,2p)//B3LYP/6-31G(d))	E _{Tot} (MPW1K/6-31G(d))	H ₂₉₈ (1.00) (MPW1K/6-31G(d))	G ₂₉₈ (1.00) (MPW1K/6-31G(d))	E _{Tot} (ROB2PLYP/6-31G(d)//B3LYP/6-31G(d))	E _{Tot} (ROB2PLYP/6-311+G(3df,2p)//B3LYP/6-31G(d))
pen 001	-195.3706781	-195.3842026	-195.2554682	-195.131341	-195.167064	-195.05894303	-195.18468902
OH	-75.7623691	-75.7655697	-75.6996746	-75.687631	-75.707852	-75.654958988	-75.71256850178
pen H abs 001	-194.7331549	-194.7468768	-194.6183422	-194.508749	-194.544200	-194.42205256	-194.5457219
pen H abs 002	-194.6877727	-194.7011229	-194.5732381	-194.463009	-194.500870	-194.38072094	-194.50249142
pen_H_abs_003	-194.6824636	-194.6957446	-194.5686466	-194.458815	-194.495028	-194.37594226	-194.49791766
H2O	-76.4584074	-76.4632079	-76.3821166	-76.356234	-76.377640	-76.3350369298	-76.409257653

Reactive Species	E _{Tot} (CBS-QB3)	H ₂₉₈ (CBS-QB3)	G ₂₉₈ (CBS-QB3)	E _{Tot} (ROB2PLYP/6- 311++G(d,p))	H ₂₉₈ (ROB2PLYP/6- 311++G(d,p))	G ₂₉₈ (ROB2PLYP/6- 311++G(d,p))	E _{Tot} (G3B3)	H ₂₉₈ (G3B3)	G ₂₉₈ (G3B3)
pen_001	-194.891095	-194.890150	-194.926091	-195.1399707	-195.0191164	-195.0549414	-195.119729	-195.118785	-195.154908
OH	-75.647359	-75.646415	-75.666647	-75.6992103	-75.6876015	-75.7078485	-75.6963668	-75.693062	-75.713309
pen_H_abs_001	-194.264788	-194.263844	-194.299484	-194.5011651	-194.3940322	-194.4296032	-194.489626	-194.488682	-194.524542
pen_H_abs_002	-194.219959	-194.219015	-194.254910	-194.4588678	-194.3516837	-194.3911139	-194.444317	-194.443372	-194.483104
pen_H_abs_003	-194.215981	-194.215037	-194.251517	-194.4544047	-194.3475194	-194.3838734	-194.441901	-194.440957	-194.477610
H2O	-76.334655	-76.333711	-76.355138	-76.3928182	-76.3678882	-76.3893352	-76.3837261	-76.379947	-76.401395

H-atom abstraction from hepta-1,3,5-triene by OH radical



Scheme S3. H-atom abstraction from hepta-1,3,5-triene by OH radical

Table S3: Energetics of conformers of hepta-1,3,5-triene.

Conformers	E _{Tot} (B3LYP/6-31G(d))	H ₂₉₈ (1.00) (B3LYP/6-31G(d))	G ₂₉₈ (1.00) (B3LYP/6-31G(d))	H ₂₉₈ (0.9806) (B3LYP/6-31G(d))	G ₂₉₈ (0.9806) (B3LYP/6-31G(d))	E _{Tot} URCCSD(T)/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2(FC)/G3MP2/ arge// B3LYP/6-31G(d)	E _{Tot} (G3(MP2)-RAD)	H ₂₉₈ (G3(MP2)-RAD)
hex_001	-272.7187404	-272.562110	-272.603644	-272.564454	-272.606153	-271.84017709	-271.7338651	-272.0617507	-272.34690969	-272.19262329
hex_002	-272.7157889	-272.558985	-272.600624	-272.555772	-272.556554	-271.83754763	-271.7311525	-272.0595647	-272.34480683	-272.18478993
hex_013	-272.713042	-272.556412	-272.598495	-272.553334	-272.554116	-271.83547602	-271.7289671	-272.0564204	-272.34177632	-272.18206832

Conformers	E _{Tot} (G3B3)	H ₂₉₈ (G3B3)	G ₂₉₈ (G3B3)	E _{Tot} (B3LYP/6-311++G(d,p)//B3LYP/6-31G(d))	E _{Tot} (B3LYP/6-311++G(3df,2p)//B3LYP/6-31G(d))	E _{Tot} (MPW1K/6-31G(d))	H ₂₉₈ (1.00) (MPW1K/6-31G(d))	G ₂₉₈ (1.00) (MPW1K/6-31G(d))	E _{Tot} (ROB2PLYP/6-31G(d)//B3LYP/6-31G(d))	E _{Tot} (ROB2PLYP/6-311++G(3df,2p)//B3LYP/6-31G(d))
hex_001	-272.459981	-272.459037	-272.501030	-272.7975444	-272.816637	-272.6386378	-272.477748	-272.519163	-272.37341867	-272.544013420
hex_002	-272.457632	-272.456688	-272.498784	-272.7947412	-272.8137044	-272.6358562	-272.474760	-272.516232	-272.370613107	-272.5413694115
hex_013	-272.454866	-272.453922	-272.496465	-272.7915917	-272.8105165	-272.633241	-272.472355	-272.514011	-272.36804973	-272.538152183

Table S4: Energetics of H-atom abstraction reactions from hepta-1,3,5-triene by OH radical.

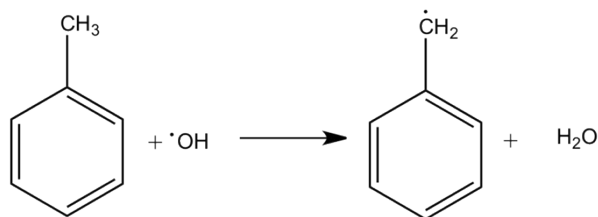
Conformers	E _{Tot} (B3LYP/6-31G(d))	H ₂₉₈ (1.00) (B3LYP/6-31G(d))	G ₂₉₈ (1.00) (B3LYP/6-31G(d))	H ₂₉₈ (0.9806) (B3LYP/6-31G(d))	G ₂₉₈ (0.9806) (B3LYP/6-31G(d))	E _{Tot} URCCSD(T)/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2/6-31G(d)// B3LYP/6-31G(d)	E _{Tot} ROMP2(FC)/G3MP2large// B3LYP/6-31G(d)	E _{Tot} (G3(MP2)-RAD)	H ₂₉₈ (G3(MP2)-RAD)
hex_H abs 001	-272.0864458	-271.943485	-271.984683	-271.945615	-271.986974	-271.21521610	-271.1115018	-271.4317056	-271.7088229	-271.5679921
hex_H abs 002	-272.0376988	-271.894638	-271.937243	-271.896766	-271.939535	-271.17068428	-271.0632746	-271.3799351	-271.66074778	-271.51981498
hex_H abs 007	-272.0356485	-271.892676	-271.936264	-271.894801	-271.938554	-271.16866355	-271.0611907	-271.3772649	-271.65814075	-271.51729325
hex_H abs 003	-272.0299844	-271.887094	-271.929269	-271.889219	-271.931558	-271.16534991	-271.0578394	-271.3739956	-271.65490911	-271.51414371
hex_001	-272.7187404	-272.562110	-272.603644	-272.564454	-272.606153	-271.84017709	-271.7338651	-272.0617507	-272.34690969	-272.19262329

Conformers	E _{Tot} (G3B3)	H ₂₉₈ (G3B3)	G ₂₉₈ (G3B3)	E _{Tot} (B3LYP/6-311++G(d,p)//B3LYP/6-31G(d))	E _{Tot} (B3LYP/6-311++G(3df,2p)//B3LYP/6-31G(d))	E _{Tot} (MPW1K/6-31G(d))	H ₂₉₈ (1.00) (MPW1K/6-31G(d))	G ₂₉₈ (1.00) (MPW1K/6-31G(d))	E _{Tot} (ROB2PLYP/6-31G(d)//B3LYP/6-31G(d))	E _{Tot} (ROB2PLYP/6-311++G(3df,2p)//B3LYP/6-31G(d))
hex_H abs 001	-271.833234	-271.832290	-271.873934	-272.165103	-272.1844086	-272.0068205	-271.860600	-271.901650	-271.7413290076	-271.90994064
hex_H abs 002	-271.789243	-271.788299	-271.831360	-272.116003	-272.1349358	-271.9584024	-271.811530	-271.853908	-271.6964345987	-271.86320125

hex H abs 007	-271.785501	-271.784557	-271.828605	-272.1137885	-272.1326938	-271.9561732	-271.809410	-271.852825	-271.6944283875	-271.86088491
hex_H_abs_003				-272.1080779	-272.1269221	-271.9513721	-271.804797	-271.846753	-271.6896353543	-271.85599852

Conformers	E _{Tot} (CBS-QB3)	H ₂₉₈ (CBS-QB3)	G ₂₉₈ (CBS-QB3)	E _{Tot} (ROB2PLYP/6-311++G(d,p))	H ₂₉₈ (ROB2PLYP/6-311++G(d,p))	G ₂₉₈ (ROB2PLYP/6-311++G(d,p))
hex H abs 001	-271.520839	-271.519895	-271.561205	-271.8475136	-271.7045528	-271.7457508
hex H abs 002	-271.472264	-271.471320	-271.514063	-271.8017024	-271.6586416	-271.7012466
hex H abs 007	-271.468195	-271.467251	-271.510955	-271.7994954	-271.6565229	-271.7001109
hex H abs 003	-271.464724	-271.463780	-271.506125	-271.794683	-271.6517926	-271.6939676
H ₂ O	-76.334655	-76.333711	-76.355138	-76.3928182	-76.3678882	-76.3893352
hex 001	-272.141332	-272.140388	-272.182078	-272.481503	-272.3248726	-272.3664066
OH	-75.647359	-75.646415	-75.666647	-75.6992103	-75.6876015	-75.7078485

H-atom abstraction from toluene by OH radical



Scheme S4. H-atom abstraction from toluene by OH radical

Table S5: Energetics of H-atom abstraction reactions from toluene by OH radical.

Species	E _{Tot} (B3LYP/6-31G(d))	H ₂₉₈ (1.00) (B3LYP/6-31G(d))	G ₂₉₈ (1.00) (B3LYP/6-31G(d))	H ₂₉₈ (0.9806) (B3LYP/6-31G(d))	G ₂₉₈ (0.9806) (B3LYP/6-31G(d))	E _{Tot} (MPW1K/6-31G(d))	H ₂₉₈ (1.00) (MPW1K/6-31G(d))	G ₂₉₈ (1.00) (MPW1K/6-31G(d))	ΔE _{Tot} (G3(MP2)-RAD)	ΔH ₂₉₈ (G3(MP2)-RAD)
tol	-271.5666503	-271.431177	-271.469177	-271.433242	-271.471361	-271.4943978	-271.355172	-271.392901	-271.19285843	-271.05945013
OH	-75.7234548	-75.711846	-75.732093	-75.711979	-75.732207	-75.6996746	-75.687628	-75.707848	-75.64391475	-75.63243895
int_1	-270.9151431	-270.793577	-270.829861	-270.795423	-270.831825	-270.8422743	-270.717626	-270.753729	-270.53737717	-270.41765707
H ₂ O	-76.408953	-76.384023	-76.405470	-76.384359	-76.405782	-76.3821167	-76.356232	-76.378293	-76.34456155	-76.31996755

Species	E _{Tot} (CBS-QB3)	H ₂₉₈ (CBS-QB3)	G ₂₉₈ (CBS-QB3)	E _{Tot} (ROB2-PLYP/6-311++G(d,p))	H ₂₉₈ (ROB2-PLYP/6-311++G(d,p))	G ₂₉₈ (ROB2-PLYP/6-311++G(d,p))	E _{Tot} (ROB2-PLYP/6-31G(d))	E _{Tot} (B3LYP/6-31G(d)/B3LYP/6-311++G(d,p))	E _{Tot} (B3LYP/6-31G(d)/B3LYP/6-311++G(3df,2p))
tol	-271.014159	-271.013215	-271.051256	-271.3382886	-271.2028153	-271.2408153	-271.2407402	-271.6388222	-271.6575589
OH	-75.647359	-75.646415	-75.666647	-75.6992103	-75.6876015	-75.7078485	-75.6549589	-75.7623691	-75.7655697
int_1	-270.372316	-270.371372	-270.407769	-270.686321	-270.5647549	-270.6010389	-270.5907883	-270.9872605	-271.006225
H ₂ O	-76.334655	-76.333711	-76.355138	-76.3928182	-76.3678882	-76.3893352	-76.3350369	-76.4584074	-76.4632079

Figure S1. PES of propene + OH reaction

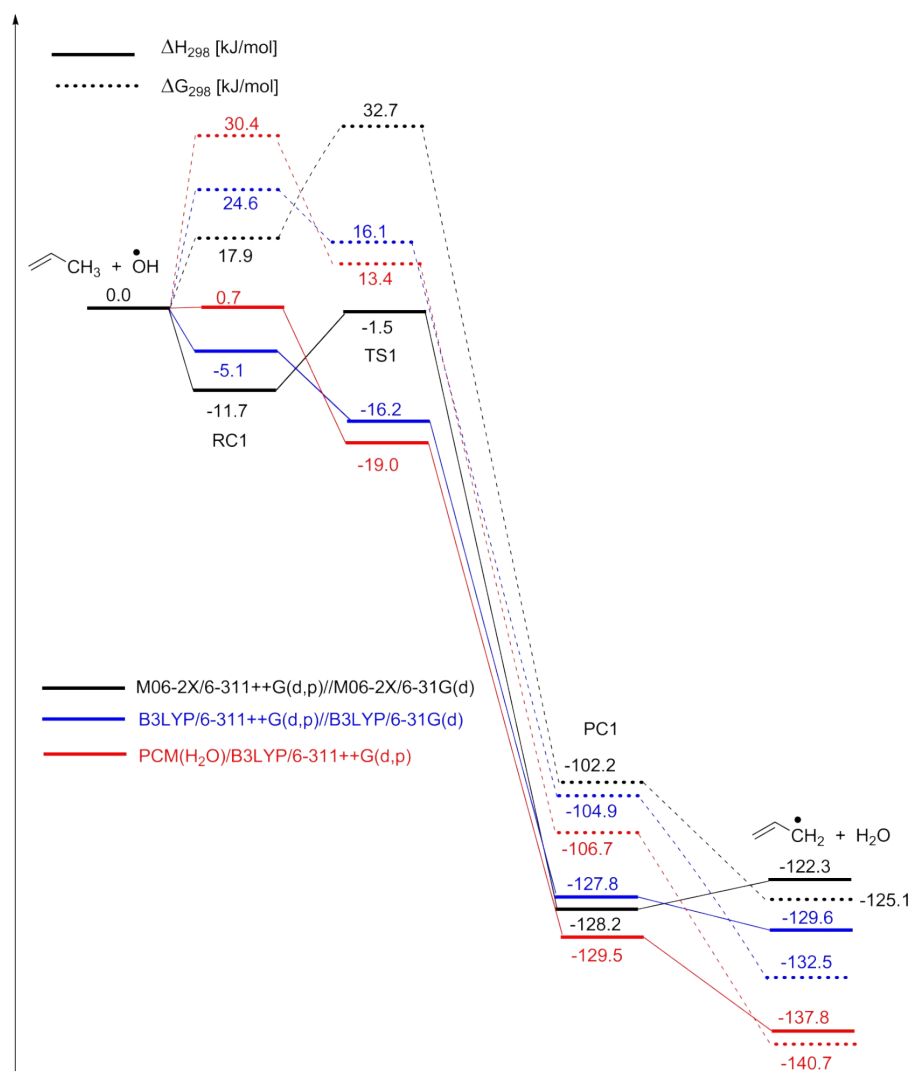


Figure S2. PES of toluene + OH reaction

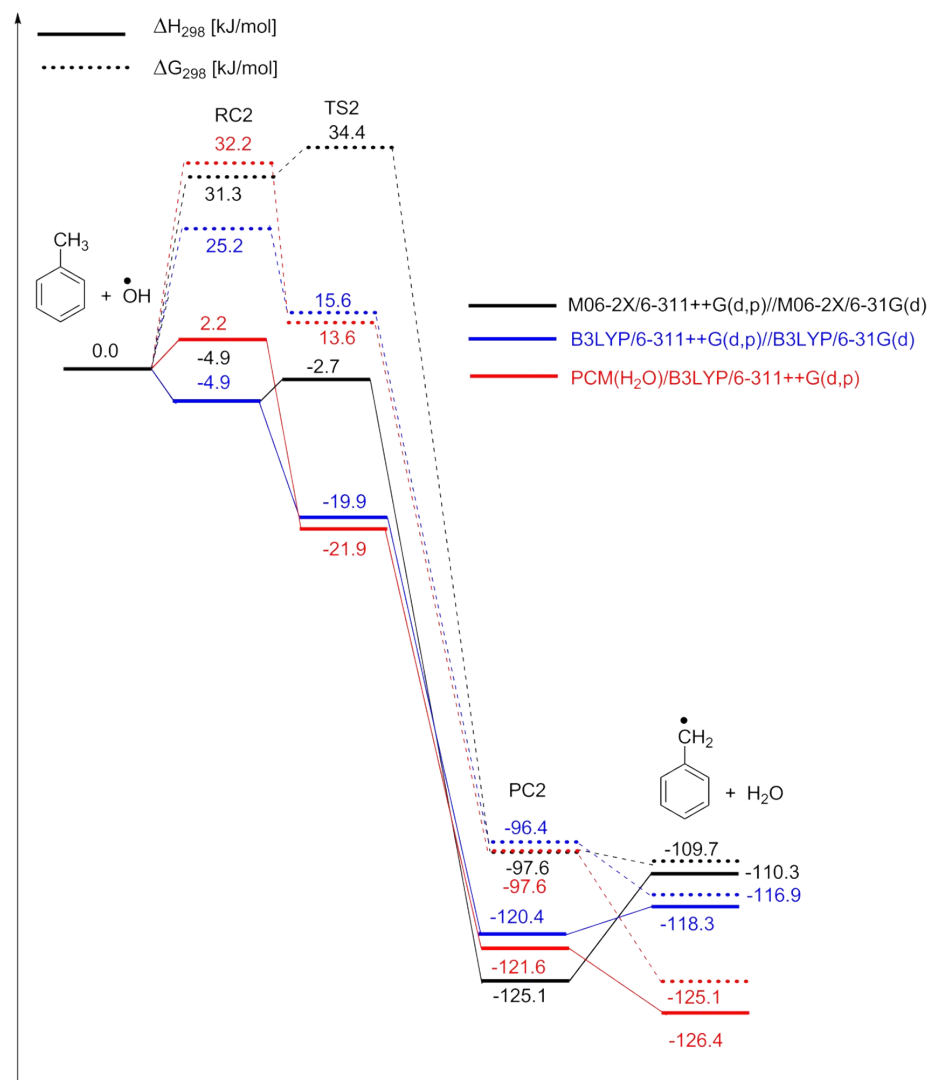


Figure S3. PES of penta-1,3-triene + OH reaction

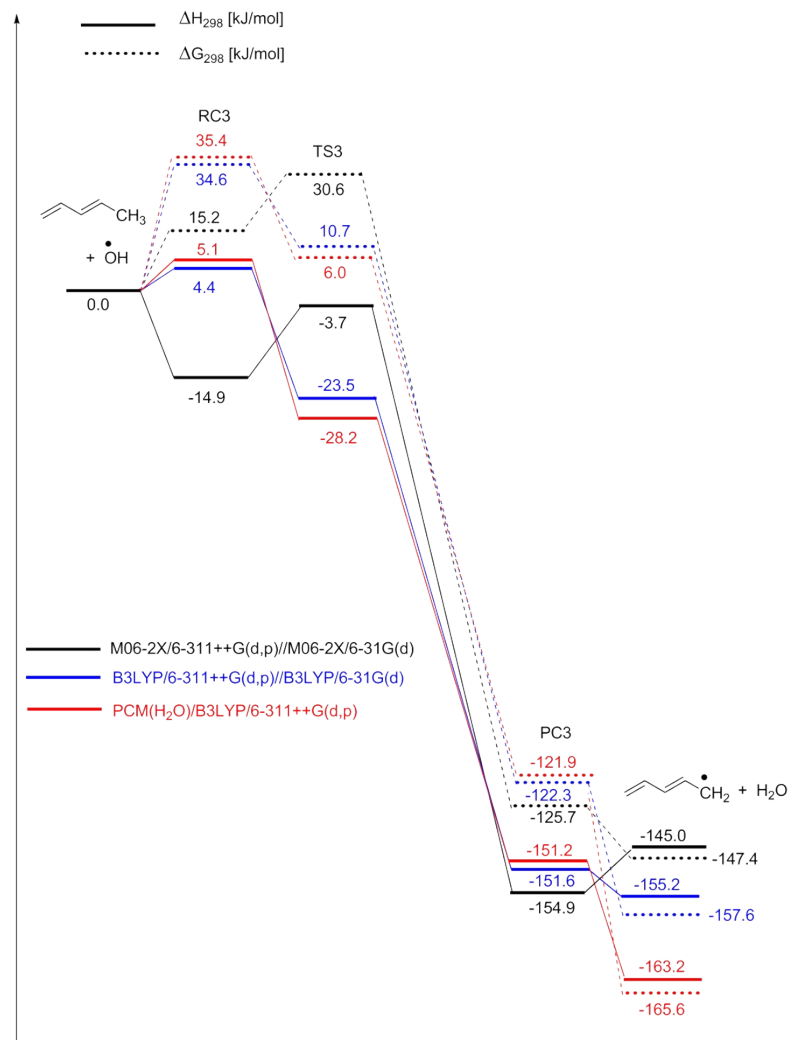


Figure S4. PES of hepta-1,3-triene + OH reaction

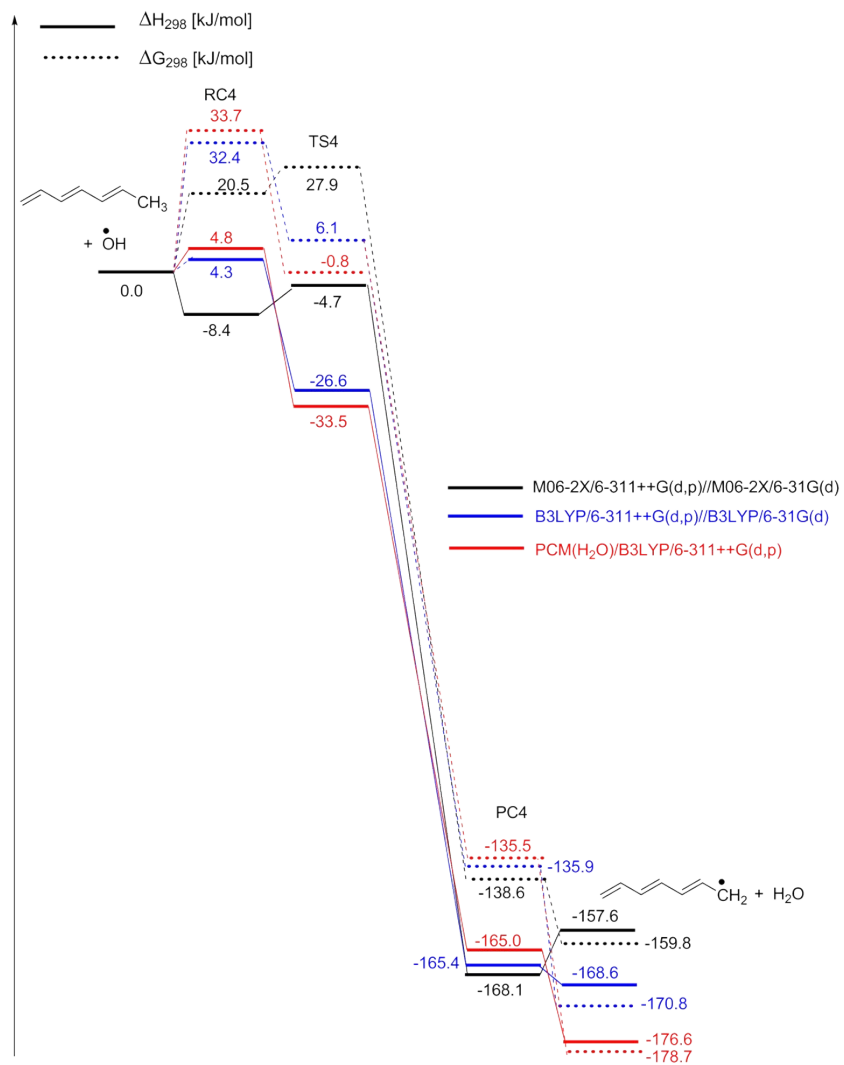
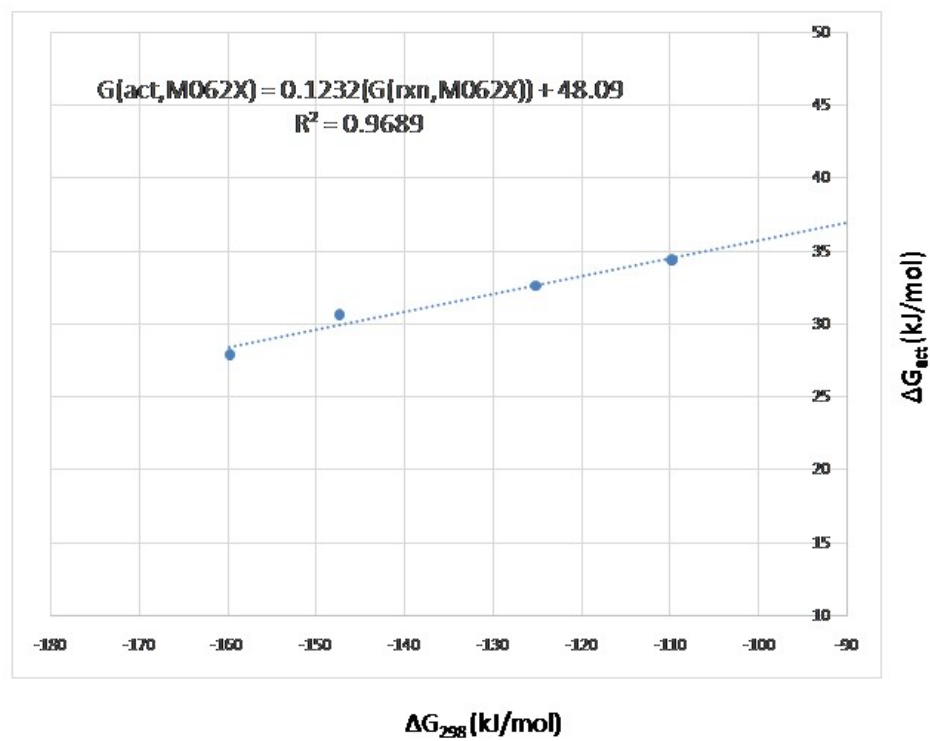
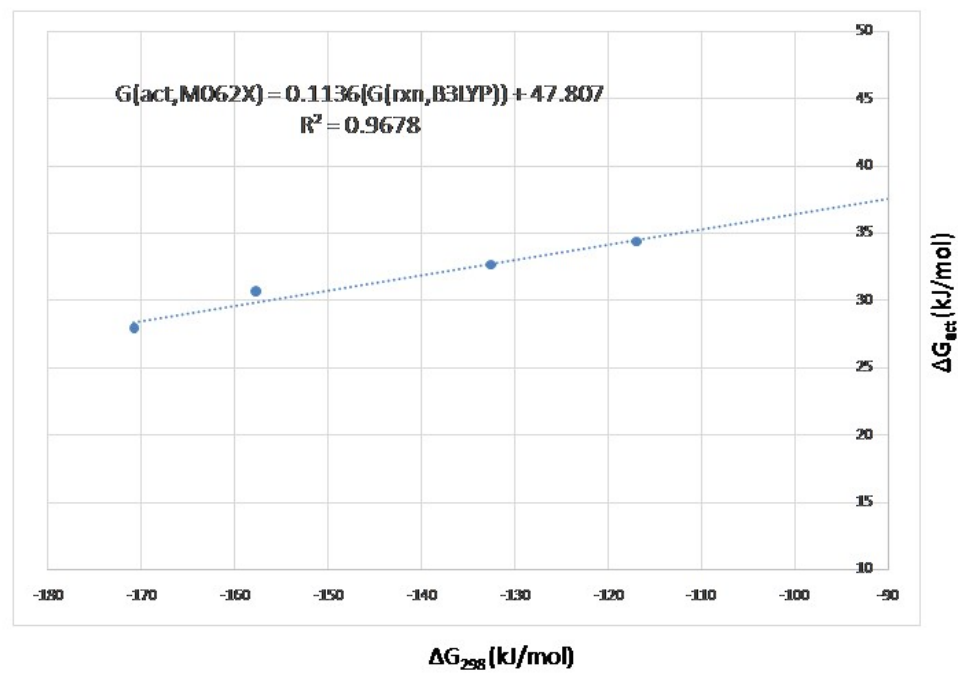


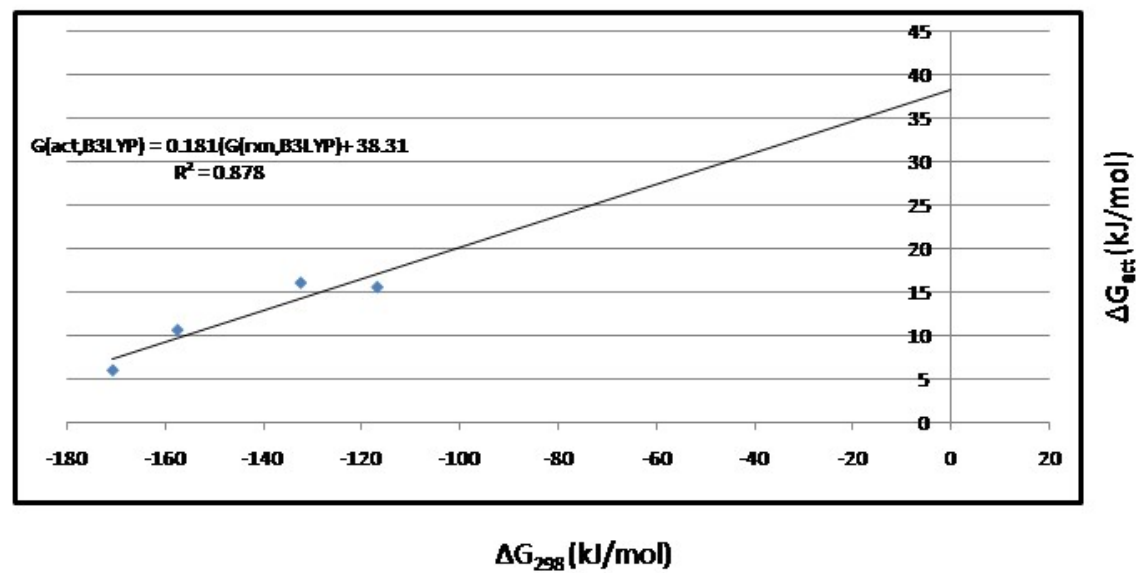
Figure S5: Regression analysis for Reaction barrier vs. Reaction energy



(a) M06-2X/6-311++G(d,p) barrier vs. M06-2X/6-311++G(d,p) reaction energy

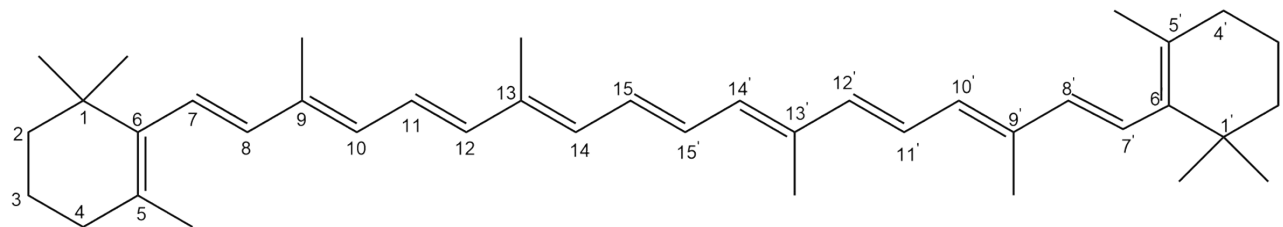


(b) M06-2X/6-311++G(d,p) barrier vs. B3LYP/6-311++G(d,p) reaction energy



(c) B3LYP/6-311++G(d,p) barrier vs. B3LYP/6-311++G(d,p) reaction energy

Energetics of the conformers and rotamers of beta-carotene



Scheme S5. Molecular Structure of beta-carotene

Table S6a: Energetics (in Hartrees) of the isomers and their conformers of beta-carotene

Isomers	Gas phase									Water Solvent (PCM)		
	B3LYP/SB			B3LYP/MB			B2PLYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
<i>all-trans (15E)</i>												
1(bet_car_030_004)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1556.559569	-1555.654393	-1555.784785	-1558.2441677	-1557.3389913	-1557.4693833
2 (bet_car_030)	-1557.9017115	-1556.996500	-1557.126500	-1558.3065541	-1557.401343	-1557.531343				-1558.2445303	-1557.339319	-1557.469319
3 (Car_H_021)	-1557.9016418	-1556.996487	-1557.126732	-1558.3064821	-1557.401328	-1557.531573	-1556.55884	-1555.653686	-1555.783931	-1558.243876	-1557.3387212	-1557.4689662
4 (Car_H_002)	-1557.9011413	-1556.995966	-1557.126407	-1558.3058906	-1557.400715	-1557.531156	-1556.558032	-1555.652857	-1555.783298	-1558.2441777	-1557.339002	-1557.469443
5 (bet_car_001)	-1557.8997584	-1556.994216	-1557.124908	-1558.3047821	-1557.39924	-1557.529932				-1558.2443961	-1557.338854	-1557.469546
6 (bet_car_007)	-1557.8997250	-1556.993957	-1557.123763	-1558.3047338	-1557.398965	-1557.528771	-1556.556411	-1555.650643	-1555.780449	-1558.244444	-1557.338676	-1557.468482
7 (bet_car_032)	-1557.8997138	-1556.994068	-1557.124408	-1558.3047009	-1557.399055	-1557.529395	-1556.556407	-1555.650762	-1555.781102	-1558.2443847	-1557.338739	-1557.469079
8 (bet_car_025)	-1557.8991466	-1556.993618	-1557.124459	-1558.3040335	-1557.398505	-1557.529346	-1556.555738	-1555.65021	-1555.781051	-1558.2442511	-1557.3387225	-1557.4695635
9 (Car_H_045)	-1557.8973707	-1556.991113	-1557.121296	-1558.3025009	-1557.396243	-1557.526426	-1556.553592	-1555.64805	-1555.778742	-1558.2442831	-1557.338025	-1557.468208
<i>15E,9Z</i>												
1 (bet_car_9)	-1557.9008134	-1556.995572	-1557.125839	-1558.3056364	-1557.400395	-1557.530662	-1556.558346	-1555.653104	-1555.783371	-1558.2415396	-1557.336298	-1557.466565
2 (Car_H_021)	-1557.9003287	-1556.995108	-1557.125212	-1558.3050964	-1557.3998757	-1557.5299797				-1558.2416233	-1557.3364026	-1557.4665066
3 (Car_H_002)	-1557.8997507	-1556.994536	-1557.124929	-1558.3044019	-1557.3991872	-1557.5295802				-1558.2416014	-1557.3363867	-1557.4667797
4 (bet_car_9_c1)	-1557.8984349	-1556.992604	-1557.121879	-1558.3034074	-1557.397576	-1557.526851				-1558.2418654	-1557.336035	-1557.46531
5 (bet_car_9_c2)	-1557.8984162	-1557.992798	-1557.123538	-1558.3034142	-1558.397796	-1557.528536				-1558.2413085	-1558.33569	-1557.46643
6 (Bet_car_032)	-1557.8984118	-1556.992640	-1557.122112	-1558.3033821	-1557.3976103	-1557.5270823				-1558.2412838	-1557.335512	-1557.464984
7 (Bet_car_025)	-1557.8979024	-1556.992262	-1557.122451	-1558.3027853	-1557.3971449	-1557.5273339						
<i>15E,13Z</i>												
1 (bet_car_13)	-1557.9005545	-1556.995458	-1557.125460	-1558.3054658	-1557.400369	-1557.530371	-1556.558099	-1555.653002	-1555.783004	-1558.2422673	-1557.337171	-1557.467173
2 (Bet_car_030)	-1557.8999879	-1556.994927	-1557.125545	-1558.3047496	-1557.3996887	-1557.5303067				-1558.2419672	-1557.3369063	-1557.4675243
3 (Car_H_021)	-1557.8999723	-1556.994890	-1557.125617							-1558.2420157	-1557.3369334	-1557.4676604
4 (Car_H_002)	-1557.8995169	-1556.994335	-1557.123967	-1558.3041807	-1557.3989988	-1557.5286308				-1558.242015	-1557.3368331	-1557.4664651
5 (bet_car_13_c2)	-1557.898148	-1556.992423	-1557.121837	-1558.303124	-1557.397399	-1557.526813				-1558.2418731	-1557.336148	-1557.465562
6 (bet_car_13_c1)	-1557.898091	-1556.992631	-1557.123498	-1558.3030737	-1557.397613	-1557.528480				-1558.242305	-1557.336845	-1557.467712
7 (Bet_car_025)	-1557.897575	-1556.991889	-1557.121840	-1558.3024481	-1557.3967621	-1557.5267131				-1558.2421601	-1557.3364741	-1557.4664251
<i>15E,8Z</i>												
1 (bet_car_8)	-1557.8972008	-1556.992256	-1557.123007	-1558.3018731	-1557.396928	-1557.527679	-1556.554457	-1555.649512	-1555.780263	-1558.238605	-1557.33366	-1557.464411

2 (bet_car_030)	-1557.8967368	-1556.991864	-1557.123454							-1558.2381687	-1557.3332959	-1557.4648859
3 (Car_H_021)	-1557.8967038	-1556.991889	-1557.123275	-1558.3013358	-1557.396521	-1557.527907				-1558.2385135	-1557.3336987	-1557.4650847
4 (Car_H_002)	-1557.8961867	-1556.991298	-1557.122549	-1558.3006717	-1557.395783	-1557.527034				-1558.2383344	-1557.3334457	-1557.4646967
5 (Car_H_100)	-1557.8947013	-1556.989393	-1557.121115	-1558.2994089	-1557.394100	-1557.525822				-1558.2380256	-1557.332717	-1557.464439
6 (Bet_car_032)	-1557.8946717	-1556.989371	-1557.121132	-1558.2994173	-1557.3941166	-1557.5258776				-1558.2381569	-1557.3328562	-1557.4646172
7 (bet_car_025)	-1557.8941683	-1556.988982	-1557.122482	-1558.2988302	-1557.3936439	-1557.5271439				-1558.2378938	-1557.3327075	-1557.4662075
8 (bet_car_8_c1)	-1557.841619	-1556.988932	-1557.121576	-1558.2988966	-1557.393666	-1557.526310				-1558.2377293	-1557.332499	-1557.465143
9 (bet_car_8_c2)	-1557.8940349	-1556.988736	-1557.120170	-1558.2986657	-1557.393367	-1557.524801	-1556.550702	-1555.645404	-1555.776838	-1558.2384388	-1557.33314	-1557.464574
15E,12Z												
1 (car_H_150)	-1557.8967934	-1556.991895	-1557.123060	-1558.301448	-1557.39655	-1557.527715	-1556.553965	-1555.649067	-1555.780232	-1558.2384017	-1557.333503	-1557.464668
2 (bet_car_12)	-1557.8967881	-1556.991932	-1556.123207	-1558.3014445	-1557.396588	-1557.527863	-1556.554134	-1555.649277	-1554.780552	-1558.2380636	-1557.333208	-1557.464483
3 (Car_H_021)	-1557.8962508	-1556.991369	-1557.122755	-1558.3008397	-1557.3959579	-1557.5273439				-1558.2383255	-1557.3334437	-1557.4648297
4 (Bet_car_030)	-1557.8962188	-1556.991304	-1557.122829	-1558.3007733	-1557.3958585	-1557.5273835				-1558.2379609	-1557.3330461	-1557.4645711
5 (Car_H_101)	-1557.8961671	-1556.991164	-1557.122833	-1558.3007321	-1557.395729	-1557.527398	-1556.553082	-1555.648079	-1555.779748	-1558.2382173	-1557.3332142	-1557.4648832
6 (bet_car_12_c1)	-1557.8943718	-1556.989062	-1557.120738	-1558.2991462	-1557.393836	-1557.525512				-1558.2379828	-1557.332673	-1557.464349
7 (Car_H_002)	-1557.8943522	-1556.988983	-1557.121381	-1558.3001468	-1557.3947776	-1557.5271756				-1558.2382081	-1557.3328389	-1557.4652369
8 (bet_car_12_c2)	-1557.8941896	-1556.989028	-1557.122811	-1558.298972	-1557.393810	-1557.527593				-1558.2380587	-1557.332897	-1557.4666800
9 (Bet_car_025)	-1557.8937869	-1556.988309	-1557.119908	-1558.2984557	-1557.3929778	-1557.5245768				-1558.2379234	-1557.3324455	-1557.4640445
15E,10Z												
1 (bet_car_10)	-1557.8945234	-1556.989222	-1557.118930	-1558.2992933	-1557.3939900	-1557.5236990	-1556.552529	-1555.647227	-1555.776935	-1558.2355302	-1557.330229	-1557.459937
2 (Bet_car_030)	-1557.8941383	-1556.988842	-1557.119161	-1558.2988174	-1557.3935211	-1557.5238401				-1558.2364052	-1557.3311089	-1557.4614279
3 (Car_H_021)	-1557.8941266	-1556.988890	-1557.119408	-1558.2987418	-1557.3935052	-1557.5240232				-1558.2364960	-1557.3312594	-1557.4617774
4 (bet_car_10_c2)	-1557.8921207	-1556.986408	-1557.116506	-1558.2969436	-1557.391230	-1557.521328				-1558.2362812	-1557.330569	-1557.460667
5 (bet_car_10_c1)	-1557.8920789	-1556.986397	-1557.117190	-1558.2969365	-1557.39122	-1557.5220470				-1558.236222	-1557.33054	-1557.461333
6 (Car_H_002)	-1557.8920424	-1556.986450	-1557.117542	-1558.2981004	-1557.392508	-1557.5236000				-1558.2363475	-1557.3307551	-1557.4618471
7 (Bet_car_025)	-1557.8914499	-1556.985785	-1557.116767	-1558.2962314	-1557.3905665	-1557.5215485				-1558.2358819	-1557.330217	-1557.461199
15E,14Z												
1 (bet_car_14)	-1557.8947094	-1556.989462	-1557.119716	-1558.2994285	-1557.394181	-1557.5244350	-1556.552639	-1555.647391	-1555.777645	-1558.23644750	-1557.3312000	-1557.4614540
2 (Car_H_021)	-1557.8941741	-1556.988880	-1557.119031							-1558.23604460	-1557.3307505	-1557.4609015
3 (Bet_car_030)	-1557.8941264	-1556.988738	-1557.119134	-1558.2987191	-1557.3933307	-1557.5237267						
4 (Car_H_002)	-1557.8936434	-1556.988303	-1557.118317	-1558.298151	-1557.3928106	-1557.5228246				-1558.2363547	-1557.3310143	-1557.4610283

5 (Bet_car_032)	-1557.8923048	-1556.986455	-1557.116462	-1558.2971293	-1557.3912795	-1557.5212865				-1558.2362812	-1557.3304314	-1557.4604384
6 (bet_car_14_c2)	-1557.8922427	-1556.986495	-1557.116914	-1558.2970901	-1557.391342	-1557.521761				-1558.2359406	-1557.3301929	-1557.4606119
7 (bet_car_14_c1)	-1557.8922038	-1556.986565	-1557.118066	-1558.2970443	-1557.391405	-1557.522906				-1558.2358694	-1557.330122	-1557.460541
8 (Bet_car_025)	-1557.8916863	-1556.985904	-1557.116436	-1558.2963841	-1557.3906018	-1557.5211338				-1558.2355605	-1557.3297782	-1557.4603102
15E,11Z												
1 (bet_car_11)	-1557.8944081	-1556.988837	-1557.119508	-1558.2993213	-1557.3937500	-1557.5244210	-1556.552058	-1555.646486	-1555.777157	-1558.2366205	-1557.330383	-1557.459878
2 (Bet_car_030)	-1557.8939295	-1556.988270	-1557.117978	-1558.2987492	-1557.3930897	-1557.5227977				-1558.2369084	-1557.3312489	-1557.4609569
3 (Car_H_021)	-1557.8939041	-1556.988277	-1557.118062							-1558.2365941	-1557.330967	-1557.460752
4 (bet_car_11_c1)	-1557.8920463	-1556.985809	-1557.115304	-1558.2970689	-1557.390831	-1557.520326				-1558.2366514	-1557.330728	-1557.461864
5 (bet_car_11_c2)	-1557.8919713	-1556.986048	-1557.117184	-1558.2969875	-1557.391064	-1557.522200				-1558.236755	-1557.3308317	-1557.4619677
6 (bet_car_032)	-1551.8919548	-1556.985855	-1557.115899	-1558.2969439	-1557.3908441	-1557.5208881						
7 (Bet_car_025)	-1557.8915161	-1556.985480	-1557.115672	-1558.296436	-1557.3903999	-1557.5205919				-1558.2367988	-1557.3307627	-1557.4609547
15E,7Z												
1 (Bet_car_032)	-1557.8939423	-1556.988698	-1557.118086	-1558.2990333	-1557.393789	-1557.523177				-1558.2370914	-1557.3318471	-1557.4612351
2 (bet_car_7)	-1557.8939308	-1556.988711	-1557.118006	-1558.2990486	-1557.393828	-1557.523123	-1556.5532891	-1555.6480693	-1555.7773643	-1558.2368486	-1557.331239	-1557.461033
3 (Car_H_021)	-1557.8937933	-1556.988618	-1557.117657							-1558.2367144	-1557.3315391	-1557.4605781
4 (Bet_car_030)	-1557.8937777	-1556.988709	-1557.118524							-1558.2367976	-1557.3317289	-1557.4615439
5 (Car_H_002)	-1557.8931673	-1557.988201	-1557.118837	-1558.2981476	-1557.3931813	-1557.5238173				-1558.2366926	-1558.3317263	-1557.4623623
6 (bet_car_7_c1)	-1557.8914745	-1556.985865	-1557.115659	-1558.296654	-1557.391044	-1557.520838				-1558.2371683	-1557.3315588	-1557.4613528
7 (Bet_car_025)	-1557.8913763	-1556.985814	-1557.115366									
15E,9Z, 9'Z												
1 (bet_car_9_91)	-1557.8994457	-1556.994476	-1557.125089	-1558.3042588	-1557.3992890	-1557.5299020				-1558.2393412	-1557.3343715	-1557.4649845
2 (bet_car_030)	-1557.8989984	-1556.993769	-1557.123267	-1558.3036898	-1557.3984604	-1557.5279584				-1558.2390508	-1557.3338214	-1557.4633194
3 (Car_H_021)	-1557.8988732	-1556.993875	-1557.124395	-1558.3035153	-1557.3985171	-1557.5290371				-1558.2390845	-1557.3340863	-1557.4646063
4 (Car_H_002)	-1557.8985047	-1556.993312	-1557.123069	-1558.3030792	-1557.3978865	-1557.5276435						
5 (bet_car_9_91c1)	-1557.8970014	-1556.991334	-1557.121275	-1558.3019203	-1557.396252	-1557.526193				-1558.2385849	-1557.3329175	-1557.4628585
6 (Bet_car_032)	-1557.8969977	-1556.991412	-1557.121678	-1558.3018993	-1557.3963136	-1557.5265796				-1558.2385024	-1557.3329167	-1557.4631827
7 (bet_car_025)	-1557.8964726	-1556.990925	-1557.122122	-1558.3012476	-1557.3957000	-1557.526897				-1558.2384877	-1557.3329401	-1557.4641371

Table S6b: Boltzmann Averaged energy of the *15E* isomer and their rotamers of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15E</i>	-1557.401365	-1557.53167	-1557.338885	-1557.469281
<i>15E,9Z</i>	-1557.399814	-1557.530084	-1557.336167	-1557.466448
<i>15E,13Z</i>	-1557.399822	-1557.530042	-1557.336849	-1557.467361
<i>15E,8Z</i>	-1557.396377	-1557.527341	-1557.33329	-1557.465317
<i>15E,12Z</i>	-1557.396122	-1557.527497	-1557.33314	-1557.465729
<i>15E,10Z</i>	-1557.393492	-1557.523664	-1557.33082	-1557.461467
<i>15E,14Z</i>	-1557.393536	-1557.523778	-1557.330728	-1557.460914
<i>15E,11Z</i>	-1557.393245	-1557.52389	-1557.330892	-1557.461513
<i>15E,7Z</i>	-1557.393626	-1557.523431	-1557.331644	-1557.461702
<i>15E,9Z, 9'Z</i>	-1557.398681	-1557.529261	-1557.333878	-1557.464435

Table S7: Relative energy [kJ/mol] of the rotamers of *15E* isomer calculated with respect to the best *15E* isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB//B3LYP/6-31G(d)		Solvent/PCM/B3LYP/MB	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
<i>all-trans (15E)</i>						
1(bet car 030 004)	0.0	0.0	0.0	0.0	0.0	0.0
2 (bet car 030)	+1.4	+2.4	+1.6	+2.7	-0.9	+0.2
3 (Car H 021)	+1.4	+1.8	+1.7	+2.1	+0.7	+1.1
4 (Car H 002)	+2.8	+2.6	+3.3	+3.2	-0.02	-0.2
5 (bet car 001)	+7.3	+6.6	+7.2	+6.4	+0.4	-0.4
6 (bet car 007)	+8.0	+9.6	+7.9	+9.4	+0.8	+2.4
7 (bet car 032)	+7.7	+7.9	+7.6	+7.8	+0.7	+0.8
8 (bet car 025)	+8.9	+7.7	+9.1	+7.9	+0.7	-0.5
9 (Car H 045)	+15.5	+16.0	+15.0	+15.6	+2.5	+3.1
<i>15E,9Z</i>						
1 (bet car 9)	+3.8	+4.1	+4.1	+4.5	+7.1	+7.4
2 (Car H 021)	+5.0	+5.8	+5.5	+6.2	+6.8	+7.5
3 (Car H 002)	+6.5	+6.5	+7.3	+7.3	+6.8	+6.8
4 (bet car 9 c1)	+11.6	+14.5	+11.5	+14.5	+7.8	+10.7
5 (bet car 9 c2)	+11.1	+10.2	+10.9	+10.0	+8.7	+7.7
6 (Bet car 032)	+11.5	+13.9	+11.4	+13.9	+9.1	+11.5
7 (Bet car 025)	+12.5	+13.0	+12.7	+13.2		
<i>15E,13Z</i>						
1 (bet car 13)	+4.1	+5.1	+4.2	+5.2	+4.8	+5.8
2 (Bet car 030)	+5.5	+4.9	+5.9	+5.4	+5.5	+4.9
3 (Car H 021)	+5.6	+4.7			+5.4	+4.5
4 (Car H 002)	+7.0	+9.0	+7.8	+9.8	+5.7	+7.7
5 (bet car 13 c2)	+12.1	+14.6	+12.0	+14.6	+7.5	+10.0
6 (bet car 13 c1)	+11.5	+10.3	+11.4	+10.2	+5.6	+4.4
7 (Bet car 025)	+13.5	+14.6	+13.7	+14.8	+6.6	+7.8
<i>15E,8Z</i>						
1 (bet car 8)	+12.5	+11.6	+13.2	+12.3	+13.9	+13.0
2 (bet car 030)	+13.5	+10.4			+14.9	+11.8

3 (Car H 021)	+13.5	+10.8	+14.3	+11.7	+13.9	+11.3
4 (Car H 002)	+15.0	+12.8	+16.2	+13.9	+14.5	+12.3
5 (Car H 100)	+20.0	+16.5	+20.7	+17.2	+16.5	+12.9
6 (Bet car 032)	+20.1	+16.5	+20.6	+17.0	+16.1	+12.5
7 (bet car 025)	+21.1	+12.9	+21.9	+13.7	+16.5	+8.3
8 (bet_car_8_c1)	+21.2	+15.3	+21.8	+15.9	+17.0	+11.1
9 (bet car 8 c2)	+21.7	+19.0	+22.6	+19.8	+15.4	+12.6
15E,12Z						
1 (bet car 12)	+13.4	+11.4	+14.2	+12.2	+14.4	+12.4
2 (Car H 150)	+13.3	+11.0	+14.1		+15.2	+12.9
3 (Car H 021)	+14.8	+12.2	+15.8	+13.2	+14.6	+11.9
4 (Bet car 030)	+15.0	+12.0	+16.0	+13.1	+15.6	+12.6
5 (Car H 101)	+15.4	+12.0	+16.4	+13.0	+15.2	+11.8
6 (bet car 12 c1)	+20.9	+17.5	+21.4	+17.9	+16.6	+13.2
7 (Car H 002)	+21.1	+15.8	+18.9	+13.6	+16.1	+10.9
8 (bet car 12 c2)	+20.9	+12.1	+21.4	+12.5	+16.0	+7.1
9 (Bet car 025)	+22.9	+19.7	+23.6	+20.4	+17.2	+14.0
15E,10Z						
1 (bet car 10)	+20.5	+22.3	+20.9	+22.7	+23.0	+24.8
2 (Bet car 030)	+21.5	+21.6	+22.2	+22.4	+20.7	+20.9
3 (Car H 021)	+21.3	+21.0	+22.2	+21.9	+20.3	+19.9
4 (bet car 10 c2)	+27.8	+28.6	+28.2	+28.9	+22.1	+22.9
5 (bet car 10 c1)	+27.9	+26.8	+28.2	+27.1	+22.2	+21.1
6 (Car H 002)	+27.7	+25.9	+24.8	+23.0	+21.6	+19.8
7 (Bet car 025)	+29.5	+27.9	+29.9	+28.4	+23.0	+21.5
15E,14Z						
1 (bet car 14)	+19.8	+20.2	+20.4	+20.8	+20.5	+20.8
2 (Car H 021)	+21.4	+21.9			+21.6	+22.3
3 (Bet car 030)	+21.7	+21.7	+22.7	+22.7		
4 (Car H 002)	+22.9	+23.9	+24.0	+25.0	+20.9	+21.9
5 (Bet car 032)	+27.7	+28.7	+28.1	+29.1	+22.5	+23.5
6 (bet car 14 c2)	+27.6	+27.5	+27.9	+27.8	+23.1	+23.0
7 (bet car 14 c1)	+27.4	+24.5	+27.7	+24.8	+23.3	+23.2
8 (Bet_car_025)	+29.2	+28.8	+29.8	+29.5	+24.2	+23.8

15E,11Z						
1 (bet_car_11)	+21.5	+20.7	+21.6	+20.8	+22.6	+24.9
2 (Bet_car_030)	+22.9	+24.7	+23.3	+25.1	+20.3	+22.1
3 (Car_H_021)	+22.9	+24.5			+21.1	+22.7
4 (bet_car_11_c1)	+29.4	+31.8	+29.2	+31.6	+21.7	+19.7
5 (bet_car_11_c2)	+28.8	+26.8	+28.6	+26.7	+21.4	+19.5
6 (bet_car_032)	+29.3	+30.2	+29.2			
7 (Bet_car_025)	+30.3	+30.8	+30.4	+30.9	+21.6	+22.1
15E,7Z						
1 (Bet_car_032)	+21.8	+24.5	+21.5	+24.1	+18.7	+21.4
2 (bet_car_7)	+21.8	+24.7	+21.4	+24.3	+20.4	+21.9
3 (Car_H_021)	+22.0	+25.6			+19.6	+23.1
4 (Bet_car_030)	+21.8	+23.3			+19.1	+20.6
5 (Car_H_002)	+23.1	+22.5	+23.1	+22.4	+19.1	+18.4
6 (bet_car_7_c1)	+29.3	+30.8	+28.7	+30.3	+19.5	+21.1
7 (Bet_car_025)	+29.4	+31.6				
15E,9Z, 9'Z						
1 (bet_car_9_91)	+6.7	+6.0	+7.0	+6.5	+12.1	+11.5
2 (bet_car_030)	+8.5	+10.9	+9.2	+11.6	+13.6	+15.9
3 (Car_H_021)	+8.3	+7.9	+9.1	+8.7	+12.9	+12.5
4 (Car_H_002)	+9.7	+11.4	+10.7	+12.4		
5 (bet_car_9_91c1)	+14.9	+16.1	+15.0	+16.2	+15.9	+17.1
6 (Bet_car_032)	+14.7	+15.0	+14.8	+15.2	+15.9	+16.3
7 (bet_car_025)	+15.9	+13.9	+16.5	+14.4	+15.9	+13.8

Table S8a: Energetics (in Hartrees) of the conformers of *15Z* isomer of beta-carotene

Isomers	Gas phase									Water Solvent (PCM)		
	B3LYP/SB			B3LYP/MB			B2PLYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
<i>15,15'-cis</i>												
1 (bet_car_trans)	-1557.898231	-1556.992788	-1557.122594	-1558.303468	-1557.398025	-1557.527831				-1558.2410021	-1557.335559	-1557.465365
2 (Car_H_021_cis)	-1557.89763	-1556.992262	-1557.122754	-1558.3027484	-1557.39738	-1557.527872	-1556.555294	-1555.649926	-1555.780418	-1558.2404994	-1557.335131	-1557.465623
3 (Car_H_002_cis)	-1557.897055	-1556.991775	-1557.122696	-1558.3020556	-1557.396775	-1557.527696	-1556.554500	-1555.64922	-1555.780141	-1558.2400613	-1557.334781	-1557.465702
4 (Bet_car_001_cis)	-1557.8957571	-1556.989954	-1557.120282	-1558.3010843	-1557.395281	-1557.525609	-1556.553154	-1555.647351	-1555.777679	-1558.240645	-1557.334842	-1557.46517
5 (Bet_car_025_cis)	-1557.8951673	-1556.989432	-1557.120450	-1558.3003734	-1557.394638	-1557.525656	-1556.552343	-1555.646608	-1555.777626	-1558.2402214	-1557.334486	-1557.465504
<i>15Z,9Z</i>												
1 (bet_car_9_15)	-1557.896844	-1556.991539	-1557.121481	-1558.302018	-1557.396713	-1557.526655	-1556.555022	-1555.649717	-1555.779659	-1558.2380705	-1557.332766	-1557.462708
2 (Car_H_021_cis)	-1557.8963522	-1556.991002	-1557.120658	-1558.3014192	-1557.396069	-1557.525725						
3 (Car_H_002_cis)	-1557.8958402	-1556.990451	-1557.120090	-1558.3008125	-1557.3954233	-1557.5250623						
4 (bet_car_9_15_c1)	-1557.894364	-1556.988729	-1557.119620	-1558.2996546	-1557.394019	-1557.524910				-1558.2378207	-1557.332186	-1557.463077
5 (bet_car_9_15_c2)	-1557.8943018	-1556.988598	-1557.119407	-1558.2996217	-1557.393918	-1557.524727				-1558.2377473	-1557.332044	-1557.462853
6 (Bet_car_025_cis)	-1557.8938094	-1556.988104	-1557.119078	-1558.2990107	-1557.3933053	-1557.5242793						
<i>15Z,13Z</i>												
1 (bet_car_13_15)	-1557.8965185	-1556.991202	-1557.121799	-1558.3017000	-1557.3963840	-1557.5269810	-1556.554490	-1555.649173	-1555.779770	-1558.2390640	-1557.3337480	-1557.4643450
2 (Car_H_021_cis)	-1557.895989	-1556.990596	-1557.121083	-1558.3010424	-1557.3956494	-1557.5261364						
3 (Car_H_002_cis)	-1557.8954546	-1556.990185	-1557.120991	-1558.3004546	-1557.395185	-1557.525991						
4 (bet_car_13_15_c2)	-1557.8941415	-1556.988246	-1557.118617	-1558.2994447	-1557.393549	-1557.52392				-1558.238719	-1557.3328235	-1557.4631945
5 (bet_car_13_15_c1)	-1557.8940896	-1556.988358	-1557.118626	-1558.2993792	-1557.393648	-1557.523916				-1558.2386773	-1557.3329460	-1557.463214
6 (bet_car_025_cis)	-1557.8935489	-1556.987643	-1557.118792	-1558.298704	-1557.3927981	-1557.5239471				-1558.238893	-1557.3329871	-1557.4641361
<i>15Z,8Z</i>												
1 (bet_car_8_15_c2)	-1557.8932411	-1556.988073	-1557.118620	-1558.2982128	-1557.3930450	-1557.523592				-1558.2350672	-1557.329572	-1557.4614560
2 (Car_H_021_cis)	-1557.8926637	-1556.987532	-1557.118886	-1558.2974909	-1557.3923592	-1557.5237132				-1558.2348206	-1557.3296889	-1557.4610429
3 (Car_H_002_cis)	-1557.8921829	-1556.986989	-1557.117901	-1558.2970173	-1557.3918234	-1557.5227354				-1558.2343058	-1557.3291119	-1557.4600239
4 (bet_car_8_15_c1)	-1557.8902078	-1556.984713	-1557.116597	-1558.2953031	-1557.389808	-1557.521692				-1558.2340542	-1557.3285110	-1557.459625
5 (bet_car_8_15)	-1557.8900219	-1556.984610	-1557.116855	-1558.2950115	-1557.389599	-1557.521844	-1556.547379	-1555.641967	-1555.774212	-1558.2351633	-1557.3299950	-1557.460542
6 (Bet_car_025_cis)	-1557.8900112	-1556.984558	-1557.117275	-1558.2949798	-1557.3895266	-1557.5222436				-1558.2342094	-1557.3287562	-1557.4614732

15Z,12Z												
1 (car_H_101_cis)	-1557.8928335	-1556.987628	-1557.118260	-1558.2978270	-1557.3926210	-1557.523253				-1558.2341285	-1557.328573	-1557.460733
2 (bet_car_12_15)	-1557.8922032	-1556.987117	-1557.119805	-1558.2970486	-1557.3919620	-1557.524650	-1556.549928	-1555.644841	-1555.777529	-1558.2342743	-1557.329069	-1557.459701
3 (Car_H_002_cis)	-1557.8917164	-1556.986570	-1557.118763	-1558.2964843	-1557.3913379	-1557.5235309				-1558.2341819	-1557.3290355	-1557.4612285
4 (bet_car_12_15_c1)	-1557.8903803	-1556.984825	-1557.116985	-1558.2954386	-1557.3898830	-1557.522043				-1558.2342679	-1557.328661	-1557.460022
5 (bet_car_12_15_c2)	-1557.8903511	-1556.984744	-1557.116105	-1558.295434	-1557.3898260	-1557.521187				-1558.2339388	-1557.3283317	-1557.4596927
6 (Bet_car_025_cis)	-1557.8898151	-1556.984328	-1557.116770	-1558.2947719	-1557.3892848	-1557.5217268				-1558.2341747	-1557.3286876	-1557.4611296
15Z,10Z												
1 (bet_car_10_15)	-1557.8905464	-1556.985042	-1557.114614	-1558.2956721	-1557.390168	-1557.5197400	-1556.5491299	-1555.6436255	-1555.7731975			
2 (Car_H_021_cis)	-1557.8900932	-1556.984677	-1557.115038	-1558.2950124	-1557.3895962	-1557.5199572				-1558.2321287	-1557.3267125	-1557.4570735
3 (Car_H_002_cis)	-1557.8895593	-1556.984043	-1557.114341	-1558.2944003	-1557.388884	-1557.519182				-1558.2321028	-1557.3265865	-1557.4568845
4 (bet_car_10_15_c1)	-1557.8881138	-1556.982146	-1557.111947	-1558.2932794	-1557.387312	-1557.517113				-1558.2325422	-1557.3265744	-1557.4563754
5 (bet_car_10_15_c2)	-1557.8880938	-1556.982207	-1557.112541	-1558.2932839	-1557.387397	-1557.517731				-1558.2322797	-1557.326312	-1557.456113
6 (Bet_car_025_cis)	-1557.8875142	-1556.981646	-1557.112139	-1558.2925622	-1557.386694	-1557.517187						
15Z,11Z												
1 (bet_car_11_15)	-1557.8904225	-1556.984676	-1557.114429	-1558.2956716	-1557.389925	-1557.519678	-1556.5487378	-1555.6429913	-1555.7727443	-1558.2332267	-1557.327137	-1557.4579530
2 (Car_H_021_cis)	-1557.889849	-1556.984104	-1557.114255	-1558.294978	-1557.389233	-1557.519384				-1558.2330715	-1557.3273265	-1557.4574775
3 (Car_H_002_cis)	-1557.8893176	-1556.983607	-1557.114393	-1558.2943567	-1557.3886461	-1557.5194321						
4 (bet_Car_11_15_c2)	-1557.8879618	-1556.981729	-1557.112411	-1558.2933451	-1557.387112	-1557.517794				-1558.2331347	-1557.3269019	-1557.4575839
5 (bet_car_11_15_c1)	-1557.88793	-1556.981840	-1557.112656	-1558.2932847	-1557.387195	-1557.518011				-1558.2328011	-1557.326568	-1557.45725
6 (Bet_car_025_cis)	-1557.8874146	-1556.981227	-1557.112210	-1558.2926588	-1557.3864712	-1557.5174542				-1558.2329273	-1557.3267397	-1557.4577227
15Z,7Z												
1 (bet_car_7_5)	-1557.8898485	-1556.984581	-1557.114992	-1557.2953017	-1557.3900340	-1557.5204450	-1556.5498556	-1555.6445881	-1555.7749991	-1558.2339123	-1557.3280100	-1557.4584260
2 (Car_H_021_cis)	-1557.889314	-1556.983918	-1557.114731	-1558.2945831	-1557.3891871	-1557.5200001				-1558.2335185	-1557.3281225	-1557.4589355
3 (Car_H_002_cis)	-1557.8891344	-1556.983799	-1557.114814	-1558.2944501	-1557.3891147	-1557.5201297				-1558.2336419	-1557.3283065	-1557.4593215
4 (bet_car_7_15_c1)	-1557.8875066	-1556.981604	-1557.112020	-1558.2929952	-1557.387092	-1557.517508				-1558.2337428	-1557.3278402	-1557.4582562
5 (Bet_car_025_cis)	-1557.8873375	-1556.981550	-1557.111340	-1558.2928384	-1557.3870509	-1557.5168409				-1558.2338941	-1557.3281066	-1557.4578966

Table S8b: Boltzmann Averaged energy of the *15Z* isomer and their rotamers of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

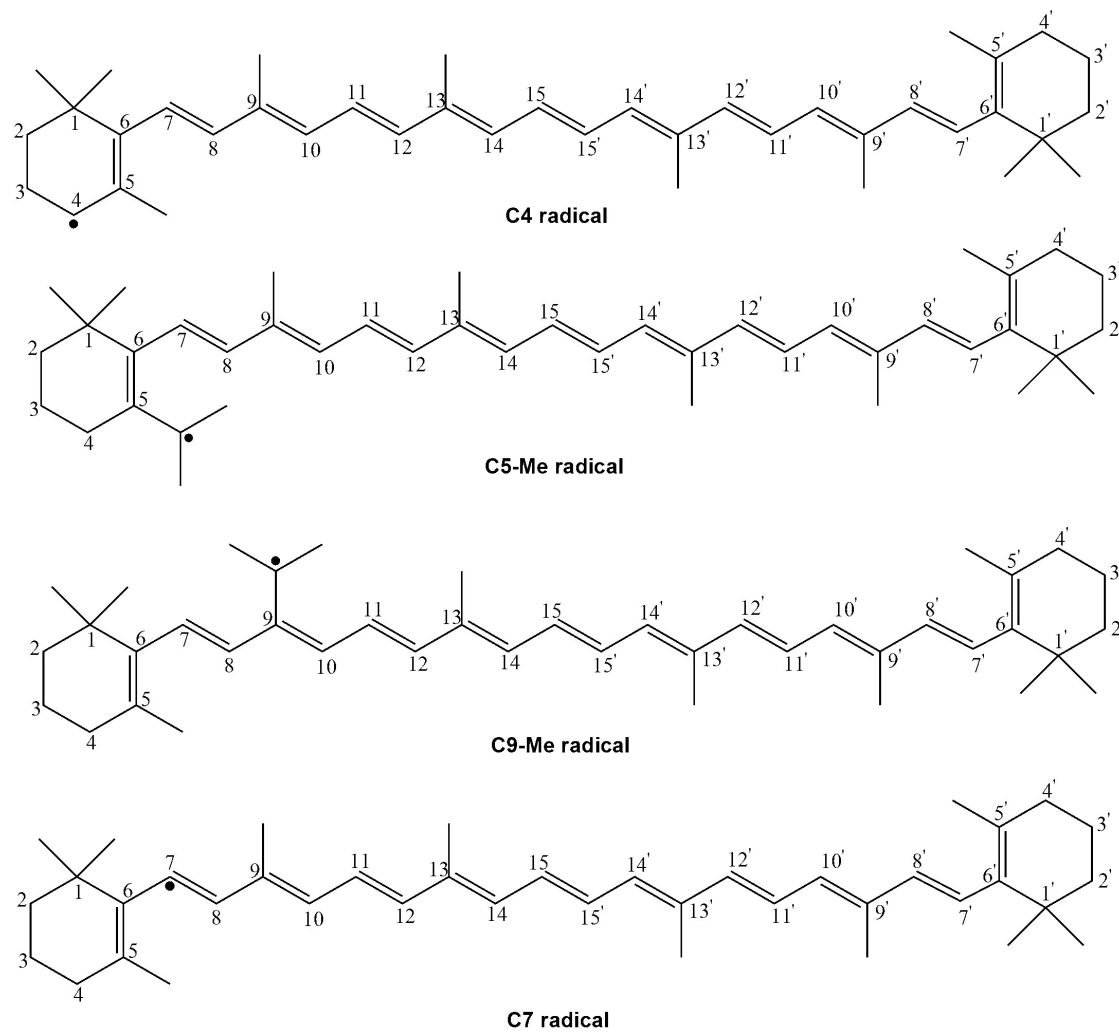
Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15Z</i>	-1557.397539	-1557.527669	-1557.335107	-1557.465509
<i>15Z,9Z</i>	-1557.396162	-1557.52595	-1557.332442	-1557.462904
<i>15Z,13Z</i>	-1557.395824	-1557.52642	-1557.33329	-1557.463991
<i>15Z,8Z</i>	-1557.392531	-1557.523247	-1557.329537	-1557.461112
<i>15Z,12Z</i>	-1557.392066	-1557.524023	-1557.328796	-1557.460811
<i>15Z,10Z</i>	-1557.389642	-1557.519541	-1557.326568	-1557.456759
<i>15Z,11Z</i>	-1557.389366	-1557.51928	-1557.327012	-1557.457656
<i>15Z,7Z</i>	-1557.389527	-1557.520149	-1557.328102	-1557.458835

Table S9: Relative energy [kJ/mol] of the rotamers of *15Z* isomer

Isomers	B3LYP/SB		B3LYP/MB		Solvent/PCM/B3LYP/MB	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
<i>15,15'-cis</i>						
1 (bet car trans)	+11.1	+12.6	+10.4	+11.9	+9.0	+10.5
2 (Car H 021 cis)	+12.5	+12.2	+12.0	+11.8	+10.1	+9.8
3 (Car H 002 cis)	+13.8	+12.4	+13.6	+12.3	+11.0	+9.7
4 (Bet car 001 cis)	+18.5	+18.7	+17.6	+17.7	+10.9	+11.1
5 (Bet car 025 cis)	+19.9	+18.3	+19.3	+17.6	+11.8	+10.2
<i>15Z,9Z</i>						
1 (bet car 9 15)	+14.4	+15.6	+13.8	+14.9	+16.3	+17.5
2 (Car H 021 cis)	+15.8	+17.7	+15.5	+17.4		
3 (Car H 002 cis)	+17.2	+19.2	+17.2	+19.2		
4 (bet car 9 15 c1)	+21.8	+20.5	+20.9	+19.6	+17.9	+16.5
5 (bet car 9 15 c2)	+22.1	+21.0	+21.1	+20.0	+18.2	+17.1
6 (Bet car 025 cis)	+23.4	+21.9	+22.7	+21.2		
<i>15Z,13Z</i>						
1 (bet car 13 15)	+15.3	+14.7	+14.7	+14.1	+13.8	+13.2
2 (Car H 021 cis)	+16.9	+16.6	+16.6	+16.4		
3 (Car H 002 cis)	+17.9	+16.8	+17.8	+16.7		
4 (bet car 13 15 c2)	+23.0	+23.1	+22.1	+22.2	+16.2	+16.2
5 (bet car 13 15 c1)	+22.7	+23.1	+21.8	+22.2	+15.9	+16.2
6 (bet car 025 cis)	+24.6	+22.6	+24.1	+22.1	+15.8	+13.8
<i>15Z,8Z</i>						
1 (bet car 8 15 c2)	+23.5	+23.1	+23.4	+23.0	+24.7	+20.8
2 (Car H 021 cis)	+24.9	+22.4	+25.2	+22.7	+24.4	+21.9
3 (Car H 002 cis)	+26.3	+24.9	+26.6	+25.3	+25.9	+24.6
4 (bet car 8 15 c1)	+32.3	+28.4	+31.9	+28.0	+27.5	+25.6
5 (bet car 8 15)	+32.6	+27.7	+32.5	+27.6	+23.6	+23.2
6 (Bet car 025 cis)	+32.7	+26.6	+32.7	+26.6	+26.9	+20.8
<i>15Z,12Z</i>						
1 (car H 101 cis)	+24.6	+24.0	+24.5	+23.9	+27.4	+22.7

2 (bet car 12 15)	+25.9	+19.9	+26.3	+20.3	+26.1	+25.4
3 (Car H 002 cis)	+27.4	+22.7	+27.9	+23.2	+26.1	+21.4
4 (bet car 12 15 c1)	+32.0	+27.4	+31.7	+27.1	+27.1	+24.6
5 (bet car 12 15 c2)	+32.2	+29.7	+31.9	+29.3	+27.9	+25.4
6 (Bet car 025 cis)	+33.3	+27.9	+33.3	+27.9	+27.1	+21.7
15Z,10Z						
1 (bet car 10 15)	+31.4	+33.6	+30.9	+33.2		
2 (Car H 021 cis)	+32.4	+32.5	+32.5	+32.6	+32.2	+32.3
3 (Car H 002 cis)	+34.1	+34.3	+34.4	+34.6	+32.6	+32.8
4 (bet car 10 15 c1)	+39.0	+40.6	+38.5	+40.0	+32.6	+34.1
5 (bet car 10 15 c2)	+38.9	+39.0	+38.3	+38.4	+33.3	+34.8
6 (Bet car 025 cis)	+40.4	+40.1	+40.1	+39.8		
15Z,11Z						
1 (bet car 11 15)	+32.4	+34.1	+31.6	+33.3	+31.1	+30.0
2 (Car H 021 cis)	+33.9	+34.5	+33.4	+34.1	+30.6	+31.2
3 (Car H 002 cis)	+35.2	+34.2	+34.9	+33.9		
4 (bet Car 11 15 c2)	+40.1	+39.4	+39.0	+38.3	+31.7	+30.9
5 (bet car 11 15 c1)	+39.8	+38.7	+38.8	+37.7	+32.6	+31.8
6 (Bet car 025 cis)	+41.5	+39.9	+40.7	+39.1	+32.2	+30.6
15Z,7Z						
1 (bet car 7 5)	+32.6	+32.6	+31.4	+31.3	+28.8	+28.8
2 (Car H 021 cis)	+34.4	+33.3	+33.6	+32.5	+28.5	+27.4
3 (Car H 002 cis)	+34.7	+33.1	+33.7	+32.1	+28.1	+26.4
4 (bet car 7 15 c1)	+40.5	+40.4	+39.1	+39.0	+29.3	+29.2
5 (Bet car 025 cis)	+40.6	+42.2	+39.2	+40.7	+28.6	+30.2

H-atom abstraction reactions



Scheme S6. Radicals formed from H-atom abstraction from various sites of beta-carotene.

Table S10a. Energetics [Hartrees] of the H-atom abstraction reactions (C4 radical) from *15E* isomer.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C4-radical									
<i>all-trans</i>									
1 (bet_car_030)	-1557.282701	-1556.391460	-1556.523256	-1557.6868092	-1556.7955682	-1556.9273642	-1557.6264566	-1556.7352156	-1556.8670116
2 (Car_H_021_002)	-1557.2824857	-1556.391061	-1556.522682	-1557.6864684	-1556.795044	-1556.926665	-1557.6266289	-1556.7352040	-1556.8668250
3 (Car_H_045_002)	-1557.2814887	-1556.389690	-1556.520893	-1557.6857192	-1556.793921	-1556.925124	-1557.6280917	-1556.7362930	-1556.8674960
4 (bet_car_007)	-1557.2809232	-1556.389086	-1556.520398	-1557.6851002	-1556.793263	-1556.924575	-1557.6269203	-1556.7350831	-1556.8663951
5 (bet_car_032)	-1557.2793401	-1556.387579	-1556.518652	-1557.6835045	-1556.7917434	-1556.9228164			
<i>15E,8Z</i>									
1(bet_car_8_c4_c1)	-1557.2819983	-1556.390581	-1556.521041	-1557.6860467	-1556.794629	-1556.925089	-1557.6260163	-1556.734599	-1556.8650590
2 (Car_H_021)	-1557.2814416	-1556.390096	-1556.521185	-1557.6854396	-1556.794094	-1556.925183	-1557.6250105	-1556.7336649	-1556.8647539
3 (bet_car_8_c4)	-1557.2814171	-1556.389992	-1556.520252	-1557.6854513	-1556.794026	-1556.924286	-1557.6247931	-1556.733368	-1556.8636280
4 (Car_H_002)	-1557.2809002	-1556.389534	-1556.520193	-1557.6848408	-1556.7934746	-1556.9241336	-1557.6245594	-1556.7331932	-1556.8638522
5 (Bet_car_032)	-1557.2793401	-1556.387579	-1556.518652	-1557.6835045	-1556.7917434	-1556.9228164	-1557.6247185	-1556.7329574	-1556.8640304
6 (bet_car_8_c4_c2)	-1557.2793185	-1556.387540	-1556.518923	-1557.6834715	-1556.791693	-1556.923076	-1557.6245956	-1556.732817	-1556.8642000
7 (Car_H_100_002)	-1557.2756488	-1556.384317	-1556.517012	-1557.679509	-1556.788178	-1556.920873	-1557.6204474	-1556.729116	-1556.8618110
<i>15E,12Z</i>									
1 (Bet_car_032)	-1557.2815492	-1556.390177	-1556.520824	-1557.6856052	-1556.7942330	-1556.924880			
2 (bet_car_12_c4_c1)	-1557.2814535	-1556.390082	-1556.521070	-1557.6855256	-1556.7941540	-1556.925142	-1557.6250947	-1556.7337232	-1556.8647112
3 (bet_car_12_c4)	-1557.2810703	-1556.389633	-1556.519886	-1557.6850926	-1556.7936550	-1556.923908	-1557.6241735	-1556.7327362	-1556.8629892
4 (Car_H_021)	-1557.2810447	-1556.389754	-1556.520883	-1557.6850594	-1556.7937687	-1556.9248977	-1557.6243916	-1556.7331009	-1556.8642299
5 (Bet_car_030)	-1557.2809887	-1556.389597	-1556.519898	-1557.6850346	-1556.7936429	-1556.9239439	-1557.6241522	-1556.7327605	-1556.8630615
6 (Car_H_002)	-1557.2805258	-1556.389033	-1556.519005	-1557.6844646	-1556.7929718	-1556.9229438	-1557.6240428	-1556.73255	-1556.862522
7 (Car_H_150_002)	-1557.2796896	-1556.388398	-1556.519317	-1557.6835233	-1556.792232	-1556.9231510	-1557.6229318	-1556.73164	-1556.862559
8 (Bet_car_025)	-1557.2788585	-1556.387133	-1556.518342	-1557.6830036	-1556.7912781	-1556.9224871	-1557.6240622	-1556.7323367	-1556.8635457
<i>15E,13Z</i>									
1 (bet_car_13_c2_c4)	-1557.280212	-1556.389262	-1556.521957	-1557.6841100	-1556.7931600	-1556.925855	-1557.6237173	-1556.7327673	-1556.8654623
2 (Bet_car_030)	-1557.2798557	-1556.388846	-1556.520778				-1557.6228400	-1556.7318303	-1556.8637623
3 (Car_H_021)	-1557.2794727	-1556.389074	-1556.517210	-1557.6832642	-1556.7928655	-1556.9210015	-1557.6230348	-1556.7326361	-1556.8607721

4 (Car_H_002)	-1557.2790163	-1556.387702	-1556.518925	-1557.6827264	-1556.7914121	-1556.9226351	-1557.6225535	-1556.7312392	-1556.8624622
5 (bet_car_13_c1_c4)	-1557.2772093	-1556.385503	-1556.516824	-1557.6811185	-1556.789412	-1556.920733	-1557.6226927	-1556.7309864	-1556.8623074
15E,9Z									
1 (bet_car_9_c4_c2)	-1557.2796833	-1556.388381	-1556.518367	-1557.6834405	-1556.7921380	-1556.9221240	-1557.6219909	-1556.7306890	-1556.8606750
2 (Car_H_021)	-1557.2789032	-1556.387708	-1556.518459	-1557.682561	-1556.7913658	-1556.9221168	-1557.6207015	-1556.7295063	-1556.8602573
3 (bet_car_9_c4)	-1557.2788963	-1556.387750	-1556.519204	-1557.6825629	-1556.791416	-1556.9228700	-1557.6207453	-1556.729599	-1556.8610530
4 (Car_H_002)	-1557.2783476	-1556.387202	-1556.519295	-1557.6819099	-1556.7907643	-1556.9228573	-1557.6207727	-1556.7296271	-1556.8617201
5 (bet_car_9_c4_c1)	-1557.2766345	-1556.385163	-1556.516377	-1557.6804236	-1556.788952	-1556.920166	-1557.6208917	-1556.7294202	-1556.8606342
15E,9Z,9'Z									
1 (bet_car_9_91_c4)	-1557.277466	-1556.386314	-1556.516507	-1557.6810361	-1556.7898841	-1556.9200771	-1557.6182217	-1556.7270697	-1556.8572627
2 (Car_H_021)	-1557.2774273	-1556.386182	-1556.516419	-1557.6810005	-1556.7897552	-1556.9199922	-1557.6183152	-1556.7270699	-1556.8573069
3 (Car_H_002)	-1557.2769156	-1556.385827	-1556.516555	-1557.680389	-1556.7893004	-1556.9200284	-1557.6182478	-1556.7271592	-1556.8578872
4 (Bet_car_030)	-1557.2768833	-1556.385685	-1556.516488	-1557.6803524	-1556.7891541	-1556.9199571	-1557.6183575	-1556.7271592	-1556.8579622
5 (Bet_car_032)	-1557.2750422	-1556.383372	-1556.513985	-1557.6787506	-1556.7870804	-1556.9176934	-1557.6176333	-1556.7259631	-1556.8565761
6 (bet_car_9_91c1_c4)	-1557.2750298	-1556.383513	-1556.514389	-1557.6787311	-1556.7872143	-1556.9180903			
15E,14Z									
1 (bet_car_14_c4_c1)	-1557.2768842	-1556.385052	-1556.515612	-1557.6808673	-1556.789412	-1556.920733	-1557.6211558	-1556.7293240	-1556.8598840
2 (bet_car_14_c4)	-1557.2763937	-1556.384497	-1556.514653	-1557.6803353	-1556.788438	-1556.918594	-1557.6201284	-1556.7282320	-1556.858388
3 (Car_H_002)	-1557.2758142	-1556.384113	-1556.515368	-1557.6796744	-1556.7879732	-1556.9192282	-1557.6197541	-1556.7280529	-1556.8593079
4 (bet_car_14_c4_c2)	-1557.2742467	-1556.382026	-1556.513322	-1557.6808673	-1556.79316	-1556.9258550	-1557.6200016	-1556.727781	-1556.859077
15E,10Z									
1 (bet_car_10_c4_c2)	-1557.2760003	-1556.384239	-1556.514451	-1557.6800339	-1556.7882730	-1556.9184850	-1557.6208257	-1556.7290644	-1556.8592764
2 (Bet_car_030)	-1557.2754367	-1556.383670	-1556.514080	-1557.6794645	-1556.7876978	-1556.9181078	-1557.6200083	-1556.7282416	-1556.8586516
3 (bet_car_10_c4)	-1557.2754356	-1556.383663	-1556.513612	-1557.6794346	-1556.787662	-1556.917611	-1557.6197097	-1556.7279371	-1556.8578861
4 (Car_H_021)	-1557.2754215	-1556.383708	-1556.514161	-1557.6794099	-1556.7876964	-1556.9181494	-1557.6197844	-1556.7280709	-1556.8585239
5 (Car_H_002)	-1557.2748783	-1556.383159	-1556.513657	-1557.6787985	-1556.7870792	-1556.9175772	-1557.6195522	-1556.7278329	-1556.8583309
6 (bet_car_10_c4_c1)	-1557.2731498	-1556.381116	-1556.512456	-1557.6772805	-1556.785247	-1556.916587			
15E,11Z									
1 (bet_car_11_c4)	-1557.2757386	-1556.384006	-1556.514300	-1557.6796527	-1556.787920	-1556.918214	-1557.6195333	-1556.7278007	-1556.8580947
2 (bet_car_11_c1_c4)	-1557.2735424	-1556.381435	-1556.511881	-1557.677575	-1556.785467	-1556.915913	-1557.6195535	-1556.7274461	-1556.8578921
15E,7Z									

1 (Car_H_021)	-1557.2749053	-1556.384013	-1556.514577	-1557.6790855	-1556.7881932	-1556.9187572	-1557.6170483	-1556.726156	-1556.85672
2 (Car_H_002)	-1557.2743642	-1556.383411	-1556.514323	-1557.6784321	-1556.7874789	-1556.9183909			
3 (bet_car_7)	-1557.2713877	-1556.380690	-1556.513054	-1557.6754388	-1556.784741	-1556.917105	-1557.6136712	-1556.722974	-1556.855338
4 (bet_car_7_c4_c1)	-1557.269384	-1556.378183	-1556.508833				-1557.6140143	-1556.722813	-1556.853463
Bet_car	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509
H2O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362

Table S10b: Boltzmann Averaged energy of the *15E* isomer and their rotamers of C4 radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15E</i>	-1556.795107	-1556.92692	-1556.735758	-1556.867095
<i>15E,8Z</i>	-1556.794132	-1556.924743	-1556.733884	-1556.864502
<i>15E,12Z</i>	-1556.793815	-1556.924644	-1556.733058	-1556.86404
<i>15E,13Z</i>	-1556.792866	-1556.925705	-1556.732368	-1556.865022
<i>15E,9Z</i>	-1556.791629	-1556.922584	-1556.730068	-1556.861155
<i>15E,9Z,9'Z</i>	-1556.789527	-1556.919909	-1556.727037	-1556.857627
<i>15E,14Z</i>	-1556.79304	-1556.925823	-1556.728773	-1556.859441
<i>15E,10Z</i>	-1556.787794	-1556.918048	-1556.728481	-1556.858759
<i>15E,11Z</i>	-1556.78775	-1556.918029	-1556.727656	-1556.858004
<i>15E,7Z</i>	-1556.78791	-1556.918468	-1556.7229	-1556.855112

Table S11a. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C4 radical) from *15E* isomer (Conformational Mobility)

Isomers	B3LYP/SB		B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C4-radical						
<i>all-trans</i>						
1 (bet car 030)	-174.9	-181.7	-200.4	-207.2	-214.5	-221.4
2 (Car H 021 002)	-173.9	-180.2	-198.9	-205.4	-214.5	-220.9
3 (Car H 045 002)	-170.3	-175.5	-196.0	-201.3	-217.3	-222.6
4 (bet car 007)	-168.7	-174.2	-194.3	-199.9	-214.2	-219.7
5 (bet car 032)	-164.7	-169.6	-190.3	-195.3		
<i>15E,8Z</i>						
1(bet car 8 c4 c1)	-172.6	-175.9	-197.9	-201.2	-212.9	-216.2
2 (Car H 021)	-171.3	-176.3	-196.5	-201.5	-210.5	-215.4
3 (bet car 8 c4)	-171.0	-173.8	-196.3	-199.1	-209.7	-212.5
4 (Car H 002)	-169.8	-173.7	-194.9	-198.7	-209.2	-213.1
5 (Bet car 032)	-164.7	-169.6	-190.3	-195.3	-208.6	-213.5
6 (bet car 8 c4 c2)	-164.6	-170.4	-190.2	-195.9	-208.2	-213.9
7 (Car H 100 002)	-156.2	-165.4	-180.9	-190.2	-198.5	-207.7
<i>15E,12Z</i>						
1 (Bet car 032)	-171.5	-175.4	-196.8	-200.7		
2 (bet car 12 c4 c1)	-171.3	-176.0	-196.6	-201.4	-210.6	-215.3
3 (bet car 12 c4)	-170.1	-172.9	-195.3	-198.1	-208.0	-210.8
4 (Car H 021)	-170.4	-175.5	-195.6	-200.7	-208.9	-214.1
5 (Bet car 030)	-170.0	-172.9	-195.3	-198.2	-208.1	-210.9
6 (Car H 002)	-168.5	-170.6	-193.5	-195.6	-207.5	-209.6
7 (Car H 150 002)	-166.9	-171.4	-191.6	-196.1	-205.1	-209.7
8 (Bet car 025)	-163.5	-168.8	-189.1	-194.4	-206.9	-212.3
<i>15E,13Z</i>						
1 (bet car 13 c2 c4)	-169.1	-178.3	-194.0	-203.2	-208.1	-217.3
2 (Bet car 030)	-168.0	-175.2			-205.6	-212.8
3 (Car H 021)	-168.6	-165.9	-193.3	-190.5	-207.7	-204.9
4 (Car H 002)	-165.0	-170.4	-189.4	-194.8	-204.1	-209.4

5 (bet_car 13 c1 c4)	-159.3	-164.8	-184.2	-189.8	-203.4	-209.0
15E,9Z						
1 (bet_car 9 c4 c2)	-166.8	-168.9	-191.4	-193.4	-202.6	-204.7
2 (Car_H 021)	-165.0	-169.2	-189.3	-193.4	-199.5	-203.6
3 (bet_car 9 c4)	-165.2	-171.1	-189.4	-195.4	-199.8	-205.7
4 (Car_H 002)	-163.7	-171.3	-187.7	-195.4	-199.8	-207.5
5 (bet_car 9 c4 c1)	-158.4	-163.7	-182.9	-188.3	-199.3	-204.6
15E,9Z,9'Z						
1 (bet_car 9 91 c4)	-161.4	-164.0	-185.4	-188.1	-193.1	-195.8
2 (Car_H 021)	-161.0	-163.8	-185.1	-187.8	-193.1	-195.9
3 (Car_H 002)	-160.1	-164.1	-183.9	-187.9	-193.4	-197.4
4 (Bet_car 030)	-159.7	-163.9	-183.5	-187.7	-193.4	-197.6
5 (Bet_car 032)	-153.7	-157.4	-178.1	-181.8	-190.2	-193.9
6 (bet_car 9 91c1 c4)	-154.0	-158.5	-178.4	-182.8		
15E,14Z						
1 (bet_car 14 c4 c1)	-158.1	-161.7	-184.2	-189.8	-199.1	-202.6
2 (bet_car 14 c4)	-156.6	-159.2	-181.6	-184.2	-196.2	-198.7
3 (Car_H 002)	-155.6	-161.0	-180.4	-185.8	-195.7	-201.1
4 (bet_car 14 c4 c2)	-150.1	-155.7	-194.0	-203.2	-195.0	-200.5
15E,10Z						
1 (bet_car 10 c4 c2)	-155.9	-158.6	-181.2	-183.9	-198.4	-201.1
2 (Bet_car 030)	-154.4	-157.6	-179.7	-182.9	-196.2	-199.4
3 (bet_car 10 c4)	-154.4	-156.4	-179.6	-181.6	-195.4	-197.4
4 (Car_H 021)	-154.5	-157.9	-179.7	-183.0	-195.8	-199.1
5 (Car_H 002)	-153.1	-156.5	-178.1	-181.5	-195.1	-198.6
6 (bet_car 10 c4 c1)	-147.7	-153.4	-173.3	-178.9		
15E,11Z						
1 (bet_car 11 c4)	-155.3	-158.2	-180.3	-183.2	-195.1	-197.9
2 (bet_car 11 c1 c4)	-148.6	-151.9	-173.8	-177.1	-194.1	-197.4
15E,7Z						
1 (Car_H 021)	-155.4	-158.9	-180.9	-184.6		
2 (Car_H 002)	-153.8	-158.3	-179.1	-183.6		
3 (bet_car 7)	-146.6	-154.9	-171.9	-180.3	-182.4	-190.7
4 (bet_car 7 c4 c1)	-140.0	-143.9			-181.9	-185.8

Table S11b. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C4 radical) calculated with respect to the best isomer (Conformational restriction)

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C4-radical				
15E	-200.4	-207.2	-216.5	-222.2
15E,8Z	-211.1	-213.2	-226.8	-224.6
15E,12Z	-210.9	-210.0	-225.0	-222.4
15E,13Z	-198.2	-208.5	-212.9	-221.7
15E,9Z	-195.5	-199.9	-209.4	-214.3
15E,9Z,9'Z	-192.5	-194.5	-205.5	-209.2
15E,14Z	-204.6	-224.0	-219.5	-223.5
15E,10Z	-202.2	-205.8	-218.7	-220.8
15E,11Z	-201.9	-204.0	-215.4	-217.4
15E,7Z	-202.4	-207.0	-201.1	-209.1

Table S11c. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C4 radical) calculated with respect to the Boltzmann Averaging of the conformers.

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C4-radical				
<i>15E</i>	-200.7	-207.9	-216.2	-221.9
<i>15E,8Z</i>	-211.3	-213.5	-226.0	-225.5
<i>15E,12Z</i>	-211.1	-212.8	-224.2	-223.2
<i>15E,13Z</i>	-198.9	-208.9	-212.7	-221.5
<i>15E,9Z</i>	-195.7	-200.6	-208.4	-213.7
<i>15E,9Z,9'Z</i>	-193.1	-195.8	-206.5	-209.7
<i>15E,14Z</i>	-215.9	-225.7	-219.3	-223.7
<i>15E,10Z</i>	-202.2	-205.6	-218.3	-220.5
<i>15E,11Z</i>	-202.7	-204.9	-215.9	-218.4
<i>15E,7Z</i>	-202.2	-207.3	-201.5	-210.3

Table S12a. Energetics [Hartrees] of the H-atom abstraction reactions (C4 radical) from *15Z* isomer.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C4-radical									
<i>15,15'</i>-cis (<i>15Z</i>)									
1 (bet_car_trans)	-1557.2783646	-1556.386851	-1556.518587	-1557.6825987	-1556.7910851	-1556.9228211	-1557.6226793	-1556.7311657	-1556.8629017
2 (car_H_002_cis)	-1557.2774338	-1556.385930	-1556.518217	-1557.6815479	-1556.7900441	-1556.9223311	-1557.6216751	-1556.7301713	-1556.8624583
3 (bet_cis_002)	-1557.2761286	-1556.384347	-1556.516750	-1557.6804229	-1556.7886413	-1556.9210443	-1557.6228064	-1556.7310248	-1556.8634278
<i>15Z,8Z</i>									
1 (bet_car_8_15_c4_c1)	-1557.2771948	-1556.385749	-1556.517055	-1557.6813560	-1556.7899100	-1556.921216	-1557.6214371	-1556.729991	-1556.861297
2 (bet_car_8_15_c4)	-1557.2767005	-1556.385263	-1556.516147	-1557.6808495	-1556.7894120	-1556.920296	-1557.6204084	-1556.728971	-1556.859855
3 (Bet_car_025_cis)	-1557.2765798	-1556.385195	-1556.517220	-1557.6806035	-1556.7892187	-1556.9212437	-1557.6209918	-1556.729607	-1556.861632
4 (Car_H_021_cis)	-1557.2760943	-1556.384717	-1556.516105	-1557.6801035	-1556.7887262	-1556.9201142	-1557.6198028	-1556.7284255	-1556.8598135
5 (Car_H_002_cis)	-1557.276082	-1556.384739	-1556.516167	-1557.6801238	-1556.7887808	-1556.9202088	-1557.6198586	-1556.7285156	-1556.8599436
6 (bet_car_8_15_c4_c2)	-1557.2744891	-1556.382722	-1556.514393	-1557.6786988	-1556.7869310	-1556.918602	-1557.6202459	-1556.728479	-1556.86015
<i>15Z,12Z</i>									
1 (bet_car_12_15_c4_c1)	-1557.2766867	-1556.385203	-1556.515852	-1557.6807839	-1556.786295	-1556.916785	-1557.6203973	-1556.7289136	-1556.8595626
2 (bet_car_12_15_c4)	-1557.2761921	-1556.384641	-1556.515502	-1557.6802763	-1556.788725	-1556.919586	-1557.6192353	-1556.7276842	-1556.8585452
3 (Bet_car_025_cis)	-1557.2761119	-1556.384628	-1556.515597	-1557.6806035	-1556.7891196	-1556.9200886	-1557.6201108	-1556.7286269	-1556.8595959
4 (Car_H_002_cis)	-1557.275677	-1556.384097	-1556.514415	-1557.6801238	-1556.7885438	-1556.9188618	-1557.619114	-1556.727534	-1556.857852
5 (bet_car_12_15_c4_c2)	-1557.274067	-1556.382135	-1556.512625	-1557.6782272	-1556.786295	-1556.916785	-1557.6192804	-1556.7273484	-1556.8578384
<i>15Z,9Z</i>									
1 (bet_car_9_15_c4_c2)	-1557.2751799	-1556.383958	-1556.515303	-1557.6792361	-1556.788014	-1556.919359	-1557.6182249	-1556.7270030	-1556.8583480
2 (Bet_car_025_cis)	-1557.2746862	-1556.383402	-1556.514525	-1557.6786196	-1556.7873354	-1556.9184584	-1557.6181513	-1556.7268671	-1556.8579901
3 (bet_car_9_15_c4)	-1557.2744049	-1556.383199	-1556.514843	-1557.6783214	-1556.787116	-1556.91876	-1557.6170516	-1556.725846	-1556.85749
4 (Car_H_002_cis)	-1557.2739287	-1556.382629	-1556.513798	-1557.677742	-1556.7864423	-1556.9176113	-1557.6170803	-1556.7257806	-1556.8569496
5 (bet_car_9_15_c4_c1)	-1557.2720297	-1556.380380	-1556.512524	-1557.6760116	-1556.784362	-1556.916506	-1557.6171766	-1556.725527	-1556.857671
<i>15Z,13Z</i>									
1 (Bet_car_025_cis)	-1557.2752468	-1556.383804	-1556.515478	-1557.6792507	-1556.7878079	-1556.9194819	-1557.619905	-1556.7284622	-1556.8601362
2 (bet_car_13_15_c4)	-1557.2750416	-1556.383437	-1556.514545	-1557.6790858	-1556.787481	-1556.918589	-1557.6186689	-1556.7270643	-1556.8581723

3 (Car_H_002_cis)	-1557.2745022	-1556.382982	-1556.514280	-1557.6784529	-1556.7869327	-1556.9182307	-1557.618559	-1556.7270388	-1556.8583368
4 (bet_car_13_15_c4_c1)	-1557.2726132	-1556.380683	-1556.512252	-1557.6767622	-1556.784832	-1556.916401	-1557.6187058	-1556.7267756	-1556.8583446
5 (bet_car_13_15_c4_c2)	-1557.2630249	-1556.371786	-1556.504100				-1557.6072282	-1556.715989	-1556.848303
15Z,11Z									
1 (bet_car_11_15_c4_c2)	-1557.2715788	-1556.379802	-1556.510964	-1557.6757631	-1556.7839860	-1556.9151480	-1557.6163343	-1556.7245575	-1556.8557195
2 (Bet_car_025_cis)	-1557.2710301	-1556.379280	-1556.510618	-1557.6750912	-1556.7833411	-1556.9146791	-1557.6159595	-1556.7242094	-1556.8555474
3 (bet_car_11_15_c4)	-1557.271013	-1556.379147	-1556.509406	-1557.6751092	-1556.783243	-1556.913502	-1557.6150382	-1556.7231722	-1556.8534312
4 (bet_car_11_15_c4_c1)	-1557.2687559	-1556.376383	-1556.506608	-1557.6729066	-1556.780534	-1556.910759	-1557.6149338	-1556.7225609	-1556.8527859
15Z,10Z									
1 (bet_car_10_15_c4_c2)	-1557.2713965	-1556.379519	-1556.511331	-1557.6755916	-1556.783714	-1556.915526	-1557.6208257	-1556.7289482	-1556.8607602
2 (Bet_car_025_cis)	-1557.2708129	-1556.378954	-1556.510655	-1557.6748895	-1556.7830306	-1556.9147316	-1557.6158946	-1556.7240357	-1556.8557367
3 (bet_car_10_15_c4)	-1557.2708098	-1556.378802	-1556.508675	-1557.6749874	-1556.78298	-1556.912853	-1557.6149835	-1556.722976	-1556.852849
4 (Car_H_021_cis)	-1557.2702289	-1556.378254	-1556.508474	-1557.6742855	-1556.7823106	-1556.9125306			
5 (Car_H_002_cis)	-1557.2701727	-1556.378256	-1556.510902	-1557.6742104	-1556.7822937	-1556.9149397	-1557.6146836	-1556.7227669	-1556.8554129
6 (bet_car_10_15_c4_c1)	-1557.2685136	-1556.376190	-1556.506528	-1557.6727906	-1556.780467	-1556.910805	-1557.6148844	-1556.7225608	-1556.8528988
15Z,7Z									
1 (Bet_car_025_cis)	-1557.2680016	-1556.376478	-1556.507118	-1557.6723914	-1556.7808678	-1556.9115078	-1557.6129883	-1556.7214647	-1556.8521047
2 (bet_car_7_15_c4)	-1557.2666336	-1556.375720	-1556.506527	-1557.6708256	-1556.779912	-1556.910719	-1557.6095642	-1556.718651	-1556.849458
Bet_car (closed shell)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509
H ₂ O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362

Table S12b: Boltzmann Averaged energy of the *15Z* isomer and their rotamers of C4 radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15Z</i>	-1556.790709	-1556.922499	-1556.730954	-1556.863092
<i>15Z,8Z</i>	-1556.78938	-1556.920841	-1556.72941	-1556.861059
<i>15Z,12Z</i>	-1556.788748	-1556.919657	-1556.728435	-1556.859241
<i>15Z,9Z</i>	-1556.78751	-1556.918851	-1556.726586	-1556.857906
<i>15Z,13Z</i>	-1556.78748	-1556.919011	-1556.726977	-1556.858291
<i>15Z,11Z</i>	-1556.783607	-1556.914805	-1556.724166	-1556.855477
<i>15Z,10Z</i>	-1556.783134	-1556.915058	-1556.728895	-1556.860714
<i>15Z,7Z</i>	-1556.780613	-1556.911269	-1556.721329	-1556.851954

Table S13a. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C4 radical) from *15Z* isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C4-radical						
<i>15,15'-cis (15Z)</i>						
1 (bet car trans)	-162.8	-169.5	-188.6	-195.3	-203.9	-210.6
2 (car H 002 cis)	-160.4	-168.5	-185.8	-193.9	-201.3	-209.4
3 (bet cis 002)	-156.2	-164.7	-182.2	-190.6	-203.5	-211.9
<i>15Z,8Z</i>						
1 (bet car 8 15 c4 c1)	-159.9	-165.5	-185.5	-191.1	-200.8	-206.4
2 (bet car 8 15 c4)	-158.6	-163.1	-184.2	-188.6	-198.1	-202.6
3 (Bet car 025 cis)	-158.4	-165.9	-183.7	-191.1	-199.8	-207.2
4 (Car H 021 cis)	-157.2	-162.9	-182.4	-188.2	-196.7	-202.5
5 (Car H 002 cis)	-157.3	-163.1	-182.5	-188.4	-196.9	-202.8
6 (bet car 8 15 c4 c2)	-151.9	-158.5	-177.7	-184.2	-196.8	-203.4
<i>15Z,12Z</i>						
1 (bet car 12 15 c4 c1)	-158.5	-162.3	-176.0	-179.4	-197.9	-201.8
2 (bet car 12 15 c4)	-157.0	-161.4	-182.4	-186.8	-194.7	-199.1
3 (Bet car 025 cis)	-156.9	-161.6	-183.4	-188.1	-197.2	-201.9
4 (Car H 002 cis)	-155.6	-158.5	-181.9	-184.9	-194.4	-197.3
5 (bet car 12 15 c4 c2)	-150.4	-153.8	-176.0	-179.4	-193.9	-197.3
<i>15Z,9Z</i>						
1 (bet car 9 15 c4 c2)	-155.2	-160.9	-180.5	-186.2	-192.9	-198.6
2 (Bet car 025 cis)	-153.7	-158.8	-178.7	-183.8	-192.6	-197.7
3 (bet car 9 15 c4)	-153.2	-159.6	-178.2	-184.6	-189.9	-196.4
4 (Car H 002 cis)	-151.7	-156.9	-176.4	-181.6	-189.7	-194.9
5 (bet car 9 15 c4 c1)	-145.8	-153.6	-170.9	-178.7	-189.1	-196.8
<i>15Z,13Z</i>						
1 (Bet car 025 cis)	-154.8	-161.3	-179.9	-186.5		
2 (bet car 13 15 c4)	-153.8	-158.9	-179.1	-184.1	-193.1	-198.2
3 (Car H 002 cis)	-152.6	-158.2	-177.7	-183.2	-193.1	-198.6
4 (bet car 13 15 c4 c1)	-146.6	-152.8	-172.2	-178.4	-192.4	-198.6
5 (bet car 13 15 c4 c2)	-123.2	-131.4			-164.0	-172.2

<i>15Z,11Z</i>						
1 (bet car 11 15 c4 c2)	-144.3	-149.5	-169.9	-175.1	-186.5	-191.7
2 (Bet car 025 cis)	-142.9	-148.6	-168.3	-173.9	-185.6	-191.3
3 (bet car 11 15 c4)	-142.6	-145.4	-168.0	-170.8	-182.9	-185.7
4 (bet car 11 15 c4 c1)	-135.3	-138.0	-160.9	-163.6	-181.3	-184.0
<i>15Z,10Z</i>						
1 (bet car 10 15 c4 c2)	-143.5	-150.4	-169.2	-176.1	-198.1	-204.9
2 (Bet car 025 cis)	-142.1	-148.7	-167.4	-174.0	-185.2	-191.8
3 (bet car 10 15 c4)	-141.7	-143.5	-167.3	-169.1	-182.4	-184.2
4 (Car H 021 cis)	-140.2	-142.9	-165.5	-168.2		
5 (Car H 002 cis)	-140.2	-149.3	-165.5	-174.6	-181.8	-190.9
6 (bet car 10 15 c4 c1)	-134.8	-137.8	-160.7	-163.7	-181.3	-184.3
<i>15Z,7Z</i>						
1 (Bet car 025 cis)	-135.6	-139.4	-161.7	-165.6	-178.4	-182.2
2 (bet car 7 15 c4)	-133.6	-137.8	-159.3	-163.5	-171.0	-175.3

Table S13b. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C4 radical) from *15Z* isomer (Conformational Restriction).

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C4-radical				
<i>15Z</i>	-198.9	-207.1	-212.9	-221.6
<i>15Z,8Z</i>	-208.9	-213.8	-224.4	-228.0
<i>15Z,12Z</i>	-207.9	-208.3	-224.0	-223.3
<i>15Z,9Z</i>	-194.3	-201.2	-209.3	-215.2
<i>15Z,13Z</i>	-194.6	-200.6	-206.9	-211.8
<i>15Z,11Z</i>	-201.6	-208.4	-217.2	-221.7
<i>15Z,10Z</i>	-200.2	-208.7	-230.6	-237.3
<i>15Z,7Z</i>	-193.1	-196.8	-206.5	-208.6

Table S13c. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C4 radical) from *15Z* isomer obtained by Boltzmann averaging of the conformers

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C4-radical				
<i>15Z</i>	-199.2	-206.8	-213.5	-221.2
<i>15Z,8Z</i>	-208.9	-214.0	-224.1	-227.5
<i>15Z,12Z</i>	-208.5	-208.9	-223.5	-223.5
<i>15Z,9Z</i>	-194.5	-201.7	-209.1	-214.5
<i>15Z,13Z</i>	-195.3	-200.9	-207.9	-212.6
<i>15Z,11Z</i>	-202.1	-208.6	-217.0	-221.9
<i>15Z,10Z</i>	-200.1	-208.6	-230.6	-238.0
<i>15Z,7Z</i>	-193.8	-197.0	-206.7	-209.5

Table S14a. Energetics [Hartrees] of the H-atom abstraction reactions (C5Me radical) from *15E* isomer.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C5-Me-radical									
<i>all-trans (15E)</i>									
1 (Car_H_021)	-1557.280049	-1556.388696	-1556.518950	-1557.6847852	-1556.7934322	-1556.9236862	-1557.6232856	-1556.7319326	-1556.8621866
2 (bet_car_030_004)	-1557.2746772	-1556.383755	-1556.515349	-1557.6794849	-1556.7885627	-1556.9201567	-1557.6179065	-1556.7269843	-1556.8585783
3 (Bet_car_030)	-1557.2740782	-1556.383057	-1556.514709	-1557.6787671	-1556.7877459	-1556.9193979	-1557.6176532	-1556.726632	-1556.858284
4 (bet_car_007)	-1557.2725593	-1556.381130	-1556.512972	-1557.6775118	-1556.7860825	-1556.9179245	-1557.6178159	-1556.7263866	-1556.8582286
5 (Car_H_045_001)	-1557.2710669	-1556.379055	-1556.509886	-1557.6760134	-1556.784002	-1556.914833	-1557.6169839	-1556.724972	-1556.855803
<i>15E,8Z</i>									
1 (Bet_car_030)	-1557.2787885	-1556.387467	-1556.517240	-1557.6835702	-1556.7922487	-1556.9220217	-1557.6215871	-1556.7302656	-1556.8600386
2 (Car_H_021)	-1557.2787423	-1556.387399	-1556.517184	-1557.6834771	-1556.7921338	-1556.9219188			
3 (Car_H_002)	-1557.2781852	-1556.386808	-1556.517014	-1557.6828594	-1556.7914822	-1556.9216882	-1557.6214115	-1556.7300343	-1556.8602403
4 (Bet_car_025)	-1557.2766399	-1556.384877	-1556.515198	-1557.6815163	-1556.7897534	-1556.9200744			
5 (bet_car_8_c5m)	-1557.2727048	-1556.382740	-1556.511864	-1557.6774611	-1556.787496	-1556.91662	-1557.6156081	-1556.725643	-1556.854767
6 (bet_car_8_c5m_c1)	-1557.2697664	-1556.378423	-1556.509742	-1557.6746712	-1556.783328	-1556.914647	-1557.6139657	-1556.722622	-1556.853941
<i>15E,12Z</i>									
1 (Car_H_021)	-1557.278229	-1556.386899	-1556.516898				-1557.6209372	-1556.7296072	-1556.8596062
2 (Car_H_002)	-1557.2775244	-1556.386095	-1556.515833	-1557.6821483	-1556.7907189	-1556.9204569	-1557.6205256	-1556.7290962	-1556.8588342
3 (Bet_car_025)	-1557.276017	-1556.384438	-1556.516002	-1557.6808265	-1556.7892475	-1556.9208115	-1557.620556	-1556.728977	-1556.860541
4 (bet_car_12_c5m)	-1557.2727142	-1556.381806	-1556.513237	-1557.6774326	-1556.786524	-1556.917955	-1557.6155361	-1556.7246279	-1556.8560589
5 (Car_H_150_001)	-1557.2713634	-1556.380487	-1556.512866	-1557.6759131	-1556.785037	-1556.917416	-1557.6139453	-1556.723069	-1556.855448
6 (bet_car_12_c5m_c1)	-1557.2692544	-1556.377915	-1556.508932	-1557.6741264	-1556.782787	-1556.913804	-1557.6131913	-1556.7218519	-1556.8528689
7 (Bet_car_032)	-1557.269342	-1556.378101	-1556.509920	-1557.67419	-1556.782949	-1556.914768	-1557.612914	-1556.721673	-1556.853492
<i>15E,13Z</i>									
1 (Bet_car_030)	-1557.276707	-1556.385722	-1556.515940	-1557.6812018	-1556.7902168	-1556.9204348	-1557.6190062	-1556.7280212	-1556.8582392
2 (Car_H_021)	-1557.2766959	-1556.385709	-1556.516113	-1557.6811937	-1556.7902068	-1556.9206108	-1557.6190191	-1556.7280322	-1556.8584362
3 (bet_car_13_c5m)	-1557.2712809	-1556.380547	-1556.513447	-1557.6758533	-1556.785119	-1556.918019	-1557.6136732	-1556.722939	-1556.855839
4 (Bet_car_032)	-1557.2698117	-1556.378527	-1556.509930	-1557.6743854	-1556.7831007	-1556.9145037	-1557.6127085	-1556.7214238	-1556.8528268
5 (bet_car_13_c5m_c1)	-1557.2690432	-1556.377824	-1556.509338	-1557.6736689	-1556.78245	-1556.913964	-1557.6138551	-1556.7226359	-1556.8541499

6 (bet_car_13_c5m_c2)	-1557.2680811	-1556.377174	-1556.508790	-1557.6727427	-1556.7818356	-1556.9134516	-1557.6116109	-1556.720704	-1556.85232
15E,9Z									
1 (Bet_car_030)	-1557.275205	-1556.384287	-1557.515786	-1557.6796737	-1556.7887557	-1556.9202547	-1557.6163892	-1556.7254712	-1556.8569702
2 (Bet_car_025)	-1557.2729776	-1556.381667	-1556.512984	-1557.6776126	-1556.786302	-1556.917619	-1557.6165515	-1556.7252409	-1556.8565579
3 (bet_car_9_c5m)	-1557.2700114	-1556.379226	-1556.510585	-1557.6745101	-1556.783725	-1556.915084			
4 (bet_car_9_c5m_c2)	-1557.268555	-1556.377237	-1556.507543	-1557.6730284	-1556.78171	-1556.912016	-1557.6105853	-1556.719267	-1556.849573
5 (bet_car_9_c5m_c1)	-1557.26776	-1556.376644	-1556.508260	-1557.6723706	-1556.781255	-1556.912871	-1557.6115926	-1556.720477	-1556.852093
15E,14Z									
1 (Car_H_021)	-1557.2734241	-1556.381685	-1556.512348	-1557.6780449	-1556.7863058	-1556.9169688	-1557.6165248	-1556.7247857	-1556.8554487
2 (bet_car_14_c5m)	-1557.2679849	-1556.376590	-1556.508406	-1557.6726622	-1556.781267	-1556.913083	-1557.6112144	-1556.71982	-1556.851636
3 (bet_car_14_c5m_c2)	-1557.2658781	-1556.374029	-1556.505261						
4 (bet_car_14_c5m_c1)	-1557.264638	-1556.373064	-1556.504586	-1557.6694144	-1556.77784	-1556.909362			
15E,11Z									
1 (Car_H_021)	-1557.2727072	-1556.381093	-1556.511169	-1557.6772753	-1556.7856611	-1556.9157371	-1557.61569	-1556.7240758	-1556.8541518
2 (Bet_car_025)	-1557.2705507	-1556.378596	-1556.508867	-1557.6752683	-1556.7833136	-1556.9135846	-1557.6160916	-1556.7241369	-1556.8544079
3 (bet_car_11_c5m)	-1557.2673132	-1556.375924	-1556.506874	-1557.6719568	-1556.780568	-1556.911518	-1557.6104147	-1556.7190255	-1556.8499755
4 (bet_car_11_c5m_c1)	-1557.2651064	-1556.373474	-1556.505489	-1557.6698769	-1556.778245	-1556.91026	-1557.610622	-1556.7189896	-1556.8510046
5 (Bet_car_032)	-1557.2640134	-1556.372314	-1556.503126	-1557.6687687	-1556.7770693	-1556.9078813			
15E,10Z									
1 (Bet_car_030)	-1557.2723409	-1556.380740	-1556.511354	-1557.6770645	-1556.7854636	-1556.9160776	-1557.6162722	-1556.7246713	-1556.8552853
2 (bet_car_10_c5m)	-1557.2669522	-1556.375633	-1556.507185	-1557.6716658	-1556.780347	-1556.911899	-1557.6108216	-1556.7195024	-1556.8510544
3 (bet_car_10_c5m_c2)	-1557.2653693	-1556.373320	-1556.503130	-1557.6701296	-1556.7780803	-1556.9078903	-1557.6097566	-1556.7177073	-1556.8475173
4 (bet_car_10_c5m_c1)	-1557.2599949	-1556.368135	-1556.499849	-1557.6649738	-1556.773114	-1556.904828	-1557.6058399	-1556.71398	-1556.845694
15E,7Z									
1 (Bet_car_030)	-1557.2693633	-1556.378220	-1556.507183	-1557.6740347	-1556.7828914	-1556.9118544	-1557.6119784	-1556.7208351	-1556.8497981
2 (Bet_car_025)	-1557.2671975	-1557.375771	-1556.505352	-1557.6719397	-1557.7805132	-1556.9100942			
3 (bet_car_7_c5m)	-1557.2659395	-1556.375928	-1556.504520	-1557.6709015	-1556.78089	-1556.909482	-1557.6103431	-1556.720332	-1556.848924
4 (bet_car_7_c5m_c1)	-1557.2618002	-1556.370618	-1556.501000	-1557.6665767	-1556.775395	-1556.905777			
Bet_car (closed shell)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509

H2O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362
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Table S14b: Boltzmann Averaged energy of the *15E* isomer and their rotamers of C5-Me radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15E</i>	-1556.793387	-1556.923548	-1556.731868	-1556.861989
<i>15E,8Z</i>	-1556.791978	-1556.921804	-1556.730229	-1556.860009
<i>15E,12Z</i>	-1556.790412	-1556.920534	-1556.729295	-1556.860092
<i>15E,13Z</i>	-1556.790197	-1556.920436	-1556.728002	-1556.858227
<i>15E,9Z</i>	-1556.788558	-1556.920079	-1556.725352	-1556.85679
<i>15E,14Z</i>	-1556.786281	-1556.916904	-1556.72476	-1556.855383
<i>15E,11Z</i>	-1556.785457	-1556.91548	-1556.724084	-1556.854226
<i>15E,10Z</i>	-1556.785438	-1556.916027	-1556.724645	-1556.855236
<i>15E,7Z</i>	-1556.78253	-1556.911471	-1556.720649	-1556.84955

Table S15a. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C5-Me radical) from the 15E isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C5-Me-radical						
<i>all-trans (15E)</i>						
1 (Car H 021)	-167.7	-170.4	-194.7	-197.5	-205.9	-208.7
2 (bet car 030 004)	-154.7	-160.9	-181.9	-188.3	-192.9	-199.2
3 (Bet car 030)	-152.8	-159.3	-179.8	-186.3	-191.9	-198.5
4 (bet car 007)	-147.8	-154.7	-175.4	-182.4	-191.3	-198.3
5 (Car H 045 001)	-142.3	-146.6	-169.9	-174.3	-187.6	-191.9
<i>15E,8Z</i>						
1 (Bet car 030)	-164.4	-165.9	-191.6	-193.2	-201.5	-203.1
2 (Car H 021)	-164.2	-165.8	-191.3	-192.9		
3 (Car H 002)	-162.7	-165.4	-189.6	-192.3		
4 (Bet car 025)	-157.6	-160.6	-185.1	-188.1		
5 (bet car 8 c5m)	-152.0	-151.8	-179.2	-178.9	-189.4	-189.2
6 (bet car 8 c5m c1)	-140.7	-146.3	-168.2	-173.8	-181.5	-187.0
<i>15E,12Z</i>						
1 (Car H 021)	-162.9	-165.0			-199.8	-201.9
2 (Car H 002)	-160.8	-162.2	-187.6	-189.1	-198.5	-199.9
3 (Bet car 025)	-156.5	-162.7	-183.7	-189.9	-198.1	-204.4
4 (bet car 12 c5m)	-149.6	-155.4	-176.6	-182.5	-186.7	-192.6
5 (Car H 150 001)	-146.1	-154.5	-172.7	-181.1	-182.6	-191.0
6 (bet car 12 c5m c1)	-139.3	-144.1	-166.8	-171.6	-179.4	-184.2
7 (Bet car 032)	-139.8	-146.7	-167.2	-174.1	-178.9	-185.9
<i>15E,13Z</i>						
1 (Bet car 030)	-159.8	-162.5	-186.3	-189.0	-195.6	-198.3
2 (Car H 021)	-159.8	-162.9	-186.3	-189.5	-195.7	-198.8
3 (bet car 13 c5m)	-146.3	-155.9	-172.9	-182.7	-182.3	-192.0
4 (Bet car 032)	-140.9	-146.7	-167.6	-173.4	-178.3	-184.1
5 (bet car 13 c5m c1)	-139.1	-145.2	-165.9	-172.0	-181.5	-187.6
6 (bet car 13 c5m c2)	-137.4	-143.8	-164.3	-170.7	-176.4	-182.8

<i>15E,9Z</i>						
1 (Bet car 030)	-156.1	-162.1	-182.5	-188.5	-188.9	-195.0
2 (Bet car 025)	-149.2	-154.8	-176.0	-181.6	-188.3	-193.9
3 (bet car 9 c5m)	-142.8	-148.5	-169.3	-174.9		
4 (bet car 9 c5m c2)	-137.6	-140.5	-163.9	-166.9	-172.6	-175.6
5 (bet car 9 c5m c1)	-136.0	-142.4	-162.8	-169.1	-175.8	-182.2
<i>15E,14Z</i>						
1 (Car H 021)	-149.2	-153.1	-176.0	-179.9	-187.1	-191.0
2 (bet car 14 c5m)	-135.9	-142.7	-162.8	-169.7	-174.1	-180.9
3 (bet car 14 c5m c2)	-129.1	-134.5				
4 (bet car 14 c5m c1)	-126.6	-132.7	-153.8	-159.9		
<i>15E,11Z</i>						
1 (Car H 021)	-147.7	-150.0	-174.3	-176.7	-185.3	-187.6
2 (Bet car 025)	-141.1	-143.9	-168.2	-171.0	-185.4	-188.3
3 (bet car 11 c5m)	-134.1	-138.7	-160.9	-165.6	-172.0	-176.6
4 (bet car 11 c5m c1)	-127.7	-135.1	-154.9	-162.3	-171.9	-179.3
5 (Bet car 032)	-124.6	-128.9	-151.8	-156.0		
<i>15E,10Z</i>						
1 (Bet car 030)	-146.7	-150.5	-173.8	-177.6	-186.8	-190.6
2 (bet car 10 c5m)	-133.4	-139.5	-160.4	-166.6	-173.3	-179.5
3 (bet car 10 c5m c2)	-127.3	-128.9	-154.4	-156.1	-168.6	-170.2
4 (bet car 10 c5m c1)	-113.7	-120.3	-141.4	-148.0	-158.8	-165.4
<i>15E,7Z</i>						
1 (Bet car 030)	-140.1	-139.5	-167.1	-166.5	-176.8	-176.2
2 (Bet car 025)	-133.7	-134.7	-160.8	-161.8		
3 (bet car 7 c5m)	-134.1	-132.5	-161.8	-160.2	-175.4	-173.9
4 (bet car 7 c5m c1)	-120.2	-123.3	-147.4	-150.5		

Table S15b. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C5-Me radical) from the 15E isomer (Conformational Restriction).

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C5-Me-radical				
15E	-194.7	-197.5	-205.9	-208.7
15E,8Z	-204.9	-204.9	-215.4	-211.4
15E,12Z	-201.8	-201.8	-214.2	-209.0
15E,13Z	-190.5	-194.7	-200.4	-203.2
15E,9Z	-186.6	-192.9	-195.7	-201.8
15E,14Z	-196.5	-200.7	-207.6	-211.8
15E,11Z	-195.9	-197.5	-205.8	-207.7
15E,10Z	-194.8	-199.5	-207.1	-210.4
15E,7Z	-188.4	-188.9	-195.5	-194.6

Table S15c. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C5-Me radical) from the 15E isomer obtained by Boltzmann Averaging of the conformers

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C5-Me-radical				
15E	-196.2	-199.0	-206.0	-208.4
15E,8Z	-205.6	-205.8	-216.4	-213.7
15E,12Z	-202.2	-202.0	-214.3	-212.8
15E,13Z	-191.9	-195.1	-201.2	-203.6
15E,9Z	-187.6	-194.1	-196.0	-202.2
15E,14Z	-198.1	-202.3	-208.8	-213.1
15E,11Z	-196.7	-198.2	-206.6	-208.5
15E,10Z	-196.0	-200.3	-208.2	-211.2
15E,7Z	-188.0	-188.9	-195.6	-195.7

Table S16a. Energetics [Hartrees] of the H-atom abstraction reactions (C5Me radical) from *15Z* isomer.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C5-Me-radical									
<i>15,15'</i>-cis (<i>15Z</i>)									
1 (Car_H_002_cis)	-1557.2748027	-1556.383439	-1556.514318	-1557.6795599	-1556.7881962	-1556.9190752	-1557.6186137	-1556.72725	-1556.858129
2 (Bet_025_cis_001)	-1557.2731813	-1556.381433	-1556.512443	-1557.6781531	-1556.786405	-1556.917415	-1557.6191022	-1556.727354	-1556.858364
3 (bet_car_trans)	-1557.2699046	-1556.378862	-1556.511265	-1557.6747994	-1556.7837568	-1556.9161598	-1557.6135233	-1556.7224807	-1556.8548837
4(car_H_021_cis)	-1557.2693309	-1556.378260	-1556.510512	-1557.674161	-1556.7830901	-1556.9153421	-1557.613216	-1556.7221451	-1556.8543971
<i>15Z,13Z</i>									
1 (Car_H_002_cis)	-1557.2715111	-1556.380230	-1556.510685	-1557.6761072	-1556.7848261	-1556.9152811	-1557.6147884	-1556.7235073	-1556.8539623
2 (bet_13_15_c5m)	-1557.2667063	-1556.375659	-1556.506744	-1557.6714598	-1556.780413	-1556.911498	-1557.6095272	-1556.7184799	-1556.8495649
3 (Car_H_021_cis)	-1557.2661504	-1556.375168	-1556.506588				-1557.6094969	-1556.7185145	-1556.8499345
4 (Bet_car_025)	-1557.2646296	-1556.373096	-1556.504147	-1557.6692974	-1556.7777638	-1556.9088148	-1557.6087713	-1556.7172377	-1556.8482887
5 (Bet_car_001_cis)	-1557.2643113	-1556.372980	-1556.505026	-1557.6691418	-1556.7778105	-1556.9098565	-1557.609624	-1556.7182927	-1556.8503387
<i>15Z,9Z</i>									
1 (Csr_H_002_cis)	-1557.2701418	-1556.378995	-1556.511572	-1557.6747426	-1556.7835958	-1556.9161728	-1557.6123885	-1556.7212417	-1556.8538187
2 (bet_9_15_c5m)	-1557.2654782	-1556.374707	-1556.507238	-1557.6702435	-1556.779472	-1556.912003	-1557.6075384	-1556.716767	-1556.849298
3 (Car_H_021)	-1557.2649989	-1556.374142	-1556.506217	-1557.6696337	-1556.7787768	-1556.9108518	-1557.6075411	-1556.7166842	-1556.8487592
4 (bet_car_9_15_c5m_c2)	-1557.2640219	-1556.372625	-1556.504482	-1557.6687741	-1556.777377	-1556.909234	-1557.6075384	-1556.716142	-1556.847999
5 (Bet_car_025_cis)	-1557.2635493	-1556.372036	-1556.503016	-1557.6681771	-1556.7766638	-1556.9076438	-1557.6067673	-1556.715254	-1556.846234
6 (bet_car_9_15_c5m_c1)	-1557.2630577	-1556.371842	-1556.504444	-1557.6678457	-1556.77663	-1556.909232	-1557.6074567	-1556.716241	-1556.848843
<i>15Z,8Z</i>									
1 (bet_car_8_15_c5m)	-1557.2684484	-1556.377467	-1556.509583	-1557.6733913	-1556.7824099	-1556.9145259	-1557.611536	-1556.7205546	-1556.8526706
2 (bet_car_8_15_c5m_c2)	-1557.2662447	-1556.374921	-1556.507211	-1557.6712651	-1556.779941	-1556.912231	-1557.6115968	-1556.720273	-1556.852563
<i>15Z,12Z</i>									
1 (bet_car_12_15_c5m)	-1557.2678941	-1556.376672	-1556.507152	-1557.6727054	-1556.781483	-1556.911963	-1557.6104106	-1556.7191885	-1556.8496685
2 (bet_car_12_15_c5m_c1)	-1557.2663505	-1556.374583	-1556.504224	-1557.6711785	-1556.779411	-1556.909052	-1557.6095141	-1556.717747	-1556.847388
3 (Bet_car_025_cis)	-1557.2657611	-1556.373995	-1556.504411	-1557.6704543	-1556.7786882	-1556.9091042	-1557.6092667	-1556.7175006	-1556.8479166
<i>15Z,11Z</i>									
1 (Car_H_002_cis)	-1557.2674511	-1556.375649	-1556.505602	-1557.6720903	-1556.7802882	-1556.9102412	-1557.611197	-1556.7193949	-1556.8493479

2 (bet_11_15_c5m)	-1557.2625889	-1556.371111	-1556.502049	-1557.6673705	-1556.775893	-1556.906831	-1557.6061425	-1556.7146646	-1556.8456026
3 (Car_H_021_cis)	-1557.2620349	-1556.370606	-1556.501859	-1557.6667435	-1556.7753146	-1556.9065676	-1557.6058033	-1556.7143744	-1556.8456274
4 (bet_car_11_15_c5m_c2)	-1557.261004	-1556.369008	-1556.499295	-1557.665851	-1556.773855	-1556.904142	-1557.6051407	-1556.7131447	-1556.8434317
5 (Bet_Car_025_cis)	-1557.2604783	-1556.368487	-1556.499132	-1557.6651951	-1556.7732038	-1556.9038488	-1557.6050256	-1556.7130343	-1556.8436793
6 (bet_car_11_15_c5m_c1)	-1557.2602805	-1556.368419	-1556.500744	-1557.6651951	-1556.773334	-1556.905659			
15Z,10Z									
1 (Car_H_002_cis)	-1557.2670745	-1556.375203	-1556.505006	-1557.6717972	-1556.7799257	-1556.9097287	-1557.6108341	-1556.7189626	-1556.8487656
2 (bet_car_10_15_c5m)	-1557.2623022	-1556.370702	-1556.501644	-1557.6672019	-1556.775602	-1556.906544	-1557.6060179	-1556.7144177	-1556.8453597
3 (Bet_car_025_cis)	-1557.2601179	-1556.367996	-1556.498094	-1557.6649319	-1556.77281	-1556.902908	-1557.6046649	-1556.712543	-1556.842641
4 (bet_car_10_15_c5m_c2)	-1557.2590065	-1556.367233	-1556.498280	-1557.6640207	-1556.772247	-1556.903294	-1557.6039729	-1556.7121994	-1556.8432464
15Z,7Z									
1 (Car_H_002_cis)	-1557.2639964	-1556.372738	-1556.502203	-1557.6686633	-1556.7774049	-1556.9068699	-1557.6074385	-1556.7161801	-1556.8456451
2 (Bet_car_025_cis)	-1557.2624268	-1556.370781	-1556.499867	-1557.6672902	-1556.7756444	-1556.9047304	-1557.6077908	-1556.716145	-1556.845231
3 (Car_H_021_cis)	-1557.2585667	-1556.367571	-1556.497966	-1557.6632389	-1556.7722432	-1556.9026382	-1557.6021316	-1556.7111359	-1556.8415309
4 (bet_7_15_c5m_c1)	-1557.2570394	-1556.365598	-1556.495462	-1557.6618798	-1556.7704384	-1556.9003024	-1557.6025372	-1556.711096	-1556.84096
Bet_car (closed shell)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509
H2O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362

Table S16b: Boltzmann Averaged energy of the *15Z* isomer and their rotamers of C5-Me radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15Z</i>	-1556.787911	-1556.918679	-1556.72728	-1556.858183
<i>15Z,13Z</i>	-1556.784777	-1556.91519	-1556.72343	-1556.853781
<i>15Z,9Z</i>	-1556.783499	-1556.916095	-1556.721111	-1556.853719
<i>15Z,8Z</i>	-1556.782242	-1556.914341	-1556.720435	-1556.85262
<i>15Z,12Z</i>	-1556.78116	-1556.911715	-1556.718759	-1556.849285
<i>15Z,11Z</i>	-1556.780207	-1556.910034	-1556.719324	-1556.849187
<i>15Z,10Z</i>	-1556.779876	-1556.909612	-1556.718914	-1556.848652
<i>15Z,7Z</i>	-1556.777147	-1556.906623	-1556.716139	-1556.845433

Table S17a. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C5-Me radical) from the *15Z* isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C5-Me-radical						
<i>15,15'-cis (15Z)</i>						
1 (Car H 002 cis)	-153.8	-158.3	-181.0	-185.4	-193.6	-198.0
2 (Bet 025 cis 001)	-148.6	-153.3	-176.3	-181.1	-193.9	-198.7
3 (bet car trans)	-141.8	-150.3	-169.3	-177.8	-181.1	-189.5
4(car H 021 cis)	-140.3	-148.3	-167.6	-175.6	-180.2	-188.2
<i>15Z,13Z</i>						
1 (Car H 002 cis)	-145.4	-148.7	-172.2	-175.5	-183.8	-187.1
2 (bet 13 15 c5m)	-133.4	-138.4	-160.6	-165.5	-170.6	-175.5
3 (Car H 021 cis)	-132.1	-137.9			-170.7	-176.5
4 (Bet car 025)	-126.7	-131.6	-153.6	-158.5	-167.3	-172.2
5 (Bet car 001 cis)	-126.4	-133.9	-153.7	-161.2	-170.1	-177.6
<i>15Z,9Z</i>						
1 (Csr H 002 cis)	-142.2	-151.1	-168.9	-177.8	-177.8	-186.7
2 (bet 9 15 c5m)	-130.9	-139.7	-158.1	-166.9	-166.1	-174.8
3 (Car H 021)	-129.4	-137.0	-156.3	-163.8	-165.9	-173.4
4 (bet car 9 15 c5m c2)	-125.4	-132.5	-152.6	-159.6	-164.4	-171.4
5 (Bet car 025 cis)	-123.9	-128.6	-150.7	-155.4	-162.1	-166.8
6 (bet car 9 15 c5m c1)	-123.4	-132.3	-150.6	-159.6	-164.7	-173.7
<i>15Z,8Z</i>						
1 (bet car 8 15 c5m)	-138.2	-145.8	-165.8	-173.5	-176.0	-183.7
2 (bet car 8 15 c5m c2)	-131.5	-139.6	-159.3	-167.5	-175.3	-183.4
<i>15Z,12Z</i>						
1 (bet car 12 15 c5m)	-136.1	-139.5	-163.4	-166.7	-172.4	-175.8
2 (bet car 12 15 c5m c1)	-130.6	-131.8	-157.9	-159.1	-168.7	-169.8
3 (Bet car 025 cis)	-129.0	-132.3	-156.0	-159.2	-168.0	-171.2
<i>15Z,11Z</i>						
1 (Car H 002 cis)	-133.4	-135.4	-160.2	-162.2	-172.9	-174.9

2 (bet 11 15 c5m)	-121.5	-126.1	-148.7	-153.3	-160.6	-165.2
3 (Car H 021 cis)	-120.2	-125.6	-147.2	-152.6	-159.8	-165.2
4 (bet car 11 15 c5m c2)	-115.9	-118.8	-143.3	-146.2	-156.6	-159.4
5 (Bet Car 025 cis)	-114.6	-118.4	-141.6	-145.4	-156.3	-160.1
6 (bet car 11 15 c5m c1)	-114.4	-122.6	-141.9	-150.2		
15Z,10Z						
1 (Car H 002 cis)	-132.2	-133.8	-159.3	-160.9	-171.8	-173.5
2 (bet car 10 15 c5m)	-120.4	-125.0	-147.9	-152.5	-159.9	-164.5
3 (Bet car 025 cis)	-113.3	-115.7	-140.6	-142.9	-155.0	-157.4
4 (bet car 10 15 c5m c2)	-111.3	-116.2	-139.1	-144.0	-154.1	-158.9
15Z,7Z						
1 (Car H 002 cis)	-125.7	-126.5	-152.7	-153.4	-164.5	-165.3
2 (Bet car 025 cis)	-120.6	-120.3	-148.0	-147.7	-164.4	-164.2
3 (Car H 021 cis)	-112.2	-115.3	-139.1	-142.3	-151.3	-154.5
4 (bet 7 15 c5m c1)	-107.0	-108.8	-134.4	-136.1	-151.2	-152.9

Table S17b. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C5-Me radical) from the *15Z* isomer (Conformational Restriction).

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C5-Me-radical				
<i>15Z</i>	-191.4	-197.2	-202.9	-208.3
<i>15Z,13Z</i>	-186.8	-189.6	-197.5	-200.3
<i>15Z,9Z</i>	-182.7	-192.8	-194.2	-203.3
<i>15Z,8Z</i>	-189.3	-196.2	-199.6	-204.5
<i>15Z,12Z</i>	-187.9	-187.0	-198.5	-197.2
<i>15Z,11Z</i>	-191.9	-195.5	-203.6	-204.9
<i>15Z,10Z</i>	-190.3	-193.5	-204.4	-205.8
<i>15Z,7Z</i>	-184.0	-184.7	-192.6	-191.7

Table S17c. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C5-Me radical) from the *15Z* isomer obtained from Boltzmann Averaging of the conformers.

Isomers	B3LYP/MB		Water Solvent (PCM)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C5-Me-radical				
<i>15Z</i>	-191.9	-196.7	-203.9	-208.4
<i>15Z,13Z</i>	-188.2	-190.8	-198.6	-200.8
<i>15Z,9Z</i>	-183.9	-194.5	-194.7	-203.5
<i>15Z,8Z</i>	-190.2	-196.9	-200.5	-205.3
<i>15Z,12Z</i>	-188.5	-188.0	-198.1	-197.3
<i>15Z,11Z</i>	-193.1	-196.0	-204.3	-205.4
<i>15Z,10Z</i>	-191.5	-194.3	-204.3	-206.3
<i>15Z,7Z</i>	-184.7	-184.8	-193.0	-192.4

Table S18a. Energetics [Hartrees] of the H-atom abstraction reactions (C9Me radical) from *15E* isomer.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C9-Me-radical									
<i>15E,9Z</i>									
1 (bet_car_9_c9m)	-1557.2697565	-1556.378792	-1556.508996	-1557.6745391	-1556.783575	-1556.913779	-1557.6102777	-1556.719313	-1556.849517
2 (bet_car_030)	-1557.269326	-1556.378441	-1556.509684	-1557.6740559	-1556.7831709	-1556.9144139	-1557.6101658	-1556.7192808	-1556.8505238
3 (bet_car_9_c9m_c1)	-1557.267786	-1556.376452	-1556.506487	-1557.6727322	-1556.781398	-1556.911433	-1557.6106034	-1556.719269	-1556.849304
4 (bet_car_025)	-1557.2672932	-1556.376057	-1556.507476	-1557.6721903	-1556.7809541	-1556.9123731	-1557.6106046	-1556.7193684	-1556.8507874
5 (bet_car_032)	-1557.2667841	-1556.375415	-1556.506237	-1557.6716447	-1556.7802756	-1556.9110976	-1557.6094455	-1556.7180764	-1556.8488984
<i>15E,8Z</i>									
1 (bet_car_8_c9m)	-1557.2687565	-1556.377776	-1556.508973	-1557.6735063	-1556.7825258	-1556.913722	-1557.6105427	-1556.719562	-1556.850759
2 (Bet_car_030)	-1557.2682357	-1556.377314	-1556.509348	-1557.6729261	-1556.7820044	-1556.9140384	-1557.6100259	-1556.7191042	-1556.8511382
3 (Bet_car_032)	-1557.2667147	-1556.375298	-1556.506854	-1557.6716009	-1556.7801842	-1556.9117402	-1557.6103267	-1556.71891	-1556.850466
4 (bet_car_8_c9m_c2)	-1557.2667098	-1556.375299	-1556.506402	-1557.6715871	-1556.780176	-1556.911279	-1557.6102326	-1556.718822	-1556.849925
5 (bet_car_025)	-1557.2663055	-1556.374890	-1556.505698	-1557.6711118	-1556.7796963	-1556.9105043	-1557.6099465	-1556.718531	-1556.849339
6 (bet_car_8_c9m_c1)	-1557.2656818	-1556.374270	-1556.505417	-1557.6705218	-1556.77911	-1556.910257	-1557.6097407	-1556.718329	-1556.849476
<i>15E,13Z</i>									
1 (bet_car_13_c9m)	-1557.2660981	-1556.375018	-1556.506047	-1557.670968	-1556.779888	-1556.910917	-1557.6082089	-1556.717129	-1556.848158
2 (Bet_car_030)	-1556.2618714	-1556.371521	-1556.502806				-1557.6036896	-1556.7133392	-1556.8446242
3 (Car_H_002)	-1557.2613799	-1557.370917	-1556.501598	-1557.6655232	-1556.7750603	-1556.9057413	-1557.6036965	-1556.7132336	-1556.8439146
4 (bet_car_13_c9m_c1)	-1557.2601067	-1556.369265	-1556.500127	-1557.6644958	-1556.773654	-1556.904516	-1557.6043262	-1556.713485	-1556.844347
5 (Bet_car_025)	-1557.2597127	-1556.368801	-1556.499644	-1557.6640629	-1556.7731512	-1556.9039942	-1557.6040455	-1556.7131338	-1556.8439768
6 (bet_car_13_c9m_c2)	-1557.2593535	-1556.368581	-1556.499853	-1557.6637138	-1556.772941	-1556.904213	-1557.6031218	-1556.712349	-1556.843621
<i>all-trans(15E)</i>									
1 (Car_H_021_003)	-1557.2654939	-1556.374820	-1556.506614	-1557.6699576	-1556.779284	-1556.911078	-1557.6075306	-1556.716857	-1556.848651
2 (bet_car_030_004)	-1557.2630131	-1557.372297	-1556.504377	-1557.6676639	-1556.7769478	-1556.9090278	-1557.6057994	-1557.7150833	-1556.8471633
3 (bet_car_030)	-1557.2625425	-1556.371683	-1556.503247	-1557.6670996	-1556.7762401	-1556.9078041	-1557.6059424	-1556.7150829	-1556.8466469
4 (bet_car_007)	-1557.26105	-1556.369808	-1556.502086	-1557.6658283	-1556.7745863	-1556.9068643	-1557.6061722	-1556.7149302	-1556.8472082
5 (bet_car_001)	-1557.2609724	-1556.369768	-1556.502174	-1557.6657696	-1556.7745652	-1556.906971			

6 (Car_H_045_004)	-1557.2606296	-1556.369212	-1556.501933	-1557.6652819	-1556.773864	-1556.906585			
7 (Bet_car_025)	-1557.2605678	-1556.369230	-1556.501277	-1557.6652597	-1556.7739219	-1556.9059689	-1557.6059638	-1556.714626	-1556.846673
8 (bet_car_032)	-1557.2605301	-1556.369257	-1556.500809	-1557.6652852	-1556.7740121	-1556.9055641			
15E,12Z									
1 (car_H_002)	-1557.2633276	-1556.372600	-1556.504758	-1557.667702	-1556.7769744	-1556.9091324	-1557.6055976	-1556.71487	-1556.847028
2 (bet_car_12_c9m)	-1557.2629364	-1556.372360	-1556.503324	-1557.6672982	-1556.776722	-1556.907686	-1557.6062051	-1556.7156287	-1556.8465927
3 (Bet_car_025)	-1557.2618483	-1556.370876	-1556.503168	-1557.6664784	-1556.7755061	-1556.9077981	-1557.6057244	-1556.7147521	-1556.8470441
4 (Bet_car_032)	-1557.2614198	-1556.370404	-1556.501894	-1557.6660182	-1556.7750024	-1556.9064924			
15E,10Z									
1 (Bet_car_030)	-1557.2614	-1556.370433	-1556.501858	-1557.6660394	-1556.7750724	-1556.9064974	-1557.6026915	-1556.7117245	-1556.8431495
2 (bet_car_10_c9m)	-1557.2610203	-1556.370010	-1556.500887	-1557.6655072	-1556.774497	-1556.905374	-1557.6018463	-1556.710836	-1556.841713
3 (Car_H_002)	-1557.2608973	-1556.369759	-1556.500483	-1557.6654148	-1556.7742765	-1556.9050005	-1557.6025749	-1556.7114366	-1556.8421606
4 (Bet_car_032)	-1557.2589785	-1556.367617	-1556.498963	-1557.663706	-1556.7723445	-1556.9036905			
5 (bet_car_10_c9m_c1)	-1557.2589496	-1556.367690	-1556.499264	-1557.6635785	-1556.772319	-1556.903893			
6 (bet_car_10_c9m_c2)	-1557.2589474	-1556.367669	-1556.499544	-1557.6636961	-1556.772418	-1556.904293			
7 (bet_car_025)	-1557.2584759	-1556.367177	-1556.499356	-1557.6630158	-1556.7717169	-1556.9038959	-1557.6021841	-1556.7108852	-1556.8430642
15E,7Z									
1 (Bet_car_032)	-1557.2604929	-1556.369817	-1556.500811	-1557.6652118	-1556.7745359	-1556.9055299			
2 (Car_H_002)	-1557.259763	-1556.369233	-1556.501433	-1557.664376	-1556.773846	-1556.906046	-1557.6030997	-1556.7125697	-1556.8447697
3 (bet_car_7_c9m_c1)	-1557.2584152	-1556.367371	-1556.498095	-1557.6633783	-1556.772334	-1556.903058	-1557.6030916	-1556.712047	-1556.842771
15E,14Z									
1 (bet_car_14_c9m)	-1557.2592885	-1556.368379	-1556.499860	-1557.663743	-1556.772834	-1556.904315	-1557.6012446	-1556.710335	-1556.841816
2 (Bet_car_030)	-1557.258832	-1556.367855	-1556.499009	-1557.6632392	-1556.7722622	-1556.9034162			
3 (Bet_car_032)	-1557.2582165	-1556.367237	-1556.499087	-1557.6608323	-1556.7698528	-1556.9017028	-1557.6005236	-1556.7095441	-1556.8413941
4 (bet_car_14_c9m_c2)	-1557.2571798	-1556.365691	-1556.497125	-1557.661692	-1556.770203	-1556.901637	-1557.6015378	-1556.710049	-1556.841483
5 (Bet_car_025)	-1557.2567383	-1556.365305	-1556.497107	-1557.6612596	-1556.7698263	-1556.9016283	-1557.6015657	-1556.7101324	-1556.8419344
15E,11Z									
1 (Bet_car_030)	-1557.2586183	-1556.367663	-1556.499185	-1557.6628801	-1556.7719248	-1556.9034468	-1557.6003764	-1556.7094211	-1556.8409431
2 (bet_car_11_c9m)	-1557.2584568	-1556.367420	-1556.499216	-1557.6628755	-1556.771839	-1556.903635	-1557.6006006	-1556.7095638	-1556.8413598
3 (Bet_car_025)	-1557.2565649	-1556.365273	-1556.497130	-1557.6609524	-1556.7696605	-1556.9015175	-1557.6003041	-1556.7090122	-1556.8408692
4 (bet_car_11_c1_c9m)	-1557.2560871	-1556.364903	-1556.496812	-1557.6603644	-1556.76918	-1556.901089	-1557.5995378	-1556.7083537	-1556.8402627

5 (Bet_car_032)	-1557.2558182	-1556.364570	-1556.496943						
Bet_car (closed shell)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509
H2O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362

Table S18b: Boltzmann Averaged energy of the *15E* isomer and their rotamers of C9-Me radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15E,9Z</i>	-1556.783172	-1556.913952	-1556.719231	-1556.850324
<i>15E,8Z</i>	-1556.782018	-1556.913655	-1556.719051	-1556.850604
<i>15E,13Z</i>	-1556.779841	-1556.910879	-1556.716854	-1556.847892
<i>15E</i>	-1556.778903	-1556.910644	-1556.716202	-1556.847989
<i>15E,12Z</i>	-1556.776619	-1556.908608	-1556.715257	-1556.846931
<i>15E,10Z</i>	-1556.774515	-1556.905749	-1556.711368	-1556.842852
<i>15E,7Z</i>	-1556.77419	-1556.905784	-1556.712379	-1556.844555
<i>15E,14Z</i>	-1556.772471	-1556.903876	-1556.710094	-1556.84171
<i>15E,11Z</i>	-1556.771714	-1556.903359	-1556.70928	-1556.841006

Table S19a. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C9-Me radical) from the *15E* isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C9-Me-radical						
<i>15E,9Z</i>						
1 (bet_car_9_c9m)	-141.6	-144.3	-168.9	-171.5	-172.8	-175.4
2 (bet_car_030)	-140.7	-146.1	-167.8	-173.2	-172.7	-178.1
3 (bet_car_9_c9m_c1)	-135.5	-137.7	-163.2	-165.4	-172.7	-174.9
4 (bet_car_025)	-134.5	-140.3	-161.9	-167.8	-172.9	-178.8
5 (bet_car_032)	-132.8	-137.1	-160.2	-164.5	-169.5	-173.8
<i>15E,8Z</i>						
1 (bet_car_8_c9m)	-138.9	-144.2	-166.1	-171.4	-173.4	-178.7
2 (Bet_car_030)	-137.7	-145.2	-164.7	-172.2	-172.2	-179.7
3 (Bet_car_032)	-132.5	-138.7	-159.9	-166.2	-171.7	-177.9
4 (bet_car_8_c9m_c2)	-132.5	-137.5	-159.9	-164.9	-171.5	-176.5
5 (bet_car_025)	-131.4	-135.6	-158.7	-162.9	-170.7	-174.9
6 (bet_car_8_c9m_c1)	-129.8	-134.9	-157.1	-162.3	-170.2	-175.3
<i>15E,13Z</i>						
1 (bet_car_13_c9m)	-131.7	-136.6	-159.2	-164.0	-167.0	-171.9
2 (Bet_car_030)	-122.5	-128.1			-157.1	-162.6
3 (Car_H_002)	-120.9	-124.9	-146.5	-150.4	-156.8	-160.7
4 (bet_car_13_c9m_c1)	-116.6	-121.0	-142.8	-147.2	-157.5	-161.8
5 (Bet_car_025)	-115.4	-119.7	-141.5	-145.8	-156.5	-160.9
6 (bet_car_13_c9m_c2)	-114.8	-120.3	-140.9	-146.4	-154.5	-159.9
<i>all-trans(15E)</i>						
1 (Car_H_021_003)	-131.2	-138.1	-157.6	-164.4	-166.3	-173.2
2 (bet_car_030_004)	-124.6	-132.2		-159.1	-161.7	-169.2
3 (bet_car_030)	-122.9	-129.2	-149.6	-155.8	-161.7	-167.9
4 (bet_car_007)	-118.1	-126.2	-145.3	-153.4	-161.3	-169.4
5 (bet_car_001)	-117.9	-126.4	-145.2	-153.6		
6 (Car_H_045_004)	-116.5	-125.8	-143.4	-152.6		

7 (Bet_car_025)	-116.5	-124.0	-143.5	-151.0	-160.5	-167.9
8 (bet_car_032)	-116.6	-122.8	-143.8	-149.9		
15E,12Z						
1 (car_H_002)	-125.4	-133.2	-151.5	-159.3	-161.1	-168.9
2 (bet_car_12_c9m)	-124.8	-129.4	-150.8	-155.5	-163.1	-167.7
3 (Bet_car_025)	-120.8	-129.0	-147.7	-155.8	-160.8	-168.9
4 (Bet_car_032)	-119.6	-125.6	-146.4	-152.4		
15E,10Z						
1 (Bet_car_030)	-119.7	-125.6	-146.5	-152.4	-152.8	-158.7
2 (bet_car_10_c9m)	-118.6	-123.0	-145.0	-149.5	-150.5	-154.9
3 (Car_H_002)	-117.9	-121.9	-144.4	-148.5	-152.1	-156.1
4 (Bet_car_032)	-112.3	-117.9	-139.4	-145.0		
5 (bet_car_10_c9m_c1)	-112.5	-118.7	-139.3	-145.6		
6 (bet_car_10_c9m_c2)	-112.4	-119.5	-139.6	-146.6		
7 (bet_car_025)	-111.1	-118.9	-137.7	-145.6	-150.6	-158.5
15E,7Z						
1 (Bet_car_032)	-118.1	-122.8	-145.1	-149.8		
2 (Car_H_002)	-116.5	-124.4	-143.3	-151.2	-155.1	-162.9
3 (bet_car_7_c9m_c1)	-111.7	-115.7	-139.3	-143.4	-153.7	-157.7
15E,14Z						
1 (bet_car_14_c9m)	-114.3	-120.3	-140.7	-146.7	-149.2	-155.2
2 (Bet_car_030)	-112.9	-118.1	-139.2	-144.3		
3 (Bet_car_032)	-111.3	-118.3			-147.1	-154.1
4 (bet_car_14_c9m_c2)	-107.2	-113.1	-133.7	-139.6	-148.4	-154.3
5 (Bet_car_025)	-106.2	-113.1	-132.7	-139.6	-148.7	-155.5
15E,11Z						
1 (Bet_car_030)	-112.4	-118.5	-138.3	-144.4	-146.8	-152.9
2 (bet_car_11_c9m)	-111.8	-118.6	-138.1	-144.9	-147.2	-154.0
3 (Bet_car_025)	-106.1	-113.2	-132.3	-139.3	-145.7	-152.7
4 (bet_car_11_c1_c9m)	-105.2	-112.3	-131.1	-138.2	-144.0	-151.1
5 (Bet_car_032)	-104.3	-112.7				

Table S19b. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C9-Me radical) from the *15E* isomer (Conformational Restriction).

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C9-Me-radical				
<i>15E,9Z</i>	-173.0	-177.7	-179.7	-185.6
<i>15E,8Z</i>	-179.4	-183.9	-187.3	-188.0
<i>15E,13Z</i>	-163.4	-169.2	-171.8	-176.3
<i>15E</i>	-161.7	-168.9	-173.1	-179.9
<i>15E,12Z</i>	-165.7	-171.1	-177.5	-176.0
<i>15E,10Z</i>	-167.5	-174.3	-173.2	-178.5
<i>15E,7Z</i>	-166.5	-173.7	-173.8	-181.4
<i>15E,14Z</i>	-161.1	-167.5	-169.7	-176.3
<i>15E,11Z</i>	-159.9	-165.7	-167.5	-173.5

Table S19c. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C9-Me radical) from the *15E* isomer obtained by Boltzmann Averaging.

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C9-Me-radical				
<i>15E,9Z</i>	-173.5	-178.0	-180.0	-185.3
<i>15E,8Z</i>	-179.5	-184.4	-187.1	-189.0
<i>15E,13Z</i>	-164.7	-170.0	-171.9	-176.5
<i>15E</i>	-158.2	-165.1	-164.9	-171.7
<i>15E,12Z</i>	-166.0	-170.7	-177.5	-178.2
<i>15E,10Z</i>	-167.3	-173.3	-173.4	-178.7
<i>15E,7Z</i>	-166.1	-174.0	-173.9	-182.6
<i>15E,14Z</i>	-161.9	-168.1	-170.3	-177.2
<i>15E,11Z</i>	-160.6	-166.4	-167.7	-173.8

Table S20a. Energetics [Hartrees] of the H-atom abstraction reactions (C9Me radical) from *15Z* isomer in gas phase.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C9-Me-radical									
<i>15Z,9Z</i>									
1 (bet_car_9_15_c9m)	-1557.2648921	-1556.373944	-1556.505656	-1557.6698171	-1556.778869	-1556.910581	-1557.606135	-1556.715187	-1556.846899
2 (Car_H_021_cis)	-1557.2643917	-1556.373412	-1556.504321	-1557.669199	-1556.7782193	-1556.9091283	-1557.6061185	-1556.7151388	-1556.8460478
3 (bet_car_9_15_c9m_c1)	-1557.2627658	-1556.371337	-1556.502541	-1557.6677584	-1556.77633	-1556.907534	-1557.6061905	-1556.714762	-1556.845966
4 (bet_car_9_15_c9m_c2)	-1557.2618988	-1556.370611	-1556.502374	-1557.6668212	-1556.7755334	-1556.907296	-1557.6058336	-1556.714546	-1556.846309
5 (Bet_car_025_cis)	-1557.2613614	-1556.369943	-1556.501688	-1557.6661655	-1556.7747471	-1556.9064921	-1557.6054171	-1556.7139987	-1556.8457437
<i>15Z,8Z</i>									
1 (bet_car_8_15_c9m)	-1557.2638085	-1556.372802	-1556.504469	-1557.6686151	-1556.7776086	-1556.909275	-1557.6057812	-1556.714775	-1556.846442
2 (Car_H_021_cis)	-1557.2632527	-1556.372198	-1556.504225	-1557.6679741	-1556.7769194	-1556.9089464	-1557.6053378	-1556.7142831	-1556.8463101
3 (bet_car_8_15_c9m_c2)	-1557.2616338	-1556.370330	-1556.502721	-1557.6665316	-1556.7752278	-1556.907618	-1557.605976	-1556.714672	-1556.847063
4 (bet_car_8_15_c9m_c1)	-1557.260771	-1556.369310	-1556.501273				-1557.6051985	-1556.713738	-1556.845701
5 (Bet_car_025_cis)	-1557.2603906	-1556.368867	-1556.500556	-1557.6651936	-1556.77367	-1556.905359	-1557.6050276	-1556.713504	-1556.845193
<i>15Z,12Z</i>									
1 (bet_car_12_15_c9m)	-1557.259006	-1556.368446	-1556.500976	-1557.6636519	-1556.773092	-1556.905622	-1557.6006018	-1556.710041	-1556.842571
2 (Car_H_021_cis)	-1557.258855	-1556.368071	-1556.499062	-1557.6633439	-1556.7725599	-1556.9035509	-1557.6008765	-1556.7100925	-1556.8410835
3 (Car_H_002_cis)	-1557.2584108	-1556.367582	-1556.498344	-1557.662865	-1556.7720362	-1556.9027982	-1557.6005984	-1556.7097696	-1556.8405316
4 (bet_car_12_15_c9m_c1)	-1557.2559532	-1556.364913	-1556.496484	-1557.6603479	-1556.769308	-1556.900879	-1557.5991608	-1556.7081206	-1556.8396916
5 (Bet_car_025)	-1557.2555341	-1556.364338	-1556.496390	-1557.6599879	-1556.7687918	-1556.9008438	-1557.5994865	-1556.7082904	-1556.8403424
<i>15,15'-cis (15Z)</i>									
1 (Bet_025_cis_003)	-1557.2577316	-1556.366744	-1556.499667	-1557.6622335	-1556.771246	-1556.904169	-1557.6029965	-1556.712009	-1556.844932
2 (Car_H_021_cis)	-1557.2572056	-1556.366374	-1556.498393	-1557.661711	-1556.7708794	-1556.9028984	-1557.5998346	-1556.709003	-1556.841022
3 (Car_H_002_cis)	-1557.256588	-1556.365835	-1556.498741	-1557.6610086	-1556.7702556	-1556.9031616	-1557.600016	-1556.709263	-1556.842169
<i>15Z,13Z</i>									
1 (bet_car_13_15_c9m)	-1557.2575238	-1556.367078	-1556.498926	-1557.6620183	-1556.771573	-1556.903421	-1557.5997422	-1556.7092964	-1556.8411444
2 (Car_H_002_cis)	-1557.2565485	-1556.366096	-1556.498162	-1557.660867	-1556.7704145	-1556.9024805	-1557.5994086	-1556.7089561	-1556.8410221
3 (Bet_car_001_cis)	-1557.2551847	-1556.364521	-1556.498039	-1557.6597529	-1556.7690892	-1556.9026072	-1557.5995	-1556.7088363	-1556.8423543
4 (bet_car_13_15_c9m_c2)	-1557.254518	-1556.363723	-1556.496125				-1557.5991586	-1556.7083636	-1556.8407656

5 (Bet_car_025_cis)	-1557.2539901	-1556.363079	-1556.494623				-1557.5990405	-1556.7081294	-1556.8396734
15Z,10Z									
1 (car_H_021_cis)	-1557.2563564	-1556.365227	-1556.496238	-1557.6609746	-1556.7698452	-1556.9008562	-1557.5980473	-1556.7069179	-1556.8379289
2 (bet_car_10_15_c9m)	-1557.2560613	-1556.365025	-1556.496476	-1557.6586332	-1556.767597	-1556.899048	-1557.5974514	-1556.706415	-1556.837866
3 (Car_H_002_cis)	-1557.2559156	-1556.364789	-1556.496473	-1557.6604725	-1556.7693459	-1556.9010299	-1557.5980602	-1556.7069336	-1556.8386176
4 (bet_car_10_15_c9m_c2)	-1557.2540299	-1556.362565	-1556.494788	-1557.6588319	-1556.767367	-1556.89959	-1557.5978574	-1556.7063925	-1556.8386155
5 (bet_car_10_15_c9m_c1)	-1557.2539502	-1556.362596	-1556.494665	-1557.6586332	-1556.767279	-1556.899348	-1557.5975253	-1556.7061711	-1556.8382401
6 (Bet_car_025)	-1557.2534939	-1556.361997	-1556.493443	-1557.6581842	-1556.7666873	-1556.8981333	-1557.5974247	-1556.7059278	-1556.8373738
15Z,7Z									
1 (bet_car_7_15_c9m)	-1557.2556456	-1556.364893	-1556.496059	-1557.6605695	-1556.769817	-1556.900983	-1557.5987043	-1556.707952	-1556.839118
2 (Car_H_021_cis)	-1557.2550633	-1556.364237	-1556.495728	-1557.6597641	-1556.7689378	-1556.9004288	-1557.5982525	-1556.7074262	-1556.8389172
3 (Car_H_002_cis)	-1557.2550493	-1556.364293	-1556.496614	-1557.6597056	-1556.7689493	-1556.9012703	-1557.5984427	-1556.7076864	-1556.8400074
4 (bet_car_7_15_c9m_c1)	-1557.2535899	-1556.362277	-1556.492895	-1557.6584513	-1556.7671384	-1556.897756	-1557.5986772	-1556.707364	-1556.837982
5 (Bet_car_025_cis)	-1557.2533157	-1556.362193	-1556.493154				-1557.5990306	-1556.7079079	-1556.8388689
15Z,11Z									
1 (bet_car_11_15_c9m)	-1557.253502	-1556.362578	-1556.493607	-1557.65805	-1556.767126	-1556.898155			
2 (Car_H_002_cis)	-1557.253201	-1556.362150	-1556.492614	-1557.6574556	-1556.7664046	-1556.8968686	-1557.5957858	-1556.7047348	-1556.8351988
3 (bet_car_11_15_c9m_c1)	-1557.2520423	-1556.360535	-1556.492029	-1557.6565486	-1556.765041	-1556.896535	-1557.5959582	-1556.7044509	-1556.8359449
4 (bet_car_11_15_c9m_c2)	-1557.2512462	-1556.359883	-1556.491468	-1557.6557232	-1556.76436	-1556.895945	-1557.5959426	-1556.7045794	-1556.8361644
Bet_car (closed shell)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509
H2O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362

Table S20b: Boltzmann Averaged energy of the *15Z* isomer and their rotamers of C9-Me radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15Z,9Z</i>	-1556.778623	-1556.910374	-1556.714909	-1556.846551
<i>15Z,8Z</i>	-1556.777379	-1556.908982	-1556.714579	-1556.846696
<i>15Z,12Z</i>	-1556.773025	-1556.905591	-1556.709819	-1556.842441
<i>15Z</i>	-1556.770952	-1556.903747	-1556.711759	-1556.844736
<i>15Z,13Z</i>	-1556.771193	-1556.903035	-1556.708905	-1556.840901
<i>15Z,10Z</i>	-1556.769327	-1556.900562	-1556.706600	-1556.838292
<i>15Z,7Z</i>	-1556.769472	-1556.901102	-1556.707780	-1556.839496
<i>15Z,11Z</i>	-1556.766689	-1556.897611	-1556.704603	-1556.835922

Table S21a. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C9-Me radical) from the *15Z* isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C9-Me-radical						
<i>15Z,9Z</i>						
1 (bet car 9 15 c9m)	-128.9	-135.5	-156.5	-163.1	-161.9	-168.5
2 (Car H 021 cis)	-127.5	-132.0				
3 (bet car 9 15 c9m c1)	-122.1	-127.3	-149.8	-155.1	-160.8	-166.1
4 (bet car 9 15 c9m c2)	-120.2	-126.9	-147.7	-154.5	-160.3	-167.0
5 (Bet car 025 cis)	-118.4	-125.1				
<i>15Z,8Z</i>						
1 (bet car 8 15 c9m)	-125.9	-132.4	-153.2	-159.7	-160.9	-167.3
2 (Car H 021 cis)	-124.3	-131.8				
3 (bet car 8 15 c9m c2)	-119.4	-127.8	-146.9	-155.4	-160.6	-168.9
4 (bet car 8 15 c9m c1)	-116.7	-124.0			-158.1	-165.4
5 (Bet car 025 cis)	-115.6	-122.1	-142.8	-149.4		
<i>15Z,12Z</i>						
1 (bet car 12 15 c9m)	-114.5	-123.2	-141.3	-150.1	-148.4	-157.2
2 (Car H 021 cis)	-113.5	-118.2				
3 (Car H 002 cis)	-112.2	-116.3				
4 (bet car 12 15 c9m c1)	-105.2	-111.5	-131.4	-137.7	-143.4	-149.6
5 (Bet car 025)	-103.7	-111.2				
<i>15,15'-cis (15Z)</i>						
1 (Bet 025 cis 003)	-110.0	-119.8	-136.5	-146.3	-153.6	-163.4
2 (Car H 021 cis)	-109.0	-116.5	-135.5	-142.9	-145.7	-153.1
3 (Car H 002 cis)	-107.6	-117.4	-133.9	-143.6	-146.4	-156.1
<i>15Z,13Z</i>						
1 (bet car 13 15 c9m)	-110.9	-117.9	-137.4	-144.3	-146.5	-153.5
2 (Car H 002 cis)	-108.3	-115.9	-134.3	-141.9	-145.6	-153.1
3 (Bet car 001 cis)	-104.2	-115.5	-130.8	-142.2		
4 (bet car 13 15 c9m c2)	-102.1	-110.5			-144.0	-152.4

5 (Bet car 025 cis)	-100.4	-106.6			-143.4	-149.6
15Z,10Z						
1 (car H 021 cis)	-106.0	-110.8	-132.8	-137.6	-140.2	-145.0
2 (bet car 10 15 c9m)	-105.5	-111.4	-126.9	-132.8	-138.9	-144.8
3 (Car H 002 cis)	-104.9	-111.4	-131.5	-138.1	-140.3	-146.8
4 (bet car 10 15 c9m c2)	-99.0	-107.0	-126.3	-134.3	-138.8	-146.8
5 (bet car 10 15 c9m c1)	-99.1	-106.7	-126.1	-133.6	-138.3	-145.8
6 (Bet car 025)	-97.5	-103.5	-124.5	-130.5	-137.6	-143.5
15Z,7Z						
1 (bet car 7 15 c9m)	-105.2	-110.3	-132.7	-137.9	-142.9	-148.1
2 (Car H 021 cis)	-103.4	-109.5				
3 (Car H 002 cis)	-103.6	-111.8	-130.5	-138.7	-142.3	-150.5
4 (bet car 7 15 c9m c1)	-98.3	-102.0	-125.7	-129.5	-141.4	-145.1
5 (Bet car 025 cis)	-98.1	-102.7			-142.8	-147.5
15Z,11Z						
1 (bet car 11 15 c9m)	-99.1	-103.9	-125.7	-130.5		
2 (Car H 002 cis)	-97.9	-101.3	-123.8	-127.1	-134.5	-137.8
3 (bet car 11 15 c9m c1)	-93.7	-99.7	-120.2	-126.3	-133.7	-139.8
4 (bet car 11 15 c9m c2)	-92.0	-98.3	-118.4	-124.7	-134.1	-140.4

Table S21b. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C9-Me radical) from the *15Z* isomer (Conformational Restriction).

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C9-Me-radical				
<i>15Z,9Z</i>	-170.3	-178.1	-178.3	-185.1
<i>15Z,8Z</i>	-176.6	-182.4	-184.5	-189.7
<i>15Z,12Z</i>	-165.9	-170.4	-174.5	-178.6
<i>15Z</i>	-146.9	-158.1	-162.6	-173.1
<i>15Z,13Z</i>	-152.0	-158.5	-160.2	-166.7
<i>15Z,10Z</i>	-163.8	-170.2	-172.8	-179.1
<i>15Z,7Z</i>	-164.1	-169.9	-171.0	-176.9
<i>15Z,11Z</i>	-157.3	-163.8	-165.1	-170.4

Table S21c. Relative enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C9-Me radical) from the *15Z* isomer obtained by Boltzmann averaging of the conformers

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C9-Me-radical				
<i>15Z,9Z</i>	-171.1	-179.4	-178.4	-184.7
<i>15Z,8Z</i>	-177.4	-182.9	-185.2	-189.7
<i>15Z,12Z</i>	-167.2	-171.9	-174.6	-179.4
<i>15Z</i>	-147.4	-157.5	-163.1	-173.1
<i>15Z,13Z</i>	-152.5	-158.9	-160.4	-167.0
<i>15Z,10Z</i>	-163.8	-170.5	-172.0	-179.1
<i>15Z,7Z</i>	-164.5	-170.3	-171.1	-176.8
<i>15Z,11Z</i>	-157.6	-163.4	-165.6	-170.5

Table S22a. Energetics [Hartrees] of the H-atom abstraction reactions (C7 radical) from *15E* isomer.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C7-radical									
<i>15E,7Z</i>									
1 (Car_H_021)	-1557.2434598	-1556.352407	-1556.485753	-1557.6472025	-1556.7561497	-1556.8894957	-1557.5831821	-1556.6921293	-1556.8254753
2 (bet_car_7_c7)	-1557.2432731	-1556.352257	-1556.486081	-1557.6469172	-1556.755901	-1556.889725	-1557.5834891	-1556.692473	-1556.826297
3 (Bet_Car_030)	-1557.2432645	-1556.352274	-1556.486077	-1557.6469496	-1556.7559591	-1556.8897621			
4 (Car_H_002)	-1557.2428308	-1556.351716	-1556.484203						
<i>all-trans</i>									
1 (bet_car_030_004)	-1557.2433388	-1556.352386	-1556.486049	-1557.6470565	-1556.7561037	-1556.8897667	-1557.5829842	-1556.6920314	-1556.8256944
2 (Car_H_021)	-1557.243243	-1556.352306	-1556.486945	-1557.6472025	-1556.7562655	-1556.8909045	-1557.5833434	-1556.6924064	-1556.8270454
3 (Car_H_021_004)	-1557.2428962	-1556.351840	-1556.484661	-1557.6465392	-1556.755483	-1556.888304	-1557.5827891	-1556.691733	-1556.824554
4 (Car_H_002)	-1557.2428451	-1556.351799	-1556.484628	-1557.6464526	-1556.7554065	-1556.8882355			
5 (Car_H_045_003)	-1557.2409597	-1556.349528	-1556.483730	-1557.6448045	-1556.753373	-1556.887575	-1557.5827499	-1556.691318	-1556.82552
6 (bet_car_025)	-1557.2408327	-1556.349390	-1556.483605	-1557.6445867	-1556.753144	-1556.887359	-1557.5829179	-1556.6914752	-1556.8256902
<i>15E,9Z</i>									
1 (bet_car_9_c7_c2)	-1557.2421949	-1556.351169	-1556.483387	-1557.6458914	-1556.7548655	-1556.8870835			
2 (Car_H_021)	-1557.2420615	-1556.351072	-1556.484167	-1557.645661	-1556.7546715	-1556.8877665	-1557.5813706	-1556.6903811	-1556.8234761
3 (bet_car_9_c7)	-1557.2419973	-1556.351057	-1556.484684	-1557.6456287	-1556.754688	-1556.888315	-1557.5807403	-1556.6898	-1556.823427
4 (Car_H_002)	-1557.241574	-1556.350672	-1556.483017	-1557.6450824	-1556.7541804	-1556.8865254	-1557.5814091	-1556.6905071	-1556.8228521
5 (bet_car_9_c7_c1)	-1557.2397001	-1556.348328	-1556.481334	-1557.6434946	-1556.752123	-1556.885129	-1557.5810495	-1556.689677	-1556.822683
6 (Bet_car_025)	-1557.2396017	-1556.348250	-1556.481464	-1557.6433321	-1556.7519804	-1556.8851944	-1557.5814132	-1556.6900615	-1556.8232755
<i>15E,13Z</i>									
1 (bet_car_13_c7_c2)	-1557.241846	-1556.350908	-1556.483894	-1557.64557	-1556.754632	-1556.887618	-1557.580802	-1556.689864	-1556.82285
2 (bet_car_13_c7)	-1557.2418374	-1556.350896	-1556.484618	-1557.6455702	-1556.754629	-1556.888351	-1557.5809116	-1556.68997	-1556.823692
3 (Bet_car_030)	-1557.2417698	-1556.350834	-1556.483978	-1557.6454346	-1556.7544988	-1556.8876428	-1557.5812997	-1556.6903639	-1556.8235079
4 (Car_H_002)	-1557.2412992	-1556.350252	-1556.482364	-1557.6448633	-1556.7538161	-1556.8859281	-1557.5813517	-1556.6903045	-1556.8224165
5 (bet_car_13_c7_c1)	-1557.2393684	-1556.347895	-1556.480532	-1557.6431971	-1556.751723	-1556.884360	-1557.5808256	-1556.689352	-1556.821989
6 (Bet_Car_025)	-1557.2393093	-1556.347804	-1556.480592	-1557.6430793	-1556.751574	-1556.884362	-1557.5814226	-1556.6899173	-1556.8227053
<i>15E,8Z</i>									

1 (bet_car_8_c7)	-1557.2391817	-1556.348346	-1556.482020	-1557.6429354	-1556.7521	-1556.885774	-1557.5782487	-1556.687413	-1556.821087
2 (bet_car_8_c7_c1)	-1557.2391814	-1556.348345	-1556.482023	-1557.642936	-1556.7521	-1556.885778	-1557.5782524	-1556.687416	-1556.821094
3 (Bet_car_030)	-1557.2391067	-1556.348325	-1556.482441	-1557.6427461	-1556.7519644	-1556.8860804	-1557.5775078	-1556.6867261	-1556.8208421
4 (Car_H_021)	-1557.2390622	-1556.348264	-1556.482055	-1557.6426801	-1556.7518819	-1556.8856729	-1557.5778715	-1556.6870733	-1556.8208643
5 (Car_H_002)	-1557.2385042	-1556.347679	-1556.481685	-1557.6420542	-1556.751229	-1556.885235	-1557.5774274	-1556.6866022	-1556.8206082
6 (bet_car_8_c7_c2)	-1557.2367134	-1556.345511	-1556.479422	-1557.6406072	-1556.749405	-1556.883316	-1557.5780485	-1556.686846	-1556.820757
7 (Bet_car_025)	-1557.2366273	-1556.345403	-1556.479633	-1557.6403355	-1556.7491112	-1556.8833412	-1557.5774164	-1556.6861921	-1556.8204221
15E,12Z									
1 (Bet_car_032)	-1557.2381144	-1556.347320	-1556.481109	-1557.6416617	-1556.7508673	-1556.8846563	-1557.5770564	-1556.686262	-1556.820051
2 (bet_car_12_c7_c1)	-1557.2380136	-1556.347256	-1556.481267	-1557.6415359	-1556.750778	-1556.884789	-1557.5770342	-1556.6862766	-1556.8202876
3 (bet_car_12_c7)	-1557.2379494	-1556.347256	-1556.481560	-1557.6414598	-1556.750766	-1556.88507	-1557.5762792	-1556.6855858	-1556.8198898
4 (Car_H_002)	-1557.2373227	-1556.346602	-1556.481604	-1557.6406341	-1556.7499134	-1556.8849154	-1557.576948	-1556.6862273	-1556.8212293
5 (Bet_car_025)	-1557.235469	-1556.344337	-1556.479917				-1557.5768722	-1556.6857402	-1556.8213202
15E,10Z									
1 (bet_car_10_c7)	-1557.236543	-1556.345347	-1556.477985	-1557.6400887	-1556.748893	-1556.881531	-1557.5759542	-1556.6847582	-1556.8173962
2 (bet_car_10_c7_c2)	-1557.2365429	-1556.345349	-1556.478001	-1557.6400893	-1556.748895	-1556.881547	-1557.5759527	-1556.684759	-1556.817411
3 (bet_car_10_c7_c1)	-1557.2340114	-1556.342501	-1556.476408	-1557.6376763	-1556.746166	-1556.880073	-1557.5758668	-1556.6843564	-1556.8182634
15E,14Z									
1 (bet_car_14_c7_c1)	-1557.2358798	-1556.344759	-1556.478416	-1557.6394616	-1556.748340	-1556.881997			
2 (bet_car_14_c7)	-1557.2358791	-1556.344758	-1556.478459	-1557.6394613	-1556.74834	-1556.882041			
3 (bet_car_14_c7_c2)	-1557.2335332	-1556.341812	-1556.475234	-1557.6371726	-1556.745451	-1556.878873	-1557.5751062	-1556.683385	-1556.816807
15E,11Z									
1 (bet_car_11_c7)	-1557.2356458	-1556.344318	-1556.477932	-1557.6393701	-1556.748042	-1556.881656	-1557.5755256	-1556.6841978	-1556.8178118
2 (bet_car_11_c1_c7)	-1557.2333796	-1556.341423	-1556.474264	-1557.6372271	-1556.745271	-1556.878112			
Bet_car (closed shell)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509
H2O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362

Table S22b: Boltzmann Averaged energy of the *15E* isomer and their rotamers of C7 radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15E,7Z</i>	-1556.756016	-1556.889675	-1556.692332	-1556.826055
<i>15E</i>	-1556.755658	-1556.889126	-1556.691960	-1556.826401
<i>15E,9Z</i>	-1556.75458	-1556.887763	-1556.690192	-1556.82324
<i>15E,13Z</i>	-1556.75442	-1556.887873	-1556.690067	-1556.823209
<i>15E,8Z</i>	-1556.751879	-1556.885707	-1556.687062	-1556.820862
<i>15E,12Z</i>	-1556.750704	-1556.884883	-1556.686101	-1556.820926
<i>15E,10Z</i>	-1556.74882	-1556.881399	-1556.68466	-1556.81788
<i>15E,14Z</i>	-1556.748274	-1556.881964	-1556.683385	-1556.816807
<i>15E,11Z</i>	-1556.747902	-1556.881575	-1556.6841978	-1556.8178118

Table S23a. Enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C7 radical) from *15E* isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C7-radical						
<i>15E,7Z</i>						
1 (Car H 021)	-72.4	-83.3	-96.9	-107.8	-101.4	-112.3
2 (bet car 7 c7)	-71.9	-84.1	-96.2	-108.4	-102.3	-114.5
3 (Bet Car 030)	-72.0	-84.1	-96.4	-108.5		
4 (Car H 002)	-70.6	-79.2				
<i>all-trans</i>						
1 (bet car 030 004)	-72.3	-84.0	-96.7	-108.5	-101.1	-112.9
2 (Car H 021)	-72.1	-86.4			-102.1	-116.4
3 (Car H 021 004)	-70.9	-80.4	-95.1	-104.6	-100.4	-109.8
4 (Car H 002)	-70.8	-80.3	-94.9	-104.5		
5 (Car H 045 003)	-64.8	-77.9	-89.6	-102.7	-99.3	-112.4
6 (bet car 025)	-64.4	-77.6	-88.9	-102.2	-99.7	-112.8
<i>15E,9Z</i>						
1 (bet car 9 c7 c2)	-69.1	-77.1	-93.5	-101.4		
2 (Car H 021)	-68.9	-79.1	-92.9	-103.2	-96.8	-107.1
3 (bet car 9 c7)	-68.8	-80.5	-93.0	-104.7	-95.3	-106.9
4 (Car H 002)	-67.8	-76.1	-91.7	-99.9	-97.1	-105.4
5 (bet car 9 c7 c1)	-61.7	-71.7	-86.3	-96.3	-94.9	-104.9
6 (Bet car 025)	-61.5	-72.0	-85.9	-96.5	-95.9	-106.5
<i>15E,13Z</i>						
1 (bet car 13 c7 c2)	-68.4	-78.4	-92.9	-102.8	-95.4	-105.4
2 (bet car 13 c7)	-68.4	-80.3	-92.8	-104.7	-95.7	-107.6
3 (Bet car 030)	-68.2	-78.6	-92.5	-102.9	-96.8	-107.1
4 (Car H 002)	-66.7	-74.4	-90.7	-98.4	-96.6	-104.3
5 (bet car 13 c7 c1)	-60.5	-69.6	-85.2	-94.3	-94.1	-103.2
6 (Bet Car 025)	-60.3	-69.7	-84.8	-94.3	-95.6	-105.0
<i>15E,8Z</i>						
1 (bet car 8 c7)	-61.7	-73.5	-86.2	-98.0	-89.0	-100.8

2 (bet car 8 c7 c1)	-61.7	-73.5	-86.2	-98.0	-89.0	-100.8
3 (Bet car 030)	-61.6	-74.6	-85.8	-98.8	-87.2	-100.1
4 (Car H 021)	-61.5	-73.6	-85.7	-97.7	-88.1	-100.2
5 (Car H 002)	-59.9	-72.6	-83.9	-96.6	-86.9	-99.5
6 (bet car 8 c7 c2)	-54.3	-66.6	-79.2	-91.5	-87.5	-99.9
7 (Bet car 025)	-53.9	-67.2	-78.4	-91.6	-85.8	-99.0
15E,12Z						
1 (Bet car 032)	-59.0	-71.1	-82.9	-95.1	-86.0	-98.1
2 (bet car 12 c7 c1)	-58.8	-71.5	-82.7	-95.4	-86.0	-98.7
3 (bet car 12 c7)	-58.8	-72.3	-82.7	-96.1	-84.2	-97.6
4 (Car H 002)	-57.1	-72.4	-80.5	-95.7	-85.9	-101.2
5 (Bet car 025)	-51.2	-67.9			-84.6	-101.4
15E,10Z						
1 (bet car 10 c7)	-53.8	-62.9	-77.8	-86.9	-82.0	-91.1
2 (bet car 10 c7 c2)	-53.8	-62.9	-77.8	-86.9	-82.0	-91.1
3 (bet car 10 c7 c1)	-46.4	-58.7	-70.6	-83.0	-80.9	-93.4
15E,14Z						
1 (bet car 14 c7 c1)	-52.3	-64.0	-76.4	-88.1		
2 (bet car 14 c7)	-52.3	-64.1	-76.4	-88.2		
3 (bet car 14 c7 c2)	-44.5	-55.7	-68.8	-79.9	-78.4	-89.5
15E,11Z						
1 (bet car 11 c7)	-51.1	-62.7	-75.6	-87.2	-80.6	-92.2
2 (bet car 11 c1 c7)	-43.5	-53.1	-68.3	-77.9		

Table S23b. Enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C7 radical) from *15E* isomer (Conformational restriction).

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C7-radical				
<i>15E,7Z</i>	-118.2	-130.9	-121.1	-132.9
<i>15E</i>	-96.7	-108.5	-101.3	-115.9
<i>15E,9Z</i>	-97.6	-109.1	-103.6	-113.9
<i>15E,13Z</i>	-97.1	-110.0	-101.5	-112.0
<i>15E,8Z</i>	-99.5	-110.5	-102.9	-109.1
<i>15E,12Z</i>	-97.1	-107.9	-100.4	-108.5
<i>15E,10Z</i>	-98.8	-108.8	-102.4	-113.2
<i>15E,14Z</i>	-96.8	-109.0	-98.9	-110.4
<i>15E,11Z</i>	-97.2	-108.0	-100.9	-111.7

Table S23c. Enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C7 radical) from *15E* isomer obtained from Boltzmann averaging of the conformers

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C7-radical				
<i>15E,7Z</i>	-118.4	-131.7	-121.2	-134.0
<i>15E</i>	-97.2	-108.6	-101.2	-115.0
<i>15E,9Z</i>	-98.4	-109.2	-103.7	-114.1
<i>15E,13Z</i>	-98.0	-109.6	-101.6	-111.7
<i>15E,8Z</i>	-100.3	-111.0	-103.1	-110.9
<i>15E,12Z</i>	-97.9	-108.4	-100.9	-110.0
<i>15E,10Z</i>	-99.9	-109.4	-103.2	-113.2
<i>15E,14Z</i>	-98.3	-110.5	-100.1	-111.8
<i>15E,11Z</i>	-98.1	-109.2	-101.8	-112.9

Table S24a. Energetics [Hartrees] of the H-atom abstraction reactions (C7 radical) from *15Z* isomer in gas phase.

Isomers	Gas phase						Solvent phase		
	B3LYP/SB			B3LYP/MB			B3LYP/MB		
	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈	E _{Tot}	H ₂₉₈	G ₂₉₈
C7-radical									
<i>15,15'-cis (15Z)</i>									
1 (bet_car_trans)	-1557.2394484	-1556.348264	-1556.481753	-1557.6435231	-1556.7523387	-1556.8858277	-1557.579735	-1556.6885506	-1556.8220396
2 (Car_H_021_cis)	-1557.2388251	-1556.347703	-1556.482387	-1557.642789	-1556.7516669	-1556.8863509	-1557.5792035	-1556.6880814	-1556.8227654
3 (bet_car_001_cis)	-1557.2369576	-1556.345394	-1556.480010	-1557.6411302	-1556.7495666	-1556.8841826			
4 (Bet_025_cis_004)	-1557.236826	-1556.345246	-1556.479878	-1557.6409243	-1556.749344	-1556.883976	-1557.5797234	-1556.688143	-1556.822775
<i>15Z,7Z</i>									
1 (Car_H_021_cis)	-1557.2386978	-1556.347575	-1556.482681				-1557.5795582	-1556.6884354	-1556.8235414
2 (bet_car_7_15_c7_c1)	-1557.236826	-1556.345242	-1556.478935	-1557.6409141	-1556.749330	-1556.883023	-1557.5796457	-1556.688062	-1556.821755
<i>15Z,9Z</i>									
1 (bet_car_9_15_c7)	-1557.2381508	-1556.347019	-1556.479904	-1557.6421266	-1556.750995	-1556.88388	-1557.5783281	-1556.687196	-1556.820081
2 (bet_car_9_15_c7_c2)	-1557.2381506	-1556.347017	-1556.479890	-1557.6421251	-1556.7509915	-1556.8838645	-1557.5783315	-1556.687198	-1556.820071
3 (Car_H_021_cis)	-1557.2376608	-1556.346443	-1556.478980	-1557.6415417	-1556.7503239	-1556.8828609	-1557.5783855	-1556.6871677	-1556.8197047
4 (Car_H_002_cis)	-1557.2375361	-1556.346376	-1556.479464	-1557.6413232	-1556.7501631	-1556.8832511	-1557.5787086	-1556.6875485	-1556.8206365
5 (bet_car_9_15_c7_c1)	-1557.2357424	-1556.343980	-1556.476553	-1557.6398311	-1556.748069	-1556.880642	-1557.5785425	-1556.68678	-1556.819353
<i>15Z,13Z</i>									
1 (bet_car_13_15_c7)	-1557.2378659	-1556.346573	-1556.479207	-1557.6418946	-1556.750601	-1556.883235	-1557.5776891	-1556.6863962	-1556.8190302
2 (Car_H_021_cis)	-1557.2373213	-1556.346076	-1556.479133	-1557.6412399	-1556.7499946	-1556.8830516	-1557.5776626	-1556.6864173	-1556.8194743
3 (Car_H_002_cis)	-1557.2372086	-1556.346026	-1556.479581	-1557.6410474	-1556.7498648	-1556.8834198	-1557.5783058	-1556.6871232	-1556.8206782
4 (bet_car_13_15_c7_c1)	-1557.2353714	-1556.343742	-1556.477150	-1557.6395018	-1556.747872	-1556.881280	-1557.5778288	-1556.6861994	-1556.8196074
<i>15Z,8Z</i>									
1 (bet_car_8_15_c7)	-1557.2351718	-1556.344145	-1556.477515	-1557.6392906	-1556.748264	-1556.881634	-1557.5743012	-1556.683274	-1556.816644
2 (Car_H_021_cis)	-1557.2346067	-1556.343523	-1556.477077	-1557.6386293	-1556.7475456	-1556.8810996	-1557.5740753	-1556.6829916	-1556.8165456
3 (Car_H_002_cis)	-1557.2344864	-1556.343486	-1556.477882	-1557.6383714	-1556.747371	-1556.881767	-1557.5736866	-1556.6826862	-1556.8170822
4 (bet_car_8_15_c7_c2)	-1557.2327695	-1556.341300	-1556.474758	-1557.6369884	-1556.745519	-1556.878977	-1557.5742532	-1556.682784	-1556.816242
<i>15Z,12Z</i>									
1 (bet_car_12_15_c7)	-1557.2340839	-1556.343091	-1556.477542	-1557.6378881	-1556.746895	-1556.881346	-1557.5728601	-1556.6818672	-1556.8163182
2 (bet_car_12_15_c7_c1)	-1557.2340838	-1556.343092	-1556.477544	-1557.6378888	-1556.746897	-1556.881349	-1557.5728603	-1556.6818685	-1556.8163205

3 (Car_H_021_cis)	-1557.2335633	-1556.342549	-1556.476876	-1557.6372636	-1556.7462493	-1556.8805763	-1557.573175	-1556.6821607	-1556.8164877
4 (Car_H_002_cis)	-1557.2334266	-1556.342559	-1556.477365	-1557.6370584	-1556.7461908	-1556.8809968	-1557.573369	-1556.6825014	-1556.8173074
5 (bet_car_12_15_c7_c2)	-1557.2316408	-1556.340279	-1556.475363	-1557.6355601	-1556.744198	-1556.879282	-1557.5724618	-1556.6811	-1556.816184
15Z,10Z									
1 (bet_car_10_15_c7)	-1557.2325734	-1556.341161	-1556.473120	-1557.6364752	-1556.745062	-1556.877021	-1557.5724345	-1556.6810221	-1556.8129811
2 (Car_H_021_cis)	-1557.2321616	-1556.340920	-1556.473897	-1557.6359008	-1556.7446592	-1556.8776362	-1557.5717986	-1556.680557	-1556.813534
3 (Car_H_002_cis)	-1557.2320935	-1556.340818	-1556.473268				-1557.5716254	-1556.6803499	-1556.8127999
4 (bet_car_10_15_c7_c1)	-1557.230104	-1556.338358	-1556.471041	-1557.634082	-1556.742336	-1556.875019	-1557.5722315	-1556.6804855	-1556.8131685
15Z,11Z									
1 (bet_car_11_15_c7)	-1557.2316946	-1556.340124	-1556.474050	-1557.6357862	-1556.744216	-1556.878142			
2 (Car_H_021_cis)	-1557.2312215	-1556.339584	-1556.472975	-1557.6351801	-1556.7435426	-1556.8769336	-1557.5720702	-1556.6804327	-1556.8138237
3 (Car_H_002_cis)	-1557.2311546	-1556.339433	-1556.472048	-1557.6350428	-1556.7433212	-1556.8759362	-1557.5727776	-1556.681056	-1556.813671
4 (bet_car_11_15_c7_c1)	-1557.2291955	-1556.337215	-1556.471972	-1557.6333555	-1556.741375	-1556.876132	-1557.5718326	-1556.6798521	-1556.8146091
Bet_car (closed shell)	-1557.9021944	-1556.997018	-1557.127410	-1558.307148	-1557.401972	-1557.532364	-1558.2441677	-1557.3389913	-1557.4693833
OH	-75.7234548	-75.711846	-75.732093	-75.7623691	-75.7507603	-75.7710073	-75.7633127	-75.7517039	-75.7719509
H2O	-76.408953	-76.384023	-76.405470	-76.4584074	-76.4334774	-76.4549244	-76.4621192	-76.4371892	-76.4586362

Table S24b: Boltzmann Averaged energy of the *15Z* isomer and their rotamers of C7 radical of beta-carotene calculated at B3LYP/6-311++G(d,p) level.

Isomers	Boltzmann Averaged			
	Gas phase		Water Solvent	
	H ₂₉₈	G ₂₉₈	H ₂₉₈	G ₂₉₈
<i>15Z</i>	-1556.751959	-1556.885946	-1556.688307	-1556.822633
<i>15Z,7Z</i>	-1556.749330	-1556.883023	-1556.688285	-1556.823308
<i>15Z,9Z</i>	-1556.75072	-1556.883605	-1556.687239	-1556.820163
<i>15Z,13Z</i>	-1556.750205	-1556.883181	-1556.686683	-1556.820133
<i>15Z,8Z</i>	-1556.747828	-1556.881523	-1556.68299	-1556.816727
<i>15Z,12Z</i>	-1556.746628	-1556.881097	-1556.682093	-1556.816739
<i>15Z,10Z</i>	-1556.744819	-1556.877331	-1556.680678	-1556.813203
<i>15Z,11Z</i>	-1556.743792	-1556.877615	-1556.68069	-1556.814227

Table S25a. Enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C7 radical) from *15Z* isomer (Conformational Mobility).

Isomers	B3LYP/SB		B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C7-radical						
<i>15,15'-cis (15Z)</i>						
1 (bet car trans)	-61.5	-72.8	-86.9	-98.1	-92.0	-103.3
2 (Car H 021 cis)	-60.0	-74.4	-85.1	-99.5	-90.8	-105.2
3 (bet car 001 cis)	-53.9	-68.2	-79.6	-93.8		
4 (Bet 025 cis 004)	-53.6	-67.8	-78.9	-93.3	-90.9	-105.2
<i>15Z,7Z</i>						
1 (Car H 021 cis)	-59.7	-75.2			-91.7	-107.2
2 (bet car 7 15 c7 c1)	-53.6	-65.4	-78.9	-90.8	-90.7	-102.5
<i>15Z,9Z</i>						
1 (bet car 9 15 c7)	-58.2	-67.9	-83.3	-93.0	-88.4	-98.2
2 (bet car 9 15 c7 c2)	-58.2	-67.9	-83.3	-92.9	-88.4	-98.1
3 (Car H 021 cis)	-56.7	-65.5	-81.6	-90.3	-88.4	-97.2
4 (Car H 002 cis)	-56.5	-66.8	-81.1	-91.4	-89.4	-99.6
5 (bet car 9 15 c7 c1)	-50.2	-59.1	-75.6	-84.5	-87.4	-96.2
<i>15Z,13Z</i>						
1 (bet car 13 15 c7)	-57.1	-66.1	-82.3	-91.3	-86.3	-95.4
2 (Car H 021 cis)	-55.7	-65.9	-80.7	-90.8	-86.4	-96.5
3 (Car H 002 cis)	-55.6	-67.1	-80.4	-91.8	-88.3	-99.7
4 (bet car 13 15 c7 c1)	-49.6	-60.7	-75.1	-86.2	-85.8	-96.9
<i>15Z,8Z</i>						
1 (bet car 8 15 c7)	-50.7	-61.6	-76.2	-87.1	-78.1	-89.1
2 (Car H 021 cis)	-49.0	-60.5	-74.3	-85.7	-77.4	-88.9
3 (Car H 002 cis)	-48.9	-62.6	-73.8	-87.5	-76.6	-90.3
4 (bet car 8 15 c7 c2)	-43.2	-54.4	-68.9	-80.2	-76.9	-88.1
<i>15Z,12Z</i>						
1 (bet car 12 15 c7)	-47.9	-61.7	-72.6	-86.4	-74.5	-88.3
2 (bet car 12 15 c7 c1)	-47.9	-61.7	-72.6	-86.4	-74.5	-88.3
3 (Car H 021 cis)	-46.5	-59.9	-70.9	-84.3	-75.2	-88.7

4 (Car_H 002 cis)	-46.5	-61.3	-70.7	-85.4	-76.1	-90.9
5 (bet car 12 15 c7 c2)	-40.5	-56.0	-65.5	-80.9	-72.4	-87.9
<i>15Z,10Z</i>						
1 (bet car 10 15 c7)	-42.8	-50.1	-67.7	-75.0	-72.2	-79.5
2 (Car_H 021 cis)	-42.2	-52.1	-66.7	-76.6	-71.0	-80.9
3 (Car_H 002 cis)	-41.9	-50.5			-70.5	-79.0
4 (bet car 10 15 c7 c1)	-35.5	-44.6	-60.6	-69.7	-70.8	-80.0
<i>15Z,11Z</i>						
1 (bet car 11 15 c7)	-40.1	-52.5	-65.5	-77.9		
2 (Car_H 021 cis)	-38.7	-49.7	-63.7	-74.8	-70.7	-81.7
3 (Car_H 002 cis)	-38.3	-47.3	-63.2	-72.2	-72.3	-81.3
4 (bet car 11 15 c7 c1)	-32.5	-47.1	-58.1	-72.7	-69.2	-83.8

Table S25b. Enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C7 radical) from *15Z* isomer (Conformational Restriction)

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C7-radical				
<i>15Z</i>	-97.2	-111.3	-101.0	-118.9
<i>15Z,7Z</i>	-110.3	-122.1	-119.8	-133.6
<i>15Z,9Z</i>	-97.1	-108.0	-105.7	-116.2
<i>15Z,13Z</i>	-96.9	-105.9	-102.0	-112.9
<i>15Z,8Z</i>	-99.6	-110.2	-101.8	-111.0
<i>15Z,12Z</i>	-97.1	-106.6	-102.2	-112.3
<i>15Z,10Z</i>	-98.7	-109.2	-104.8	-113.3
<i>15Z,11Z</i>	-97.2	-111.3	-102.9	-113.8

Table S25c. Enthalpy, ΔH_{298} and free energy, ΔG_{298} [kJ/mol] of the H-atom abstraction reactions (C7 radical) from *15Z* isomer obtained from Boltzmann averaging of the conformers

Isomers	B3LYP/MB		PCM (Water)	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
C7-radical				
<i>15Z</i>	-97.5	-110.8	-101.6	-115.0
<i>15Z,7Z</i>	-111.6	-122.9	-119.9	-134.3
<i>15Z,9Z</i>	-97.9	-109.1	-105.8	-115.4
<i>15Z,13Z</i>	-97.4	-106.8	-102.1	-112.4
<i>15Z,8Z</i>	-99.8	-110.8	-102.2	-111.1
<i>15Z,12Z</i>	-97.9	-107.6	-101.8	-111.9
<i>15Z,10Z</i>	-99.5	-109.5	-104.0	-113.2
<i>15Z,11Z</i>	-97.5	-110.9	-102.8	-113.6

Table S26. Relative enthalpies (ΔH_{298} , kJ/mol) and free energies (ΔG_{298} , kJ/mol) of the isomers of β -carotene in the gas phase and in water.

Isomers	B3LYP/MB ^(a)		B3LYP/MB ^(b)		B3LYP/MB ^(c)		B3LYP/MB ^(d)	
	Gas phase		Water		Gas phase		Water	
	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}	ΔH_{298}	ΔG_{298}
<i>all-trans (15E)</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>15E,9Z</i>	+4.1	+4.5	+7.1	+7.4	+3.7	+5.2	+3.8	+5.3
<i>15E,13Z</i>	+4.2	+5.2	+4.8	+5.8	+4.2	+5.4	+4.3	+5.5
<i>15E, 9Z,9'Z</i>	+7.0	+6.5	+12.1	+11.5	+7.6	+9.1	+7.7	+9.2
<i>15E,8Z</i>	+13.2	+12.3	+13.9	+13.0	+13.4	+12.2	+13.6	+12.4
<i>15,15'-cis (15Z)</i>	+10.4	+11.9	+9.0	+10.5	+10.7	+12.3	+9.6	+9.3
<i>15Z,9Z</i>	+13.8	+14.9	+16.3	+17.5	+14.0	+16.2	+14.0	+16.2
<i>15Z,13Z</i>	+14.7	+14.1	+13.8	+13.2	+14.3	+14.9	+14.7	+16.1

^(a) B3LYP/MB = B3LYP/6-311++G(d,p)//B3LYP/6-31G(d); ^(b) Geometries optimized at B3LYP/6-31G(d) level in the gas phase and energetics in water are obtained from these gas phase geometries at B3LYP/6-311++G(d,p) level using the PCM solvent model for water; ^(c) B3LYP/MB = B3LYP/6-311++G(d,p)//PCM(H₂O)B3LYP/6-31G(d); ^(d) Geometries optimized at B3LYP/6-31G(d) level in the solvent phase and energetics in water are obtained from these solvent phase geometries at B3LYP/6-311++G(d,p) level using the PCM solvent model for water.

Structures of the 15E isomers and rotamers of beta-carotene:

all-trans (15E)

1(bet_car_030_004)

1\1\GINC-T2\FOpt\RB3LYP\6-31G(d)\C40H56\ROOT\17-Sep-2014\0\#P Becke3L
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5,-0.1344611004,-0.0067323494\C,-8.4811678068,-2.9716841131,2.25945953
66\C,-13.8378702358,-0.4635833571,1.420577182\C,-13.8596530028,-1.2311
167652,-0.9666817704\C,-7.7124895836,-4.1131903068,2.6658854922\C,-6.7
431122784,-4.0540021138,3.6246898438\C,-5.9279829238,-5.1481779309,4.0
937040409\C,-6.1410706377,-6.5156951589,3.4888808895\C,-4.9948435503,-
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,0.1236908907\C,-11.7727119678,2.4199718568,-0.3087860496\C,-11.098964
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2\C,3.8275171939,-12.3265697626,12.5194733109\C,6.566990667,-10.795918
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3273436,-12.4678678236,12.8157693901\C,4.5010287413,-13.6789491265,12.
6422580423\C,2.3257326911,-12.4108104967,12.6677542561\C,5.9660458649,
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15E,9Z

l (bet_car_9)

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[X(C40H56)]\\@

15E,13Z

1 (bet_car_13)

1\1\GINC-S1\FOpt\RB3LYP/6-31G(d)\C40H56\SANDHIYA\13-May-2016\0\\#P Bec
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 2297\H,-9.4987877253,4.2743801882,-9.6196323184\H,-6.3163825348,2.4758
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 ,2.5588494872,-11.2876587984\H,-8.4531550593,1.4189779114,-9.981910173
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15E,8Z

1 (bet_car_8)

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 2,12.816289409,12.0278771559\C,-0.4577870252,9.0172803811,7.9660292898
 \C,-0.8504582541,8.3373884588,6.8497748085\C,-2.0343063822,7.525979706
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 4,8.9471135657\C,5.8404772121,14.3018300884,8.1515037187\C,4.531063693
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 ,3.4687009419\C,-4.768674624,4.0745030918,2.2586108276\C,-5.9676535245
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,1.4872904751,-0.1427908021\H,-12.3082521558,0.6311054876,-1.508366090
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[X(C40H56)]\\@

15E,12Z

1 (Car_H_150)

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8544372,-19.0029047839\\C,-22.3786972188,2.805920626,-19.5861906745\\C,-
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15E,10Z

l (bet_car_10)

I\I\GINC-S1\FOpt\RB3LYP\6-31G(d)\C40H56\SANDHIYA\14-May-2016\0\#P Bec
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881497\H,3.9116145699,9.715547345,7.7588071063\H,2.8280186455,8.320963
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40707,3.1916825679,2.965846501\H,-5.3874795115,2.0110240302,2.05708074
7\H,-1.7218218238,2.5717397283,-0.1572754786\H,-2.5942934091,1.0533706
769,-0.3964485038\H,-3.2240382037,2.5489206297,-1.0846979172\H,-4.9755
146837,0.9939096631,-0.8034724926\H,-7.2532983325,0.3914418533,-0.8178
03444\H,-9.180399031,-0.4227197002,-0.1410342475\H,-5.9981767749,0.021
9260741,2.6909303805\H,-7.436420494,0.9073235496,3.2206796076\H,-7.460
3920277,-0.8544448687,3.1610377531\H,-9.5566290834,-0.9057630065,2.853
2570453\H,-9.6340508731,-3.6220373906,1.5979767734\H,-10.8977227268,-4
.8010775295,2.0021807537\H,-10.9144809951,-3.9703302706,0.4337382015\H
,-11.768611278,-1.8255490846,4.1223890435\H,-11.6988188564,-3.59639119
16,4.1100738057\H,-10.2208921125,-2.6630565445,3.8839180988\H,-13.6468
308135,-2.4220248549,2.6400850911\H,-13.5127666195,-1.0556313552,-0.85
5036073\H,-14.1656888069,-0.6692080369,0.7192929498\H,-12.6740036115,1
.2931808173,0.1695610824\H,-10.9511874501,1.2006814053,0.5954656382\H,
-11.5204090862,0.6453986316,-0.9865778794\H,-14.6070462572,-3.02451118
86,0.4065634474\H,-12.9890770273,-3.3353432702,-0.2089923599\H,-13.244
0613162,-4.0796184853,2.2038239704\H,11.8347172963,9.9958738156,5.4313
415593\H,9.991555606,11.4149071621,4.7613723027\Version=ES64L-G09RevD
.01\State=1-A\HF=-1557.8945324\RMSD=5.821e-09\RMSF=1.995e-06\Dipole=0.
0109902,0.1008945,0.0911201\Quadrupole=6.0883695,-7.5142906,1.425921,7
.2403071,-0.2212141,3.5690057\PG=C01 [X(C40H56)]\@

15E,14Z

1 (bet_car_14)

1\1\GINC-S3\FOpt\RB3LYP\6-31G(d)\C40H56\SANDHIYA\14-May-2016\0\#P Bec
ke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\\
0,1\C,12.044810888,3.3080462745,-3.9454812066\C,6.4364991787,1.1949122
592,-2.95331696\C,11.2205834109,4.5851483912,-4.2366459076\C,12.347173
3892,2.6094213742,-5.2933383763\C,5.1459042461,0.6968005139,-3.3346650
312\C,4.0405296665,0.8127654009,-2.5430663953\C,2.7097513257,0.3445496
279,-2.8481416722\C,2.4782972233,-0.3530825523,-4.1679535398\C,1.71575

19197,0.559581689,-1.9253130882\C,0.3348868693,0.1933483081,-2.0089161
482\C,13.405176558,3.6882303509,-3.3155650546\C,13.2914846963,4.050728
1635,-1.8372184479\C,12.7734261745,2.8414350202,-1.0610877031\C,11.600
2317241,2.145589769,-1.7219319998\C,10.9308920605,1.1437240191,-0.8094
147147\C,11.2337810021,2.3801306561,-3.0081044426\C,10.0333544504,1.77
45104676,-3.6152272101\C,8.8000712727,1.7185656166,-3.0565816982\C,7.6
094242756,1.1378941066,-3.6562770429\C,7.7302449835,0.5048982141,-5.02
13669788\C,-0.5562074116,0.4562401765,-1.0020585985\C,-1.9609920981,0.
1656366737,-0.912364359\C,-2.8885176254,-0.1279552928,-1.8844812903\C,
-4.2348069133,-0.4291702927,-1.4562945219\C,-2.5620529783,-0.120589170
3,-3.3585583465\C,-5.290211199,-0.8047686351,-2.2355307431\C,-6.590387
4995,-1.0888893619,-1.6988169498\C,-7.7194734242,-1.474363712,-2.36962
15798\C,-8.9323625096,-1.7019368511,-1.6006605597\C,-7.7714757888,-1.6
717270341,-3.865097407\C,-10.1422717708,-2.0561905584,-2.0975603678\C,
-11.3724841614,-2.2667821252,-1.3113102113\C,-12.6395472096,-1.5832976
375,-1.8818814074\C,-11.3935955657,-3.0012872758,-0.1697362584\C,-12.4
908897319,-0.0478951417,-1.7583340288\C,-12.8306765218,-1.9326414886,-
3.3776263129\C,-13.912558156,-2.0522676443,-1.1390100917\C,-12.6289337
521,-3.1358135427,0.6979129217\C,-10.226870112,-3.8074610398,0.3531604
287\C,-13.7229215021,-2.1200800506,0.3743369037\H,6.4756545828,1.67881
71269,-1.9762552866\H,10.2407376875,4.3316264452,-4.6553526115\H,11.04
68029662,5.1693028283,-3.3265133044\H,11.7435092312,5.2261235737,-4.95
79906542\H,13.0439762593,3.2235105067,-5.876749612\H,12.8127002052,1.6
28693499,-5.1391200847\H,11.4507567515,2.4710168514,-5.9063349827\H,5.
0488548017,0.20615746,-4.2991428074\H,4.1589209057,1.3095612363,-1.579
1333514\H,3.1127818043,-1.2441625383,-4.2552870175\H,1.4429893245,-0.6
706876005,-4.3019924703\H,2.7350902464,0.3050540357,-5.0078322993\H,2.
004964278,1.0777555906,-1.0098319994\H,-0.0009216027,-0.3401292867,-2.
8907153292\H,13.8442692681,4.5138982934,-3.8909036838\H,14.0946323946,
2.8371227498,-3.4149473141\H,12.6056672654,4.8977165174,-1.7067734128\
H,12.4798161255,3.1355456624,-0.0423360284\H,11.6952594133,0.576610086
,-0.2596349316\H,10.3129912775,1.6402436058,-0.0472344626\H,10.2955210
507,0.4365077507,-1.3455555166\H,10.1489417075,1.3901394938,-4.6260732
47\H,8.6584337025,2.1614463498,-2.0716162219\H,8.0744351381,1.23777766
16,-5.7626984945\H,8.4688712357,-0.3066086255,-5.0118564975\H,6.786421
1695,0.0908398907,-5.3801476135\H,-0.1402657378,0.9220340193,-0.106982
4767\H,-2.351205545,0.2083492924,0.1047940073\H,-4.4087631833,-0.36175
28489,-0.3814712237\H,-1.7816323609,0.6123112015,-3.5825544512\H,-2.20
56158074,-1.1002863426,-3.7056195933\H,-3.4395222602,0.1367047718,-3.9

587677353\H,-5.1466965033,-0.9035318328,-3.3076730193\H,-6.6787790487,
-0.9798144839,-0.6168854935\H,-8.8403953605,-1.5483229154,-0.526307246
9\H,-6.8103113967,-1.4901694343,-4.3490186075\H,-8.0822492814,-2.69443
15068,-4.1135290236\H,-8.5065331819,-0.9971142586,-4.3231787134\H,-10.
2418146138,-2.1410394122,-3.1773314826\H,-11.5744340867,0.297997949,-2
.2483899195\H,-13.3416084842,0.4612426767,-2.2290870013\H,-12.44153201
41,0.2701072194,-0.7112170132\H,-12.8073763757,-3.0167793479,-3.539972
201\H,-13.8050970392,-1.563125795,-3.7197707208\H,-12.0701718824,-1.47
38033782,-4.0176584832\H,-14.1898377499,-3.0528282518,-1.5017015823\H,
-12.3283202405,-3.0542134751,1.7531198712\H,-13.0253931146,-4.15965960
65,0.5925220158\H,-10.5818765783,-4.7895864608,0.6959016439\H,-9.44658
77004,-3.9640560186,-0.3938666804\H,-9.7634440843,-3.3288147019,1.2280
672438\H,-14.6608201411,-2.3975266668,0.871075134\H,-13.4412547642,-1.
1336928168,0.7650315679\H,-14.742970683,-1.3840998173,-1.402753745\H,1
4.2628122698,4.3711330866,-1.440653144\H,13.5862479458,2.1087087754,-0
.9228548337\\Version=ES64L-G09RevD.01\State=1-A\HF=-1557.8947094\RMSD=
8.115e-09\RMSF=2.990e-06\Dipole=0.0091449,-0.1443112,-0.2191584\Quadru
pole=9.4573173,-10.7054676,1.2481502,5.0166595,-1.0853398,2.7409239\PG
=C01 [X(C40H56)]\@

15E,11Z

l (bet_car_11)

1\1\GINC-T4\FOpt\RB3LYP\6-31G(d)\C40H56\SANDHIYA\13-May-2016\0\#P Bec
ke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\\
0,1\C,9.350803452,-4.3326148066,9.5540658739\C,4.4981209578,-3.4707822
763,6.0154375658\C,9.4755601871,-2.8180464381,9.261628154\C,10.2762933
442,-5.0928809096,8.5738112767\C,3.7984706089,-3.2822615861,4.77703192
84\C,2.6022546579,-2.6303599067,4.6937985909\C,1.8273224309,-2.3991145
272,3.4993016973\C,2.3548028823,-2.924902598,2.1851690948\C,0.64439601
41,-1.7093318376,3.6128888311\C,-0.2834320416,-1.3669041953,2.58207563
39\C,9.8544966665,-4.6385547679,10.9844204539\C,8.8344438735,-4.277498
2247,12.060989242\C,7.5706052315,-5.1104428827,11.8550270208\C,7.09892
73617,-5.1587907543,10.4154001865\C,5.7054591212,-5.7283480971,10.2801
708709\C,7.8759541232,-4.7671819773,9.3732499741\C,7.3748765509,-4.717
0835254,7.9862734039\C,6.201932373,-4.1668124145,7.5895253808\C,5.6963
926321,-4.0971305487,6.2282601781\C,6.5178374603,-4.7162972831,5.12393
1224\C,-1.4344911039,-0.6596859121,2.804119514\C,-2.3598988337,-0.3190

685212,1.7705602446\C,-3.5335270118,0.3929033223,1.8688305764\C,-4.279
7912404,0.5933838903,0.6456334735\C,-4.0287998467,0.9399793481,3.18572
8878\C,-5.4446722822,1.2551737389,0.3572746829\C,-6.3281117991,2.00969
31368,1.202050736\C,-7.4821724107,2.646515969,0.8239130443\C,-8.223045
0088,3.3770731326,1.8402415466\C,-8.0269835194,2.6417323718,-0.5837245
043\C,-9.3582158731,4.0917400717,1.6474780336\C,-10.0872461904,4.85460
88585,2.678640363\C,-10.4814103269,6.2949468056,2.269013386\C,-10.3843
885302,4.3377321323,3.8980433039\C,-9.2020695528,7.1571303028,2.146301
1132\C,-11.2045118709,6.3054122958,0.9006491461\C,-11.4481221726,6.925
4369801,3.2988304414\C,-11.0439248547,5.1480485795,4.9961312581\C,-10.
1471392702,2.9001135803,4.2998612546\C,-11.0343028407,6.654569836,4.74
29212108\H,4.0001525065,-3.0586439789,6.8943597653\H,9.0987867198,-2.5
803763782,8.2610077592\H,8.9020255411,-2.2192238948,9.9775395763\H,10.
5246568318,-2.5000373199,9.3149244798\H,11.3239735098,-4.8779037704,8.
8172273882\H,10.1303324172,-6.1770390149,8.6477335844\H,10.1213567433,
-4.7957712535,7.5316423464\H,4.243342853,-3.6784578381,3.8682417714\H,
2.1760634382,-2.2382814526,5.6182291493\H,2.4839036786,-4.0140107805,2.
.2231981325\H,1.6949662703,-2.6990283213,1.3460513686\H,3.3386068324,-
2.4943955775,1.9588657179\H,0.3703325738,-1.3749522752,4.6145542014\H,
-0.0716211822,-1.6804324155,1.5614031075\H,10.8031821805,-4.1101096232
,11.1466916823\H,10.0783307715,-5.7126221719,11.0620495223\H,8.5880174
552,-3.2093305817,12.0060290773\H,6.7512608955,-4.7265944406,12.481029
6265\H,5.5982615623,-6.6002393431,10.9408408862\H,4.940560938,-5.00667
13181,10.6016355627\H,5.4670399745,-6.0358250259,9.2605589494\H,8.0380
564147,-5.1103609231,7.2187444704\H,5.5659423177,-3.7105398879,8.34698
82697\H,7.5054319414,-4.2412983364,5.0578103233\H,6.6914298385,-5.7826
650418,5.3159962696\H,6.0430971723,-4.6276174807,4.1452573374\H,-1.642
8327181,-0.3433587195,3.8244832099\H,-2.0872498455,-0.672929611,0.7755
037383\H,-3.8125467265,0.1184118954,-0.2167897275\H,-3.3807835209,0.66
36689892,4.0192711049\H,-4.0856770144,2.0351972368,3.1630946435\H,-5.0
345216075,0.5669850983,3.4126932121\H,-5.7330048697,1.2004047762,-0.68
98167383\H,-6.0640293968,2.1011035584,2.2498537817\H,-7.7930223135,3.3
532574227,2.8408155226\H,-7.4190519849,2.0562793492,-1.2747229429\H,-9
.0441947822,2.2308011302,-0.6049698859\H,-8.0899932643,3.6634805684,-0
.9803248943\H,-9.7448209621,4.1661007835,0.6335186229\H,-8.4934510051,
6.7068102743,1.4429838484\H,-9.4479520603,8.1633984019,1.7837232653\H,
-8.6882362562,7.2582729566,3.1084112001\H,-12.0475409921,5.6043591909,
0.889573016\H,-11.6002685079,7.3089262138,0.701885242\H,-10.537597795,
6.0531763841,0.0698846652\H,-12.4559524057,6.514057417,3.1409734593\H,

-10.5484091418,4.9159272805,5.9506822209\H,-12.0816388992,4.7955876237
,5.1205781044\H,-11.0265427949,2.5172262233,4.8366735966\H,-9.95006485
16,2.245943315,3.4487569738\H,-9.3014937102,2.8096810267,4.9970131437\
H,-11.7101512575,7.163030064,5.4415629164\H,-10.0303226075,7.056362540
4,4.9309537143\H,-11.5184429298,8.0039838808,3.1053466624\H,9.24850345
89,-4.4522532473,13.0617405331\H,7.740024518,-6.1417462793,12.20761945
15\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-1557.8944081\\RMSD=4.009e-09
\\RMSF=2.097e-06\\Dipole=-0.0452602,0.0026635,0.1086506\\Quadrupole=4.209
6867,-6.9545008,2.7448141,-10.0156333,0.818171,1.1093905\\PG=C01 [X(C40
H56)]\\@

15E,7Z

1 (bet_car_032)

1\\GINC-LXA13\\FOpt\\UB3LYP\\6-31G(d)\\C40H56\\DI49BOQ\\15-Nov-2016\\0\\#p u
b3lyp/6-31g(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\0
,1\\C,-12.6986780663,-0.5819578391,1.3718223615\\C,-7.0839887324,0.69109
54795,1.3431374217\\C,-13.658485843,-1.74471064,1.7163654095\\C,-13.4098
053361,0.3132059614,0.3290150164\\C,-5.9704204197,0.6109355879,2.245623
6428\\C,-4.7825415428,1.240246571,2.0112304337\\C,-3.6130573176,1.219661
663,2.8560869694\\C,-3.6650207642,0.4257011264,4.1399280488\\C,-2.506564
7314,1.9272587056,2.4534633515\\C,-1.2492446177,2.0615592076,3.11911331
65\\C,-12.4358793956,0.2776188048,2.6307922156\\C,-12.9585973859,-2.8975
257711,2.4325205675\\C,-11.878211617,-3.4792131198,1.5210098206\\C,-11.0
247663069,-2.4279894949,0.8391794736\\C,-9.807341695,-3.0046819693,0.15
62812789\\C,-11.3578554888,-1.1162970697,0.8092766601\\C,-10.5134613781,
-0.1046678253,0.1237505634\\C,-9.2684753469,0.3650591581,0.3839168116\\C
, -8.3204821731,0.1149048131,1.4658663341\\C,-8.7111202558,-0.7033983974
,2.6726637918\\C,-0.2097917086,2.8027697484,2.6258077308\\C,1.0469538226
,2.9446204434,3.2907179152\\C,2.1461466474,3.6632380382,2.8869708845\\C,
3.3138678847,3.6643471514,3.7342009248\\C,2.1894564375,4.4536298682,1.6
003337075\\C,4.4884522617,4.3190182589,3.5010906686\\C,5.6031834782,4.26
98637828,4.4031021225\\C,6.8205761918,4.8837185805,4.2814573418\\C,7.799
2966556,4.6859358492,5.338152087\\C,7.1977105943,5.7546932626,3.1078447
501\\C,9.054782862,5.1944132417,5.3756427968\\C,10.0452041091,4.97603115
91,6.447070848\\C,11.4669452283,4.6030327867,5.9604698634\\C,9.734014259
1,5.0892553797,7.7637671797\\C,11.4359378463,3.1903990786,5.3298477561\\
C,11.9666813906,5.6013736256,4.888562569\\C,12.4845872396,4.6409777082,

7.1250947088\C,10.7156612852,4.7664808313,8.8722326599\C,8.408859737,5
 .5889673502,8.291846753\C,11.9484023794,3.9971747654,8.4010444813\H,-6
 .9050036032,1.2850455056,0.4458040274\H,-14.1019581133,-2.1285182309,0
 .7859843177\H,-12.0346472026,-0.3209012597,3.4560287593\H,-14.48886732
 94,-1.3536895393,2.319153424\H,-14.4083759977,0.5813845146,0.694959181
 2\H,-12.8661383088,1.2452640618,0.1449723134\H,-13.5329245811,-0.20793
 31735,-0.628061204\H,-6.0803551452,0.0180190629,3.1494009927\H,-4.6936
 212111,1.8250203164,1.0946086037\H,-3.8761060835,-0.6318308244,3.93665
 56242\H,-2.7314967345,0.474326783,4.7026654702\H,-4.4670885958,0.79129
 73689,4.7936397136\H,-2.5891230571,2.4616350227,1.5058966573\H,-1.1024
 632067,1.553017159,4.0703126946\H,-13.3671076549,0.7439695071,2.977007
 1523\H,-11.718265351,1.0770993359,2.4169295257\H,-13.6802011011,-3.674
 939565,2.7122896066\H,-12.3426962644,-4.1129717519,0.7474228485\H,-9.2
 61885337,-2.2667336915,-0.4335176053\H,-9.1100949502,-3.4438452726,0.8
 839650426\H,-10.1084987371,-3.8270323895,-0.5088534793\H,-10.989731952
 3,0.3543254021,-0.7438164677\H,-8.8952966567,1.0866471037,-0.344334857
 4\H,-8.0180333179,-0.554425958,3.5039615946\H,-9.7111442329,-0.4304771
 903,3.0192461427\H,-8.7372585061,-1.7750734912,2.4472420703\H,-0.35870
 70143,3.310790569,1.6746898401\H,1.1339250672,2.4129765444,4.239408712
 7\H,3.234559669,3.0797127458,4.6517456198\H,1.2596294814,4.3863866109,
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\@

15E,9Z, 9'Z

l (bet_car_9_91)

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Structures of *15Z* isomer and rotamers

15,15'-cis

l(bet_car_trans)

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15Z,9Z

1 (bet_car_9_15)

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931,-2.6176668678\H,5.5011387049,2.527873203,-6.7533274894\H,6.308297,
4.0234732137,-6.2502255419\H,7.2449545392,2.5431708545,-6.4422984468\H



,8.3268024811,3.9938367935,-4.9284029845\H,10.1108295035,1.898873671,-
 3.853245126\H,11.8216601303,2.2069847999,-3.4965653315\H,10.6488037032
 ,2.0261460622,-2.1768428901\H,10.5859222614,5.5166075676,-4.7754549202
 \H,11.9569716006,4.3944964796,-4.8148963032\H,10.3894351963,3.87921626
 59,-5.4342912046\H,11.5289593206,5.7489155282,-2.5149088683\H,9.217830
 7655,4.9787092729,0.3361632096\H,9.7657620861,6.3244356924,-0.63532087
 9\H,7.2601895532,6.2756988414,-0.9827872267\H,6.5958414912,5.245819602
 ,-2.2694268827\H,6.8145240359,4.6138140621,-0.6295279119\H,11.75474227
 32,5.0460062553,-0.1206152861\H,10.9705116518,3.516097171,-0.494350914
 \H,12.4979082353,4.2854557667,-2.3725381383\H,-7.7619108962,-5.8908974
 839,-12.2934658986\H,-6.3177472093,-7.454928928,-11.1490601318\Versio
 n=ES64L-G09RevD.01\State=1-A\HF=-1557.896844\RMSD=6.467e-09\RMSF=1.974
 e-06\Dipole=0.0952268,0.0444199,0.1211744\Quadrupole=2.6764335,-6.9564
 599,4.2800265,10.8131754,2.5756169,1.877662\PG=C01 [X(C40H56)]\@

15Z,13Z

1 (bet_car_13_15)

1\1\GINC-T3\FOpt\RB3LYP\6-31G(d)\C40H56\SANDHIYA\14-May-2016\0\#P Bec
 ke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\\
 0,1\C,8.9787828974,5.9271349428,-8.5028242737\C,4.5900576481,5.6076563
 396,-4.3241230657\C,8.7076199622,4.403603912,-8.4993477259\C,10.196413
 2121,6.2042336056,-7.588575029\C,4.0343956816,5.363764093,-3.023096944
 4\C,2.7273242523,5.0258899165,-2.8283213295\C,2.078283627,4.7722517802
 ,-1.5630388363\C,2.8988788575,4.8946147119,-0.3009230804\C,0.747777131
 2,4.4331010903,-1.5736816824\C,-0.0930399735,4.1497802459,-0.449471674
 8\C,9.3638647164,6.3935864438,-9.9264548521\C,8.1577080405,6.526555656
 1,-10.8526135671\C,7.2052921492,7.5798161991,-10.289339363\C,6.9550198
 859,7.4458429084,-8.8006118301\C,5.8040137607,8.3038331311,-8.32782706
 42\C,7.7205688945,6.6699419185,-7.9914780007\C,7.4111672045,6.46873610
 29,-6.5625036173\C,6.1956532742,6.1551800275,-6.0528494906\C,5.8748859
 746,5.9473707634,-4.6496547941\C,6.9736703931,6.1187602447,-3.62935572
 85\C,-1.4179060735,3.79632652,-0.4821958848\C,-2.2292139718,3.61628621
 8,-1.6507880212\C,-3.5601921351,3.2771536034,-1.7072008944\C,-4.369839
 8918,3.0697800628,-0.5294378188\C,-4.2130850247,3.1170301134,-3.062101
 8714\C,-5.6886292166,2.7217484379,-0.5173248431\C,-6.4402165958,2.5450
 376175,0.6935006169\C,-7.7569204419,2.1991358162,0.8294157792\C,-8.305
 8268085,2.0923005266,2.1722311872\C,-8.6701324423,1.9285921734,-0.3417

798416\C,-9.5869195629,1.7891654379,2.4920311154\C,-10.1443894851,1.71
 08370331,3.8559720319\C,-11.4906728354,2.4496731269,4.0554639413\C,-9.
 5228730556,1.0464689101,4.8633947016\C,-11.2578639914,3.9748408106,3.9
 356425166\C,-12.5185164871,2.0303947431,2.9767781379\C,-12.1148385325,
 2.1157350459,5.4307691747\C,-10.0362636064,1.0487470347,6.2894169674\C
 ,-8.287577468,0.1923349788,4.693408\C,-11.0911012831,2.1190221086,6.56
 30288182\H,3.8864242851,5.5099253433,-5.1521922903\H,8.4056863514,4.06
 23246245,-7.5032956119\H,7.9046637462,4.1346421373,-9.1941874106\H,9.6
 095795312,3.8499749073,-8.7902908969\H,11.1017722183,5.7877306522,-8.0
 467476568\H,10.3548813634,7.2804255931,-7.450807589\H,10.0947865054,5.
 7429988218,-6.6010067407\H,4.6868412576,5.4558996668,-2.1590407487\H,2
 .0932337146,4.9356355148,-3.7113893166\H,3.3235007816,5.9022113248,-0.
 2084174373\H,2.3194878785,4.6956520816,0.6017935371\H,3.7424753117,4.1
 927801982,-0.3150180183\H,0.2811630389,4.3784191418,-2.5556501802\H,0.
 3557423737,4.2228383738,0.5379295983\H,10.1037191841,5.695940234,-10.3
 408742941\H,9.8616434637,7.3721370883,-9.8591011583\H,7.6382398849,5.5
 634610598,-10.9382781216\H,6.2386982689,7.5435226463,-10.8136602278\H,
 5.8592916465,9.2914526422,-8.8072093725\H,4.834024589,7.8769235915,-8.
 6212016007\H,5.7930495771,8.4454585755,-7.2458002227\H,8.2514059508,6.
 5289345213,-5.8740149621\H,5.3646447576,6.0263327104,-6.7451849776\H,7
 .7958825635,5.4163656171,-3.8188045933\H,7.4011829689,7.1281045626,-3.
 6811335081\H,6.629110725,5.9551245005,-2.6068514029\H,-1.8889457188,3.
 6304376811,0.4833546176\H,-1.7326234637,3.7570869478,-2.6083765714\H,-
 3.8883537736,3.2098195858,0.4361075812\H,-3.5017442848,3.3110301881,-3
 .8698177436\H,-4.6080146387,2.1018302263,-3.199727886\H,-5.0584689514,
 3.8066196228,-3.1844783295\H,-6.2003692007,2.5730609613,-1.4638795458\
 H,-5.8811179006,2.7140839115,1.6149739393\H,-7.6069425107,2.3025427124
 ,2.9807508434\H,-8.1641724186,2.0280176765,-1.3034146855\H,-9.08619067
 05,0.9146668493,-0.28674353\H,-9.5217579097,2.6212053894,-0.3410122343
 \H,-10.2920879031,1.645857035,1.6762815361\H,-10.7896931034,4.22500161
 04,2.9775655778\H,-12.2098924425,4.5169711387,4.0010914489\H,-10.59948
 17628,4.346950579,4.7280402262\H,-12.6215106037,0.939946945,2.92687343
 68\H,-13.501568039,2.4492150557,3.2243275315\H,-12.2559575735,2.396910
 2187,1.9792706259\H,-12.576516961,1.118621077,5.3808980565\H,-9.181113
 9349,1.1686110904,6.9711717121\H,-10.4468186595,0.0511112298,6.5190600
 014\H,-8.4080423318,-0.7452750169,5.2541710006\H,-8.0779668367,-0.0535
 560714,3.6509016902\H,-7.3961638966,0.6837071964,5.1094806159\H,-11.57
 98552311,1.9352312088,7.5277387466\H,-10.6115179732,3.103496593,6.6375
 459142\H,-12.9279278882,2.8254902993,5.6327348928\H,8.4753390305,6.801

9746341,-11.8658456267\H,7.6015525943,8.5891647121,-10.4913099316\\Ver
sion=ES64L-G09RevD.01\State=1-A\HF=-1557.8965185\RMSD=8.041e-09\RMSF=1
.460e-06\Dipole=-0.1102011,-0.021543,0.0576218\Quadrupole=6.9780051,-1
2.1681922,5.1901871,5.3417712,-2.8245523,-2.8848757\PG=C01 [X(C40H56)]
\\@

15Z,8Z

l (bet_car_8_15)

1\1\GINC-R1\FOpt\RB3LYP\6-31G(d)\C40H56\SANDHIYA\07-Jun-2016\0\#P Bec
ke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\\
0,1\C,-7.2127396068,-2.7873034685,-10.3242586349\C,-3.5400482882,-1.96
5099728,-5.565290624\C,-7.7979503576,-1.4791112082,-9.7404001665\C,-8.
0601558657,-3.9725648551,-9.8026111939\C,-3.1640342608,-2.0034082671,-
4.1806088164\C,-2.2357169457,-1.1611727631,-3.6418238808\C,-1.79151735
96,-1.1290328129,-2.2684421068\C,-2.3895641613,-2.1214427031,-1.299488
3559\C,-0.8476158995,-0.196395701,-1.9129948786\C,-0.2632814735,0.0088
244995,-0.6228923185\C,-7.3379026504,-2.7810261606,-11.865943182\C,-6.
2777151037,-1.9142756525,-12.5409326563\C,-4.8928731243,-2.4715921589,
-12.2176379937\C,-4.7016008613,-2.8260013079,-10.7564304868\C,-3.25565
54998,-3.0962573657,-10.4095089356\C,-5.7353093182,-2.9273115041,-9.88
23296584\C,-5.5334373198,-3.1752950543,-8.4416128999\C,-4.6579328651,-
2.5207214467,-7.6412504195\C,-4.4533728959,-2.7464890587,-6.2193786687
\C,-5.2572659327,-3.8295623711,-5.5420483436\C,0.6697518141,0.95725401
63,-0.2840388259\C,1.2405268193,1.9468609063,-1.1462220215\C,2.1755765
207,2.9004209221,-0.8248072099\C,2.6038848387,3.8146334706,-1.85762397
22\C,2.7771104369,3.0459372632,0.5530593612\C,3.5172447326,4.819370833
3,-1.7284372474\C,3.8841184983,5.689984659,-2.8108105864\C,4.765948257
2,6.7322992836,-2.7807873807\C,5.0852093686,7.5031387652,-3.9832830529
\C,5.4729362969,7.1902255399,-1.5246152682\C,5.0082113612,7.076179742,
-5.265880138\C,5.3203220275,7.8731000243,-6.4657987425\C,6.1817039893,
7.1470884156,-7.5286470577\C,4.8914766549,9.1519959453,-6.6266008809\C
,7.6011965879,6.9097049712,-6.960034022\C,5.5697700221,5.7723389664,-7
.8920236261\C,6.2656358871,7.9656560921,-8.8383540449\C,5.3023588033,1
0.0131770917,-7.8040339312\C,3.9294324288,9.860273124,-5.7006767225\C,
6.4860714224,9.4557554299,-8.5918282465\H,-3.0229551253,-1.2135024372,
-6.1636811227\H,-7.6944369077,-1.4557684983,-8.6502462084\H,-7.2854081
719,-0.595879135,-10.1366206395\H,-8.8647072582,-1.3912851491,-9.98331

86308\H,-9.0625016351,-3.9321590139,-10.2462852086\H,-7.6108989016,-4.9346057412,-10.0763205431\H,-8.1885910308,-3.9504495051,-8.7157236294\H,-3.6418721791,-2.7378046196,-3.5379069094\H,-1.7721442556,-0.430776923,-4.3063860373\H,-2.1985118406,-3.1510615127,-1.6276791214\H,-1.9930458854,-2.0170265642,-0.2885749726\H,-3.4789383182,-2.0016862631,-1.2424939176\H,-0.5056905856,0.4598445453,-2.7114439963\H,-0.5830774963,-0.651845276,0.1789854547\H,-8.349081822,-2.4507856787,-12.1382886501\H,-7.2356829722,-3.811350659,-12.2371162298\H,-6.3541651528,-0.8787084592,-12.1853101576\H,-4.1119958337,-1.7541797123,-12.5110836151\H,-2.7938616108,-3.7032882452,-11.2010242686\H,-2.6710607476,-2.1662736744,-10.3588725857\H,-3.1353628521,-3.6186327285,-9.4589629031\H,-6.1875278666,-3.9137457644,-7.9829652341\H,-4.0477181834,-1.7329270521,-8.0812601067\H,-6.3332852394,-3.6285779471,-5.6262335896\H,-5.0789935766,-4.8030266255,-6.0162417001\H,-5.022217218,-3.9281685371,-4.4809063948\H,0.9999852912,0.9501101269,0.7516561486\H,0.8924627946,1.952988974,-2.1777414735\H,2.1408795819,3.6755907308,-2.8355297613\H,2.3871249467,2.3163526255,1.2641090573\H,3.8671924903,2.9245371507,0.5171359448\H,2.5806928011,4.0457009517,0.9605718571\H,3.9972252708,4.970561888,-0.7653133679\H,3.3803647566,5.4926038759,-3.7567343098\H,5.4672065641,8.5080899245,-3.8037616177\H,5.075882209,6.7335933614,-0.6156784781\H,6.5476884889,6.9670567964,-1.57188861\H,5.3851865403,8.2789166204,-1.41382695\H,4.7571985064,6.0299972841,-5.4308847756\H,7.5569835007,6.3538061608,-6.0172645388\H,8.208295725,6.3309588899,-7.6677709998\H,8.1197471184,7.8536534018,-6.7597398183\H,4.5147741119,5.8679710713,-8.1748736492\H,6.1087253643,5.3453378024,-8.7466877995\H,5.641665958,5.0485322756,-7.0740073068\H,5.3274369826,7.8400031791,-9.3984102936\H,5.5268618223,11.0258398974,-7.4370155627\H,4.4333980532,10.1379304661,-8.4717804734\H,3.1857289142,10.4100730618,-6.2945868661\H,3.402028862,9.1805997864,-5.0291203283\H,4.4419949914,10.6122359669,-5.083452072\H,6.5999851451,9.9934652951,-9.5411783527\H,7.4152401015,9.6135058132,-8.0290302954\H,7.0622562865,7.5470423071,-9.4673077207\H,-6.4338749936,-1.8850194335,-13.6263605176\H,-4.6990048228,-3.3697557291,-12.8277854044\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-1557.8932411\\RMSD=9.056e-09\\RMSF=2.862e-06\\Dipole=0.138956,0.1662129,-0.0400482\\Quadrupole=-4.4585932,0.5537443,3.9048489,10.4925201,2.6168917,-1.8990583\\PG=C01 [X(C40H56)]\\@

15Z,12Z

1 (bet_car_12_15)

I\1\GINC-HP3\FOpt\RB3LYP\6-31G(d)\C40H56\SANDHIYA\09-Jun-2016\0\#P Be
 cke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\
 \0,1\C,-5.0953350207,-8.6236031426,6.9818512535\C,-3.2209220697,-3.903
 3920022,3.649719298\C,-3.6064553001,-8.9978329472,6.787213651\C,-5.928
 5326508,-9.3840805446,5.9219223286\C,-2.8282793699,-3.2376491418,2.440
 440847\C,-2.0151293122,-2.1420618496,2.4267996175\C,-1.5673624034,-1.4
 140182499,1.2631059704\C,-2.0236131778,-1.8885542744,-0.0965060277\C,-
 0.7491569679,-0.3266558523,1.4518046783\C,-0.1898645296,0.5320280069,0
 .4531221601\C,-5.5844157807,-9.1005892255,8.3695817485\C,-5.1312105144
 ,-8.1853098436,9.5033530839\C,-5.720206451,-6.7922292008,9.2889675367\
 C,-5.589753992,-6.2854719409,7.8663574547\C,-5.9089610293,-4.813311669
 9,7.7436812258\C,-5.2623457248,-7.0919884882,6.8243773108\C,-5.0327319
 828,-6.5772831953,5.4609610234\C,-4.2803602336,-5.4986933676,5.1339494
 376\C,-4.030016248,-4.9979382944,3.7919670049\C,-4.6733861443,-5.71250
 07021,2.6284201516\C,0.6243084497,1.6175883314,0.6631794556\C,1.085203
 1347,2.1164299088,1.923338162\C,1.8795343817,3.2142136143,2.1341100466
 \C,2.3339768599,3.5900135731,3.4623111854\C,2.3427542664,4.1241923712,
 1.0163755902\C,2.3627407601,2.8183718163,4.5859602345\C,2.8074356546,3
 .306037308,5.8597106627\C,2.8806701468,2.6277631004,7.0464565636\C,3.3
 563422313,3.34250459,8.2198611858\C,2.48489122,1.1793557868,7.20129136
 76\C,3.4621416909,2.8411529614,9.4743892398\C,3.9191985412,3.579133926
 3,10.6669174986\C,3.0342096902,3.4017163814,11.9254539128\C,5.02862752
 31,4.361494421,10.6623765839\C,1.6678280071,4.0880516108,11.6881232763
 \C,2.7794775905,1.9033791099,12.2183804752\C,3.7172973015,3.9989315199
 ,13.1781512888\C,5.4470728476,5.2025040307,11.8516193498\C,6.005563834
 5,4.4584232205,9.5130593029\C,4.3584229074,5.3583369699,12.912032651\H
 ,-2.8162760573,-3.4727729307,4.5668904815\H,-3.2372802622,-8.642468675
 2,5.8191759291\H,-2.9730959354,-8.5529679992,7.5624596996\H,-3.4740371
 038,-10.0867728485,6.8229235289\H,-5.9141276374,-10.4579387917,6.14498
 6907\H,-6.9744402877,-9.0549259028,5.9259597337\H,-5.5342427472,-9.261
 8606088,4.9079001202\H,-3.1964764102,-3.627560839,1.495490769\H,-1.658
 10734,-1.766598405,3.3868499582\H,-3.1188173104,-1.8792374394,-0.16511
 74389\H,-1.6367830346,-1.2745288286,-0.9110017143\H,-1.7014165598,-2.9
 219459779,-0.2771181962\H,-0.5019646845,-0.0949498988,2.486420611\H,-0
 .4256521553,0.308399708,-0.5841225018\H,-5.2398976797,-10.1303418513,8
 .532383812\H,-6.6837689368,-9.1360415117,8.3677912805\H,-4.0354678566,
 -8.126011535,9.5268980252\H,-5.2465757575,-6.0657071025,9.9660693501\H
 ,-6.7941701556,-4.5765220742,8.3507353935\H,-5.0942418214,-4.188005140

5,8.1367697141\H,-6.1021096034,-4.5028385799,6.7154195971\H,-5.4648336
515,-7.1587794633,4.6496149077\H,-3.7890936676,-4.9497663404,5.9362488
085\H,-4.3503866788,-6.7608842604,2.5867366659\H,-5.7658422415,-5.7212
624465,2.731543425\H,-4.4341350798,-5.2543841611,1.6672718123\H,0.9566
222969,2.1427427154,-0.2287367868\H,0.7616682067,1.5726787365,2.807252
4353\H,2.7189299415,4.6071523155,3.552934273\H,1.7615779272,4.00768314
34,0.0994424239\H,2.2671304838,5.1743575064,1.3239515351\H,3.398080361
2,3.9432708801,0.7700114238\H,2.046337479,1.7807292679,4.5157046843\H,
3.120778035,4.3509572656,5.8727269044\H,3.6262370217,4.3848088,8.05555
37899\H,2.1452738109,0.7318637947,6.2658820037\H,3.3278554398,0.581481
0168,7.5701812537\H,1.6750964917,1.072213098,7.9346516764\H,3.12767409
02,1.8197269856,9.6412086315\H,1.1856079934,3.6966500259,10.7859574209
\H,0.9950855854,3.9129695281,12.5374195402\H,1.7763445217,5.1701947311
,11.557706557\H,3.7194697062,1.3406216223,12.262884625\H,2.2795262077,
1.7986111578,13.1890369486\H,2.1320700346,1.4319067947,11.4719874576\H
,4.4982347499,3.3055708976,13.5233280182\H,5.773205296,6.1884035163,11
.4878774021\H,6.3477794853,4.7527902374,12.3022158758\H,7.0335825846,4
.4305557743,9.9008343579\H,5.8896181989,3.6542514902,8.7843089899\H,5.
9076754741,5.4142532324,8.9782145774\H,4.7814648013,5.7747407808,13.83
45090624\H,3.600862299,6.0728592077,12.564976272\H,2.9786187497,4.0643
656972,13.9879415787\H,-5.4440485638,-8.5868951729,10.4750908299\H,-6.
7869919397,-6.7897661183,9.5694449311\\Version=ES64L-G09RevD.01\\State=
1-A\\HF=-1557.8928335\\RMSD=7.269e-09\\RMSF=1.385e-06\\Dipole=0.0727154,0.
008619,0.1396972\\Quadrupole=-5.8169723,0.284246,5.5327263,9.0381147,2.
0762476,0.4107177\\PG=C01 [X(C40H56)]\\@

15Z,10Z

1 (bet_car_10_15)

1\1\GINC-T4\FOpt\RB3LYP\6-31G(d)\C40H56\SANDHIYA\07-Jun-2016\0\\#P Bec
ke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
0,1\C,-5.2333497677,-10.3364587323,4.127929961\C,-3.4097528873,-4.9270
412721,2.0765448758\C,-3.7480782306,-10.6368041276,3.8139744387\C,-6.0
87001872,-10.8027415583,2.9241687828\C,-3.0487832402,-3.9671352967,1.0
723976001\C,-2.1912716472,-2.9326586508,1.3083687979\C,-1.7696315179,-
1.9286669576,0.3598312062\C,-2.3255664663,-1.9932334489,-1.0432278305\
C,-0.881127223,-0.9692795287,0.7802680835\C,-0.3278822709,0.1048406585
,0.0127158295\C,-5.691953859,-11.1580413852,5.3556734256\C,-5.21427754

62,-10.5628841258,6.6775877623\C,-5.8055590371,-9.1640523692,6.8419059
008\C,-5.7070915988,-8.3075736339,5.5953725593\C,-6.0268975566,-6.8549
255955,5.862868179\C,-5.4058417308,-8.8173884732,4.3738416677\C,-5.212
780107,-7.9654901022,3.1843823243\C,-4.4532988704,-6.8450355283,3.1268
818085\C,-4.2420707617,-6.0066412193,1.9574769038\C,-4.949104518,-6.37
4244446,0.6755026019\C,0.5711718949,1.0480806357,0.443472919\C,1.13853
46362,1.1586115662,1.7535535699\C,2.0540301604,2.0810972649,2.19606146
13\C,2.4902187123,2.0010214425,3.5743353839\C,2.6290486396,3.168956694
3,1.3208109393\C,3.4301381868,2.794986011,4.1623781513\C,3.913935667,2
.7597337376,5.5249640078\C,3.309222478,2.3378943354,6.6773241025\C,4.0
933965094,2.3766248706,7.9052893576\C,1.8742788043,1.8748084435,6.7401
664236\C,3.6968673824,1.9718794897,9.1345072372\C,4.5108282965,2.03103
54794,10.3657783874\C,3.8055443753,2.6716264581,11.5861992118\C,5.7837
662519,1.5650107478,10.4225053285\C,3.6157110997,4.1854249217,11.32682
06398\C,2.4106757675,2.0415680199,11.8141078812\C,4.6218599048,2.45331
28279,12.8813347139\C,6.6563215348,1.7046142021,11.6543425382\C,6.4710
219098,0.8139369485,9.3054016931\C,6.1167587868,2.6938881612,12.685813
2283\H,-2.9547836872,-4.7663728786,3.0550418192\H,-3.4003431059,-10.04
31697982,2.9616992618\H,-3.0996087079,-10.399627897,4.6643508105\H,-3.
6123920644,-11.6977947696,3.5679295916\H,-6.0664646731,-11.897584832,2
.8605906958\H,-7.1331200984,-10.4929323155,3.0334944032\H,-5.713420394
3,-10.4186492649,1.9694508752\H,-3.4780184643,-4.0751867439,0.08009057
74\H,-1.7694670299,-2.8447708181,2.3105533886\H,-3.4208495079,-1.92678
65965,-1.0314037672\H,-1.952747375,-1.192954517,-1.6839739672\H,-2.068
9193738,-2.9475977753,-1.5202955672\H,-0.5599328284,-1.0426185419,1.81
78834846\H,-0.6431153187,0.1879481484,-1.0242341799\H,-5.3431446838,-1
2.1927556181,5.2402766798\H,-6.7910558792,-11.1989678713,5.3676018894\H,
-4.118184099,-10.5075237744,6.6930525963\H,-5.3149658715,-8.63475352
36,7.6724256608\H,-6.9018370639,-6.7857314055,6.5245996031\H,-5.204921
4917,-6.3505902889,6.3912439724\H,-6.2361464278,-6.2896616768,4.953175
5855\H,-5.6822247687,-8.3082384711,2.264808727\H,-3.9253552512,-6.5332
813995,4.0272257806\H,-4.6545995571,-7.377582542,0.3411903006\H,-6.036
4367823,-6.3956531791,0.821828446\H,-4.7364431634,-5.6794079933,-0.138
6875453\H,0.8804083924,1.7823406299,-0.2959748258\H,0.809464249,0.4261
500396,2.4886272847\H,2.0387029268,1.2028425724,4.1582829323\H,2.20813
86522,3.1681105527,0.3144478741\H,2.446927292,4.158299315,1.7582512327
\H,3.716922993,3.058697709,1.2244342406\H,3.9389354348,3.5226324506,3.
5311791439\H,4.9206284594,3.1632634416,5.6427324752\H,5.1015026765,2.7
757859901,7.7992703451\H,1.292472018,2.2726991522,5.9052408786\H,1.793

4718917,0.7794052603,6.7130571746\H,1.3988438253,2.2071721765,7.669113
0738\H,2.6768133485,1.61285543,9.251469272\H,3.0603293796,4.3562347381
,10.398393377\H,3.0564985971,4.6508390767,12.1486556176\H,4.576611315,
4.7028169884,11.2334541842\H,2.4718296465,0.9483902199,11.8752258427\H
,1.9915142102,2.4069586829,12.7595961665\H,1.6988177408,2.3019318917,1
1.024297319\H,4.4756767063,1.4188841716,13.2255017387\H,7.6693245065,1
.9948116461,11.3377328898\H,6.7761893353,0.7100463552,12.1158672744\H,
6.9993311065,-0.0578920562,9.7166070652\H,5.7797554972,0.4670959228,8.
5354593863\H,7.2378147122,1.4316869985,8.8158324186\H,6.6545616993,2.5
857201174,13.6358172067\H,6.2922035542,3.721472567,12.3423825135\H,4.2
179272986,3.1034448924,13.6686211146\H,-5.507188805,-11.2025311079,7.5
192753007\H,-6.8656026109,-9.2379141153,7.1375252162\\Version=ES64L-G0
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.6263809,7.3554526,3.7760144,-2.3951186\PG=C01 [X(C40H56)]\\@

15Z,11Z

l (bet_car_11_15)

l\1\GINC-T4\FOpt\RB3LYP/6-31G(d)\C40H56\SANDHIYA\14-May-2016\0\#P Bec
ke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\\
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255793,4.4932036469\C,-6.1571778994,-8.2278700786,8.8513222893\C,-8.53
4915235,-8.0655507826,8.0720934367\C,-3.8955549297,-4.3696694249,3.158
0444691\C,-2.7430575779,-3.6946088799,2.8795821774\C,-2.1746206482,-3.
4597536199,1.5732278786\C,-2.9114954476,-3.9914207777,0.3665999059\C,-
0.9913494033,-2.7659692541,1.4953441253\C,-0.2573302344,-2.4189571418,
0.3172346067\C,-7.9600172116,-7.2892251784,10.3661724201\C,-7.16513281
16,-6.3121662641,11.228617348\C,-7.291749229,-4.906203608,10.644520306
\C,-7.108245005,-4.8482917689,9.1410054251\C,-6.9508377931,-3.43486593
74,8.6294789374\C,-7.1309070333,-5.9537157241,8.3534584022\C,-6.854897
8017,-5.9006479535,6.904545189\C,-5.8099813182,-5.265486768,6.32147252
27\C,-5.5164474052,-5.2150216744,4.8979861282\C,-6.4683227367,-5.89630
05009,3.944951861\C,0.9335418159,-1.7373600279,0.2581671116\C,1.693105
7235,-1.2444093722,1.3658239977\C,2.8867022165,-0.5600193034,1.3369741
652\C,3.4533533347,-0.1856612349,2.616096156\C,3.5848839203,-0.2095912
134,0.0452238218\C,4.5978919485,0.4758250703,2.9762626812\C,5.64984089
1,1.0354789403,2.1737009574\C,6.7698281809,1.6868224385,2.6224629199\C

,7.7140310096,2.1791261675,1.6315977483\C,7.0814542472,1.9264031737,4.0797008224\C,8.8573368916,2.8630092766,1.8793423306\C,9.7931153061,3.3763513234,0.8608780524\C,10.2393363323,4.8456081787,1.0626961896\C,10.2259967058,2.6209336483,-0.1808765985\C,9.0291348142,5.7824005976,0.8328331781\C,10.7614393972,5.0729456768,2.5019412751\C,11.3885249876,5.2200148892,0.0974146664\C,11.0988759243,3.1736354289,-1.2897587946\C,9.9417399447,1.1458176651,-0.3473566376\C,11.1639257122,4.6992625023,-1.3196252878\H,-3.7779549973,-4.1049794932,5.2778619055\H,-5.7604193329,-8.2692225339,7.8312803769\H,-5.3674772281,-7.8228843832,9.4932847205\H,-6.3677390733,-9.2547101614,9.1767402735\H,-8.8384400939,-8.9951727956,8.5687437666\H,-9.4251934652,-7.4336848961,7.9699084988\H,-8.18815034,-8.3352167329,7.0694201686\H,-4.4683667048,-4.7889992587,2.3355999907\H,-2.1820225619,-3.2854975543,3.7209322342\H,-3.9246685229,-3.5733273612,0.313531737\H,-2.40829942,-3.7599162812,-0.5732010665\H,-3.0190493184,-5.0819953662,0.4253612106\H,-0.5681355861,-2.4447543996,2.4454080012\H,-0.6790229695,-2.7214203739,-0.6378938237\H,-7.9471425282,-8.2979393529,10.7997274321\H,-9.0119787239,-6.9683601552,10.353007676\H,-6.1085865629,-6.6081206113,11.2596413401\H,-6.5637212794,-4.2281750651,11.1144449189\H,-7.6760948203,-2.7784400198,9.1308544391\H,-5.9571859437,-3.0276821629,8.8662128235\H,-7.09773869,-3.3525635575,7.5512994739\H,-7.5252449792,-6.4701083926,6.2644034239\H,-5.0976899247,-4.7498306553,6.9644145243\H,-6.5300218759,-6.9718727327,4.1562703105\H,-7.4834897883,-5.4937314922,4.0522010996\H,-6.1738652779,-5.7819862027,2.9003443624\H,1.331821026,-1.5660916166,-0.7384413212\H,1.2818862721,-1.4374620206,2.3547324245\H,2.8379270797,-0.500398988,3.4585746424\H,3.030066108,-0.544381758,-0.8326352726\H,3.7200989194,0.8747628998,-0.045749572\H,4.5808369571,-0.6664242478,-0.0010276451\H,4.7196399295,0.5889672953,4.0509977041\H,5.5638435724,0.9395856073,1.0971897285\H,7.4459490709,1.9858365693,0.5937335481\H,6.3235578699,1.5198320535,4.7505942136\H,8.0442180276,1.4751720746,4.3510064374\H,7.1657371689,3.0009784796,4.2875847437\H,9.0867896357,3.1127894933,2.9128097762\H,8.1946621511,5.5121356259,1.4888232517\H,9.3027937045,6.8244832917,1.0419264101\H,8.6653926655,5.7269869712,-0.198918635\H,11.5363856936,4.3431517245,2.7648539246\H,11.2034924521,6.0738619189,2.5786914943\H,9.9664377378,5.0148958928,3.2523905069\H,12.3288480732,4.7966763963,0.4800398041\H,10.7326121503,2.7854724009,-2.2518790028\H,12.1145340742,2.7571705716,-1.1823475578\H,10.859054459,0.62717706,-0.6598957007\H,9.5737150345,0.6752895356,0.566095181\H,9.2032096605,0.9629439933,-1.1413593219\H,11.9672809836,5.0340629886,-1.987400468\H,10.2286745083,5.1032833261,-1.7280

455765\H,11.5134808335,6.3108484785,0.1014435727\H,-7.5248803574,-6.32
86841706,12.2648473996\H,-8.2788245237,-4.4833696232,10.896371245\\Ver
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15Z,7Z

1 (bet_car_7_5)

1\1\GINC-Q1\FOpt\RB3LYP\6-31G(d)\C40H56\ROOT\14-May-2016\0\#P Becke3L
YP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\0,1\
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118,-5.3451483569\C,-8.3259006178,-2.1580880628,-9.4653305384\C,-8.959
5881248,-4.5779187203,-9.2894474472\C,-3.6269490256,-2.9021075807,-3.9
697742394\C,-2.55767127,-2.1794413927,-3.5271966463\C,-2.0782317117,-2
.0944930053,-2.1677952024\C,-2.8032867778,-2.8846808274,-1.1038839127\
C,-0.9899497696,-1.2965276709,-1.9104848129\C,-0.3563295157,-1.0648040
994,-0.6484994965\C,-8.1327439812,-3.7020681545,-11.4669335254\C,-6.97
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242,-4.4981293123,-10.0625570503\C,-6.5073426828,-3.908544858,-9.50767
50023\C,-6.2983017805,-4.0505402889,-8.0541146683\C,-5.3004684279,-3.4
791710424,-7.3373441064\C,-5.0881269062,-3.6029983092,-5.9042063234\C,
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,-0.4021460672\C,1.4293594465,0.5498792147,-1.3551572445\C,2.488459336
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.6201201389,-3.4252378655\C,5.873111588,5.169184842,-4.7460444289\C,6.
3780795265,5.0327233034,-2.2128335551\C,6.6537459863,6.1996494683,-5.1
546261044\C,7.4202217441,7.2164315805,-4.3927487122\C,8.9420141468,7.2
530563237,-4.6824261846\C,6.8087163899,8.1177817714,-3.5877778957\C,9.
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1480041\C,9.5834578814,8.5473891848,-4.1289104031\C,7.5697797972,9.164
4723582,-2.7988109233\C,5.3112839405,8.2274639401,-3.4231218154\C,9.07
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\H,-9.9577046973,-4.4238333345,-9.7174177408\H,-8.6693536684,-5.617765
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 28164\H,6.2750958142,4.3117167839,-1.3982183454\H,7.4404715976,5.10780
 09843,-2.4587692951\H,6.072097412,6.0128338057,-1.8311522011\H,6.73074
 51296,6.3006698589,-6.237995151\H,9.1482840655,5.0901668995,-4.3946383
 053\H,10.6846730603,5.9742559689,-4.3508932881\H,9.5851948123,6.035985
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 046\H,9.3549231143,9.3794145698,-4.8108437722\H,7.1463468992,9.2207116
 38,-1.7849205764\H,7.3765214929,10.1542484359,-3.2448016308\H,4.994932
 7177,9.2654002642,-3.6012509238\H,4.7590364926,7.5774187058,-4.1030230
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 7,-2.3503252954\H,9.2841401865,8.0928363065,-2.0321617771\H,10.6755134
 545,8.432664237,-4.132788173\H,-7.1633351191,-3.1208919014,-13.3213394
 057\H,-5.6418831843,-4.7684306441,-12.4167717623\\Version=ES64L-G09Rev
 D.01\State=1-A\HF=-1557.8898485\RMSD=4.805e-09\RMSF=1.809e-06\Dipole=0
 .0098737,0.0901019,0.1447955\Quadrupole=-0.8718779,-2.794851,3.6667289
 ,11.5939046,3.4346448,1.0659384\PG=C01 [X(C40H56)]\@

Structures of the rotamers of *15E* isomer of C4 radical

all-trans

1 (bet_car_030)

I\1\GINC-LXA167\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\11-Nov-2016\0\
#p UB3LYP/6-31g(d) opt freq scf=tight\Beta_Carotene (-30) optimizatio
n\0,2\C,-12.9460926946,-0.6904537,-0.3694179397\C,-6.662811552,-0.386
9852904,-0.1282481846\C,-13.6385198505,-1.1364559188,0.943195757\C,-12
.7927631986,-1.9322479779,-1.2680270012\C,-5.4245603398,-0.9916480433,
-0.2341797808\C,-4.2059234243,-0.2934646578,-0.1012303522\C,-2.9194004
66,-0.8361649844,-0.1837890965\C,-2.7436996505,-2.3185730183,-0.439037
1388\C,-1.8153590665,0.0283413205,-0.0273595788\C,-0.4548479927,-0.285
6066851,-0.0657535604\C,-13.8370491176,0.3197135556,-1.136655936\C,-14
.1197509321,1.5907535506,-0.3348017604\C,-12.906479291,2.0620695777,0.
4052973577\C,-11.7465539541,1.3743801425,0.5278717859\C,-10.629300254,
2.0258195454,1.3228804815\C,-11.6101550247,0.0131250504,-0.0319401032\
C,-10.4314210486,-0.6681287901,-0.2171624862\C,-9.0706270759,-0.239408
8803,-0.0917337307\C,-7.9396036845,-1.0208599011,-0.2488187906\C,-7.97
99460298,-2.5060530659,-0.5332009835\C,0.562771663,0.6552275999,0.0999
836264\C,1.9306342465,0.3340793441,0.0678666257\C,3.0237883771,1.18523
07221,0.2158051328\C,4.3331588078,0.6229285763,0.154642558\C,2.8738482
554,2.6721145812,0.4387335792\C,5.5260442249,1.2990736778,0.2733438228
\C,6.7937359442,0.6496576344,0.2074338264\C,8.0467753534,1.2079315941,
0.3058494744\C,9.1965628521,0.3300953086,0.2181011339\C,8.2800077311,2
.6861870913,0.501033209\C,10.5013642645,0.7030017348,0.2653093705\C,11
.6611899027,-0.2012195779,0.1678406142\C,12.7875106194,0.2741692878,-0
.7825718234\C,11.7372288977,-1.3690952655,0.8575629655\C,12.2770474081
,0.2283403874,-2.2426481029\C,13.2062530862,1.729084834,-0.4605878316\
C,14.0521735463,-0.6046727868,-0.6369790904\C,12.8726900544,-2.3566411
947,0.6802421526\C,10.7462123985,-1.8103538584,1.9099631907\C,13.73106
5033,-2.0948444475,-0.55606694\H,-6.6762488356,0.6855608526,0.06968514
38\H,-13.0391963202,-1.9029765541,1.4474683581\H,-13.7682912722,-0.305
624378,1.6425244792\H,-14.6268068699,-1.5649248074,0.7319334397\H,-13.
7862784387,-2.3022714306,-1.5474539311\H,-12.2475176399,-1.7022819448,
-2.1903383076\H,-12.2783970897,-2.7564553206,-0.761792044\H,-5.3818634
549,-2.0604449593,-0.4286585514\H,-4.276823444,0.7785999375,0.08584289
75\H,-3.1642003611,-2.6036896875,-1.4114255683\H,-1.6959878232,-2.6234
921573,-0.4342067166\H,-3.2614753114,-2.9136565063,0.3227628214\H,-2.0
590964815,1.0773987715,0.1466179172\H,-0.1502731929,-1.3174665009,-0.2
329603324\H,-14.7799341759,-0.1668617828,-1.4180235331\H,-13.326154252

,0.5857553418,-2.0716487556\H,-14.9356840619,1.4175179035,0.3855988073
 \H,-12.9820378329,3.0361020248,0.8879771961\H,-9.8631569158,2.47416080
 71,0.6784783357\H,-11.0327956362,2.8321957231,1.9436561549\H,-10.12572
 54212,1.3103596651,1.9810705784\H,-10.5406634596,-1.6922551761,-0.5531
 45376\H,-8.8811112235,0.8066747257,0.1139480447\H,-8.9953000081,-2.900
 0961755,-0.5920390914\H,-7.4769505043,-2.7376293652,-1.4804337701\H,-7
 .4570205294,-3.0665810482,0.251731552\H,0.2619177525,1.6885600303,0.26
 30865546\H,2.1650548772,-0.7194447878,-0.0929390692\H,4.384659356,-0.4
 555602945,-0.0014927841\H,1.8303863542,2.9903696193,0.4641414193\H,3.3
 360966815,2.9757208113,1.3866500483\H,3.3730751385,3.2403801356,-0.356
 4030418\H,5.5015047503,2.3745280211,0.4259250532\H,6.7549392424,-0.431
 2072232,0.0627844728\H,8.9686008154,-0.726548382,0.0849728199\H,7.3502
 686237,3.2539755393,0.566100818\H,8.8522063792,2.8751919861,1.41823598
 9\H,8.8653234802,3.1028993256,-0.3291464976\H,10.7224328184,1.76623831
 38,0.3257376169\H,11.3658155315,0.8250545193,-2.3581610105\H,13.034733
 7749,0.6274390475,-2.9291497128\H,12.0399392347,-0.7943106308,-2.55531
 28012\H,13.4520506279,1.8468997905,0.6014381446\H,14.0979069847,1.9922
 640174,-1.0426946294\H,12.4297855248,2.4573113658,-0.7158136693\H,14.5
 867365723,-0.3121660828,0.2786504914\H,12.4529385181,-3.3732521487,0.6
 482514635\H,13.5033663474,-2.337256731,1.5849431265\H,11.2859239643,-2
 .2269388897,2.7721197037\H,10.1076130625,-0.9983556859,2.2621740721\H,
 10.0938841071,-2.6153528055,1.541415922\H,14.6524278359,-2.6887550632,
 -0.5140658621\H,13.1924428521,-2.4154122119,-1.4572661244\H,14.7299492
 483,-0.3923568515,-1.4744167934\H,-14.4889799184,2.386956235,-0.997210
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 .0117062,0.0184959\Quadrupole=16.9901656,-0.2041815,-16.785984,-1.0509
 085,1.4401176,2.5095615\PG=C01 [X(C40H55)]\@

15E,8Z

l(bet_car_8_c4_c1)

I\1\GINC-HP2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\10-Jun-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizati
 on\0,2\C,-12.4478527031,0.3969128346,-0.9001658138\C,-6.4552751501,0.
 6336051278,0.1339145403\C,-11.9217491061,0.1847895714,-2.3401004796\C,
 -12.810585335,1.8921783833,-0.731770377\C,-5.1646404964,1.2334479549,0
 .1553310863\C,-3.9985070563,0.4974521036,0.1172438768\C,-2.6697833771,

1.0034817087,0.1411741349\C,-2.4493954355,2.4957784749,0.2238132485\C,
-1.612380012,0.0898572956,0.0855091793\C,-0.236474646,0.345827852,0.09
66403743\C,-13.748866119,-0.4122377838,-0.6886391092\C,-13.4901434893,
-1.8980489744,-0.4528033762\C,-12.6591084131,-2.0670274947,0.817746078
2\C,-11.4844318712,-1.1144446313,0.9117932633\C,-10.5241260448,-1.4880
458187,2.0174280653\C,-11.3530223704,-0.025062574,0.1106862724\C,-10.1
589966696,0.8380570845,0.1359893074\C,-8.8690930753,0.4116377664,0.142
7499389\C,-7.687234986,1.2482994071,0.1616009923\C,-7.8621283308,2.746
3655103,0.2110767414\C,0.7356944066,-0.6630701218,0.0275028077\C,2.105
6005252,-0.4317499639,0.0365389243\C,3.1286563325,-1.4140849862,-0.039
8447844\C,4.4539935091,-0.9943322512,-0.0186617057\C,2.7382895913,-2.8
72370033,-0.1435618249\C,5.6268447273,-1.7879511416,-0.0908347053\C,6.
8977420155,-1.2596876162,-0.060714556\C,8.1196859923,-2.0062429008,-0.
1485400606\C,9.3699149417,-1.4222697001,-0.0896089232\C,8.0344700528,-
3.5073214802,-0.330231864\C,9.6657414853,-0.0413013117,0.1732917373\C,
10.8662898876,0.6257043275,0.1554187903\C,12.2005400952,-0.0034322292,
-0.3133886154\C,10.8950352699,2.0021025995,0.6925432916\C,12.725660324
1,-0.9794881625,0.7683761739\C,12.0601344882,-0.7401663447,-1.66865896
95\C,13.2649628174,1.0970496853,-0.5628571654\C,12.056744869,2.6546902
08,0.9249902274\C,9.5994930445,2.6912829105,1.0732405339\C,13.40418960
14,2.1023089894,0.5772304961\H,-6.4604838688,-0.4567940801,0.092819554
7\H,-10.9832691612,0.7268566493,-2.4990080962\H,-11.7268012423,-0.8730
857011,-2.5472413861\H,-12.6523452551,0.5463646397,-3.0750631959\H,-13
.6826868381,2.1307597555,-1.3527917261\H,-13.0658569916,2.1252759924,0
.3087560618\H,-12.0014600691,2.5600088102,-1.0443993758\H,-5.094952962
6,2.3166360981,0.205496303\H,-4.0980141085,-0.5875577429,0.0626844547\
H,-2.9137518322,2.9119399319,1.1268094944\H,-1.3917459185,2.7639870851
,0.2445994088\H,-2.9031446461,3.00806874,-0.6341728517\H,-1.897468169,
-0.9616739441,0.023873454\H,0.118016408,1.3730925677,0.160135331\H,-14
.4063262675,-0.2590730306,-1.5546233048\H,-14.2828322237,-0.0079200624
,0.1837849219\H,-12.9533712327,-2.3290989838,-1.3077253165\H,-12.28328
96416,-3.0980932644,0.8969909007\H,-11.0902057426,-1.7888963784,2.9103
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736211019,2.2935056044\H,-10.3378157713,1.9098605524,0.0892860742\H,-8
.6825176544,-0.6609615528,0.1141390942\H,-8.4197893885,3.1042475054,-0
.6643750355\H,-8.4373967706,3.0448451203,1.0966670578\H,-6.9109447992,
3.2809168966,0.2366085433\H,0.3779420134,-1.6897849758,-0.0391612077\H
,2.4338602177,0.6059346817,0.1065891462\H,4.6161797461,0.0814877835,0.
0613474646\H,2.1383360989,-3.1802193344,0.7217720528\H,2.1280856324,-3

.0525695153,-1.0372382172\H,3.6023110826,-3.5364789891,-0.1963442902\H,
5.5159870587,-2.8651866,-0.1766127636\H,6.9757291084,-0.1774901684,0.
0195290674\H,10.2060816711,-2.1014934982,-0.2071489216\H,7.5239504146,
-3.986234293,0.5156077753\H,7.4715895107,-3.7732482201,-1.2342236668\H,
9.0297745848,-3.9534675685,-0.4120548034\H,8.8097670384,0.5426362217,
0.4919817067\H,12.0204128152,-1.7949991144,0.9537629228\H,13.679811364
1,-1.4213300639,0.4534105301\H,12.8878288666,-0.4683362529,1.723441434
7\H,11.6003408613,-0.0859654914,-2.4176767046\H,13.0550506492,-1.02305
07373,-2.0345995684\H,11.4628630315,-1.650806757,-1.6154674666\H,12.98
69963704,1.6493510844,-1.4704448012\H,12.0194740699,3.6389009066,1.389
1260624\H,9.7972848822,3.7155175619,1.4021100222\H,8.9012942023,2.7420
128517,0.2284116842\H,9.0804524528,2.1753610502,1.8908578883\H,14.0815
553082,2.9148974353,0.2825456619\H,13.8718059865,1.636440876,1.4595933
367\H,14.2262313075,0.6098324351,-0.7704076834\H,-14.4355256605,-2.447
7990043,-0.3669227666\H,-13.2991506432,-1.9279813684,1.7051983522\\Ver
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.0700644\Quadrupole=12.2696254,2.5402545,-14.8098799,0.7700843,0.01551
78,1.1397752\PG=C01 [X(C40H55)]\\@

15E,12Z

l (bet_car_032)

l\l\GINC-LXA123\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\22-Nov-2016\0\\
#p ub3lyp/6-31g(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
n\\0,2\C,-11.8358569685,0.5481480976,-0.1316658766\C,-6.4914296267,1.1
557523932,0.1073372368\C,-13.3281893634,0.2965846712,-0.4728360193\C,-
11.3243199815,1.4878280202,-1.2517243545\C,-5.1193822546,1.200382644,0
.0933181718\C,-4.3848311982,2.4077823637,0.2555568888\C,-3.0064906321,
2.5872536253,0.2627643618\C,-2.4687033016,3.9905567135,0.4550584104\C,
-2.0873118448,1.5142411729,0.0980936929\C,-0.7044378314,1.620118489,0.
0954887832\C,-11.7450138481,1.2590701902,1.2410098916\C,-13.9856279834
,-0.801646698,0.3587931854\C,-13.151844468,-2.0433494718,0.2951135507\
C,-11.8210967433,-2.0416005954,0.0519425427\C,-11.1035653737,-3.375980
4606,-0.0055008662\C,-11.0533161249,-0.7864003578,-0.0804057742\C,-9.6
814486813,-0.8753034004,-0.0726679758\C,-8.6862026419,0.1545934602,-0.
0005124945\C,-7.3182337778,-0.0104249279,-0.0457574282\C,-6.6410950661
,-1.346109679,-0.2515490016\C,0.1706014685,0.5327530994,-0.0709447786\

C,1.5622947123,0.6574616751,-0.0683193275\C,2.5278132454,-0.3456075824
,-0.2228045838\C,3.8978747127,0.0254414706,-0.1763410917\C,2.161313006
7,-1.7966478553,-0.4314552391\C,4.986255242,-0.8150800896,-0.302249055
\C,6.3297311569,-0.3528564279,-0.2386650709\C,7.4934050457,-1.08314172
86,-0.3460006461\C,8.7542223078,-0.379908032,-0.2414644222\C,7.5130793
751,-2.5765501585,-0.5625126756\C,9.993282297,-0.9362803592,-0.2861746
305\C,11.2711013513,-0.2146323552,-0.1584244418\C,12.3078742668,-0.878
6694385,0.7816570896\C,11.5237202794,0.9497347274,-0.811564855\C,11.79
35808407,-0.8107291459,2.2393665732\C,12.5187194773,-2.366472902,0.410
4420506\C,13.6867205369,-0.1849807936,0.6758946717\C,12.7885059084,1.7
558017736,-0.5957101129\C,10.618153924,1.5615474624,-1.8556119059\C,13
.5814087476,1.337362952,0.6407523439\H,-7.0200287479,2.099172066,0.250
9571975\H,-13.39945913,0.0088478125,-1.5303073359\H,-12.167799635,0.64
04543,2.0400514824\H,-13.8726008684,1.2435170571,-0.3656099808\H,-12.0
136364937,2.3346798958,-1.3587180482\H,-10.3323440347,1.9008172802,-1.
0654508046\H,-11.2893330956,0.9605589179,-2.2114858847\H,-4.5702651717
,0.2729933272,-0.0470133164\H,-4.9906973435,3.3038453747,0.391342278\H
,-1.8364852769,4.0616347878,1.3494670339\H,-1.853386169,4.3066737577,-
0.397005194\H,-3.2821315507,4.7134678775,0.5645703564\H,-2.4976885522,
0.5155042348,-0.0387575681\H,-0.2514958241,2.601344205,0.2303235737\H,
-12.2979874518,2.2069635638,1.2175697195\H,-10.7092004905,1.4784235464
,1.5155022323\H,-14.9969346615,-1.0049096933,-0.017749597\H,-13.652736
1091,-2.9968775746,0.4539907284\H,-10.392376953,-3.4997778419,0.821011
2702\H,-11.8237966114,-4.1970364227,0.0537618197\H,-10.5384986252,-3.4
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.6094575619\H,-7.3492279851,-2.1619097196,-0.4029394907\H,-5.984433418
6,-1.3157573644,-1.1299048691\H,-0.2802088858,-0.4487959733,-0.2061755
852\H,1.9481957688,1.6681723511,0.0743075608\H,4.1042695199,1.08555774
77,-0.0224201637\H,1.0825100051,-1.9545123904,-0.4771665076\H,2.590409
4168,-2.1796597651,-1.3659102357\H,2.5531583308,-2.4223846149,0.380668
5718\H,4.8077688894,-1.8759689398,-0.4544881948\H,6.4459610664,0.72094
473,-0.0832075207\H,8.6787958117,0.6959840814,-0.0904221345\H,6.512282
2273,-3.002578733,-0.6521470719\H,8.0671576178,-2.8324036982,-1.474522
6025\H,8.0176052494,-3.0870576376,0.2684352959\H,10.0581440402,-2.0193
012218,-0.3615603892\H,10.8029121872,-1.2696353694,2.3272044536\H,12.4
76036653,-1.3425092697,2.9146513437\H,11.7073422185,0.2238452952,2.588
9407878\H,12.7542798037,-2.4820455012,-0.6541077609\H,13.3590177792,-2
.7729480575,0.9864581222\H,11.6448891096,-2.9857085883,0.6373247214\H,

14.1869950484,-0.5218499246,-0.2438248299\H,12.5206425775,2.8214734192
 , -0.5385341112\H,13.422337234,1.6690397391,-1.4942736023\H,11.22225085
 14,1.9260027257,-2.6983828387\H,9.8759443991,0.860213984,-2.2412720709
 \H,10.0814520128,2.4380697464,-1.4644484147\H,14.5780716176,1.79553221
 01,0.6284883629\H,13.079157649,1.7035065196,1.5455925475\H,14.31570917
 68,-0.5178296222,1.5121191437\H,-14.1212505965,-0.4790719395,1.4037001
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 .1974384,-0.0058254\Quadrupole=14.6103114,0.9429768,-15.5532882,1.8133
 598,-1.5410736,1.3209411\PG=C01 [X(C40H55)]\@

15E,13Z

1 (bet_car_13_c2_c4)

1\1\GINC-R2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\10-Jun-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
 n\\0,2\C,-10.7630282733,-1.8841290672,-0.7217440302\C,-5.6508779216,1.
 3260492323,0.098074077\C,-10.285285382,-1.7859653576,-2.1900913908\C,-
 11.8188348555,-0.7784498583,-0.4792949436\C,-4.8357934995,2.5007861086
 ,0.0842466511\C,-3.4660889527,2.4554545657,0.0400075085\C,-2.570474162
 2,3.5746015188,0.0340928383\C,-3.1488098492,4.96975072,0.0654949051\C,
 -1.2084844912,3.3264894757,0.0057659564\C,-0.1447404077,4.2605430768,0
 .0065514475\C,-11.4658549256,-3.241122975,-0.4837894187\C,-10.48174145
 35,-4.3955685869,-0.3155391651\C,-9.6125891112,-4.1358258292,0.9132946
 062\C,-9.0747037551,-2.7211808557,0.9939248416\C,-8.0018213063,-2.5701
 962173,2.0478761691\C,-9.5491453272,-1.707150512,0.2245433069\C,-8.948
 0311282,-0.3613561431,0.2245171105\C,-7.6211596386,-0.0824689391,0.173
 0797091\C,-7.0189666407,1.2377913742,0.1602238978\C,-7.9251644325,2.44
 32159127,0.2197136991\C,1.1905260815,3.8988341891,-0.0103273127\C,2.25
 17665377,4.8276471727,0.0000224304\C,3.6302858589,4.5754135552,-0.0067
 578738\C,4.1705585192,3.2720321327,-0.0343715165\C,4.5679036158,5.7662
 508561,0.0179013294\C,5.5301493937,2.9470926551,-0.0350105507\C,6.0011
 914017,1.6346612472,-0.0670459528\C,7.3428067703,1.1804286901,-0.06772
 17493\C,7.5727151752,-0.1955050064,-0.1056141197\C,8.5047824562,2.1516
 790808,-0.0267207484\C,8.8526365814,-0.8115523025,-0.0618383395\C,9.21
 48197395,-2.1461242818,-0.1222865958\C,8.2182590295,-3.2965482195,-0.3
 943419239\C,10.6156345941,-2.4874179944,0.1704111409\C,7.3461709126,-3
 .5405045743,0.8622794766\C,7.3122776389,-3.0145264926,-1.6190609367\C,

8.9743251452,-4.6033949661,-0.7494409045\C,11.0159978711,-3.7685719793
,0.3618809668\C,11.6448666301,-1.3868227734,0.343761462\C,10.110716301
2,-4.9508772134,0.2090014748\H,-5.1043603524,0.3824305257,0.0602330457
\H,-9.7578979698,-0.8426652988,-2.3683921305\H,-9.5965436983,-2.598650
9424,-2.4450427817\H,-11.1389015077,-1.8345158307,-2.8783156125\H,-12.
7264372854,-1.005462834,-1.0519816794\H,-12.0965912698,-0.7185618156,0
.5796665631\H,-11.4759979308,0.210309162,-0.8004371438\H,-5.3257272973
,3.4702339765,0.1158462385\H,-2.9981602292,1.4704328203,0.0116130841\H
, -3.754224055,5.122992914,0.9679892483\H,-2.3800226544,5.7439229529,0.
0486277818\H,-3.8088705862,5.139316038,-0.7946096963\H,-0.9107129313,2
.2770073963,-0.0145038034\H,-0.374625485,5.3244602185,0.0260510272\H,-
12.1593278384,-3.4313285618,-1.3135339207\H,-12.0795755381,-3.17063934
94,0.4261514906\H,-9.8481474408,-4.4865984875,-1.207343243\H,-8.764321
9686,-4.8361831336,0.9400915408\H,-8.2910755003,-3.1292976216,2.948926
7724\H,-7.0444977245,-2.9991706357,1.7179562834\H,-7.8225400929,-1.530
9955107,2.3294469998\H,-9.6422874754,0.475872642,0.208253457\H,-6.9212
012914,-0.9150172898,0.1189475077\H,-8.6213689976,2.4507194868,-0.6290
551989\H,-8.5368599016,2.4287947629,1.1308438226\H,-7.3747715832,3.385
4443557,0.203687985\H,1.4185505592,2.8339453018,-0.0283152517\H,1.9546
171036,5.8763662838,0.0193310131\H,3.4742713737,2.4358140787,-0.057055
5217\H,4.0114997751,6.7077800119,0.03149659\H,5.2166640674,5.750742319
2,0.9030415402\H,5.2253195721,5.780658958,-0.8607295339\H,6.2479509995
,3.7622350266,-0.0073909943\H,5.2402120924,0.8533815239,-0.0947964914\
H,6.6872254032,-0.8200543335,-0.1330018366\H,8.1823820724,3.1915670853
, -0.0993500704\H,9.0734852077,2.0498358478,0.9063573701\H,9.2025858581
,1.967583051,-0.851469863\H,9.6685078091,-0.1135447891,0.0899298831\H,
6.7717911969,-2.6502996178,1.1346967953\H,6.6380683864,-4.3595885771,0
.6819004606\H,7.9597902838,-3.8081882909,1.7292491538\H,7.9155636879,-
2.7342431882,-2.4896484152\H,6.7547478966,-3.9239862764,-1.8753309632\
H,6.5805920834,-2.2226962996,-1.4550087381\H,9.4010533416,-4.494679166
3,-1.7554904063\H,12.0501401245,-3.9565418539,0.6453829464\H,12.638027
6867,-1.8174179306,0.500515383\H,11.6997935232,-0.7364944126,-0.537997
1726\H,11.4229710997,-0.7445259008,1.2052739188\H,10.674280233,-5.8135
090566,-0.1706549028\H,9.7177251361,-5.2659166101,1.1892676713\H,8.246
3730997,-5.4230188079,-0.8008907988\H,-11.0152029397,-5.3484554454,-0.
2115917819\H,-10.1874448673,-4.3490302898,1.8302298459\\Version=ES64L-
G09RevD.01\State=2-A\HF=-1557.280212\S2=0.937894\S2-1=0.\S2A=0.777333\
RMSD=6.105e-09\RMSF=2.332e-06\Dipole=0.2694562,-0.1164584,0.0918244\Qu
adripole=10.8761277,4.9483374,-15.8244651,-1.5593168,0.7539278,-0.3448

885\PG=C01 [X(C40H55)]\@

15E,9Z

l (bet_car_9_c4_c2)

l\1\GINC-HP1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\11-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizati
on\0,2\C,-12.2424515999,0.613207371,0.8068001852\C,-6.4089136313,-0.7
908045956,-0.2119830707\C,-11.7126947955,0.6143223171,2.26084335\C,-12
.8964648632,-0.7622953253,0.5302896941\C,-5.2743697214,-1.6598172524,-
0.2354840742\C,-3.9815269609,-1.2049014176,-0.1773884261\C,-2.79362694
12,-2.0059518783,-0.1874859851\C,-2.9308723283,-3.5085189132,-0.263923
2023\C,-1.566010782,-1.3659183043,-0.1264222107\C,-0.2757610306,-1.944
4986336,-0.1159491263\C,-13.3496511243,1.6813330739,0.6472260001\C,-12
.7928679282,3.0967081707,0.5192012107\C,-11.922772707,3.1808157164,-0.
7332371837\C,-10.9621484081,2.0191073919,-0.8895897693\C,-9.9253121199
,2.2657111459,-1.9612366993\C,-11.0658732712,0.8741981007,-0.166200761
\C,-10.0690748165,-0.2090407035,-0.2420287915\C,-8.7206001351,-0.05915
6981,-0.219200301\C,-7.738755655,-1.1266983445,-0.2682615677\C,-8.2290
031667,-2.5503389891,-0.3754843112\C,0.8963860297,-1.2080531338,-0.057
8487881\C,2.1796736223,-1.787925183,-0.0416259359\C,3.421428987,-1.149
6842261,0.0104111174\C,4.5867882128,-1.9502841243,0.0241942981\C,3.555
9402327,0.3567614084,0.0533948183\C,5.9061054651,-1.5018248818,0.07097
38932\C,7.0043117171,-2.3670865008,0.0876979873\C,8.3860367502,-2.0465
64035,0.1283460694\C,8.8554158714,-0.7319047037,0.1471930094\C,9.36175
41336,-3.2086592747,0.1502896212\C,10.227350625,-0.367454726,0.1483455
158\C,10.8318224508,0.8798546806,0.1629777305\C,10.0554999403,2.209548
4041,0.3072036318\C,12.2841651173,0.9354476065,-0.0576216593\C,9.28417
88338,2.5109381074,-1.0018233344\C,9.0738644459,2.1860246701,1.5056702
71\C,11.025220032,3.3831378139,0.6056492622\C,12.9246155146,2.10280256
63,-0.3152224719\C,13.0993094947,-0.34355483,-0.0784695743\C,12.244661
5821,3.4362536691,-0.3112392747\H,-6.1783762521,0.2731449565,-0.138516
0217\H,-10.9070636016,-0.1173736445,2.3850370912\H,-11.3111743627,1.59
3498085,2.5435959005\H,-12.5156569374,0.359527349,2.9644139159\H,-13.8
116080049,-0.8595911526,1.1269793735\H,-13.1714128483,-0.8678210242,-0.
.5258167382\H,-12.2463005788,-1.6003338803,0.8010524952\H,-5.446309135
6,-2.7305356125,-0.300476931\H,-3.8305837606,-0.126277875,-0.115380129
9\H,-3.4580265219,-3.8073829348,-1.1789463902\H,-1.9673569517,-4.02059

07256,-0.2573419113\H,-3.5159233134,-3.8920690962,0.581545235\H,-1.593
5307093,-0.276162365,-0.0795133504\H,-0.1824337321,-3.0283267897,-0.15
40521674\H,-14.0409945278,1.6049412361,1.496895875\H,-13.9375562226,1.
454643668,-0.2542805809\H,-12.1952799367,3.3500240412,1.4044375503\H,-
11.3453449002,4.1174224016,-0.7381671125\H,-10.4012413523,2.7383202384
,-2.8320121512\H,-9.1490693648,2.9664875981,-1.6210806386\H,-9.4286089
526,1.352274006,-2.2932008248\H,-10.4627507804,-1.2225970252,-0.257676
2611\H,-8.3134983747,0.947251637,-0.1332345429\H,-8.872079379,-2.80773
58589,0.4761975726\H,-8.8326703629,-2.6891036444,-1.2814372041\H,-7.41
45681597,-3.2760325183,-0.4051942618\H,0.8035125566,-0.1238926071,-0.0
225732546\H,2.2055315722,-2.8781366903,-0.0728135238\H,4.4347012996,-3
.0299115118,-0.0040191447\H,2.5908759635,0.8652610201,0.0255441028\H,4
.072623847,0.6795361192,0.965776791\H,4.1450663803,0.7228473214,-0.796
4846323\H,6.0808383783,-0.4289234465,0.0965418521\H,6.7644596492,-3.43
03697951,0.0680775602\H,8.1106174319,0.0525939979,0.1225523399\H,8.833
9057516,-4.1665617404,0.1486142375\H,10.0265143371,-3.1972546983,-0.72
29617739\H,10.0018586702,-3.184937162,1.0407632832\H,10.9050305755,-1.
2110895224,0.0796410342\H,8.5711406306,1.7173478849,-1.2429713886\H,8.
7270969643,3.4520725291,-0.9082475769\H,9.9654910087,2.6043480398,-1.8
544475801\H,9.5892204311,1.874942057,2.4210496652\H,8.6753622268,3.194
9270657,1.670053508\H,8.2218337157,1.5201923887,1.3648039161\H,11.3832
176686,3.2838146062,1.6390612429\H,13.9893167931,2.0770596217,-0.54044
09783\H,14.1632769343,-0.1135121011,-0.1854850624\H,12.9742754297,-0.9
212695927,0.8455336747\H,12.8183607708,-1.0011800489,-0.910815745\H,12
.9392308379,4.2154112378,0.0297658299\H,11.9569284899,3.72760262,-1.33
43905539\H,10.4600007897,4.3225159663,0.5552326029\H,-13.6062420605,3.
831038576,0.4694646504\H,-12.5618000913,3.2351925388,-1.6306400141\\Ve
rsion=ES64L-G09RevD.01\State=2-A\HF=-1557.2796833\S2=0.954461\S2-1=0.\
S2A=0.78138\RMSD=7.207e-09\RMSF=2.177e-06\Dipole=0.1655444,0.1395415,-
0.0708831\Quadrupole=12.55472,2.9032113,-15.4579313,2.4450139,-0.45833
27,-0.1799219\PG=C01 [X(C40H55)]\\@

15E,9Z,9'Z

l (bet_car_9_91_c4)

l\1\GINC-Q1\FOp\UB3LYP/6-31G(d)\C40H55(2)\ROOT\07-Jul-2016\0\\#P Beck
e3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\0
,2\C,-1.0172806731,0.3526704036,-0.0958885009\C,0.5773750063,-0.125722

497,5.9946690225\C,0.1545685784,0.7697850477,-1.0205681349\C,-1.763345
1541,1.6327868823,0.3284771214\C,0.8522639591,-1.4546416705,6.32468947
8\C,1.1981130099,-1.8622158403,7.6138621615\C,1.4824365151,-3.18048617
5,8.0352256054\C,1.4264944422,-4.309536477,7.0289857735\C,1.804183692,
-3.3929780991,9.3789081841\C,2.1124384696,-4.6056381247,10.0244184857\
C,-2.0300931994,-0.5279554791,-0.8703682958\C,-1.4097616775,-1.8224724
164,-1.3964868729\C,-0.4956212646,-2.4458018561,-0.3882826558\C,-0.081
4404917,-1.8599701373,0.7628123579\C,0.8330474857,-2.6689821953,1.6635
770873\C,-0.4609914856,-0.4742124595,1.0875280307\C,-0.3075300984,0.14
24193722,2.3143378016\C,0.0920511229,-0.3606160653,3.5848458495\C,0.21
24293339,0.4195634093,4.7335881745\C,-0.0461235665,1.9145937235,4.6824
927049\C,2.413201269,-4.700876032,11.3737647706\C,2.7157255972,-5.9195
556286,12.0246906787\C,3.023470802,-6.1275604534,13.359218241\C,3.2897
161286,-7.466718319,13.7970896112\C,3.0871547604,-5.0066617891,14.3700
945608\C,3.6028799009,-7.8633176498,15.0708650358\C,3.8474741785,-9.23
02165051,15.4213479999\C,4.163472994,-9.7525517908,16.6513638754\C,4.3
065753565,-8.9271776755,17.837248187\C,4.3702301948,-11.2436105203,16.
7827929279\C,4.5826188013,-9.3776967975,19.0860387445\C,4.7141682244,-
8.5408961746,20.2942775602\C,3.9296687202,-9.0460999565,21.5296588412\
C,5.4624010875,-7.4083485729,20.3200980716\C,2.4121306261,-8.901629282
3,21.2632414106\C,4.2328806507,-10.5382021763,21.8073381778\C,4.320706
1129,-8.2582214172,22.8021865084\C,5.5231310197,-6.4910031608,21.52524
66843\C,6.3581341494,-6.9465420248,19.1937004365\C,4.4283966301,-6.755
2567594,22.5574868316\H,0.649045473,0.5871673422,6.8163329482\H,0.8351
391185,1.4450199153,-0.4897012682\H,0.7398686565,-0.0909708058,-1.3570
013428\H,-0.2213358307,1.2966597757,-1.9073175395\H,-2.2216272063,2.09
43949119,-0.5540844025\H,-2.5609955098,1.417895539,1.0485325334\H,-1.0
970449486,2.3826090221,0.7684611008\H,0.7922907234,-2.2132878847,5.547
9681292\H,1.2516335437,-1.0853696175,8.3775184822\H,2.1284451641,-4.13
5601369,6.20412739\H,1.6725551529,-5.2769355324,7.4696566241\H,0.42571
77843,-4.3934390347,6.5874095946\H,1.8150248172,-2.5046417898,10.01212
44102\H,2.1160239075,-5.5283013794,9.4465874035\H,-2.4569956211,0.0511
223083,-1.6994032794\H,-2.8598773763,-0.7723123182,-0.1936897612\H,-0.
8487731929,-1.6309851636,-2.3257111676\H,1.2444086297,-3.5207722206,1.
1127539133\H,1.6704749959,-2.0717149928,2.0390611899\H,0.3040211626,-3
.077502988,2.5335904549\H,-0.5674085715,1.1944236811,2.331083248\H,0.2
92952277,-1.4169711556,3.6902278894\H,0.6181225013,2.4192561651,3.9702
341888\H,-1.0756523984,2.1386127404,4.3755891458\H,0.1108146174,2.3746
897774,5.6623417753\H,2.4097687371,-3.7789142591,11.9523209605\H,2.700

8364732,-6.8073571958,11.390498608\H,3.2314166475,-8.2406178467,13.030335141\H,2.8737481847,-4.0308252504,13.9310060946\H,2.3668818107,-5.1699139047,15.1818961707\H,4.0813424681,-4.952114119,14.8316115595\H,3.6647162145,-7.1090033072,15.8502583995\H,3.7672207998,-9.9377351361,14.5953461063\H,4.1627564239,-7.8574716518,17.7111665856\H,4.2443923446,-11.7472856329,15.8200568854\H,5.3743320062,-11.4791316127,17.1593153003\H,3.6560238803,-11.6877168111,17.4893004192\H,4.6616738446,-10.4523755095,19.2333889293\H,2.1224326717,-9.4302533573,20.3487518048\H,1.8326499006,-9.3197143613,22.0962969054\H,2.1223019542,-7.8524728714,21.1404168323\H,5.3121542716,-10.7207841835,21.8710590714\H,3.7858028252,-10.8309907204,22.7651159649\H,3.8167928438,-11.2015799929,21.0424577571\H,5.2927979271,-8.6241772699,23.1637216999\H,5.4792567484,-5.4483462347,21.17669149\H,6.5150018783,-6.5924831466,21.9968238267\H,7.3262161172,-6.6233197147,19.6018802587\H,6.5393593833,-7.7212511337,18.4468839611\H,5.9388105363,-6.0711456931,18.6768548525\H,4.6490691872,-6.2251233542,23.4921974898\H,3.4706961109,-6.361581681,22.1930366107\H,3.5911654694,-8.4775577308,23.5928925247\H,-2.1966651788,-2.5359029118,-1.680714475\H,-0.1392808777,-3.4507045517,-0.61254175\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.277466\S2=0.942493\S2-1=0.\S2A=0.777655\RMSE=5.246e-09\RMSF=1.863e-06\Dipole=-0.0624857,0.0914697,-0.237593\Quadrupole=-13.8452791,-1.5183392,15.3636183,-2.2985654,8.0936491,-1.0274515\PG=C01 [X(C40H55)]\\@

15E,14Z

1 (bet_car_14_c4_c1)

1\1\GINC-S4\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\14-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
n\\0,2\C,-12.5987556596,-0.3725691525,0.8438512606\C,-6.640024195,-0.2344505621,-0.3501000781\C,-12.0243545484,-0.3552710074,2.2804115423\C,-12.920486258,-1.8391079283,0.4674343766\C,-5.333668783,-0.798368473,-0.4176574998\C,-4.184092419,-0.0453650012,-0.3168260044\C,-2.8450737996,-0.5297115536,-0.3503884829\C,-2.6050322638,-2.0127216828,-0.5128852342\C,-1.8032606433,0.3907969305,-0.2232227247\C,-0.4213055274,0.1446647312,-0.2063462996\C,-13.9329963255,0.4095431709,0.7995726582\C,-13.7310826224,1.9220606908,0.7730357267\C,-12.9636135511,2.3019119186,-0.4913620822\C,-11.762322215,1.4191939436,-0.7640838954\C,-10.8596976256,1.9826291794,-1.8373981778\C,-11.5588592068,0.2348125257,-0.1305066039

\C,-10.3337990642,-0.5644657439,-0.3075816408\C,-9.0607825989,-0.09027
15799,-0.3001545485\C,-7.8531044492,-0.8798623305,-0.4292074851\C,-7.9
832720952,-2.3700960281,-0.6308305753\C,0.5157694871,1.1798146979,-0.0
740023865\C,1.913085517,1.1633947158,-0.0223368864\C,2.8568618236,0.10
23116251,-0.0572373212\C,4.2075948206,0.4453259056,0.0104086704\C,2.41
14537742,-1.3373634201,-0.1577145324\C,5.3360228767,-0.4081319548,0.00
18709175\C,6.6313148608,0.0604374768,0.0692849511\C,7.828676333,-0.726
164112,0.0686109433\C,9.0410722957,-0.064979379,0.1320193389\C,7.69957
25587,-2.2312186493,0.0005410588\C,10.3446405934,-0.6530938809,0.08643
79591\C,11.5892779542,-0.0704234544,0.1687317344\C,11.8270597136,1.430
1258677,0.4631842708\C,12.7606595419,-0.9183359036,-0.1276804732\C,11.
4519389459,2.27236905,-0.7812917732\C,11.0286744311,1.9223209181,1.696
103203\C,13.313884222,1.6898317961,0.8214493172\C,13.9942597089,-0.393
7531327,-0.3140895476\C,12.5868645769,-2.4137338524,-0.3102121295\C,14
.312247881,1.0592337945,-0.145746214\H,-6.6747455769,0.8469687292,-0.2
089070192\H,-11.0630898557,-0.8784859928,2.3235443463\H,-11.8568981595
,0.6672840264,2.6358317235\H,-12.7128527173,-0.8498381204,2.9774714963
\H,-13.7636246577,-2.196355611,1.0713328128\H,-13.2029117401,-1.927052
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5737561\H,-3.0637106832,-2.3850654378,-1.4375907665\H,-1.5442396269,-2
.2663987967,-0.5487092332\H,-3.0524472731,-2.5768473821,0.3155027459\H
,-2.1013962011,1.4353174015,-0.1185382701\H,-0.0773404209,-0.877257920
2,-0.2991461326\H,-14.5485915132,0.1084728498,1.657507506\H,-14.490169
9161,0.1160921384,-0.1022105644\H,-13.1704647221,2.2453666301,1.659681
3555\H,-12.6257719389,3.3476555205,-0.4367926818\H,-11.4706131951,2.38
81561034,-2.6561713605\H,-10.257401082,2.8228645079,-1.4623012315\H,-1
0.1755467221,1.2403234465,-2.2525772831\H,-10.46914326,-1.6409287902,-
0.3820348958\H,-8.9090982939,0.9781895265,-0.1539088093\H,-8.504398477
5,-2.8369210639,0.2153659861\H,-8.5741946326,-2.592727089,-1.528316786
1\H,-7.017660927,-2.8669308982,-0.7386730053\H,0.0804135341,2.17760857
76,-0.0010690002\H,2.3634723552,2.1513595995,0.066974849\H,4.427994018
9,1.5113141949,0.0793362219\H,1.7402181682,-1.5985414281,0.6693530935\
H,1.8619664454,-1.5156641248,-1.0904527511\H,3.2490801809,-2.036452972
5,-0.1329916914\H,5.1784329553,-1.4811112289,-0.0619153723\H,6.7680500
446,1.1410264386,0.1270599235\H,8.9711495426,1.0158237222,0.1787503185
\H,7.0794748472,-2.6047841636,0.8247427469\H,7.2126689701,-2.541886399
7,-0.9326404833\H,8.6609606395,-2.743248752,0.0599544262\H,10.34208408
48,-1.7214276733,-0.0945559967\H,10.4001178461,2.1460494709,-1.0536386

479\H,11.6266190084,3.3383866011,-0.5867781648\H,12.0489302408,1.98489
 89184,-1.6535210663\H,11.2104456155,1.2715676745,2.5586023057\H,11.359
 3541369,2.933908903,1.9626820031\H,9.9507474094,1.966857414,1.53695727
 97\H,13.5062557109,1.2791633649,1.8216087291\H,14.8068694443,-1.058910
 2765,-0.6013848067\H,13.5585473797,-2.8920587437,-0.4631137233\H,12.12
 06219448,-2.8803558402,0.5664103789\H,11.9594590208,-2.655883471,-1.17
 73839926\H,15.3348076975,1.1811536489,0.2355837081\H,14.29965099,1.574
 968649,-1.1195123876\H,13.4701154906,2.7740472125,0.8886657124\H,-14.6
 95932379,2.4430191602,0.8052660723\H,-13.6374279799,2.2652144591,-1.36
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 382\S2-1=0.\S2A=0.773806\RMSD=5.710e-09\RMSF=2.362e-06\Dipole=0.290670
 6,-0.2840574,-0.0678951\Quadrupole=16.0233231,0.3769629,-16.400286,-0.
 6798232,-0.6927937,1.1637962\PG=C01 [X(C40H55)]\@

15E,10Z

1 (bet_car_10_c4_c2)

I\1\GINC-HP1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\10-Jun-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizati
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 031104,-0.31707309\C,11.8820454848,0.4446789301,2.373733709\C,12.77831
 19818,2.0742990411,0.690851741\C,5.2146863222,1.0106118304,-0.36432692
 74\C,4.0776965873,0.2380426045,-0.3291942316\C,2.7286087931,0.70590012
 62,-0.349995059\C,2.471151694,2.1930851529,-0.4190037708\C,1.702073028
 6,-0.2319290472,-0.2982687048\C,0.3127325763,-0.0060450381,-0.28589130
 54\C,13.8161704447,-0.1812686793,0.8609112362\C,13.6334984473,-1.68973
 3266,0.7178815814\C,12.8833782466,-1.9819816018,-0.579832765\C,11.6745
 190695,-1.0946276386,-0.7987836332\C,10.7901019106,-1.5857127252,-1.92
 17066018\C,11.4504567139,0.0362438225,-0.0804897713\C,10.2176159878,0.
 8331016111,-0.2128355546\C,8.9513909063,0.3444927677,-0.2490167311\C,7
 .7333064186,1.1257532567,-0.3375774222\C,7.8458037074,2.6276843454,-0.
 436520425\C,-0.6343677306,-1.0261547885,-0.2288798776\C,-2.0155044342,
 -0.7998694081,-0.2009828078\C,-3.0581800417,-1.743847852,-0.1411208233
 \C,-4.3795134517,-1.267804639,-0.1012009923\C,-2.7831307303,-3.2320985
 82,-0.1131498619\C,-5.5328795973,-2.0751081775,-0.0402295433\C,-6.8821
 502772,-1.7395034131,0.0186584934\C,-7.5673012683,-0.4849360193,0.0777
 485809\C,-8.9553103163,-0.5271534021,0.1025062501\C,-6.7984308397,0.81
 42860051,0.1277375166\C,-9.8496265756,0.5860249884,0.0917220378\C,-11.

2267747826,0.6251201467,0.1562030725\C,-12.1186096342,-0.6161631296,0.3956864228\C,-11.885983314,1.9189275833,-0.1024195906\C,-12.1598129808,-1.4844675213,-0.8860960323\C,-11.6362086478,-1.4676787377,1.5964687234\C,-13.5631945361,-0.1887105419,0.7647734624\C,-13.223249171,2.0157461782,-0.293102125\C,-11.0537616164,3.1791193626,-0.240715007\C,-14.1645915342,0.8583688295,-0.1685267438\H,6.578256593,-0.6270950098,-0.2481956289\H,10.9137229989,0.9514444714,2.4455647151\H,11.7240309759,-0.6041776032,2.6473831718\H,12.556509408,0.8922841479,3.1148467893\H,13.6099366037,2.3944411902,1.3304675936\H,13.0711844276,2.2468023283,-0.3515525363\H,11.9288386306,2.7254208262,0.9207614423\H,5.1075514737,2.0902922561,-0.4219385411\H,4.2091379726,-0.8434305215,-0.2722533126\H,2.9310547952,2.6290347823,-1.3148807511\H,1.4075165569,2.4353068869,-0.4453689539\H,2.9070209073,2.7077679655,0.446814749\H,2.0110797363,-1.2775963757,-0.2562972129\H,-0.0594782087,1.0163959327,-0.3165477026\H,14.4193664107,0.0610980624,1.745844295\H,14.378453538,0.1863221284,-0.0099785429\H,13.0681975199,-2.0857592651,1.5714644606\H,12.557519403,-3.0325644658,-0.6075224536\H,11.4143738571,-1.9188610362,-2.76278067\H,10.1963261106,-2.4603092,-1.618500753\H,10.0993703354,-0.8230044831,-2.2858058971\H,10.3411972979,1.9136333861,-0.2137145983\H,8.8123296969,-0.7332642772,-0.1769113251\H,8.3549002103,3.0421026546,0.4435832212\H,8.4403974976,2.9179340236,-1.3120133439\H,6.8747517828,3.1189304668,-0.5180884787\H,-0.2604074822,-2.0482164818,-0.2004106342\H,-2.3254061303,0.2460077041,-0.2230844704\H,-4.4920376528,-0.1899053144,-0.12449343\H,-1.7189354684,-3.4613287246,-0.1868771645\H,-3.1545262562,-3.6858930604,0.8138769158\H,-3.2853591799,-3.7414696463,-0.9443978631\H,-5.351456221,-3.1483387879,-0.0465719542\H,-7.5507671161,-2.5999281567,0.0235134292\H,-9.3841131347,-1.5224614202,0.0815492089\H,-6.0765079487,0.8039765885,0.9524804156\H,-6.2314185426,0.9773402687,-0.7973656601\H,-7.4465180474,1.6793022911,0.2762587716\H,-9.3652547018,1.5457031047,-0.0441445548\H,-11.1634959406,-1.836687186,-1.1687024511\H,-12.7992326993,-2.3630887229,-0.731079362\H,-12.558182321,-0.9217240347,-1.7372263876\H,-11.508600913,-0.8423986616,2.4870635465\H,-12.3907446446,-2.2301361679,1.8263390721\H,-10.6941915206,-1.987834527,1.4202441659\H,-13.5526531218,0.228922267,1.7804206804\H,-13.6455600789,2.9853280325,-0.5514737764\H,-11.702550252,4.0489628148,-0.377747837\H,-10.4373697426,3.3611958322,0.6484492799\H,-10.3745318721,3.1345997879,-1.101338757\H,-15.1335394444,1.1987201184,0.2203768034\H,-14.3814096197,0.4274390787,-1.1592853998\H,-14.1934410371,-1.0865881046,0.7985073967\H,14.6044130434,-2.200317637,0.721162202\H,13.5654002406,-1.8723079411,-1.43978973

45\\Version=ES64L-G09RevD.01\\State=2-A\\HF=-1557.2760003\\S2=0.936598\\S2
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553693,-0.0400596\\Quadrupole=14.7511823,1.148248,-15.8994303,-1.855658
,0.4853614,-0.2971913\\PG=C01 [X(C40H55)]\\@

15E,11Z

1 (bet_car_11_c4)

1\\GINC-HP2\\FOpt\\UB3LYP\\6-31G(d)\\C40H55(2)\\SANDHIYA\\15-May-2016\\0\\#P
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920855041,-0.1460913379\\C,-11.4695305998,1.4289484067,2.0995474773\\C,-
12.8935463383,-0.1271962205,0.7422248062\\C,-5.4256713456,-1.9486481552
,-0.0359361444\\C,-4.0938376657,-1.6009032572,-0.0639937836\\C,-2.978812
0417,-2.4838202979,0.0329864515\\C,-3.2265127984,-3.9674957097,0.175605
1776\\C,-1.6967883824,-1.9373481013,-0.0080058\\C,-0.4614231843,-2.60190
41826,0.0616720226\\C,-13.0771382247,2.3245825298,0.3569807275\\C,-12.38
13689057,3.6064986192,-0.0929328244\\C,-11.5866478279,3.3248849407,-1.3
666728821\\C,-10.7627478215,2.0543779753,-1.3033966135\\C,-9.7680918856,
1.9505553513,-2.4365717988\\C,-10.9443600926,1.1060300172,-0.3481386635
\\C,-10.0688079365,-0.0736456307,-0.2249089534\\C,-8.7115623114,-0.06079
80892,-0.2603459618\\C,-7.8352958332,-1.2070876147,-0.1253970927\\C,-8.4
532070607,-2.5745819209,0.0341495053\\C,0.7706510582,-1.9446507991,0.01
81754929\\C,2.0008723616,-2.600033547,0.0837565636\\C,3.29945925,-2.0394
532388,0.0547833122\\C,4.3826506277,-2.922706775,0.1425393012\\C,3.49864
25141,-0.547613979,-0.0733765289\\C,5.7864148212,-2.7133009571,0.160013
9014\\C,6.5270852826,-1.5455680083,0.1689025032\\C,7.959982417,-1.469933
0894,0.1824581017\\C,8.5384449271,-0.214144108,0.2101207746\\C,8.7580014
971,-2.7543535209,0.1708745644\\C,9.939394187,0.0860198114,0.1706237334
\\C,10.6042980497,1.2854649641,0.2453158156\\C,12.1373845086,1.308905372
2,0.0400216178\\C,9.9975230282,2.5951015855,0.5653245333\\C,12.837929659
3,1.4683237429,1.412501117\\C,12.699294312,0.0422083315,-0.6335217064\\C
,12.4764177686,2.506254584,-0.8845596073\\C,10.6703333133,3.7465793617,
0.332526508\\C,8.6378983375,2.7028207242,1.2319090979\\C,12.0188352717,3
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,2.1534309103\\H,-12.252084298,1.4229605572,2.8690522801\\H,-13.77437614
15,0.0058207648,1.3822007938\\H,-13.2444771544,-0.4121693522,-0.2566586

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\H,-13.7178850972,2.5086131321,1.2294194634\H,-13.7410179328,1.9859039
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,0.9387100254\H,-9.1100789176,-2.8092806983,-0.8130056979\H,-7.7070359
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68,0.2030305906\H,2.5607695167,-0.0145427773,-0.2382616967\H,3.9599610
784,-0.1301045951,0.8305551281\H,4.1627204983,-0.3136081794,-0.9136331
89\H,6.3565951616,-3.6402620591,0.1811343362\H,6.0157716164,-0.5893952
097,0.1754782376\H,7.8400921087,0.613452086,0.2259390835\H,8.544360380
8,-3.3435132731,-0.7297126812\H,9.8347571774,-2.5844795638,0.208380452
6\H,8.497652572,-3.3820689912,1.0321663332\H,10.5703573628,-0.78023433
8,0.0132756755\H,12.6491020805,0.5896817459,2.0396402544\H,13.92378761
45,1.5641687745,1.2832119193\H,12.4791412632,2.3462490588,1.9570973398
\H,12.1971246424,-0.1709175336,-1.5840111358\H,13.7662193393,0.1847848
713,-0.8417099077\H,12.6162077025,-0.8445059026,0.0045157274\H,11.9879
778809,2.3393861234,-1.8539623642\H,10.2101144385,4.684621546,0.641861
3485\H,8.5318565238,3.681715818,1.7104230854\H,7.8119251329,2.60844577
37,0.5162484357\H,8.4966845242,1.9334085149,1.9978890029\H,12.00342006
6,4.6157690115,-1.0974035909\H,12.7447058656,4.2153971923,0.4330190214
\H,13.5575193161,2.5254530992,-1.0735755542\H,-13.1135901368,4.4045066
682,-0.267636845\H,-12.2715242345,3.2614874338,-2.229017367\Version=E
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964\Quadrupole=13.8807883,1.9059618,-15.7867501,4.0866854,-0.3754839,-
1.5960382\PG=C01 [X(C40H55)]\@

15E,7Z

l(car_H_021)

I\1\GINC-LXA152\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\24-Nov-2016\0\
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 7200597282,-1.0236549927\C,-11.4107687069,-0.1542899139,0.1280948556\C
 ,-12.8559467374,0.0051536795,0.6472694524\C,-13.0741188035,1.524013669
 4,0.8833988123\C,-12.8736487538,2.3690894112,-0.3801867841\C,-10.03970
 76783,0.2760065179,-2.046565072\C,-10.576303763,-1.0765165029,0.677433
 932\C,-9.1467032309,-1.3098388819,0.5103515555\C,-8.1087496595,-0.4231
 526657,0.6034555774\C,-6.7627414424,-0.9229066223,0.4349685165\C,-5.60
 68359261,-0.1894072871,0.4830669716\C,-4.3163804494,-0.7595498768,0.28
 71885073\C,-3.08403299,-0.1279059023,0.3191556557\C,-1.9151893109,-0.9
 088423655,0.0825919532\C,-0.6050144151,-0.4587663893,0.085158691\C,0.5
 103659363,-1.2789467443,-0.1645481194\C,1.8276816956,-0.8165147538,-0.
 1477354603\C,3.0067708957,-1.5366118483,-0.3848471502\C,4.2463872934,-
 0.8515129596,-0.2905083472\C,5.5035738119,-1.3906000632,-0.4843555328\
 C,6.699125619,-0.632053471,-0.3556628841\C,-13.1168099473,-0.714574709
 3,1.9822589815\C,-13.8653825442,-0.534951053,-0.3942708033\C,8.0015189
 832,-1.0526699998,-0.5199686268\C,-8.3091907328,1.0406751492,0.9176997
 128\C,-2.9306568477,1.3515395358,0.5957020154\C,2.9998978933,-3.008118
 8077,-0.7288078245\C,9.0631965672,-0.0899793831,-0.3191697223\C,8.3694
 070232,-2.468112223,-0.8925596943\C,10.3975665491,-0.3347055836,-0.405
 1300657\C,11.4751097014,0.6414538863,-0.1700540905\C,12.6485544484,0.1
 222568693,0.698413299\C,13.8255609896,1.1262233703,0.7117013899\C,13.3
 661810654,2.5734758027,0.8640108239\C,12.4905497099,2.9478198955,-0.32
 96728111\C,11.4446100673,1.9048760965,-0.6695853878\C,10.4110893541,2.
 4161005735,-1.6466183787\C,13.1988649376,-1.2137477334,0.1433717841\C,
 12.1470939786,-0.1215141371,2.1419378321\H,-11.5269682637,2.4454299052
 ,-2.131262715\H,-12.3678750868,1.851684181,1.6579389484\H,-14.08178886
 06,1.6877892852,1.2874375836\H,-13.7971793013,2.3815546522,-0.98118156
 04\H,-12.6971354582,3.4203527957,-0.1100736708\H,-10.1977046438,-0.773
 4369906,-2.3225777089\H,-10.1267969317,0.8831035701,-2.9535655124\H,-9
 .0097195032,0.3506557215,-1.6901430593\H,-11.0272301945,-1.7832913554,
 1.37351041\H,-8.8698829647,-2.3620020383,0.4111950707\H,-6.6740359416,
 -1.9918303437,0.2363229088\H,-5.6769925597,0.8782184868,0.6724276219\H
 ,-4.3038924476,-1.8314747465,0.0849711318\H,-2.0763764383,-1.96810614,
 -0.1211253673\H,-0.4093589705,0.5926280375,0.2922438904\H,0.3126165492
 ,-2.3278921911,-0.3778229333\H,1.9575482808,0.2421040995,0.0831684402\
 H,4.1938837627,0.2072972631,-0.0330290118\H,5.5813456619,-2.4431357155
 ,-0.7423767845\H,6.5599860251,0.4167828993,-0.0886048005\H,-14.1238461

33,-0.4691032923,2.3397732305\H,-13.0687587794,-1.8046066524,1.8822299
528\H,-12.4013064769,-0.4106408468,2.7544490958\H,-14.8953665044,-0.35
09521724,-0.0630400419\H,-13.7341229626,-0.0695924199,-1.3751697233\H,
-13.741114169,-1.6167171776,-0.5199367606\H,-8.0697536101,1.6811301628
,0.0588005845\H,-9.3410912035,1.2455943169,1.2057718176\H,-7.652793788
2,1.3484641278,1.7405005416\H,-3.8883977462,1.8519063138,0.7469775416\H,
-2.3238024455,1.5216390787,1.4938454562\H,-2.4214618607,1.8554511406
,-0.2351118775\H,3.5343228959,-3.5930700002,0.0307393331\H,1.990937840
7,-3.4160529397,-0.8090151453\H,3.5047770366,-3.1895085023,-1.68596060
71\H,8.7404427464,0.9145348972,-0.049695105\H,8.9921168453,-2.92947492
45,-0.1148153891\H,7.496032244,-3.10626623,-1.03732712\H,8.9547170718,
-2.4888199715,-1.820593186\H,10.710442598,-1.3574177979,-0.6023103205\H,
14.3843467031,1.0347200681,-0.2311795304\H,14.5206299252,0.845556559
6,1.5139220099\H,14.2275769311,3.2492339903,0.9330045026\H,12.79723819
28,2.694464736,1.7948871787\H,13.1217805379,3.1212210967,-1.2175001576
\H,11.9837487544,3.90767156,-0.1492023358\H,9.6935746944,3.0938449362,
-1.1615217305\H,10.9060951414,3.0073866201,-2.4298317168\H,9.843569236
1,1.6159850207,-2.1253112176\H,14.1178087405,-1.4823397342,0.678631833
2\H,12.498240184,-2.0450227391,0.2721411202\H,13.4425531814,-1.1318446
242,-0.9224481247\H,11.8213728658,0.8094829679,2.6186538646\H,11.29433
98283,-0.8089054828,2.1500633851\H,12.9427581901,-0.5594329828,2.75814
55122\Version=AS64L-G09RevD.01\State=2-A\HF=-1557.2749053\S2=0.887443
\S2-1=0.\S2A=0.764561\RMSD=4.391e-09\RMSF=1.216e-06\Dipole=-0.311049,0
.2104564,-0.0262791\Quadrupole=15.0336275,-0.2327273,-14.8009002,-4.09
71115,-1.4075476,1.5992629\PG=C01 [X(C40H55)]\@

Structures of the rotamers of 15Z isomer and rotamers of C4 radical

15,15'-cis (15Z)

1 (bet_car_trans)

1\1\GINC-MPP2R02C03S07\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\11-Nov-2
016\0\#p ub3lyp/6-31g(d) opt freq scf=tight\Beta_Carotene (-30) opti
mization\0,2\C,10.0775174332,-2.5102045675,0.6675970578\C,5.653916619
9,1.5590448266,-0.2451842956\C,9.5211851409,-2.3834532114,2.1059681607
\C,11.3180276398,-1.5928516449,0.5444627071\C,5.0540604547,2.852089267

9,-0.2034449856\C,3.6916982829,3.0424910049,-0.1640482905\C,3.00432795
 23,4.2918539674,-0.1174017903\C,3.8107317685,5.5695562047,-0.117105055
 4\C,1.6113362888,4.2764714061,-0.0696201673\C,0.7374127574,5.375571583
 7,-0.0109225555\C,10.5561190904,-3.9589152605,0.4125236475\C,9.4040588
 293,-4.9198039303,0.1295619576\C,8.6787754522,-4.4723642712,-1.1378133
 714\C,8.3930492754,-2.9847032691,-1.1854027557\C,7.4332428637,-2.61327
 2352,-2.2920557693\C,8.9801297251,-2.0949078016,-0.3435701029\C,8.6193
 623231,-0.6658502776,-0.3209432632\C,7.3579062779,-0.1637165244,-0.316
 9895943\C,6.9906492443,1.2378611824,-0.278392495\C,8.0896772529,2.2721
 835787,-0.2735463137\C,-0.6660080082,5.3297520851,0.044819806\C,-1.477
 3371526,4.1954125759,0.047528805\C,-2.8918950937,4.1833663219,0.115576
 8562\C,-3.5445638877,2.9508345015,0.1106265399\C,-3.6431724098,5.49488
 51483,0.1933566048\C,-4.9334255946,2.6919380633,0.1809576442\C,-5.4644
 717839,1.4192964765,0.1675503913\C,-6.8525976148,1.0692640516,0.240677
 1707\C,-7.1866895661,-0.2714443835,0.2099634036\C,-7.8659107162,2.1868
 231111,0.3503540301\C,-8.510362357,-0.8212393819,0.2369095289\C,-8.953
 7948493,-2.1210658362,0.230279472\C,-10.4769715524,-2.3904696491,0.168
 0296115\C,-8.1098352659,-3.3305628876,0.3316996207\C,-10.9821215972,-2
 .7953965008,1.5755116263\C,-11.310104075,-1.1833110282,-0.3042006003\C
 ,-10.7217265481,-3.535816116,-0.8470721027\C,-8.6098024246,-4.55343919
 45,0.0352168388\C,-6.677921449,-3.2660726487,0.8301121188\C,-9.9918163
 207,-4.825819651,-0.4726303451\H,4.9540404318,0.72192094,-0.2503518776
 \H,9.1537820807,-1.3693486304,2.2965533348\H,8.6861601499,-3.071310497
 4,2.2774725659\H,10.3030255671,-2.6065266242,2.8432637864\H,12.1338251
 436,-1.9926425947,1.1591647465\H,11.6733244186,-1.5403242741,-0.491479
 3516\H,11.1235113072,-0.5735191156,0.8928400028\H,5.7024159422,3.72400
 72995,-0.2004649579\H,3.0639188471,2.1503006781,-0.1648338609\H,4.4450
 845465,5.6322673741,-1.0102984256\H,3.1848942336,6.4629241751,-0.09509
 14545\H,4.4785561547,5.6116350738,0.7528222882\H,1.1562253054,3.286821
 7311,-0.0750658682\H,1.1732870799,6.3714344629,-0.0027525022\H,11.1468
 606056,-4.2941550983,1.2752537636\H,11.2359909047,-3.9640792082,-0.452
 0386951\H,9.7734390521,-5.9465072307,0.0164211797\H,9.272083103,-4.748
 2003444,-2.0258222791\H,7.6898854662,-3.1701737938,-3.2043091001\H,6.3
 996143009,-2.8951400672,-2.0441639452\H,7.4422915194,-1.5470206446,-2.
 524602232\H,9.4446554571,0.0382289038,-0.2422587789\H,6.5248206786,-0.
 8653048585,-0.3226316264\H,8.7395312493,2.1490533759,0.6028193489\H,8.
 7293846737,2.1681914071,-1.1591579375\H,7.7064749373,3.2939159213,-0.2
 587181484\H,-1.1628756384,6.2963568109,0.0932195407\H,-0.9966884602,3.
 2197697071,-0.0044252246\H,-2.903577188,2.0703151214,0.0473747925\H,-3

.4253928701,6.1248072864,-0.6778879693\H,-4.7246804914,5.3565520987,0.2347953476\H,-3.3492499981,6.0651429766,1.0831927354\H,-5.6153664901,3.5348313801,0.2506215885\H,-4.7635294799,0.5868227936,0.094416035\H,-6.3482220709,-0.9513701236,0.1284141836\H,-7.8092458056,2.8533795065,-0.5195190227\H,-8.8928297426,1.8266397618,0.4231889575\H,-7.6708743821,2.8019928396,1.2375992427\H,-9.2927692546,-0.0726084379,0.2247584062\H,-10.869026804,-1.9592842453,2.2748271774\H,-12.0453360469,-3.0664155438,1.541407704\H,-10.425375928,-3.6441494196,1.9827158722\H,-10.9619128541,-0.8015237689,-1.2706477292\H,-12.356608768,-1.4886511635,-0.4207157309\H,-11.2993836152,-0.3571708921,0.4151858222\H,-11.7998693321,-3.722887637,-0.9328313199\H,-7.9677633838,-5.4217909786,0.1804242097\H,-6.3457898028,-4.2609582374,1.1433833972\H,-5.9806180945,-2.927786107,0.0539094103\H,-6.5714027371,-2.5894787607,1.6845169779\H,-10.556350803,-5.3774521644,0.2965799442\H,8.7039009369,-4.929476829,0.9748029733\H,7.7290463853,-5.0165452046,-1.2497788246\H,-9.9475679306,-5.5052012158,-1.335965993\H,-10.3790979126,-3.1973288834,-1.8341082253\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2783646\S2=0.917028\S2-1=0.\S2A=0.772122\RMSD=9.125e-09\RMSF=1.572e-06\Dipole=-0.3197424,-0.2070263,-0.0266316\Quadrupole=11.0093572,5.0504502,-16.0598074,2.7420685,0.0252683,1.3546701\PG=C01 [X(C40H55)]\\@

15Z,8Z

1 (bet_car_8_15_c4_c1)

1\1\GINC-T1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\11-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
n\\0,2\C,9.4604127715,-2.359501653,0.6929768958\C,5.0634570298,1.73874
92696,-0.2178429045\C,8.9046554306,-2.2296379389,2.131276674\C,10.7074
196025,-1.4509151877,0.5704748382\C,4.4709357572,3.0349381272,-0.17304
35394\C,3.1092125653,3.2315059241,-0.1365925348\C,2.4263899787,4.48303
41484,-0.0877866032\C,3.2363180067,5.7583674063,-0.0794890491\C,1.0328
923987,4.4710613229,-0.0469961994\C,0.1602620518,5.5709045039,0.008960
1058\C,9.9288768322,-3.8114641941,0.4373882417\C,8.7701831342,-4.76395
64086,0.1532118856\C,8.0491119935,-4.3107624205,-1.1145332953\C,7.7736
247009,-2.8211421307,-1.1612879629\C,6.8170933464,-2.4423090282,-2.268
2468885\C,8.3662071088,-1.9360500532,-0.3183074126\C,8.0146912168,-0.5
04775103,-0.2938503409\C,6.7564935005,0.0055818177,-0.2908841307\C,6.3
983484297,1.4093783368,-0.2488208983\C,7.5037161038,2.4368066281,-0.23

77224064\C,-1.2440405289,5.5244481049,0.0556101044\C,-2.0522557089,4.3
885602977,0.0532253704\C,-3.4679193606,4.3705740255,0.1078225727\C,-4.
1126187906,3.1346110903,0.0989591417\C,-4.2265985732,5.6781760739,0.17
47538321\C,-5.5008922377,2.8648551302,0.1532014709\C,-6.0171761696,1.5
863192242,0.1376872482\C,-7.4057153138,1.2374240554,0.1860076367\C,-7.
8599194068,-0.0688785794,0.1828955974\C,-8.4284430841,2.3536586066,0.2
330242023\C,-7.0577419864,-1.2581610058,0.2268513215\C,-7.4228067311,-
2.5807597841,0.1513974328\C,-8.8630073554,-3.0687853801,-0.1355105862\
C,-6.3889209025,-3.594671428,0.4456413642\C,-9.7423499874,-2.862839468
5,1.1225057076\C,-9.5000365007,-2.3507405807,-1.3510731599\C,-8.865521
5458,-4.5731586589,-0.5142630409\C,-6.6960605784,-4.90059143,0.6193780
75\C,-4.9466666206,-3.1686952148,0.6387520134\C,-8.0727337535,-5.46125
59095,0.440986231\H,4.3586189134,0.9058645905,-0.2276810932\H,8.543624
4626,-1.2133081929,2.3222109766\H,8.0653008701,-2.9122860294,2.3024743
609\H,9.6849561726,-2.4578135385,2.8686120456\H,11.5200308572,-1.85655
5243,1.1855503833\H,11.0635758515,-1.4008952505,-0.4652938254\H,10.520
0799231,-0.4302247801,0.9188476847\H,5.1236978027,3.9035611121,-0.1655
795544\H,2.4778918589,2.3418646081,-0.1426892933\H,3.8667046023,5.8277
406682,-0.9750323264\H,2.6129895371,6.6531660909,-0.0459688533\H,3.908
1848782,5.790364452,0.7876649984\H,0.5762187689,3.4822520464,-0.057979
2859\H,0.5964436129,6.5665857424,0.0207968144\H,10.5166787105,-4.15137
30632,1.3002750711\H,10.609182616,-3.8210011148,-0.4267790331\H,8.0692
697268,-4.7689030562,0.9978636517\H,7.0956944202,-4.8481920039,-1.2277
077222\H,7.0710320651,-2.9997165311,-3.1809309434\H,5.7815501292,-2.71
81191096,-2.0215498026\H,6.8330248784,-1.3758746231,-2.4995516705\H,8.
844373659,0.1937666053,-0.2120381198\H,5.9188551406,-0.6904968852,-0.2
998060165\H,8.1523310543,2.3044588923,0.6381689758\H,8.1431262671,2.33
39640635,-1.1236820613\H,7.1267934841,3.46077439,-0.2171083855\H,-1.74
25947555,6.4903878766,0.1001828112\H,-1.5682636807,3.4143393121,0.0073
087934\H,-3.465161323,2.2581901421,0.045785781\H,-4.0017485753,6.30771
10594,-0.6949087107\H,-5.307766361,5.5340938008,0.2040488731\H,-3.9458
458991,6.2511441256,1.0670950916\H,-6.1907133045,3.7021531974,0.210600
1103\H,-5.2974644223,0.7733274876,0.0704699627\H,-8.9371525013,-0.1857
53353,0.1944698803\H,-8.3020674508,2.9769206238,1.1279148124\H,-8.3394
621854,3.0199857873,-0.6346811118\H,-9.4476074156,1.9565926026,0.24660
99933\H,-6.0043036063,-1.0749221873,0.4037237667\H,-9.7945343312,-1.80
89953413,1.4114135754\H,-10.765263173,-3.2147503399,0.9358455208\H,-9.
3460529736,-3.4148866292,1.9816300464\H,-8.8376266096,-2.4044845756,-2
.2221236791\H,-10.441892108,-2.8482309363,-1.6136131823\H,-9.727898186

3,-1.299186521,-1.1737902374\H,-8.4299438231,-4.6792877396,-1.51682489
5\H,-5.9033535915,-5.5903463669,0.9043774788\H,-4.3109385976,-4.044038
5513,0.8000910565\H,-4.5590193008,-2.6326732933,-0.2365257325\H,-4.823
2518262,-2.5059978581,1.5045664757\H,-8.0166739548,-6.4843381909,0.045
8235775\H,-8.5833764472,-5.5502963448,1.4133903089\H,-9.9072430569,-4.
9114134722,-0.584619082\H,9.1322432115,-5.7932308544,0.0399051537\H,8.
641215163,-4.5900738366,-2.0022444245\\Version=ES64L-G09RevD.01\State=
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MSF=1.215e-06\Dipole=-0.0030043,-0.0834019,0.0208358\Quadrupole=7.6507
573,6.9445441,-14.5953013,0.9422266,-0.7158071,0.5731004\PG=C01 [X(C40
H55)]\@

15Z,12Z

1 (bet_car_12_15_c4_c1)

1\1\GINC-S4FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\16-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
n\\0,2\C,-8.7067513524,-2.7556975259,-0.8073710815\C,-4.6882344657,1.7
171931473,0.1098146937\C,-8.1603659478,-2.5797438902,-2.2444662048\C,-
10.0293264461,-1.9600683397,-0.6908911943\C,-4.2187091335,3.0613820917
,0.0599718441\C,-2.8807141928,3.3889484515,0.0411420946\C,-2.327345286
2,4.7011373579,-0.0081494009\C,-3.2628948385,5.8873378207,-0.043118694
4\C,-0.9374726175,4.8338922328,-0.0226696487\C,-0.1873446155,6.0183705
491,-0.0676082492\C,-9.0487601483,-4.2421491555,-0.5495707525\C,-7.814
9351077,-5.0912647429,-0.2574396087\C,-7.1394320299,-4.5736380226,1.01
09474708\C,-6.9922621223,-3.0658251364,1.0528446385\C,-6.0736451282,-2
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,2.1903132832,0.1009022762\C,1.2169082406,6.1292685026,-0.0796886785\C
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2.4133499514\H,-8.9158311178,-2.8752802843,-2.9837272249\H,-10.8005371
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1133\H,-9.9329944834,-0.9271346212,-1.0408004305\H,-4.9496363229,3.864
8198075,0.0351021581\H,-2.165036692,2.5659022092,0.0654951719\H,-3.918
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6795857\H,2.9770679394,0.2032531896,-0.8998790044\H,3.45285774,-1.2047
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2865659,-0.7000311149,-1.1767634508\H,10.2062785133,-1.2980952063,-0.7
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.7977721087,2.44379155\H,9.7551619551,-1.2272657412,1.8332141677\H,8.2
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903608\H,7.5836007295,-6.0514157185,-0.6962778854\H,5.3923380755,-5.70
14978531,-0.530250222\H,4.8062547006,-4.3909658358,0.5030323453\H,4.91
82835582,-4.1554776155,-1.2431209981\H,9.8467621428,-5.5705817257,0.10
574161\H,9.7402769088,-4.4678350946,-1.2494006598\H,10.5002549972,-3.2
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\RMSF=2.359e-06\Dipole=-0.0283173,-0.2848627,-0.0115959\Quadrupole=8.3

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X(C40H55)]\@

15Z,9Z

l (bet_car_9_15_c4_c2)

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.0562596429,-0.3155457695,0.7864245935\C,4.9671593464,2.5553213331,-0.
0728768597\C,3.6032730092,2.4318538108,-0.0634826118\C,2.6460270925,3.
5016787999,-0.0161330936\C,3.1552242285,4.923413413,0.0270192581\C,1.3
016708458,3.1782354581,-0.0112336079\C,0.1952303185,4.0659003091,0.033
0937331\C,11.9011328186,-2.7902594759,0.5669916512\C,11.0299697116,-3.
9964161852,0.2258211078\C,10.2423463686,-3.7044075165,-1.0501617753\C,
9.6050731653,-2.3295495763,-1.0762114051\C,8.6072339018,-2.1742843052,
-2.2008501396\C,9.941073713,-1.3449044748,-0.2040746837\C,9.2513343571
,-0.0414926214,-0.1724696317\C,7.9089315189,0.1500256598,-0.1830460553
\C,7.2229691526,1.4290719112,-0.1328306977\C,8.0534752219,2.6887789591
,-0.0936445932\C,-1.1492712392,3.7217655898,0.0386178772\C,-1.69428282
01,2.4185110017,0.0005020344\C,-3.0405737595,2.05667369,0.0082767703\C
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\C,-11.7182036234,0.3360594086,-0.420409089\C,-12.2522104159,-1.843500
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 \H,-7.3158288886,-0.1923870674,-0.0371779836\H,-5.0407412274,-3.817077
 2953,-0.1417408948\H,-6.5311056809,-3.8912653386,0.8036974207\H,-6.608
 1953909,-3.8661554134,-0.9583790647\H,-8.5541353357,-2.9929312401,0.10
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 ,-0.0187735305,-1.4345314233\H,-13.0194618209,-2.5613218102,0.89500448
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15Z,13Z

l (bet_car_025_cis)

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,0.4376567491,-0.0213659974\C,1.1152677611,-0.9700243754,-0.1307771802
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H,-10.8098880751,0.3498980037,2.6543984231\H,-12.3069316836,-0.5496295
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1686946,0.6855386\PG=C01 [X(C40H55)]\@

15Z,11Z

1 (bet_car_11_15_c4_c2)

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,-12.4089789156,-0.0350310586,-0.8210344209\C,-5.149751163,2.379930546
,0.0798434175\C,-3.7930745107,2.1671058141,0.0800948705\C,-2.771824108
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\C,-1.4452821536,2.7553026349,0.0268422107\C,-0.2894920661,3.563006836
7,-0.0267647633\C,-12.4010597591,-2.5139298561,-0.5984556084\C,-11.605
8896782,-3.7665545766,-0.2392975412\C,-10.8250364428,-3.5133318545,1.0
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\C,-9.5951082992,0.0720992318,0.1554598979\C,-8.2425379555,0.176529610
4,0.1863825543\C,-7.4752436936,1.406517215,0.1289910093\C,-8.221148200
4,2.7171077871,0.0620653412\C,1.040008823,3.1301373393,-0.0276818853\C
,1.4975358968,1.8063833848,0.0298781912\C,2.8308944911,1.3492624162,0.
0243692801\C,3.0332011082,-0.040723005,0.1003772055\C,3.9922303854,2.3
108700845,-0.0652797791\C,4.2039275584,-0.8340716536,0.1214999291\C,5.
5444743183,-0.4783201181,0.1011075845\C,6.6446761562,-1.3922342093,0.1
126339977\C,7.9262493168,-0.8638117799,0.0819066529\C,6.3658456677,-2.
8781188711,0.1567739807\C,9.1540380555,-1.590753462,0.011947533\C,10.4
576499003,-1.1415128896,0.015521403\C,10.8634295789,0.3344302708,0.240
4944457\C,11.5180099236,-2.11850356,-0.2945420469\C,10.530662377,1.167
646314,-1.0220397636\C,10.1708096111,0.9531662765,1.4804238498\C,12.38
26265854,0.4463650799,0.5347407204\C,12.7926094656,-1.7364235355,-0.54
50404661\C,11.17728963,-3.5908732254,-0.4194820165\C,13.2691139472,-0.
3210723179,-0.4426748645\H,-5.6818277371,0.3144609029,0.1827160796\H,-
10.2045359328,-0.5362985055,-2.4661688725\H,-10.2811904245,-2.29818433
98,-2.3906601908\H,-11.6540781178,-1.3821623313,-3.0438885813\H,-13.28
10437024,-0.1950828774,-1.4666743182\H,-12.7741589581,0.159063002,0.19
44263285\H,-11.9032565,0.8661480405,-1.1821634035\H,-5.5156231983,3.40
1805685,0.0344676083\H,-3.448095844,1.1331147296,0.1246362685\H,-3.785
8574204,4.894467951,0.8361285648\H,-2.329678502,5.2999830435,-0.075638
6667\H,-3.7989870524,4.8147231372,-0.9254072049\H,-1.291350698,1.67816
76742,0.0739668263\H,-0.4295360114,4.6398286462,-0.0747792578\H,-13.03
11070335,-2.6865094147,-1.480991205\H,-13.0838561739,-2.2832859932,0.2
323443326\H,-10.9115980457,-4.0198533509,-1.0509651869\H,-10.089482209
6,-4.3142436475,1.2165717859\H,-9.5580667281,-2.4976866015,3.126030267
9\H,-8.2081614808,-2.6679214471,2.0145022967\H,-8.8064612143,-1.050967
7022,2.4184338856\H,-10.1702634348,0.9872295678,0.0340134707\H,-7.6560
340668,-0.7399022838,0.2371691508\H,-8.8609978418,2.7576950247,-0.8291
433057\H,-8.8805104051,2.8371885532,0.931045391\H,-7.555050771,3.58087
29348,0.0288862585\H,1.7833224979,3.9219021978,-0.0773357672\H,0.74184
30533,1.024839231,0.0883174607\H,2.113075759,-0.6222551063,0.148689638
8\H,3.6706656906,3.3480932264,-0.1710473075\H,4.6237817043,2.251856012
8,0.8298380109\H,4.6282203498,2.074762215,-0.9267250242\H,3.9964550145
, -1.9018334956,0.1617677072\H,5.8162226154,0.5708218264,0.0726348125\H
,7.9753555339,0.2191520701,0.064266991\H,5.7396432985,-3.1307441224,1.
0209796627\H,5.8228727599,-3.2059513513,-0.7386509223\H,7.2753926434,-
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,9.4623760115,1.1400194892,-1.2556266786\H,10.8182019684,2.2163856048,
 -0.8732479083\H,11.0644816585,0.7920573476,-1.9017059922\H,10.30988905
 38,0.3142006489,2.3594396958\H,10.6223069815,1.9288080249,1.6990469547
 \H,9.0994867088,1.1136786212,1.3546590172\H,12.5707385011,0.053475927,
 1.5429183805\H,13.5174275083,-2.4938027653,-0.8386543944\H,12.08340307
 68,-4.1762840369,-0.6000778988\H,10.7061736607,-3.9794725085,0.4919101
 452\H,10.4863532253,-3.7865676747,-1.2491565712\H,14.313244827,-0.2966
 373461,-0.1034523961\H,13.2720111428,0.159063958,-1.4345818073\H,12.65
 51827509,1.5093903553,0.5535475986\H,-12.2736377868,-4.6284523384,-0.1
 181768774\H,-11.5053927982,-3.5650382607,1.9156330892\\Version=ES64L-G
 09RevD.01\State=2-A\HF=-1557.2715788\S2=0.928131\S2-1=0.\S2A=0.77505\R
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 drupole=13.8469717,2.2240038,-16.0709755,0.1739988,-1.6171791,-0.91321
 \PG=C01 [X(C40H55)]\\@

15Z,10Z

l (bet_car_10_15_c4_c2)

I\1\GINC-S3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\12-Jun-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
 n\\0,2\C,9.3192690175,-2.5728270564,0.6824965423\C,5.082160356,1.70275
 54434,-0.148628355\C,8.7653356285,-2.4495556173,2.1221576622\C,10.5980
 919691,-1.7072938006,0.5788288864\C,4.5404726843,3.0233224514,-0.07940
 42488\C,3.1918809452,3.2743617488,-0.0411066558\C,2.5603665953,4.55790
 69581,0.0294398849\C,3.4296185627,5.7929395856,0.0654484076\C,1.174220
 0582,4.60633185,0.0622094976\C,0.3483145155,5.7511707627,0.132421893\C
 ,9.7370091681,-4.0353079652,0.4003010327\C,8.5466067554,-4.9419400487,
 0.0993770471\C,7.8402233029,-4.4408736162,-1.15881236\C,7.6184225978,-
 2.9416607279,-1.1792943562\C,6.674823586,-2.509790749,-2.2779558515\C,
 8.2426348344,-2.0929748336,-0.3222914041\C,7.9432272595,-0.6499098948,
 -0.2737035843\C,6.7056599492,-0.0940956555,-0.2560343614\C,6.400896389
 9,1.3230856246,-0.1887358609\C,7.5468423661,2.3051043329,-0.1632457503
 \C,-1.0465774205,5.7753647856,0.1652249462\C,-1.9112271002,4.668414588
 1,0.133247062\C,-3.3149165931,4.6672387507,0.1671913158\C,-3.975406691
 2,3.4228419465,0.1236059937\C,-4.1193198966,5.9467681658,0.2486471484\
 C,-5.3687106897,3.24000344,0.160281364\C,-6.1407809812,2.0790638321,0.
 1229685535\C,-5.8028922189,0.6975991055,-0.0078964875\C,-6.8522815239,
 -0.2145145352,0.0328157223\C,-4.3675249715,0.2658322495,-0.1963345469\

C,-6.7540050112,-1.6370623783,-0.0030757448\C,-7.7411074138,-2.6019647
049,0.0030117136\C,-9.2546992985,-2.293075415,-0.0812319875\C,-7.32311
0575,-4.0038130748,0.1840795844\C,-9.7452618226,-1.7087243972,1.266713
3313\C,-9.5919092041,-1.3168296513,-1.235666509\C,-10.0607204285,-3.58
0016623,-0.3980643885\C,-8.2155752108,-4.9897307287,0.4410751917\C,-5.
8502161597,-4.3649299451,0.1626757312\C,-9.6972057657,-4.7791892499,0.
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248825897,2.3301185011\H,7.9028224861,-3.106044377,2.280294096\H,9.535
851763,-2.7169602206,2.8565953278\H,11.3939694922,-2.1526213327,1.1882
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0454065,2.4136155755,-0.0652834949\H,4.065588196,5.8494599673,-0.82709
82084\H,2.8499634064,6.7157897745,0.1158976784\H,4.0996696684,5.774410
9403,0.9343846973\H,0.6720720698,3.6404298455,0.0300839534\H,0.8352976
309,6.7224548953,0.1660104138\H,10.3124830719,-4.4112392579,1.25650547
3\H,10.416846023,-4.0524576348,-0.4641779536\H,7.8464158252,-4.9390790
594,0.944586561\H,6.8679949329,-4.9418169746,-1.2793495771\H,6.9089916
72,-3.058331128,-3.2012542615\H,5.6307057659,-2.7548932035,-2.03498957
7\H,6.7268501292,-1.4403541718,-2.4890500346\H,8.7983849012,0.01646906
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9234,2.1323336878,0.7093412536\H,8.1804087177,2.1896364771,-1.05179653
49\H,7.2122606869,3.3432084769,-0.1262618427\H,-1.4937663633,6.7648196
293,0.2217883424\H,-1.4497833289,3.6838731494,0.0749040856\H,-3.331935
2979,2.5524995824,0.0674527464\H,-3.4894931204,6.8372288531,0.26607538
83\H,-4.7977008483,6.0407248718,-0.6079183856\H,-4.7392706717,5.965391
6246,1.1533780437\H,-5.9584305271,4.1510356107,0.2436108994\H,-7.21181
1291,2.2592270663,0.2111806507\H,-7.8362906512,0.2243413542,0.15143329
63\H,-3.913156157,0.7953794406,-1.0415328358\H,-3.7629151713,0.4916633
309,0.6910576306\H,-4.2741018968,-0.8025764234,-0.3969283186\H,-5.7388
702744,-2.0143191158,0.0256168435\H,-9.2245497669,-0.78088437,1.520566
2102\H,-10.8202756706,-1.4920141607,1.2197506748\H,-9.5772862555,-2.41
01444561,2.091085833\H,-9.1674903559,-1.6745254709,-2.1803446379\H,-10
.6808218501,-1.2596329846,-1.356985251\H,-9.2302315416,-0.3008095933,-
1.0749946488\H,-9.8773340291,-3.855122171,-1.4453016692\H,-7.843011887
7,-5.9940028284,0.6358610396\H,-5.7242134859,-5.4474229246,0.255550944
8\H,-5.3671192681,-4.0526953023,-0.7714790048\H,-5.2961339223,-3.89598
7627,0.9856217464\H,-10.2155159124,-5.6778491441,0.1136201046\H,-10.04
54510574,-4.635668961,1.5093317358\H,-11.1301947477,-3.3485772296,-0.3
141243483\H,8.8732624364,-5.9806628994,-0.0337037169\H,8.4203786405,-4

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6\\Dipole=-0.0558942,-0.2504681,0.0125582\\Quadrupole=8.327557,5.8139831
,-14.1415401,3.3153953,-1.1452494,0.7556814\\PG=C01 [X(C40H55)]\\@
15Z,7Z

l (bet_car_025_cis)

l\\GINC-P3\\FOpt\\UB3LYP\\6-31G(d)\\C40H55(2)\\SANDHIYA\\09-Feb-2016\\0\\#P
UB3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
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48195,0.13420428\\C,-7.974839833,-3.3461717105,0.9083686051\\C,-8.030319
1539,-2.864624191,-1.5808374981\\C,-5.1535504535,2.6926792625,0.2019889
336\\C,-3.7742439122,2.7538791104,0.1689115047\\C,-2.9755563225,3.928200
9537,0.22093786\\C,-3.6545678917,5.2734976942,0.3380385264\\C,-1.5845277
627,3.7887541418,0.1505773394\\C,-0.6186001722,4.8011341467,0.163688961
2\\C,-9.8187398214,-4.2246850015,-0.5597591123\\C,-10.9848647131,-4.3110
420492,0.4178388223\\C,-11.8530696547,-3.0670253616,0.2567797282\\C,-11.
0657464457,-1.7785926858,0.1633702989\\C,-11.9380097054,-0.547602311,0.
3369167898\\C,-9.7114298771,-1.7290047205,-0.0287644071\\C,-9.0667891569
,-0.4176426886,0.0335587629\\C,-7.7474517237,-0.0684170445,0.0492960695
\\C,-7.244485382,1.2829085721,0.1387342408\\C,-8.2262789195,2.4268108695
,0.2254260516\\C,0.7815362797,4.6361223317,0.081884654\\C,1.4879342533,3
.4453660853,-0.0165850394\\C,2.9029753506,3.3166925146,-0.1097638524\\C,
3.444183994,2.0429948197,-0.2062606567\\C,3.7584205471,4.564562253,-0.1
036817227\\C,4.8130241388,1.6720971633,-0.3223071151\\C,5.2315694219,0.3
693131926,-0.4063548524\\C,6.5960018514,-0.0894752693,-0.5307841754\\C,6
.8246286523,-1.4383143619,-0.5844431139\\C,7.6996073164,0.9348618621,-0
.652227811\\C,8.0767043368,-2.1606344578,-0.7697357225\\C,9.2888401349,-
2.0549709801,-0.1620288025\\C,10.5145034471,-2.8090475349,-0.7211839993
\\C,9.5500470983,-1.2920496018,1.0861452198\\C,10.9043518649,-3.97649286
76,0.217448204\\C,10.2980905426,-3.3847077011,-2.131927042\\C,11.6654425
008,-1.771395258,-0.8118808139\\C,10.8026778237,-0.8923276614,1.3896243
143\\C,8.4445875152,-1.0837957762,2.1026915411\\C,12.0136444588,-1.13232
30551,0.5372829869\\H,-5.2651257312,0.5709575635,0.0640247163\\H,-7.3112
715054,-2.519808331,1.17265332\\H,-8.5666009541,-3.579924681,1.79984383
31\\H,-7.3506013464,-4.2192017217,0.6795755219\\H,-7.5794151426,-3.83303
916,-1.831764223\\H,-8.654576589,-2.5560710151,-2.4271839759\\H,-7.22045
89252,-2.1399233245,-1.487448862\\H,-5.7099001142,3.6226523007,0.277463

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396\H,-0.9605941802,5.8303548244,0.2370707788\H,-9.2129758846,-5.13979
77043,-0.5341707328\H,-10.2245609364,-4.149140573,-1.5790192128\H,-10.
615892442,-4.3765232637,1.4492738414\H,-12.5650170462,-2.9816054992,1.
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2086814\H,-8.8862139424,2.4458024175,-0.6514264925\H,-8.87180106,2.324
3905805,1.1072255944\H,-7.7344947317,3.3987729388,0.2885520742\H,1.358
0760667,5.5587034612,0.0970066138\H,0.9275060247,2.5117914304,-0.02832
55873\H,2.7336658387,1.2152538761,-0.1963425554\H,3.504553773,5.219952
8009,-0.946014953\H,3.5987947509,5.1445405185,0.8135774775\H,4.8244982
436,4.3420460197,-0.1696545242\H,5.5621332147,2.4589419125,-0.34397877
63\H,4.4687626938,-0.4094555848,-0.3681037975\H,5.9345715133,-2.070818
8045,-0.6177493499\H,7.4471155836,1.678041666,-1.4180379395\H,7.855775
5283,1.4817367709,0.2867442429\H,8.6466637567,0.4674366266,-0.92445709
97\H,7.9942349215,-2.9164102755,-1.5503477392\H,10.1126244853,-4.73433
45593,0.2312926322\H,11.8260568761,-4.4591249901,-0.1317895976\H,11.06
27365531,-3.6428847513,1.2467238254\H,9.9767282694,-2.6135053708,-2.84
0911085\H,11.2379321265,-3.8120907755,-2.5012526492\H,9.554299169,-4.1
89209331,-2.142521825\H,11.3609503673,-0.9890057083,-1.5198472827\H,10
.9740195526,-0.3934451306,2.3433510971\H,8.8682821884,-0.7515385324,3.
0560250625\H,7.698709366,-0.3488927676,1.7918233371\H,7.9024272509,-2.
0207855181,2.2785174315\H,12.5634377529,-0.192677528,0.3820899186\H,12
.7085111514,-1.7789245763,1.0969037378\H,12.5552248306,-2.2525931672,-
1.2386625513\H,-11.5767214298,-5.2170452562,0.2388898824\H,-12.4824211
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149e-06\Dipole=-0.0874015,-0.0539236,0.0458749\Quadrupole=23.277718,-3
.9248218,-19.3528962,0.7795949,-1.1280507,1.6289837\PG=C01 [X(C40H55)]
\\@

Structures of the rotamers of *15E* isomer of C5-Me radical

15E

1 (Car_H_021)

I\1\GINC-LXA29\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\12-Nov-2016\0\#
p ub3lyp/6-31g(d) opt freq scf=tight\Beta_Carotene (-30) optimization
\0,2\C,-12.3103052896,2.2961827872,0.5450821717\C,-11.5004973344,1.43
06759345,-0.4021056828\C,-11.5721589203,-0.0331435406,-0.1442804828\C,
-13.0022847702,-0.5908730073,-0.0222255262\C,-13.801575322,0.300283067
2,0.9733827705\C,-13.7609064444,1.7981334886,0.6496393152\C,-10.813568
299,1.9566606518,-1.4272472236\C,-10.4651748964,-0.8182906448,-0.02002
81516\C,-9.0928189686,-0.3819859234,-0.0226999152\C,-7.9690601072,-1.1
71989407,0.023968288\C,-6.6839987268,-0.5255288009,0.0694583173\C,-5.4
568650685,-1.1421450123,0.1052907315\C,-4.2302518871,-0.4276864106,0.1
563748685\C,-2.9383199774,-0.9354802096,0.1810038903\C,-1.8515481407,-
0.0200292529,0.2398024811\C,-0.5005428455,-0.3370271527,0.2602876821\C
,0.5297448354,0.6152149393,0.3224045988\C,1.8888236834,0.2864377452,0.
328818385\C,2.9911060628,1.14737831,0.3872043763\C,4.294160799,0.58077
22279,0.3625494614\C,5.4907892133,1.2674058043,0.4047937893\C,6.758368
2363,0.6233294344,0.3521396156\C,-13.0528598131,-2.0378947872,0.497277
0085\C,-13.6683930195,-0.557996311,-1.4215621539\C,8.0097059556,1.1992
736688,0.3736228202\C,-8.0102988314,-2.6837922875,0.0207728004\C,-2.64
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5085\C,13.9859724258,-0.4939782072,-0.8700754747\C,13.7141957625,-1.98
95688856,-0.7327779862\C,12.9516044121,-2.2427377413,0.5659470823\C,11
.7988465031,-1.2855714861,0.7944981389\C,10.8898064251,-1.7283917629,1
.9176540272\C,13.0904133372,1.8189237239,-0.6823682772\C,12.0859191827
,0.2575353589,-2.369273571\H,-12.2771981474,3.3441133524,0.225483092\H
, -11.8519604957,2.2496920772,1.5450085244\H,-13.3905311023,0.143423733
8,1.9811984865\H,-14.8418735508,-0.0509352839,1.0022343927\H,-14.28433
36875,1.997127599,-0.2940422561\H,-14.2941085439,2.3604608894,1.426562
5802\H,-10.7913318325,3.0303323509,-1.6006966989\H,-10.2636601919,1.33
47626848,-2.1273558216\H,-10.6289179366,-1.878401277,0.141606812\H,-8.
9316732538,0.6932336342,-0.0453281925\H,-6.6995565268,0.5650102229,0.0
761426446\H,-5.4223622862,-2.2281221337,0.0950967997\H,-4.3206230227,0
.6593056181,0.1781382156\H,-2.1126923865,1.0384282554,0.2709015725\H,-
0.2050164328,-1.3849363012,0.2247664781\H,0.2319635856,1.6613832716,0.
3638691332\H,2.1207439924,-0.7786568683,0.277571805\H,4.3456579207,-0.

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70613834,-0.4647867328,0.2760025839\H,-14.0969592028,-2.3514562617,0.6
135295224\H,-12.5794257327,-2.740980933,-0.1971739046\H,-12.5621862548
,-2.1357829044,1.4722847049\H,-14.716972433,-0.8747197604,-1.356218993
6\H,-13.6399074095,0.4391655534,-1.8698895357\H,-13.1492776927,-1.2391
60361,-2.1053485026\H,-7.539399659,-3.0921790537,0.9239195611\H,-9.026
0806095,-3.0782829774,-0.0320523564\H,-7.4575632375,-3.0864803037,-0.8
374154385\H,-2.0238684284,-2.6759709547,-0.7208648979\H,-2.0915861835,
-2.7318208024,1.0405925531\H,-3.5509053561,-3.0250557154,0.091272503\H
,3.326531658,3.1397425366,-0.3843207133\H,1.7980829015,2.9672190156,0.
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7526\H,10.6595361672,1.8056562646,0.2293238505\H,14.5743409024,-0.1652
928615,-0.0007791118\H,14.5977969393,-0.2840814536,-1.7573249903\H,14.
6531931578,-2.5566798121,-0.7409070975\H,13.1246069375,-2.3478101345,-
1.5864784297\H,13.6418135886,-2.1778613345,1.4239589532\H,12.563886196
4,-3.2721910872,0.5900125471\H,10.2407421832,-2.5614544087,1.610688525
1\H,11.4948587184,-2.1063825238,2.7538019216\H,10.2501091101,-0.926063
9149,2.2898068941\H,13.937028659,2.0903990915,-1.3248361447\H,12.28187
78838,2.5228720656,-0.9036605736\H,13.3992957106,1.9662240865,0.359304
1424\H,11.8620290894,-0.7776756573,-2.6489665463\H,11.1498118397,0.822
6219785,-2.4327207225\H,12.7825143262,0.6679913903,-3.1114804297\\Vers
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.0946571\Quadrupole=19.5654486,-1.3515449,-18.2139037,-0.4614289,-2.49
72381,0.1651522\PG=C01 [X(C40H55)]\@

15E,8Z

1 (bet_car_030)

1\1\GINC-R2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\27-Nov-2016\0\\#P
UB3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
0,2\C,11.1342575792,-1.9178251809,0.4242534578\C,6.9173506511,1.346438
1456,-0.336937512\C,11.5273010837,-2.7809724058,-0.8019038045\C,9.8934
206732,-2.5512763291,1.0758787967\C,5.6510588084,1.8757455236,-0.38959
21794\C,4.4753178196,1.0886902837,-0.2539116063\C,3.1522473015,1.50586
10071,-0.2809124996\C,2.7570344409,2.9544694012,-0.4663890371\C,2.1298

206846,0.5278825189,-0.1274701771\C,0.7614790037,0.7557929288,-0.12345
38719\C,12.2824506145,-1.9273201531,1.4761669533\C,13.5681738104,-1.23
4968035,1.0095357145\C,13.2811279001,0.2046658619,0.5519186062\C,12.14
81267968,0.2447662755,-0.456225919\C,12.2822958862,0.8406799639,-1.650
2094395\C,10.9084581294,-0.4681100456,-0.0427782075\C,9.6798292273,0.1
176038626,-0.0575573703\C,9.3866868304,1.4931350606,-0.3808226663\C,8.
1474729291,2.0810210935,-0.4752280517\C,8.0698027396,3.568504521,-0.74
70905285\C,-0.2061675317,-0.2517655904,0.0259154675\C,-1.5817864157,-0
.0036210111,0.0317674545\C,-2.6325664706,-0.9193519602,0.1656156126\C,
-3.9640010382,-0.4238816804,0.1494175746\C,-2.3984577557,-2.4033737987
,0.3256485248\C,-5.123471048,-1.1648034705,0.2609446294\C,-6.418886094
7,-0.5769870713,0.2446987451\C,-7.6442106969,-1.1992275097,0.341004887
5\C,-8.8340098672,-0.3746989471,0.313547844\C,-7.8031286294,-2.6940471
419,0.4736479019\C,-10.1193978289,-0.8120865032,0.3655740144\C,-11.322
5186677,0.0380305821,0.3300954008\C,-12.4379982789,-0.4413359905,-0.63
13601818\C,-11.4447867995,1.163300556,1.0814129334\C,-11.9503581645,-0
.2917101928,-2.092519301\C,-12.780246832,-1.9305425674,-0.3847044235\C
,-13.7418712973,0.3642029659,-0.4240826905\C,-12.6317470963,2.09906864
55,0.9734902548\C,-10.4598955469,1.5981634592,2.1421017378\C,-13.49354
20953,1.861955187,-0.2652388954\H,6.9922345199,0.2714558824,-0.1860575
947\H,10.695195517,-2.8321377597,-1.5133737049\H,12.3896825389,-2.3734
141495,-1.3370110201\H,11.770733195,-3.8041893357,-0.4889054238\H,10.1
377009548,-3.5593921941,1.430751642\H,9.5446892791,-1.9683043194,1.935
8295962\H,9.0624536683,-2.649037542,0.3682863597\H,5.5411873161,2.9458
298144,-0.5417055153\H,4.6396634404,0.0197846976,-0.1102036397\H,3.618
6617844,3.6139824808,-0.581051233\H,2.1254702581,3.0780564929,-1.35484
82416\H,2.1768302603,3.3156780196,0.3918889951\H,2.4621637613,-0.50324
38658,-0.0014468823\H,0.3983057525,1.7757696363,-0.2433562555\H,12.495
0132317,-2.9682150454,1.7551801961\H,11.9187410094,-1.4275655177,2.385
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697669582,0.132856528\H,11.4814811046,0.8384322187,-2.3837215736\H,13.
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7942882\H,-1.8757787796,1.0410136556,-0.0829692573\H,-4.0738010345,0.6
557816022,0.0379118605\H,-1.3387347375,-2.6640017139,0.3262555926\H,-2
.8297023486,-2.7702835877,1.2657068885\H,-2.8760363322,-2.9662698772,-
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,0.5096068939,0.1459260949\H,-8.6591576065,0.6966521742,0.2248813761\H
 , -6.8465726512, -3.2189478896, 0.4986397381\H, -8.3494826894, -2.950526584
 2, 1.3901882595\H, -8.3826362169, -3.1018458313, -0.3650618735\H, -10.28860
 63168, -1.8864007228, 0.3785939558\H, -11.0099280616, -0.8309938223, -2.249
 2538835\H, -12.6947521455, -0.6949233391, -2.7910739555\H, -11.7726323496,
 0.7572057999, -2.3537132798\H, -13.0082979368, -2.1172179366, 0.6714090632
 \H, -13.6641629628, -2.2064646086, -0.9727165388\H, -11.9715033639, -2.6043
 427981, -0.6853164952\H, -14.2486948655, -0.0034278368, 0.480220792\H, -12.
 2653441927, 3.1363372663, 0.9941071042\H, -13.2470636135, 1.9960373844, 1.8
 830977923\H, -11.0054386922, 1.9350666325, 3.0349290575\H, -9.7716607246, 0
 .8044043794, 2.437797639\H, -9.8595896771, 2.4576717359, 1.810136899\H, -14
 .4424556884, 2.405738146, -0.1801722166\H, -12.984144472, 2.2575424103, -1.
 1533644006\H, -14.419791344, 0.1638550812, -1.264296305\H, 14.3028313965, -
 1.2280092095, 1.8246554546\H, 12.9910574729, 0.7992159315, 1.4319499628\\V
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 4153076, -1.9954147\PG=C01 [X(C40H55)]\\@

15E,12Z

1 (car_H_021)

1\1\GINC-R2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\25-Nov-2016\0\\#P
 UB3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
 0,2\C,-12.6629486169,0.9635058587,1.006568055\C,-11.6497553414,0.69854
 81049,-0.0908187838\C,-11.0237841318,-0.6519215594,-0.0593268973\C,-12
 .030364274,-1.8154609619,0.0027906327\C,-13.0444578697,-1.5325462189,1
 .1502629389\C,-13.715163651,-0.15591643,1.0726324587\C,-11.3840698016,
 1.6046513346,-1.0431125067\C,-9.6751731412,-0.8425701324,-0.0648148154
 \C,-8.6633757045,0.1829599821,-0.0250100307\C,-7.3026060287,0.01540728
 82,-0.0816871262\C,-6.4699984037,1.1882469877,0.0260572954\C,-5.101223
 3257,1.2297263712,-0.0014035801\C,-4.3626602858,2.443994898,0.11558315
 63\C,-2.9870729024,2.6216171422,0.1136786207\C,-2.0677057657,1.5396312
 977,-0.0106553025\C,-0.6866994309,1.6431575821,-0.0146708455\C,0.18898
 85111,0.5477223775,-0.1363274271\C,1.5791300061,0.6712631736,-0.131736
 8256\C,2.5461246915,-0.338491426,-0.2412171872\C,3.9147770852,0.033331
 9146,-0.1989615751\C,5.004816899,-0.8120511104,-0.2814016109\C,6.34693

12333,-0.3470914067,-0.2250548929\C,-11.3745683482,-3.1788362509,0.279
4267353\C,-12.7713391223,-1.9053760115,-1.3556156353\C,7.5124951966,-1
.0802608873,-0.2913497112\C,-6.629125551,-1.3266410941,-0.2561870671\C
,-2.4450557587,4.0293984319,0.2527797427\C,2.1790193132,-1.796217603,-
0.3952106304\C,8.771442742,-0.3718622287,-0.2059101083\C,7.5348866832,
-2.5814219899,-0.4445439636\C,10.0117698972,-0.9275764907,-0.217466916
8\C,11.287370039,-0.1985900452,-0.1105849081\C,12.3169429178,-0.818089
4966,0.8670462787\C,13.6959483584,-0.1282767946,0.740999071\C,13.58949
28637,1.3909116638,0.6376162915\C,12.8057942339,1.7531713497,-0.622262
1662\C,11.5438192103,0.9362490748,-0.8124259536\C,10.6462547764,1.4996
361201,-1.8900797182\C,12.5318727116,-2.320982423,0.5657402357\C,11.79
06357265,-0.6844453852,2.3159003669\H,-13.1379165237,1.9403381982,0.85
93509366\H,-12.1351136165,1.0038862319,1.9718130827\H,-12.5102594077,-
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,-14.3637054766,-0.0997262588,0.1893042142\H,-14.3634071954,-0.0089628
33,1.9457069367\H,-11.8700152786,2.5778884271,-1.0479977459\H,-10.6841
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09067\H,-0.2319953889,2.6279135026,0.0837992749\H,-0.2628653276,-0.437
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3168246455\H,-13.239298694,-0.9574258062,-1.6353800788\H,-12.069719218
3,-2.1724151342,-2.1540806695\H,-5.9738708735,-1.5510279716,0.59519771
61\H,-7.3416879398,-2.1473025281,-0.3524294201\H,-5.9981945235,-1.3315
829216,-1.15400665\H,-3.2563730697,4.7583447786,0.3346293125\H,-1.8124
821032,4.132321599,1.1439086563\H,-1.8285408977,4.310970339,-0.6105329
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68,-0.4530075904\H,2.6227203281,-2.2189953849,-1.305333545\H,8.6936587
337,0.7093245732,-0.1006518029\H,8.0341851942,-3.0558905438,0.41058768
2\H,6.5349940549,-3.0118652144,-0.5226631537\H,8.095250138,-2.87512530
19,-1.3412260703\H,10.0788158433,-2.0127022082,-0.2468053814\H,14.2033
39666,-0.5049744727,-0.1591614065\H,14.318959098,-0.4229037861,1.59585
44802\H,14.5857722432,1.8494277305,0.6128362904\H,13.0797779034,1.7960
145979,1.5214442463\H,13.4468417777,1.6279142057,-1.511125807\H,12.536

2003013,2.8199173447,-0.6141789558\H,10.1066303049,2.3929034631,-1.543
 3360481\H,11.2567575869,1.8256177704,-2.743962195\H,9.9069931367,0.781
 2807455,-2.249097098\H,13.3674556379,-2.7000206778,1.1667974281\H,11.6
 564264391,-2.9300292567,0.8130111307\H,12.7766212479,-2.4845904129,-0.
 4904034696\H,11.7007185484,0.3648955733,2.6172726229\H,10.7996478042,-
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 7571845,0.6999827\PG=C01 [X(C40H55)]\@

15E,13Z

1 (bet_car_030)

1\1\GINC-R2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\25-Nov-2016\0\\#P
 UB3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
 0,2\C,-10.6015436519,-2.6483537717,0.0485878431\C,-5.9468211058,1.6193
 325419,0.0606096232\C,-11.0714956717,-3.1626157142,-1.3365534638\C,-11
 .6283287154,-1.6183037672,0.5496138815\C,-5.463336022,2.9134090575,0.1
 123660585\C,-4.0901125242,3.2317391449,0.142992301\C,-3.5469128604,4.5
 207720756,0.2018456625\C,-4.4725332802,5.7221515457,0.2383977385\C,-2.
 1570684383,4.7680605794,0.2320470257\C,-1.1051005548,3.8413678868,0.20
 15603746\C,-10.5667927198,-3.8218641007,1.0714973756\C,-9.5131913864,-
 4.8924978221,0.7653864077\C,-8.1164008779,-4.2641185099,0.6332182876\C
 ,-8.1269904447,-3.0996251278,-0.3397975184\C,-7.2738727537,-3.03484056
 16,-1.3731190321\C,-9.1793315848,-2.0772252571,-0.0943049065\C,-8.9070
 818504,-0.7437466309,0.0086131671\C,-7.6091873905,-0.1278029302,-0.012
 6526635\C,-7.3222099867,1.2205046732,0.0339026016\C,-8.3857907867,2.29
 63663285,0.0528771424\C,0.2378462218,4.1986211511,0.2431215054\C,1.294
 6572047,3.2660154842,0.2108846407\C,2.6621191638,3.509929012,0.2525941
 496\C,3.5529260698,2.393123853,0.2066634723\C,3.2402579513,4.902566167
 6,0.3463151412\C,4.9258569059,2.4345745508,0.2455346614\C,5.738764939,
 1.2621833886,0.1934667632\C,7.1092112148,1.1710136831,0.2311550424\C,7
 .7110687981,-0.1464165919,0.1614449237\C,8.0158586058,2.3726941293,0.3
 395847225\C,9.0394474501,-0.4258072437,0.1645692993\C,9.6399554148,-1.
 7686064375,0.0709180277\C,10.8228344217,-1.8897388463,-0.9220708436\C,
 9.1887925193,-2.8251464904,0.7956733033\C,10.2994399575,-1.7042852544,

-2.3663482039\C,11.887953448,-0.80056372,-0.648002214\C,11.5296190661,
 -3.2590939804,-0.7881370397\C,9.7222403037,-4.2323948176,0.6169321007\
 C,8.1490120902,-2.734310607,1.8888550706\C,10.5479552022,-4.420260484,
 -0.6542152924\H,-5.2133320533,0.8124590422,0.0418987292\H,-11.16259215
 54,-2.3279111651,-2.0408565674\H,-10.3704341809,-3.8811138064,-1.77067
 76187\H,-12.0526235888,-3.6471873895,-1.2538353551\H,-12.6020077186,-2
 .1038328389,0.6843394793\H,-11.3326541195,-1.1868566185,1.5126617806\H
 ,-11.771572124,-0.7987146989,-0.1635551145\H,-6.1764334041,3.733661414
 2,0.1335424836\H,-3.4024108065,2.3882345819,0.1212938675\H,-5.13813199
 22,5.6935228375,1.1103540753\H,-3.906208208,6.6567641471,0.2851505353\
 H,-5.1124571756,5.7664859425,-0.6519656934\H,-1.8593596382,5.815407153
 8,0.286126558\H,-1.3346941517,2.7781392593,0.1421104378\H,-11.56502303
 43,-4.277894462,1.1168900366\H,-10.368446103,-3.4027483352,2.068578630
 1\H,-9.7661746345,-5.4203404353,-0.1628387377\H,-7.3772836852,-5.01182
 57605,0.3234695546\H,-7.3035078245,-2.2198250202,-2.0902989869\H,-6.52
 4200124,-3.8060944342,-1.5361888056\H,-9.7505790085,-0.0801056287,0.16
 7174622\H,-6.7582145309,-0.8037368131,-0.0482110071\H,-9.3968340012,1.
 8908907706,-0.0086773693\H,-8.3224776489,2.8974862195,0.9687796914\H,-
 8.2578682649,2.9857954085,-0.7909178805\H,0.4684531091,5.2607679894,0.
 3044986471\H,0.9965429307,2.2183848214,0.1461302729\H,3.084475903,1.41
 05875959,0.1340311708\H,2.4711353358,5.6763737471,0.3651811581\H,3.846
 0614367,5.0155713515,1.2544838893\H,3.8995391539,5.1116712214,-0.50565
 81291\H,5.4163313827,3.401350811,0.3200519133\H,5.1920278039,0.3211814
 387,0.1146788029\H,7.0105575472,-0.9761751132,0.0781930608\H,7.4648364
 009,3.3134871698,0.3872519376\H,8.6456369235,2.3085175971,1.2361323401
 \H,8.6950887104,2.4288966804,-0.5211165718\H,9.7328859924,0.4121661776
 ,0.1768488215\H,9.7666722477,-0.7530632257,-2.4710874622\H,11.13118351
 05,-1.7094895074,-3.0824280138\H,9.60314447,-2.5014681929,-2.648472918
 \H,12.2013227922,-0.8056191272,0.4026817632\H,12.7753336699,-0.9913633
 375,-1.2639746363\H,11.5354835853,0.2057326637,-0.895964565\H,12.17422
 98032,-3.2429330395,0.1028420576\H,8.8747302866,-4.933999972,0.6326511
 918\H,10.3282685003,-4.4972314058,1.4997296647\H,8.4671810457,-3.33955
 16157,2.7495092168\H,7.9768002671,-1.7121323731,2.2306027924\H,7.18273
 94729,-3.1485181413,1.5662031701\H,11.0813270475,-5.3784256345,-0.6254
 919794\H,9.8834225718,-4.4569955716,-1.5271531611\H,12.1938424276,-3.4
 010594118,-1.6508218551\H,-9.5093179711,-5.6473079172,1.5618020182\H,-
 7.8056445233,-3.8939166358,1.6223139209\Version=ES64L-G09RevD.01\Stat
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 MSF=1.880e-06\Dipole=-0.504917,-0.2664105,0.136332\Quadrupole=12.81390

47,3.4517224,-16.2656271,3.4713702,-1.9947498,-0.7243139\PG=C01 [X(C40
H55)]\@

15E,9Z

1 (bet_car_030)

1\1\GINC-Q1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\26-Nov-2016\0\#P
UB3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\
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011,0.3063578903\C,12.7746362882,1.4369088474,-1.3736633457\C,13.01073
63374,0.0347664584,0.68259808\C,5.8599085164,-1.5282390152,0.217628833
9\C,4.5299233964,-1.9713292964,0.2547660357\C,3.3753930084,-1.17199739
05,0.1763563007\C,3.5139827311,0.3285504875,0.032717052\C,2.1227384822
, -1.8028124592,0.2391512057\C,0.8482176141,-1.2193306153,0.1881518183\
C,12.3715289483,2.4390219522,0.9335219882\C,11.5365288504,3.6433733787
,0.484073332\C,10.0491400793,3.2694243279,0.3824663614\C,9.8508371212,
2.0235174902,-0.4615347733\C,9.0001994506,2.0045328508,-1.4994954018\C
,10.6983296991,0.8604163795,-0.0887146406\C,10.1873437568,-0.390708505
6,0.1237335165\C,8.8072675477,-0.7745337279,0.1168849959\C,8.341617161
9,-2.0668395121,0.2790758467\C,9.3136191451,-3.2242717864,0.4312149672
\C,-0.3345469882,-1.9463017257,0.2665006837\C,-1.6164782059,-1.3614675
87,0.2178723991\C,-2.8535033178,-1.989558888,0.2940225526\C,-4.0319331
712,-1.1830646787,0.2230855205\C,-3.0016046166,-3.4849552783,0.4507895
065\C,-5.3313465471,-1.6245618041,0.2894405059\C,-6.4565811189,-0.7496
493832,0.2083540525\C,-7.7911296969,-1.0708667216,0.2685901543\C,-8.76
22562497,0.0007127573,0.1578622853\C,-8.2944801844,-2.4833454479,0.442
1147726\C,-10.1126774796,-0.1361651268,0.1767624007\C,-11.0990101789,0
.9503160409,0.0396141957\C,-12.2715537388,0.6507464929,-0.9273515853\C
, -10.9901799743,2.1293473455,0.7053330813\C,-11.7319595666,0.572100420
9,-2.3755963607\C,-12.9407324501,-0.7025058712,-0.5851785093\C,-13.369
470683,1.7358827926,-0.8311331767\C,-11.9388808086,3.2901491311,0.4829
376959\C,-9.9591569065,2.4203554154,1.7714670178\C,-12.7998973211,3.15
06277224,-0.7707433541\H,6.7090071869,-3.4463780404,0.413407824\H,12.7
17105264,0.5269560192,-1.9817838712\H,12.2248052404,2.2192248967,-1.90
44989795\H,13.8278186783,1.7391576801,-1.3118047219\H,14.0549109303,0.
3473555667,0.8005316546\H,12.6253784284,-0.2298558842,1.673809557\H,13
.011625002,-0.8688182443,0.0628993027\H,6.0396780724,-0.4604336944,0.1

186799787\H,4.3745369049,-3.0459500441,0.3575199767\H,4.0950083761,0.5
 861974723,-0.86111364\H,2.5495862973,0.8327398077,-0.0478699023\H,4.04
 00438941,0.7595220995,0.893529987\H,2.1438884754,-2.8885547273,0.34382
 23044\H,0.7614090157,-0.1390250385,0.0843280781\H,13.436241328,2.70759
 91058,0.9614512507\H,12.0883997958,2.1746926388,1.9626697334\H,11.8893
 929822,4.009182505,-0.4884253473\H,9.4621011775,4.101230793,-0.0236573
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 09,0.5093135133\H,-0.2483247563,-3.0261681894,0.3727478803\H,-1.636190
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 31561\H,-8.3456428254,0.9982005105,0.0257224931\H,-7.4864546184,-3.213
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 318562711,-2.7779285722,-0.4018147881\H,-10.5154784369,-1.1443370358,0
 .2385161951\H,-10.9324056161,-0.1722644383,-2.4560098278\H,-12.5324945
 972,0.288645274,-3.0709230972\H,-11.3193402176,1.5317472986,-2.7054245
 187\H,-13.2240002376,-0.7506302929,0.4728975431\H,-13.8525808624,-0.82
 19783151,-1.1829097446\H,-12.2967980526,-1.5594400664,-0.8073468985\H,
 -13.9665464113,1.5610068251,0.0758927556\H,-11.3529166636,4.220717622,
 0.4455060513\H,-12.5844582184,3.3953450139,1.3711206111\H,-10.43735509
 03,2.9400685469,2.6137146215\H,-9.4733223882,1.5203793891,2.1526834807
 \H,-9.1740004523,3.0964530512,1.4029841354\H,-13.6064185327,3.89414587
 17,-0.7650203263\H,-12.1930651913,3.353032462,-1.6627819978\H,-14.0550
 260784,1.6226496216,-1.6813838381\H,11.6660281093,4.4704539899,1.19357
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 41e-09\RMSF=2.374e-06\Dipole=0.4983922,0.2490947,0.1207062\Quadrupole=
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 [X(C40H55)]\@

15E,14Z

1 (car_H_021)

1\1\GINC-S3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\25-Nov-2016\0\#P
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 0,2\C,12.4529504092,-2.0750228968,1.1722911156\C,11.6029505352,-1.4973
 046827,0.0561010942\C,11.5127546509,-0.0117881584,0.032574382\C,12.872
 1692348,0.7097105023,0.0782764095\C,13.7160062528,0.1125006579,1.24287
 83469\C,13.8406019217,-1.4150378422,1.2114146057\C,11.0231707121,-2.27
 83742115,-0.8674779504\C,10.32610451,0.6572416027,-0.0158875926\C,9.00
 9768276,0.0761676155,0.0271157352\C,7.8047310396,0.72730373,-0.0903009
 475\C,6.6004762015,-0.0511199525,0.0266140866\C,5.3095056362,0.4104875
 343,-0.0722955284\C,4.176139065,-0.4347132305,0.0552350661\C,2.8287113
 765,-0.0989845363,-0.0310486193\C,1.8824179035,-1.1508192179,0.1351559
 293\C,0.4878551247,-1.1721998992,0.1009362645\C,-0.4539690763,-0.15383
 73482,-0.125656582\C,-1.833109738,-0.4021685464,-0.110568669\C,-2.8796
 02626,0.5017025134,-0.3181456769\C,-4.2153739689,0.0191227825,-0.23995
 60759\C,-5.3687431325,0.7569653329,-0.4068489164\C,-6.6719794973,0.195
 3082839,-0.2959126381\C,12.7543416495,2.2252257764,0.3135405067\C,13.5
 961518811,0.4874639272,-1.2743368899\C,-7.8886314064,0.8260961824,-0.4
 317020613\C,7.6775954841,2.2121853074,-0.3461173948\C,2.3807056255,1.3
 2032179,-0.2885379316\C,-2.6422968801,1.9642509313,-0.6157758299\C,-9.
 0923069293,0.0415485511,-0.2513464894\C,-8.0247541672,2.2954971283,-0.
 7491973373\C,-10.3686930777,0.5043735033,-0.3043762806\C,-11.589033755
 9,-0.2914693499,-0.0844571938\C,-12.6457142217,0.3721142674,0.83349920
 23\C,-13.9727367368,-0.4233699129,0.8287441765\C,-13.7587804295,-1.932
 4391823,0.9077012243\C,-12.9724264548,-2.3910636269,-0.3185201769\C,-1
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 ,-1.6581817431\C,-12.9755600764,1.8057860992,0.3519834262\C,-12.087987
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 82545,2.1930012145\H,14.7132161316,0.5725821213,1.2258737702\H,14.4205
 147834,-1.7310439704,0.335107173\H,14.3944008057,-1.7607657362,2.09336
 53054\H,11.1204282472,-3.361274234,-0.8328233379\H,10.444849653,-1.863
 5073504,-1.6877268027\H,10.3714724008,1.7407176839,-0.0499539139\H,8.9
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 6875,0.2435604004\H,2.335681341,-2.1229116144,0.3263653712\H,0.0533072
 629,-2.1569583508,0.2795007833\H,-0.1115220043,0.8544750013,-0.3186285
 413\H,-2.129129373,-1.4327984578,0.0921043944\H,-4.3310251268,-1.04307
 02212,-0.0197221557\H,-5.2784390551,1.8171766577,-0.6265314071\H,-6.70
 25947918,-0.8713430805,-0.0678911105\H,13.7556696077,2.6645924089,0.39

26953849\H,12.2435369943,2.7314029209,-0.5132425997\H,12.2143930554,2.4507412351,1.240113017\H,14.6029756485,0.9232186376,-1.2480171553\H,13.6888225521,-0.5732382131,-1.5240688668\H,13.0387913499,0.9676218548,-2.0867097023\H,7.1187584799,2.7031751383,0.4606344379\H,8.6444042918,2.7108035215,-0.4313064128\H,7.1276643022,2.4019056974,-1.2766071055\H,3.2189276677,2.0149214255,-0.3655020402\H,1.8092204112,1.3899766732,-1.2224861521\H,1.7295658941,1.6786434243,0.518017702\H,-3.1003490917,2.6013753767,0.1515787239\H,-1.5818408333,2.2173655399,-0.6629011161\H,-3.0915695338,2.2472002396,-1.5761600516\H,-8.935481725,-1.0122442114,-0.0254106225\H,-8.5580702677,2.8226611486,0.0528332049\H,-7.0605652824,2.7886235504,-0.8835419924\H,-8.6064372116,2.4451738107,-1.6676462185\H,-10.5117274797,1.571468352,-0.4581026094\H,-14.5220657133,-0.1972383367,-0.0969836171\H,-14.6006367298,-0.069939051,1.6573141027\H,-14.7200329047,-2.4580622571,0.9635081919\H,-13.2072038664,-2.190073822,1.821073091\H,-13.6356863374,-2.4199954822,-1.1994377747\H,-12.6270887496,-3.427636541,-0.1883763293\H,-10.2504360882,-2.953406137,-1.2181683938\H,-11.4529418152,-2.6146366429,-2.4533153609\H,-10.1723987052,-1.4294819216,-2.1166751313\H,-13.8279326916,2.1967415222,0.9210203082\H,-12.1446924721,2.5027827614,0.500869931\H,-13.2475739841,1.8167209886,-0.7100791968\H,-11.9130182784,-0.5326053506,2.701345985\H,-11.1331410215,0.9970546368,2.2912658121\H,-12.7899791218,0.9940756281,2.9277425554\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2734241\S2=0.902071\S2-1=0\S2A=0.768023\RMSD=4.076e-09\RMSF=1.028e-06\Dipole=0.6681556,0.2984282,0.0438392\Quadrupole=20.5632508,-2.8818776,-17.6813732,1.3288101,3.5477456,-2.4598395\PG=C01 [X(C40H55)]\@

15E,11Z

1 (car_H_021)

1\1\GINC-P2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\09-Oct-2014\0\#PUB3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\\0,2\C,-10.1194883827,3.5730580424,0.4757404855\C,-9.867606106,2.354033377,-0.3922616761\C,-10.6283301515,1.134142635,-0.0080957938\C,-12.1436084095,1.353458512,0.1554054953\C,-12.3729685263,2.5933809801,1.0685986101\C,-11.6243551369,3.8530994318,0.6189158653\C,-9.0540821748,2.4015903161,-1.4577886484\C,-10.0355019364,-0.0774557479,0.1913670455\C,-8.6261760654,-0.3641382736,0.1484783607\C,-8.0181039472,-1.5924721079,0

.2747742519\C,-6.5795520966,-1.6385133842,0.2437847638\C,-5.8164788247
,-2.783966738,0.3333099159\C,-4.4053872477,-2.9669123841,0.3110917168\
C,-3.3414374994,-2.0620935118,0.2759837549\C,-2.030804077,-2.601115087
6,0.2352563749\C,-0.8150713479,-1.9233115977,0.1810697538\C,0.42794632
02,-2.5647645197,0.1360567238\C,1.6520605986,-1.8826312638,0.079860909
5\C,2.9404742019,-2.4175119419,0.024221211\C,4.0450626151,-1.519977093
8,-0.0233094375\C,5.3790847493,-1.8593088503,-0.0867988247\C,6.4241529
61,-0.8922031685,-0.1287558367\C,-12.870859171,0.1584825433,0.79529968
16\C,-12.7619019496,1.5990906736,-1.2448163934\C,7.7823635591,-1.10416
87919,-0.1977451238\C,-8.7863870545,-2.8855789159,0.4311794516\C,-3.56
5100415,-0.5682423192,0.2869599887\C,3.2014851204,-3.9058928637,0.0117
444729\C,8.6560414016,0.0507708935,-0.2281686299\C,8.4015088327,-2.479
8001124,-0.2429158376\C,10.0135673607,0.0317841315,-0.2742604781\C,10.
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1.143789124,2.1304805706\H,-9.5951319353,4.4451709967,0.0684016505\H,-
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0871812811\H,-13.4512661979,2.7950184909,1.1238795935\H,-12.0225206456
,4.2106887654,-0.3391120603\H,-11.7865693137,4.6602813461,1.3443933579
\H,-8.5231504633,3.3133572399,-1.7226306618\H,-8.9017708819,1.54025043
51,-2.1013744664\H,-10.6861258515,-0.9064363478,0.4485486088\H,-7.9687
116444,0.4918607758,0.0164718753\H,-6.0926684425,-0.6767224138,0.12652
30284\H,-6.3665467073,-3.7191019936,0.4222946123\H,-4.1041622686,-4.01
39745247,0.3291888132\H,-1.9693835051,-3.6901638348,0.2404637788\H,-0.
8077578867,-0.8347608902,0.1665941669\H,0.4238861142,-3.6531665521,0.1
451123148\H,1.588131111,-0.7932678693,0.0786536834\H,3.8011650832,-0.4
567840523,-0.0073408586\H,5.6462827045,-2.9123055323,-0.105671303\H,6.
0970735927,0.1485048936,-0.103781675\H,-13.9308473163,0.4027492472,0.9
317384752\H,-12.8233599151,-0.7374813451,0.166248112\H,-12.4549878018,
-0.0903050606,1.7782560563\H,-13.8302014179,1.8345436399,-1.1577900935
\H,-12.2726425691,2.421039107,-1.7749969347\H,-12.6609820039,0.7026174
411,-1.8671716555\H,-8.5209666884,-3.391447683,1.3679539106\H,-9.86705
84128,-2.7358226267,0.429849235\H,-8.5517527869,-3.5812228879,-0.38431
06958\H,-4.2114610803,-0.2773190755,1.1231046575\H,-2.6330801636,-0.00
84568746,0.3827899319\H,-4.057545584,-0.2330961609,-0.6347705698\H,3.8
170093456,-4.2044175055,0.8698825433\H,2.2826949637,-4.4935153114,0.04

57044453\H,3.7487719387,-4.2010326196,-0.8925410076\H,8.1554369643,1.0171335629,-0.1887440263\H,9.0800508622,-2.6321958094,0.6065789147\H,7.6573545267,-3.2776244648,-0.2175121243\H,8.9998053562,-2.6105753835,-1.153644098\H,10.5063185475,-0.9372402912,-0.2414520061\H,13.6953480909,2.0672772969,-0.4897785869\H,13.8255949526,2.3199572803,1.2477704942\H,13.1428661324,4.4340334529,0.1220744356\H,11.8119079805,3.8653811279,1.122403439\H,12.1128929479,3.6252742467,-1.9125322743\H,10.836258707,4.4295750276,-1.0304469933\H,8.741279348,3.0145526659,-1.7849858687\H,9.9816219212,2.8598693324,-3.0195807669\H,9.1737532077,1.4077820291,-2.3899085874\H,13.8406042773,-0.169365684,1.0015013384\H,12.3500072738,-1.0800649034,0.7716132274\H,13.1537145198,-0.3324671317,-0.6242525524\H,11.1397584106,2.0914248149,2.3771819304\H,10.9068816909,0.3428257518,2.3152547225\H,12.4734027218,1.0072293363,2.8203708643\\Version=AM64L-G09RevC.01\State=2-A\HF=-1557.2727072\S2=0.910224\S2-I=0.\S2A=0.769694\RMSD=9.613e-09\RMSF=2.409e-06\Dipole=-0.5074419,0.2798596,0.051793\Quadrupole=16.2690561,0.4669869,-16.736043,-4.1789523,-3.3796613,-0.333978\PG=C01 [X(C40H55)]\\@

15E,10Z

1 (Bet_car_030)

1\1\GINC-UV3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\24-Nov-2016\0\#p
ub3lyp/6-31g(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
0,2\C,12.1484166206,-1.6549166019,0.2470223567\C,6.8425289532,1.718352152,-0.2231261597\C,12.8235018614,-2.0780674852,-1.0828600966\C,11.4056998084,-2.875798685,0.8162057496\C,5.4929425148,2.0296831172,-0.2564486293\C,4.3451456657,1.2026880821,-0.2188688181\C,3.0221707242,1.658915379,-0.2416210399\C,2.7250036886,3.1423490193,-0.3104452653\C,1.9849916152,0.700687052,-0.189773759\C,0.6062025995,0.9163709539,-0.1705495469\C,13.2281943077,-1.2288633197,1.2846929623\C,13.9958554739,0.0428797901,0.9060499448\C,13.0285945476,1.2082625014,0.6433085883\C,11.9467333816,0.8129397071,-0.3447993977\C,11.6991433694,1.5345075676,-1.4482637276\C,11.228877397,-0.4513565873,-0.0281600426\C,9.8683072952,-0.5381686793,0.0254381512\C,8.9336376415,0.5449344984,-0.116843245\C,7.556000922,0.4725270837,-0.1312139852\C,6.812907823,-0.8411000644,-0.0624227249\C,-0.3412874384,-0.1090124271,-0.121665458\C,-1.7267747738,0.1196234081,-0.0896063856\C,-2.7604911096,-0.8148280057,-0.0480208275\C,-4.

1028080779,-0.33613807,-0.0076836055\C,-2.5113621025,-2.3048404985,-0.042407664\C,-5.2496389037,-1.0969906348,0.0291575343\C,-6.5543149994,-0.5250147699,0.0826875223\C,-7.7703230167,-1.1668414403,0.1164333529\C,-8.9697364326,-0.356578297,0.1892222662\C,-7.9145211681,-2.6686155368,0.0846018497\C,-10.2497784606,-0.8095303386,0.2039133285\C,-11.4594725951,0.0295827023,0.2769534618\C,-12.5808253561,-0.3437344394,-0.7237357561\C,-11.581724579,1.0586381898,1.1551638454\C,-12.1076562744,-0.0249989985,-2.1623690106\C,-12.9115650283,-1.853847971,-0.6459226114\C,-13.8873871317,0.4239176147,-0.4145920385\C,-12.7752872949,1.9921935431,1.166165539\C,-10.5901870761,1.3742220443,2.2512520133\C,-13.6457643656,1.8947719836,-0.0853598071\H,7.4994248617,2.5863387434,-0.2692432077\H,12.0715568574,-2.4446218406,-1.7909424146\H,13.3467177131,-1.2466882932,-1.5637394999\H,13.547282957,-2.8839690098,-0.9073357367\H,12.1244417601,-3.6730271494,1.0392497246\H,10.8765603832,-2.6313093997,1.7442132659\H,10.6795502284,-3.2844039603,0.1045235629\H,5.2930700599,3.0977298417,-0.3192436832\H,4.4740685386,0.1277493888,-0.1628180033\H,3.220022293,3.6040219864,-1.1727801104\H,1.6576631034,3.349780605,-0.4008485809\H,3.0873650924,3.6615101151,0.5854629001\H,2.3063202531,-0.3413733889,-0.154495242\H,0.226079386,1.9363582668,-0.1900522365\H,13.9280715341,-2.0633032109,1.4273270163\H,12.730297591,-1.0691026847,2.2520384785\H,14.6065848867,-0.1344423481,0.0118738884\H,13.5670791939,2.0924437365,0.2834537081\H,10.9491794609,1.2326735104,-2.173386975\H,12.2505488595,2.4474491172,-1.6624206031\H,9.4463695715,-1.5135932214,0.2427910178\H,9.367346117,1.5381909135,-0.2015177364\H,7.4849264324,-1.6994127017,-0.0095283313\H,6.1562887182,-0.8783916454,0.8152681061\H,6.1791216407,-0.9783695536,-0.94685141\H,0.0316599383,-1.131569387,-0.106246185\H,-2.0322945814,1.1671964159,-0.0970626625\H,-4.2244363513,0.7479980657,-0.0038665376\H,-1.4493875085,-2.5535787595,-0.0782924622\H,-2.9304647093,-2.769945158,0.8589578373\H,-2.9922451115,-2.7862272588,-0.9034888507\H,-5.1572673364,-2.1796521181,0.0208455314\H,-6.5824600858,0.5655872718,0.10407954\H,-8.8057339519,0.7197661667,0.2196090795\H,-6.9533857905,-3.1835243462,0.0365470554\H,-8.4442486644,-3.0306180996,0.9749909403\H,-8.5040431456,-2.9862430359,-0.7854756333\H,-10.4106421332,-1.8801764409,0.099662706\H,-11.1651981038,-0.5358234052,-2.3872881764\H,-12.8558452905,-0.3517161252,-2.8959568585\H,-11.9391393857,1.0481218955,-2.3039408305\H,-13.1294171249,-2.1614742965,0.3837198166\H,-13.7986877716,-2.0676088449,-1.2546785808\H,-12.1009628548,-2.4829510309,-1.0276177354\H,-14.3844798549,-0.0490268314,0.4450494906\H,-12.4149723845,3.0225610857,1.3044124289\H,-13.3824301928,1.7798473502,2.06

21959314\H,-11.1299019529,1.5998148711,3.1819119353\H,-9.8937624984,0.
 5567886027,2.445926425\H,-9.9988100285,2.2714401232,2.0175177371\H,-14
 .5968611796,2.4191851562,0.0689041594\H,-13.1454290757,2.3935444915,-0
 .9254261893\H,-14.5712740299,0.3175932843,-1.2670435635\H,14.692027043
 8,0.3097822578,1.7111313124\H,12.5513715971,1.4868217433,1.5955205769\
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 0.\S2A=0.770711\RMSD=4.231e-09\RMSF=2.570e-06\Dipole=0.5951917,-0.2093
 46,0.1742083\Quadrupole=18.7335408,-1.7611552,-16.9723856,-2.4943034,2
 .5572881,-0.0123308\PG=C01 [X(C40H55)]\@

15E,7Z

1 (bet_car_030)

I\I\GINC-LXA162\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\25-Nov-2016\0\
 #p ub3lyp/6-31g(d) opt freq scf=tight\Beta_Carotene (-30) optimizatio
 n\0,2\C,12.9331642685,-0.0666200089,0.3682056825\C,6.7634823923,-0.72
 29183251,0.6297233174\C,13.676552582,-0.8378366717,-0.7514027707\C,13.
 3274753811,-0.684266709,1.7212087892\C,5.6107278988,0.0118705978,0.541
 0372799\C,4.3170111333,-0.5818419722,0.4956676559\C,3.0839436638,0.044
 0324625,0.4137875373\C,2.9319123705,1.5481438173,0.3613471493\C,1.9130
 494713,-0.7679998703,0.3821719829\C,0.6007467939,-0.3285089275,0.31448
 49663\C,13.3845199533,1.4228241646,0.3826408225\C,12.9863927682,2.2137
 98839,-0.8678497878\C,11.4691604408,2.1351879863,-1.0999845965\C,10.98
 49419969,0.6980059129,-1.0857468612\C,10.2887681306,0.1781936303,-2.10
 58671721\C,11.4164166142,-0.1228263621,0.0833506241\C,10.5847468358,-0
 .9219753566,0.7959821532\C,9.1397245417,-1.1199975573,0.7243911353\C,8
 .1161070779,-0.2155684869,0.6716433332\C,8.3421257874,1.2749235866,0.6
 867613814\C,-0.5137801876,-1.1863450265,0.2883982095\C,-1.8354501468,-
 0.73908008,0.2326411199\C,-3.0108191715,-1.5026329867,0.2078115169\C,-
 4.2574133749,-0.8246593731,0.1689069808\C,-2.9923991224,-3.0137753734,
 0.2272838312\C,-5.5105110594,-1.4058831857,0.1531246277\C,-6.716076756
 6,-0.6527922801,0.1222243301\C,-8.0136201141,-1.1180808699,0.110025630
 4\C,-9.0900638819,-0.1510245886,0.0855269096\C,-8.3616881837,-2.586763
 5656,0.1211087159\C,-10.4198303448,-0.4310707566,0.0543097587\C,-11.51
 65467598,0.5511390254,0.010343735\C,-12.6446445214,0.2276404511,-1.001
 0277461\C,-11.541645447,1.6610962942,0.7938802355\C,-12.094465018,0.36

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,2.6240009072,-0.5966082915\H,6.6646883791,-1.8089944365,0.6580024646\
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131328,-0.5286135292,1.8988334895\H,12.7773865783,-0.225051424,2.55027
69919\H,13.1506433044,-1.7650548329,1.7510163439\H,5.6853349958,1.0949
749831,0.4968631027\H,4.3018283646,-1.6720737051,0.5322883993\H,2.4094
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0514\H,3.8909953682,2.0681083896,0.3847585379\H,2.0734607652,-1.846211
5597,0.4175940987\H,0.4037846081,0.7423323728,0.2817313391\H,14.473731
2166,1.4566020966,0.5191063785\H,12.9442163168,1.9081848306,1.26604021
21\H,13.5125780126,1.823435166,-1.7479983584\H,11.1905543495,2.6194080
83,-2.0429976735\H,10.012703735,0.7834662691,-2.9665039674\H,9.9680966
348,-0.8588576545,-2.1116043978\H,11.0539688125,-1.5814905603,1.525525
9592\H,8.8431844916,-2.1671977113,0.8164854843\H,9.3508986901,1.512786
3769,1.0311495222\H,8.2205829814,1.7106043479,-0.3131141059\H,7.628760
9195,1.771230438,1.3544071202\H,-0.3113897782,-2.2553992258,0.31856748
56\H,-1.9720577161,0.3433832777,0.210534727\H,-4.2136442952,0.26531991
62,0.1542432469\H,-1.9801900631,-3.4211632259,0.2205594434\H,-3.499801
5707,-3.4032864982,1.1192157707\H,-3.5178583566,-3.4236382002,-0.64440
03186\H,-5.5774402321,-2.490138364,0.1695631797\H,-6.5904735512,0.4311
085141,0.1105846865\H,-8.7819046851,0.8934151357,0.0712882469\H,-7.479
4440293,-3.2289392811,0.1297365098\H,-8.9677573393,-2.8406385952,1.000
2390161\H,-8.9568657043,-2.8540588564,-0.7618373549\H,-10.7115369068,-
1.4771182067,-0.0031153504\H,-11.2167342653,-0.2747724483,-2.587110568
\H,-12.8557895846,0.0691748694,-3.1745939348\H,-11.7906172556,1.392960
0741,-2.6617242729\H,-13.4350650518,-1.4136308479,0.2292292001\H,-14.0
55138808,-1.3723750024,-1.4306111319\H,-12.4275825151,-1.9719884798,-1
.1222188107\H,-14.431913668,0.8358382198,0.0684199449\H,-12.1298810519
,3.716314614,0.7394369369\H,-13.2657287756,2.6728448576,1.5613096056\H
, -11.0901522578,2.3335479522,2.7812189786\H,-9.9801682519,1.0728288303
,2.2016017042\H,-9.840993515,2.7370298755,1.613523344\H,-14.333371203,
3.2689953072,-0.5251010825\H,-12.8678595448,2.9832552639,-1.455814613\
H,-14.5246941654,1.0684876464,-1.6744214834\H,13.2943829762,3.26142588
18,-0.7591263262\H,10.9668802108,2.6915393592,-0.2938936708\\Version=A
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4789\\RMSD=5.093e-09\\RMSF=3.978e-06\\Dipole=0.5894466,0.2129422,-0.00190

61\Quadrupole=18.2248049,-1.3948018,-16.8300031,4.0137983,0.0567812,-0.5264182\PG=C01 [X(C40H55)]\@

Structures of the rotamers of 15Z isomer of C5-Me radical.

15,15'-cis (15Z)

l(car_H_002_cis)

l\1\GINC-UV3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\12-Nov-2016\0\#p
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017574,-2.5353760296,-0.0812987839\C,-10.3565440879,-3.7110177633,-1.1
026077449\C,-9.3484275395,-4.8197314531,-0.7788952152\C,-7.0834991489,
-3.0480166984,1.4011328465\C,-8.5983421004,-0.6984650109,-0.0203429342
\C,-7.2745811618,-0.1352271188,0.019923411\C,-6.9313731352,1.195768039
9,-0.0275820552\C,-5.5343751578,1.5354959702,-0.0333346724\C,-4.994546
186,2.799868377,-0.0823541313\C,-3.5975597999,3.0431196842,-0.09483755
11\C,-2.9313646189,4.2637358068,-0.1495544915\C,-1.5122798555,4.255652
8923,-0.1619777243\C,-0.6857906003,5.374330466,-0.2242464247\C,0.72162
81861,5.3965000634,-0.2448227098\C,1.5773500199,4.2848111128,-0.198239
0278\C,2.9724182726,4.2737369243,-0.2275265531\C,3.6374465951,3.014112
9136,-0.1724491813\C,4.996805078,2.7957802746,-0.2023545757\C,5.571469
5861,1.4926639086,-0.1444657905\C,-11.3429241125,-1.4676909559,-0.6001
945535\C,-10.8764660734,-3.0296611105,1.2960562514\C,6.9008788569,1.14
10133562,-0.1808452065\C,-7.9438370786,2.3183647534,-0.0699649026\C,-3
.6659444504,5.5856861875,-0.200460096\C,3.799744829,5.5346364883,-0.31
93304011\C,7.2391659908,-0.2663664593,-0.1065122661\C,8.0188194134,2.1
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84613991,-2.2213299121,-0.0140519115\C,10.0217299083,-2.5193675521,0.9
507012746\C,10.0931413855,-4.026420224,1.2885073114\C,9.9468745373,-4.
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7539617933\C,9.8358781194,-1.7568636931,2.282371608\C,11.3536837936,-2
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4,-2.0966514905\H,-11.3700026794,-4.1300995282,-1.163926624\H,-9.63605

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102287\H,-6.3673896415,-3.8473202963,1.5793139696\H,-7.0969745332,-2.2
322825529,2.1180001043\H,-9.4114826468,-0.0021407867,-0.1961052378\H,-
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,-1.1682018165,6.3485943322,-0.2661313419\H,1.1726001961,6.3838622292,
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127263\H,-10.2103868957,-3.7738747268,1.7417324134\H,-10.94747568,-2.1
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83079469,2.0938035125,0.57166911\H,8.6338539463,1.9494688078,-1.183858
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,6.1577390578,-3.2490479865,-1.3714335571\H,7.0713124591,-1.8952596918
,-2.0505376616\H,10.6311575781,-2.0320746971,2.9866608599\H,9.87169578
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7\H,11.5644338259,-2.6118858606,-0.6196053049\H,11.3408079095,-0.99685
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15Z,13Z

1 (Car_H_002_cis)

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 95401483,-0.3289714023\C,11.0118751625,0.1865940232,0.0917745025\C,12.
 4327484361,0.7283786353,0.3329612692\C,13.1976135998,-0.2655942112,1.2
 558556349\C,13.1738454896,-1.7200266878,0.7715238276\C,10.3255520571,-
 1.6518728158,-1.4370597196\C,9.8940968256,0.952847704,0.2583760768\C,8
 .5298708239,0.5216758635,0.1374590496\C,7.3930517916,1.297512618,0.248
 9350566\C,6.12138964,0.6541116908,0.1269340591\C,4.8777846937,1.259241
 0851,0.2006946119\C,3.6643525636,0.5604889062,0.0628814352\C,2.3784074
 826,1.1211831513,0.1281771213\C,1.1992246308,0.3672205768,-0.027070244
 \C,1.0843915847,-1.0137268244,-0.2765431928\C,-0.090999473,-1.74504076
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 9793,-1.95570055,-0.495039429\C,-3.8340474818,-1.2406469749,-0.3702400
 135\C,-5.0982952462,-1.760845146,-0.4740272532\C,-6.2784435548,-0.9657
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 1442819,0.3777551166\C,-2.6438866364,-3.439250525,-0.7759676211\C,-8.6
 223265459,-0.359591538,-0.2229909199\C,-8.0094032229,-2.7876068625,-0.
 676839481\C,-9.9613959408,-0.5726563986,-0.2305107739\C,-11.013959924,
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 C,-12.9691124492,1.2052960423,1.4288309103\C,-13.3639513693,2.13510743
 25,0.2845259871\C,-12.1072986945,2.6808895746,-0.3950695713\C,-11.0321
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 73199\C,-11.5269286966,-0.6660779749,2.2186755889\C,-13.0529950482,-1.
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 4,-0.1098862964\H,0.2712119197,0.9293712253,0.0541333853\H,2.004575795
 6,-1.5867276896,-0.3675744111\H,0.0376629752,-2.8070882371,-0.61839782
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 1851410444,0.158273788\H,-8.6429815962,-2.8473485363,-1.5708650967\H,-
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 2.1595846629\H,-13.8577457105,0.8414318541,1.9618712001\H,-13.98457432
 23,2.9606691333,0.6545500154\H,-13.9735540033,1.5926196021,-0.44940330
 03\H,-11.6738644447,3.4877169873,0.2201351228\H,-12.37048175,3.1599752
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 22148\H,-12.3224238962,-0.9122454545,2.9334325491\H,-10.9904661269,-1.
 5916190706,1.9862320114\H,-10.8221483116,0.0101115879,2.7159635671\H,-
 13.5486587514,-0.6108104299,-0.6181101426\H,-12.4924077391,-1.91822626
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15Z,9Z

1 (Csr_H_002_cis)

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1.3443577376\C,-12.2592600118,0.2145765244,0.9904871689\C,-9.461824737
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7\C,-7.3341618845,-1.2260998813,0.1218898279\C,-6.1145649854,-1.881538
5757,0.1610205988\C,-4.86596138,-1.1910981018,0.1005310952\C,-4.636620
9744,0.1791854454,0.0093625267\C,-3.3546458261,0.7357315509,-0.0515921
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.2269772136,2.0370893487\H,12.4720699725,-2.7619740031,1.9111186572\H,
11.9895898184,-4.7107361465,0.433433379\H,12.4074326311,-3.3184387312,
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26\H,7.6185111223,-3.0437741744,-1.4349720783\H,8.1848696691,-1.508282
0966,-2.1057817469\H,11.4969523715,-0.7193606011,3.0339815384\H,10.456
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32,-1.1718356\PG=C01 [X(C40H55)]\\@

15Z,8Z

1 (bet_car_8_15_c5m)

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(C40H55)]\@

15Z,12Z

1 (bet_car_12_15_c5m)

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15Z,11Z

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15Z,10Z

1 (car_H_002_cis)

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 7306\H,-3.5096378327,6.8116575983,0.2451684849\H,4.0215740626,5.803510
 7878,-0.9423294542\H,2.8122266356,6.7015866946,-0.0216899082\H,4.08125
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 267,0.057633774\H,10.1929251725,-4.5344075697,-0.8727073372\H,7.232706
 5323,-4.9866236496,-0.2720389885\H,8.0039942014,-4.8791830143,-1.83660
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 1024463908,-2.0318184609,2.8937378319\H,9.3601807,-0.6226305002,2.1225
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15Z,7Z

1 (car_H_002_cis)

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 1135615273,-0.8854995543\C,-9.3243835649,-2.0172543305,0.27413448\C,-1
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439,-1.0934682555,-1.9627165114\C,-8.1287603976,-2.1205090493,0.905333
0085\C,-6.8845476399,-1.3736249262,0.743669387\C,-6.6551137192,-0.0275
226461,0.6673479224\C,-5.290679195,0.4236256174,0.5235673066\C,-4.8662
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33949,4.7864265473,-0.3768900022\C,1.530774133,3.7682084747,-0.3281094
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2,1.4149832042,-0.3401302135\C,-10.3514970807,-3.6402594248,1.99411402
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205407,-2.9606327025,-0.7045474148\C,7.8960772379,-2.9171325046,-1.722
5821283\C,10.4326361449,-1.1231911438,2.1890332246\C,11.9737233373,-1.
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Structures of the rotamers of *15E* isomer and rotamers of C9-Me radical

15E,9Z

1 (bet_car_9_c9m)

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,0.0903383568\H,11.1670279315,3.7588550464,2.0375769563\H,-13.08090809
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15E,8Z

l (bet_car_8_c9m)

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4636792966,-0.4830186452\C,-11.6860294311,-1.443549478,2.2063148206\C,
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0.8574145106\C,-3.9165956424,-0.2821668185,-0.5742454486\C,-2.60297599
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,7.3745237005,4.2432023635,-0.5661381841\H,9.1918006035,4.1648557602,-
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7,-0.0023588641,2.6028426369\H,10.9160496634,-1.3384902149,3.424563296
\H,11.8507345442,-0.0687320215,2.609228639\H,9.5104298275,-2.946240813
2,0.3336002856\H,9.7955640077,-3.1919732241,2.0652845651\H,8.745210255
5,-1.8809779439,1.5314838831\H,11.9553115897,-3.2311300536,0.433247363
7\H,14.0192958065,-0.3837932282,-0.8792113885\H,13.3121964036,-1.89300
75505,-1.4056132256\H,12.2778872489,-0.1551766032,-2.9311161361\H,10.8
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133357617\H,14.2807018762,-2.3588021163,0.7608812605\H,13.6306655679,-

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 ,-14.2950141091,1.7625578457,1.9189170998\H,-13.2910742437,2.345596813
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15E,13Z

l (bet_car_13_c9m)

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 4766837,-0.0455415178\C,9.9649962544,-2.0018559831,2.0220334569\C,11.4
 842779382,-1.014284765,0.2868171749\C,4.6481971266,2.5954383062,0.0490
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 55\H,-9.9615658956,-1.0902870173,1.7433096112\H,-11.1773272052,-2.3381
 166633,2.0828649813\H,-9.4690258548,-2.6204594232,2.4730827806\H,-10.8
 285507941,-2.4479080862,-1.6569152546\H,-12.0018205268,-2.5455783288,-
 0.3322042781\H,-11.0595273061,-1.073367892,-0.556984124\H,-10.34234890
 51,-4.6497395014,-0.6661303133\H,-6.8375749858,-5.1728058494,0.5550204
 083\H,-7.8257771015,-5.4143063183,-0.8664771975\H,-5.9523040251,-3.910
 7037447,-1.6507497505\H,-6.1392216766,-2.1521525541,-1.4761531731\H,-5
 .3970463829,-3.1129173837,-0.1872481481\H,-9.1920951672,-6.1288571506,
 0.9978355691\H,-8.7672582704,-4.7183055458,1.9598026476\H,-11.08001389
 29,-4.506722603,0.9265047752\H,10.4542580368,-5.5305031867,-0.08617701
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 1 [X(C40H55)]\\@

all-trans(15E)

1 (Car_H_021_003)

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99603285\C,-10.3758480479,-0.5532830167,-0.4702730304\C,-9.0776432716,
-0.1848533229,-0.3151414546\C,-7.9181400547,-0.907182672,-0.7949437485
\C,-6.6694221202,-0.4017494945,-0.5038380243\C,-5.3978522477,-0.933012
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3323716364\C,-0.4464534621,-0.2967536631,-0.493925077\C,0.5675096881,0
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368681807,-1.5679027871,-0.3720588309\C,8.0330042743,1.3911538791,0.59
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\H,-7.1950028813,-2.6271229496,-1.9170710329\H,-3.1907434264,-1.983622
9546,-2.5714471764\H,-1.6758503625,-2.3269510656,-1.7334411192\H,-3.20
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,2.0103603433,-1.6437858892\H,13.3507018432,1.8965172206,-0.4444148387
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96882\Quadrupole=12.1632667,-1.5462003,-10.6170663,-3.9775408,0.584163
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15E,12Z

1 (car_H_002)

1\1\GINC-Q1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\01-Dec-2016\0\#P
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12.1546040065,-0.8492292677,0.8073651313\C,-13.5419177832,-0.259411619
6,0.4635988825\C,-13.9708925808,-0.550588421,-0.9721123848\C,-10.55773

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41997579,0.2374090548\C,-6.4808349071,0.9762623796,0.5380046653\C,-5.1
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-5.7964144897,-1.6770083954,0.7018525462\H,-7.3790953141,-2.3305420851
,0.0066267166\H,-3.3368651064,4.5139215783,1.4876354096\H,-1.882697762

3,3.7779919994,2.1785287721\H,-1.9059245527,4.2503410952,0.4794416731\H,2.59338515,-2.4891452321,0.4109959905\H,1.0878900941,-1.9439065219,-0.3313697748\H,2.564314747,-2.0378884477,-1.2938761727\H,8.6700913089,0.6987700772,0.2742669914\H,6.5158472975,-2.9483511637,-0.5851182488\H,8.0220837699,-2.6762577295,-1.4668713426\H,8.0693090262,-3.0969159815,0.2438863136\H,10.0557196205,-1.922877895,-0.475490931\H,13.0695810986,1.4578620663,-1.5843786943\H,14.2430959282,0.1648212529,-1.8074446146\H,14.8298542491,1.5436974129,0.1857889365\H,14.4047382011,-0.0816605131,0.7028666799\H,12.7091633797,2.4523603119,0.8780083642\H,13.2056493637,1.4032950373,2.1842601282\H,11.1919735875,0.9292319333,3.1241491364\H,10.1814247478,1.9348546641,2.0969128341\H,9.8197302444,0.2106857304,2.256920128\H,12.3789745421,-0.6327612982,-3.2956846767\H,10.8695046599,-1.2643317048,-2.6228574397\H,11.1390446318,0.4822461978,-2.6887867867\H,13.4235852507,-1.9952947484,0.0634194894\H,12.0984652158,-2.6933771556,-0.8714861263\H,13.5807643663,-2.1944800437,-1.6935221347\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2633276\S2=0.881677\S2-1=0.\S2A=0.763438\RMSD=4.029e-09\RMSF=1.590e-06\Dipole=0.2237339,0.0211867,-0.0876422\Quadrupole=14.4504556,-1.0844723,-13.3659832,-1.2104254,2.6476652,2.8150825\PG=C01 [X(C40H55)]\@

15E,10Z

1 (bet_car_30)

1\1\GINC-Q1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\02-Dec-2016\0\#PUB3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\\0,2\C,12.233116274,-0.734940826,0.7469402699\C,6.8862871513,1.7972227972,1.2293319162\C,12.2414013786,-2.1885106474,1.2821905785\C,12.1302651987,0.2299208669,1.9502238082\C,5.5788026367,2.1884440889,1.2550328309\C,4.4322699926,1.4006773893,0.9110113143\C,3.1035311791,1.7565618649,1.0268457776\C,2.6482683649,3.0585876411,1.6476026065\C,2.1126205238,0.8421170928,0.5466070119\C,0.7424128617,1.0120874704,0.5912672024\C,13.5663130084,-0.4365553376,0.0237411944\C,13.6454026515,-1.0757021806,-1.3601035712\C,12.5192388852,-0.5361076442,-2.2425534\C,11.1674448796,-0.4714083811,-1.5549732873\C,10.0179191828,-0.337051219,-2.5271218436\C,11.0304135657,-0.5351094815,-0.2066727744\C,9.7215957219,-0.467238932,0.4742967657\C,8.7440863954,0.4373277733,0.2708274372\C,7.4444754018,0.4595785546,0.9796668207\C,6.8455593587,-0.6800550518,1.3965935361

\C,-0.1859397168,0.073726057,0.0937124259\C,-1.5666523569,0.2489556103
,0.1566701543\C,-2.5774279774,-0.6107242023,-0.3043816109\C,-3.9276162
01,-0.2286808589,-0.1061314409\C,-2.2706051221,-1.9202779567,-0.993394
4108\C,-5.0524069451,-0.93882889,-0.4855912189\C,-6.3736456124,-0.4851
982816,-0.2280579821\C,-7.5681844133,-1.0929777248,-0.55418729\C,-8.79
71577066,-0.4371160301,-0.164502216\C,-7.6499930433,-2.4059184387,-1.2
937671392\C,-10.060292116,-0.8673047686,-0.4235396565\C,-11.3014011055
, -0.1818410874,-0.0230973482\C,-12.37640082,-0.0665986006,-1.131892074
4\C,-11.4890750833,0.3188237694,1.2258732159\C,-11.8667786778,0.888076
5916,-2.2379286749\C,-12.6597881727,-1.4462208623,-1.7739146472\C,-13.
7178869454,0.4523625924,-0.5619389823\C,-12.7133226822,1.1227123023,1.
6140586347\C,-10.5464009993,0.1035232263,2.387606631\C,-13.5373366886,
1.6052976527,0.4218240811\H,7.6301568665,2.5768620982,1.3920379234\H,1
1.3132453232,-2.4319780446,1.8108206465\H,12.3601057198,-2.9175948298,
0.4740613132\H,13.0669432758,-2.3275771726,1.9917023175\H,13.019042617
4,0.1320838505,2.5862810902\H,12.0669672651,1.2714924783,1.6147245214\
H,11.2516635694,0.0270935071,2.5709463523\H,5.405181924,3.2313444313,1
.5127717927\H,4.638151647,0.4240291047,0.4780624176\H,2.0698349997,3.6
549296915,0.9310454156\H,1.9954114635,2.8719445787,2.5092921202\H,3.48
08176677,3.6706899408,1.9974385672\H,2.4868256409,-0.0801601315,0.1009
624677\H,0.3363240733,1.9202956055,1.0350859752\H,14.398219951,-0.7701
217379,0.6583278605\H,13.6742633755,0.6523916377,-0.0847531801\H,13.55
83341868,-2.166624124,-1.2777041227\H,12.4281212969,-1.1424156181,-3.1
544691207\H,9.9937523665,0.6661420511,-2.9776055708\H,10.1448813859,-1
.0426044209,-3.3591404906\H,9.0453286651,-0.5162063697,-2.0668324462\H
,9.5642970856,-1.1917089925,1.2747045181\H,8.9165057324,1.2504014398,-
0.4330159137\H,7.2558338503,-1.6545392728,1.14907481\H,5.9533429133,-0
.6631131413,2.0128672914\H,0.2216814274,-0.8297666716,-0.3560032004\H,
-1.9095880765,1.1711509578,0.6286863236\H,-4.0902274092,0.722263494,0.
4031132057\H,-1.1993225413,-2.0930443229,-1.1081970556\H,-2.6844535856
, -2.7676333017,-0.431942659\H,-2.7178407157,-1.9511537974,-1.994936117
8\H,-4.917919299,-1.8871811733,-0.9984622823\H,-6.4450661872,0.4663538
016,0.3012042779\H,-8.6764318535,0.5014890979,0.3745710528\H,-6.667360
2935,-2.8181486125,-1.5292310466\H,-8.1948727414,-3.1546886375,-0.7048
92558\H,-8.1950334248,-2.2889040561,-2.2396758164\H,-10.17701875,-1.76
43014251,-1.0276809146\H,-10.9032533732,0.5489733408,-2.6333974282\H,-
12.5805549109,0.930999725,-3.0704717328\H,-11.7246011324,1.9059435392,
-1.8589417172\H,-12.9001668692,-2.197768466,-1.0125894925\H,-13.519755
1189,-1.367217211,-2.4502893198\H,-11.8179129349,-1.8163846169,-2.3677

965893\H,-14.2288563469,-0.3720587695,-0.0431007751\H,-12.3926176727,1
.9759028295,2.2303289121\H,-13.3428779541,0.5100364043,2.2811367921\H,
-11.1250972543,-0.1378810931,3.2903890817\H,-9.8286791699,-0.700019808
6,2.2132378712\H,-9.9794402245,1.0155436493,2.6244869413\H,-14.5104616
408,1.9835346484,0.7584667225\H,-13.0272049623,2.4449920534,-0.0676429
269\H,-14.36807836,0.7445545239,-1.3971340505\H,14.6194861448,-0.87544
18266,-1.8233136348\H,12.7770751416,0.476339227,-2.5962710636\\Version
=ES64L-G09RevD.01\State=2-A\HF=-1557.2614\S2=0.875837\S2-1=0.\S2A=0.76
2004\RMSD=9.993e-09\RMSF=1.327e-06\Dipole=-0.0085343,-0.0332705,-0.132
352\Quadrupole=12.7041182,-2.8125432,-9.891575,-0.0146035,-4.2815007,4
.6593605\PG=C01 [X(C40H55)]\\@

15E,7Z

1 (bet_car_032)

I\1\GINC-Q1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\03-Dec-2016\0\\#P
UB3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
0,2\C,-12.6805014087,0.0407277984,-0.3735298695\C,-6.8378095145,-0.888
9858567,-0.5538116508\C,-13.6335348718,1.1288874453,0.1742272208\C,-13
.4290201969,-1.310762627,-0.2844292298\C,-5.6855495238,-0.1616851213,-
0.4864159699\C,-4.387036114,-0.7526926243,-0.47816292\C,-3.1590267084,
-0.1206560468,-0.3955557781\C,-3.0158128585,1.3818473705,-0.2939460723
\C,-1.9800728717,-0.9244393041,-0.4122106961\C,-0.6723669026,-0.474707
2792,-0.3444188627\C,-12.3611064104,0.3110276707,-1.8634534546\C,-12.9
190730282,2.4405445273,0.4917771233\C,-11.8634687521,2.1960726145,1.56
98177475\C,-11.0249249165,0.9557517596,1.3339855517\C,-9.7908307525,0.
9006538528,2.1983479982\C,-11.3604842126,0.0011097249,0.4346348753\C,-
10.5252864008,-1.2036747731,0.2049986825\C,-9.2431200634,-1.3440881344
,-0.193146905\C,-8.2064592852,-0.362688837,-0.5884110046\C,-8.47802390
58,0.8971639898,-1.0078772413\C,0.4529423258,-1.3196637451,-0.37171524
15\C,1.7679609005,-0.856477757,-0.3061841472\C,2.9554755025,-1.6018654
593,-0.3342129936\C,4.1904306562,-0.9065198434,-0.2608748706\C,2.96050
5567,-3.1090735708,-0.4439136274\C,5.4536773146,-1.4656324943,-0.28880
56098\C,6.6452167787,-0.6947842532,-0.2080833001\C,7.9512767173,-1.135
8266187,-0.2334045233\C,9.0093532711,-0.1538604362,-0.1318944091\C,8.3
261352422,-2.5924565609,-0.3595868223\C,10.3440841838,-0.4119891968,-0
.1219386198\C,11.4245747095,0.5800602272,0.0064126783\C,12.5639275771,

0.1828395273,0.9784944398\C,11.4277248907,1.7578970011,-0.6716121889\C,
12.0197971265,0.1733997811,2.427094883\C,13.1041708753,-1.2309924679,
0.6541002506\C,13.7592965858,1.1588691684,0.8702158239\C,12.4798274182,
2.8275567853,-0.4584739487\C,10.4303444578,2.1325043748,-1.7436523653
\C,13.3253367185,2.6201103524,0.7960692252\H,-6.7464163006,-1.97571824
99,-0.5526592506\H,-14.1057959317,0.7569955191,1.0952568139\H,-11.9223
906892,1.3036428796,-2.0121430504\H,-14.4440712275,1.2883406546,-0.549
2750917\H,-14.4188897635,-1.2125107592,-0.7463724233\H,-12.9035560855,
-2.1144060027,-0.8100238405\H,-13.5751036753,-1.6188931028,0.757862933
2\H,-5.7630076315,0.9209731952,-0.4198158908\H,-4.3676502187,-1.841073
9726,-0.5474886136\H,-3.9780784167,1.895793045,-0.2763899265\H,-2.4752
488863,1.6622907231,0.6184370391\H,-2.4430259136,1.7794676759,-1.14101
20741\H,-2.1322142503,-2.0016447901,-0.4886468934\H,-0.4858295997,0.59
5675799,-0.2671838259\H,-13.2739787034,0.2514633698,-2.4698892072\H,-1
1.6490950291,-0.4263183036,-2.2498366022\H,-13.6363086384,3.2005877862
,0.8252891479\H,-12.347563054,2.111756232,2.5568407765\H,-9.3531416599
,-0.0980575329,2.2494137132\H,-9.0169161203,1.5808453593,1.8144095031\
H,-10.0281647102,1.2331125187,3.2179621837\H,-11.0484467745,-2.1469612
123,0.3646796984\H,-8.8877217604,-2.3743040278,-0.240316668\H,-9.48717
8778,1.2888339339,-1.0169362776\H,-7.6919441349,1.5504145063,-1.373805
0411\H,0.2639067303,-2.3885595573,-0.4516764633\H,1.8888905645,0.22508
57406,-0.2262647052\H,4.1285434145,0.1793039424,-0.1758039156\H,1.9548
742773,-3.5323362734,-0.4584734269\H,3.4696980926,-3.4359905104,-1.359
6098434\H,3.4963888104,-3.5620482912,0.3995783323\H,5.5395710426,-2.54
4974612,-0.3783351821\H,6.5001614297,0.3827284351,-0.1155448749\H,8.68
18136184,0.8798774571,-0.03248038\H,7.4560435386,-3.2476157269,-0.4265
932443\H,8.9414739499,-2.7634501662,-1.2521072138\H,8.9213717071,-2.91
9210143,0.5030461769\H,10.6534234099,-1.4540731615,-0.1500483319\H,11.
1542556799,-0.491946554,2.5161257348\H,12.7903165063,-0.1753841826,3.1
265395919\H,11.6992650383,1.171460483,2.7448955257\H,13.3759890903,-1.
3206913295,-0.4042662063\H,14.0046806633,-1.4248297897,1.2495396084\H,
12.3866151895,-2.0226174567,0.8924703025\H,14.3354726605,0.9192351728,
-0.0354953272\H,11.9824536141,3.8086410783,-0.4296521877\H,13.13172701
81,2.864622802,-1.3475001866\H,10.9547454899,2.6081470922,-2.584265011
4\H,9.8723777766,1.2756968886,-2.1258314393\H,9.7027030094,2.872861019
9,-1.3805743619\H,14.1983906747,3.2841049361,0.7819383678\H,12.7423479
686,2.8881329096,1.6866579833\H,14.4325098901,0.9900141986,1.721054490
5\H,-12.4408847317,2.8388054825,-0.4125407943\H,-11.1923082916,3.06358
79085,1.6539396721\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.260492

9\S2=0.893984\S2-1=0.\S2A=0.766042\RMSD=4.888e-09\RMSF=2.445e-06\Dipol
e=0.2204326,0.113306,0.0684308\Quadrupole=10.4259197,2.9817611,-13.407
6808,-2.2706266,-2.336736,0.5490011\PG=C01 [X(C40H55)]\@

15E,14Z

l (bet_car_14_c9m)

1\1\GINC-S3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\18-May-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizatio
n\0,2\C,12.618898458,0.5570522858,0.6837305643\C,6.6185775531,0.22166
9255,-0.2653250323\C,12.1025503873,1.1564317746,2.0137662124\C,12.9767
815402,1.7245070072,-0.2674058653\C,5.3296534567,0.7242081586,-0.59687
01248\C,4.1604509285,0.1363752281,-0.1574780678\C,2.835422252,0.561998
5536,-0.4436199819\C,2.6222360119,1.7738685877,-1.3207335698\C,1.77213
73185,-0.1655225339,0.1049439342\C,0.398735928,0.0594840338,-0.0401842
897\C,13.9204604131,-0.2405777885,0.9332084446\C,13.663872521,-1.61796
33402,1.5394152368\C,12.8234173153,-2.4447886026,0.5680170948\C,11.645
505223,-1.6917367931,-0.0163247764\C,10.6773716905,-2.6016851906,-0.73
68870963\C,11.5178806034,-0.3419573911,0.0690807899\C,10.3225229428,0.
3736382635,-0.4106772064\C,9.0328254665,0.0171712076,-0.1748932667\C,7
.8507964231,0.7159934947,-0.6335771297\C,8.0238652528,1.9468476547,-1.
489234935\C,-0.5584418632,-0.7631706598,0.5843209105\C,-1.9501873158,-
0.7312510069,0.5770359934\C,-2.8881175837,0.1304289106,-0.0702590784\C
,-4.2347832995,-0.1236094472,0.1450843134\C,-2.4230118665,1.2665409415
,-0.9499875885\C,-5.3628338818,0.5715813174,-0.3785946609\C,-6.6521136
717,0.2170002464,-0.0996472924\C,-7.8699561603,0.878230531,-0.57114662
91\C,-9.1166798538,0.1000652414,-0.4032403984\C,-7.8773094032,2.116583
2531,-1.1244288208\C,-10.3446099683,0.6194899873,-0.2080851619\C,-11.5
975239645,-0.1468200884,-0.047248802\C,-12.4730034231,0.2743349408,1.1
568320329\C,-11.9475261627,-1.1511129361,-0.8894624538\C,-11.750921671
8,-0.1092051594,2.4708162131\C,-12.7077559128,1.8040986362,1.163201145
8\C,-13.8640285887,-0.4001231965,1.0998229845\C,-13.1823075674,-2.0049
097392,-0.678956847\C,-11.1982674445,-1.5179366717,-2.14989629\C,-13.7
911683551,-1.8759343846,0.7163477949\C,6.6235285276,-0.6727019441,0.35
97304108\C,11.1639113361,1.6997113129,1.860168657\C,11.9107305788,0.37
80572739,2.7604096852\C,12.8365289012,1.8565978719,2.4327134939\C,13.8
533642018,2.258390679,0.1195884611\C,13.223086991,1.3593734393,-1.2714

877689\H,12.1689156947,2.4577367117,-0.3576297786\H,5.2624225533,1.608
 4182369,-1.2246776679\H,4.2556330735,-0.7471314459,0.4751953299\H,3.08
 2662538,1.6316174458,-2.306592036\H,1.5659253858,1.9960933423,-1.48090
 18106\H,3.0835044271,2.6659309265,-0.8780654747\H,2.0521779813,-1.0181
 57581,0.7257914018\H,0.0699026436,0.8913509114,-0.6493310209\H,14.5834
 989734,0.3550016918,1.5745633191\H,14.4476287391,-0.3726875562,-0.0230
 119137\H,13.1352305322,-1.5178265975,2.4961712272\H,12.4498614106,-3.3
 54747619,1.0609427184\H,11.2372798254,-3.3394334124,-1.3287593496\H,10
 .0633370522,-3.1803728951,-0.0316003791\H,10.0018293057,-2.0647422998,
 -1.4051133235\H,10.5010224274,1.2995246521,-0.9528621061\H,8.847310047
 3,-0.8681861896,0.4315772001\H,8.5913622171,2.7191585146,-0.9536236928
 \H,8.5880835745,1.7142165604,-2.401296837\H,7.0720137998,2.3873281685,
 -1.7907061201\H,-0.1349045583,-1.5705508134,1.1835690481\H,-2.41528915
 63,-1.5132099642,1.1761699748\H,-4.4700859948,-0.964340556,0.798505642
 1\H,-1.8086840671,1.9764226537,-0.3827184562\H,-1.8084937255,0.8941049
 583,-1.7785731612\H,-3.2536929702,1.8256971585,-1.3835221596\H,-5.1931
 073281,1.4155869734,-1.0428243823\H,-6.806956452,-0.6601796423,0.52916
 49607\H,-9.0018352878,-0.9833450736,-0.4021341115\H,-8.7842644052,2.54
 26297838,-1.5401608572\H,-6.9834614128,2.73021113,-1.1759629043\H,-10.
 4142877554,1.7010191674,-0.097637621\H,-10.7513995928,0.3367281951,2.5
 12480747\H,-12.3181790525,0.2466520109,3.3402982585\H,-11.6304852551,-
 1.1940085635,2.5644759103\H,-13.0941517377,2.1523508539,0.1979231686\H
 ,-13.4475116294,2.05885918,1.9319092209\H,-11.7983943524,2.3686023217,
 1.392904424\H,-14.4843317216,0.1235710322,0.3577388293\H,-12.925440478
 7,-3.0532948018,-0.8910469968\H,-13.9317965049,-1.7344972267,-1.441463
 2365\H,-11.9128150832,-1.6803914998,-2.9691419247\H,-10.4822126009,-0.
 7555709324,-2.4607058938\H,-10.651254994,-2.4641331403,-2.030368424\H,
 -14.7883181446,-2.3324717907,0.7412501023\H,-13.177265166,-2.425279597
 4,1.4416769549\H,-14.3617344851,-0.2696453203,2.0697429919\H,14.610092
 2938,-2.128779148,1.7562176195\H,13.4561241531,-2.8079381277,-0.259285
 6484\\Version=ES64L-G09RevD.01\\State=2-A\\HF=-1557.2592885\\S2=0.897339\\
 S2-1=0.\\S2A=0.766692\\RMSD=7.484e-09\\RMSF=1.728e-06\\Dipole=0.1871813,0.
 0078528,-0.161523\\Quadrupole=13.1014868,-2.7304714,-10.3710155,2.64628
 77,-0.3845183,-5.5012266\\PG=C01 [X(C40H55)]\\@

15E,11Z

l(bet_car_030)

I\1\GINC-R2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\04-Dec-2016\0\#P
 UB3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\
 0,2\C,10.8304908148,2.2095059441,0.9993095529\C,6.6500008497,-1.861282
 7472,-0.1530783008\C,12.0684030021,1.6039989794,1.706416637\C,9.662278
 0377,2.2562642429,2.0107447787\C,5.9325700154,-3.0172785794,-0.2773922
 222\C,4.5146228168,-3.2170267873,-0.3574820257\C,3.4557135478,-2.38619
 63433,-0.0236206291\C,3.6596708488,-1.0261364462,0.601828957\C,2.13487
 02116,-2.8697060306,-0.2677314624\C,0.9376501318,-2.2049755661,-0.0586
 688134\C,11.1325405125,3.6639811269,0.5709663282\C,12.0297509513,3.745
 5187264,-0.6611643845\C,11.3481907142,3.0546206465,-1.8427243068\C,10.
 712450299,1.7192864432,-1.500101901\C,10.4199505269,0.8768055928,-2.72
 03895953\C,10.4501083426,1.3409480839,-0.2238807911\C,9.8199094841,0.0
 507994995,0.121476881\C,8.7084394708,-0.4824459777,-0.4219313738\C,8.1
 108055759,-1.7807097667,-0.0406769599\C,8.874794246,-2.8129356078,0.39
 1613865\C,-0.3249969868,-2.7633816607,-0.3289409345\C,-1.5277378174,-2
 .0832518072,-0.126968628\C,-2.8338733109,-2.539583153,-0.3514399253\C,
 -3.9122078818,-1.6563024546,-0.0822076193\C,-3.1274944846,-3.929100045
 ,-0.8679126765\C,-5.2576574194,-1.9269639754,-0.2393618588\C,-6.277099
 5661,-0.9764283612,0.0410919118\C,-7.6421651608,-1.128073991,-0.075939
 8773\C,-8.4881500904,-0.0006745275,0.2525156287\C,-8.2917284776,-2.410
 1529518,-0.5370054206\C,-9.8438444769,0.0382516766,0.1625219809\C,-10.
 7035048944,1.1951131082,0.465480137\C,-11.8192369368,1.4681535529,-0.5
 737884781\C,-10.5323905475,1.9703390494,1.5682118274\C,-11.1755991532,
 1.9226327999,-1.9056651797\C,-12.6483941962,0.189974176,-0.8471357807\
 C,-12.8061408762,2.5475165583,-0.0688751772\C,-11.34042518,3.226874985
 ,1.822937102\C,-9.5652464059,1.6651041537,2.6887329675\C,-12.103692977
 1,3.7268902788,0.5982796173\H,6.1350517502,-0.9061367787,-0.1907796701
 \H,11.8850485848,0.5749219913,2.0343029722\H,12.9437397941,1.588233964
 5,1.0490075852\H,12.3216792848,2.1909647854,2.5983422995\H,9.910821520
 8,2.9312861057,2.8393028128\H,8.7460280636,2.6260874126,1.5362849109\H
 ,9.4420927013,1.272217262,2.4366632111\H,6.5129030978,-3.9344476035,-0
 .380463603\H,4.2299545849,-4.201866394,-0.7276808796\H,3.8187451194,-0
 .2476200405,-0.1563771573\H,2.7963423237,-0.7259314184,1.2015166192\H,
 4.5359334462,-1.0272873559,1.2569150197\H,2.0680233967,-3.8764404467,-
 0.681935603\H,0.9522576089,-1.18752551,0.3288827866\H,11.5810896593,4.
 1991729806,1.418669564\H,10.1829342978,4.1723272642,0.3491035844\H,12.
 9946090147,3.2632889783,-0.4588152116\H,12.0652833999,2.9092785785,-2.
 6625567936\H,9.5808349202,1.2910376857,-3.2986276013\H,11.2866364131,0

.8806013302,-3.3949906601\H,10.1751637319,-0.1580097878,-2.4770204747\
H,10.2685169323,-0.4898634646,0.9562982002\H,8.1640119647,0.0893461337
,-1.172662428\H,9.9584166345,-2.7558381757,0.3801833594\H,8.437208148,
-3.7324022169,0.7672933057\H,-0.3420974544,-3.7800892847,-0.7170216772
\H,-1.4406460032,-1.0647136385,0.2547635835\H,-3.6434770545,-0.6638690
741,0.2823205318\H,-2.2225325986,-4.51607137,-1.0327880655\H,-3.756694
8888,-4.4855633054,-0.1617330203\H,-3.6731371149,-3.8881292773,-1.8191
4767\H,-5.5492525228,-2.9100173629,-0.5984162166\H,-5.9262936537,-0.00
35191898,0.3888955703\H,-7.9663415262,0.8990900756,0.574889833\H,-7.56
76603417,-3.2027789638,-0.7326769776\H,-8.9980936118,-2.7831839424,0.2
15327056\H,-8.8658202053,-2.249916082,-1.459099464\H,-10.3467678001,-0
.8422617208,-0.2300162964\H,-10.4542401047,1.1806983322,-2.2647271408\
H,-11.9422907264,2.0538379424,-2.6798783028\H,-10.6398079088,2.8714706
962,-1.7931415732\H,-13.0165950572,-0.2530202777,0.08573701\H,-13.5187
174416,0.4428220004,-1.4649727775\H,-12.0818360252,-0.5736419395,-1.38
96418921\H,-13.4918397762,2.0920349938,0.6607028036\H,-10.664243828,4.
0085031164,2.2003975663\H,-12.0441830484,3.0348109292,2.6503207764\H,-
10.0522768669,1.8513185469,3.6562197397\H,-9.2080344892,0.6338017791,2
.6751504671\H,-8.6868434612,2.3260432015,2.6577254169\H,-12.8289297468
,4.4971794079,0.8881461087\H,-11.4073449302,4.2007228655,-0.1054662571
\H,-13.4260624014,2.882510203,-0.9109812003\H,12.2510026828,4.79104262
99,-0.9092080342\H,10.5674169524,3.7136915842,-2.2583878962\Version=E
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65129\RMSD=5.972e-09\RMSF=3.112e-06\Dipole=-0.3862792,0.288813,-0.0635
245\Quadrupole=7.8452527,1.5191313,-9.364384,5.6829969,-0.7000819,3.00
08759\PG=C01 [X(C40H55)]\@

Structure of the *15Z* isomer and rotamers of C9-Me radical

15Z,9Z

l (bet_car_9_15_c9m)

l\1\GINC-Q1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\ROOT\17-May-2016\0\#P Beck
e3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimization\0
,2\C,11.1208947935,-1.192526081,1.0669697263\C,5.7928862352,1.22201763
88,-0.5653870061\C,10.5074416708,-0.8966152903,2.4566052603\C,12.06545
44676,-0.0239606281,0.6958933974\C,4.8735289826,2.2862722159,-0.787439

8058\C,3.5058903162,2.1252538248,-0.7164513686\C,2.5210209268,3.133333
9162,-0.9151247795\C,2.967464266,4.5377214318,-1.2497592729\C,1.174511
8964,2.7788049839,-0.7845421158\C,0.0519162232,3.6040763535,-0.9224314
368\C,11.9867438818,-2.4728728481,1.1328602118\C,11.1533976308,-3.7517
960774,1.1228580534\C,10.3607270652,-3.8255497871,-0.1809469709\C,9.67
91334536,-2.5253937018,-0.5576891198\C,8.6786897348,-2.6975818658,-1.6
77288926\C,9.9817872925,-1.3380220733,0.028219793\C,9.2475839036,-0.09
49722088,-0.269141819\C,7.8972559454,0.0399741628,-0.324964914\C,7.168
7564955,1.2627284887,-0.594644487\C,7.9516295139,2.5197584872,-0.88675
40108\C,-1.3000396026,3.2231788356,-0.775695671\C,-1.7938252119,1.9607
834363,-0.4795275128\C,-3.1678105299,1.6130013197,-0.3259337373\C,-3.4
831588592,0.2965341977,-0.0319582033\C,-4.2217346712,2.686505211,-0.48
57346594\C,-4.7723841274,-0.279030148,0.1703764914\C,-4.9633976227,-1.
6015695556,0.4544126227\C,-6.2417539218,-2.2595471908,0.6851902601\C,-
7.4668555332,-1.4372215187,0.7915026794\C,-6.2880442188,-3.6083859949,
0.8243258043\C,-8.6748913213,-1.7918941232,0.3142706075\C,-9.921259043
,-1.0049884941,0.4357632981\C,-10.7065012743,-0.8118460166,-0.88329582
64\C,-10.338092867,-0.4870433927,1.6176620044\C,-9.8976214965,0.107551
0415,-1.8292814704\C,-10.9274409346,-2.1668649593,-1.5977490132\C,-12.
103010233,-0.2015462424,-0.6178918305\C,-11.562353154,0.3988884458,1.7
381190128\C,-9.6833354938,-0.7546324373,2.9536161913\C,-12.0680492491,
0.9357901738,0.400099243\H,5.3415830292,0.2544489035,-0.3401978619\H,9
.8680777861,-0.0079704442,2.4213247028\H,9.8904348071,-1.7293522074,2.
8110865451\H,11.2974535035,-0.7184494135,3.197352523\H,12.9398650384,-
0.0349360087,1.3578800398\H,12.4247079241,-0.1136884829,-0.3361423337\H,
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1.0188369977\H,3.1330074553,1.1278916698,-0.4791739289\H,3.5717942461,
4.5484677762,-2.1655337368\H,2.1313093049,5.2220465041,-1.4005018453\H
,3.5932901739,4.9516308958,-0.4488123713\H,0.9917454652,1.733008748,-0
.5402423725\H,0.2159276794,4.6516026738,-1.1617243409\H,12.6234698023,
-2.4244983465,2.0260764675\H,12.6645353689,-2.4903771268,0.26681926\H,
10.4647996756,-3.7615281041,1.9776139201\H,9.5996848776,-4.6181287117,
-0.1238038782\H,9.0980474214,-3.3604293463,-2.4473117149\H,7.757390712
7,-3.1841982472,-1.3256040976\H,8.3993799683,-1.7538392052,-2.14880275
3\H,9.850517497,0.8014634718,-0.394590831\H,7.2838748267,-0.8383783632
,-0.128461979\H,8.5932574894,2.788067306,-0.0371492674\H,8.6131362895,
2.3768574222,-1.7505386108\H,7.3100863548,3.3768026126,-1.0983896411\H
,-2.0240964036,4.023536619,-0.9127687233\H,-1.083806036,1.1459975945,-
0.346771185\H,-2.6434364823,-0.3936315783,0.059362163\H,-4.1877856091,

3.1237222079,-1.4912963722\H,-5.2325775946,2.3083752356,-0.3261812984\H,-4.0583952132,3.5050583239,0.2258513031\H,-5.6459321015,0.3621496442,0.0865415522\H,-4.0853570163,-2.2454855481,0.5089298337\H,-7.3607923997,-0.4731109795,1.285872672\H,-7.2129563425,-4.1260665055,1.0558304408\H,-5.3944028519,-4.2176643563,0.7178510239\H,-8.7299997301,-2.715156464,-0.2614726977\H,-8.892595993,-0.2929107594,-2.0000956333\H,-10.3982773129,0.1953495473,-2.8018616905\H,-9.7840815722,1.1146867691,-1.4135067504\H,-11.3801778999,-2.903701817,-0.9236640013\H,-11.6070151741,-2.0274415181,-2.4472435124\H,-9.9985261953,-2.5889033122,-1.9940815543\H,-12.7705997153,-0.9893844846,-0.2393595268\H,-11.3303995488,1.2282310936,2.4225093412\H,-12.3621380106,-0.1708122443,2.2400564138\H,-10.4555558521,-0.9772770567,3.7034446301\H,-8.9769138996,-1.5855658704,2.9266124141\H,-9.1470851206,0.1314311555,3.3224722998\H,-13.0638102915,1.3804108256,0.5189826991\H,-11.4069729116,1.7383090562,0.0480947987\H,-12.5292293814,0.1366074387,-1.5716061835\H,11.7962562672,-4.6343158872,1.2291576821\H,11.0258656457,-4.1282579479,-1.0071283777\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2648921\S2=0.890333\S2-1=0.\S2A=0.765117\RMSD=7.046e-09\RMSF=1.269e-06\Dipole=0.0027678,0.2479596,-0.0070339\Quadrupole=12.0830729,1.1011551,-13.184228,-3.6406392,-1.4471128,-1.6120272\PG=C01 [X(C40H55)]\\@

15Z,8Z

1 (bet_car_8_15_c9m)

1\1\GINC-R2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\11-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
n\\0,2\C,9.7407379573,-2.13776902,1.0019459601\C,5.1086106296,1.5834635417,-0.3462416429\C,9.3736066831,-1.6541892616,2.4253049991\C,10.9297453249,-1.2874338337,0.4924066527\C,4.4812455112,2.8436849169,-0.5542775722\C,3.119889445,3.0309482914,-0.4295238408\C,2.406009552,4.2460756778,-0.618677401\C,3.1674228068,5.4947668995,-0.9980919079\C,1.017522251,4.2307250948,-0.4418380787\C,0.1216496049,5.2969399191,-0.5720295013\C,10.2227103945,-3.6066884861,1.0509029514\C,9.0720184579,-4.6034111202,1.1639615108\C,8.1816574723,-4.4793200381,-0.0704285892\C,7.8477755118,-3.0485766161,-0.4416605762\C,6.7461467875,-2.9600406963,-1.4724914833\C,8.5095326918,-1.9799561999,0.0747704085\C,8.1117515865,-0.5889389745,-0.2015035965\C,6.8433175657,-0.1018222489,-0.1825112502\C,6.4459274498,1.2666440066,-0.4386792724\C,7.5111637757,2.2756363419,-0.791

8448853\C,-1.2793630729,5.2484537624,-0.3850551455\C,-2.0431624745,4.1
 451871203,-0.0390394907\C,-3.4588953192,4.1260499457,0.1457450595\C,-4
 .0564089106,2.9300016703,0.4996539211\C,-4.243065154,5.4051989743,-0.0
 46488879\C,-5.4400734281,2.6691420013,0.7446941398\C,-5.9215121889,1.4
 378674714,1.0739020057\C,-7.3196117077,1.1203426161,1.3880730726\C,-7.
 8309437415,-0.2250881734,1.0798403977\C,-8.1411480012,2.018547032,1.98
 29896365\C,-7.219376427,-1.1482989173,0.310708904\C,-7.7423018751,-2.4
 959474676,-0.001251781\C,-7.7679510044,-2.8569609393,-1.5056398159\C,-
 8.1706327856,-3.3477639155,0.9625113424\C,-8.8438239331,-2.0000373081,
 -2.215347264\C,-6.4016350928,-2.5620621117,-2.1699444836\C,-8.06478716
 28,-4.3605335768,-1.7132730263\C,-8.7799902918,-4.7005215361,0.6500139
 236\C,-8.056304284,-3.0913570629,2.4477283803\C,-9.1865779952,-4.87214
 46541,-0.8127521922\H,4.4356871214,0.7665747134,-0.0807490936\H,9.0012
 680518,-0.6242647322,2.4052379166\H,8.5910298497,-2.2759028956,2.87357
 1489\H,10.2518329316,-1.686019073,3.0828737841\H,11.8292483166,-1.5297
 129721,1.0715284992\H,11.1442560936,-1.4941839664,-0.5627381742\H,10.7
 576394976,-0.2120523772,0.6032636736\H,5.1010500221,3.694535835,-0.823
 4887872\H,2.5221990492,2.1600329066,-0.1569531182\H,3.7210328109,5.346
 5779814,-1.9337870582\H,2.5169454016,6.3599425428,-1.1348475653\H,3.90
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 0944659\H,0.5216984692,6.2707528531,-0.8426117597\H,10.9273473952,-3.7
 200875791,1.8852970174\H,10.78729708,-3.8283498923,0.1333918532\H,8.48
 41206527,-4.4019250685,2.0687175952\H,7.2420752937,-5.0329076126,0.075
 7727211\H,6.8959178339,-3.7347061975,-2.2376857535\H,5.758677581,-3.15
 64740783,-1.0301222515\H,6.7026438565,-1.9889500447,-1.968864646\H,8.9
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 9121619,-1.689104919\H,7.1039849786,3.2707838267,-0.9787688776\H,-1.80
 01457533,6.192221523,-0.5327843714\H,-1.5366274276,3.1933743227,0.1129
 830946\H,-3.3936130293,2.0708641044,0.6100314234\H,-4.103821033,5.8008
 476383,-1.0599953344\H,-5.3143614734,5.267742942,0.1075923603\H,-3.904
 6810198,6.181759856,0.6505785245\H,-6.1504852259,3.4872385989,0.650643
 2467\H,-5.2178143838,0.6071109604,1.1129110212\H,-8.8061697702,-0.4604
 48556,1.5032543121\H,-7.7955650558,3.0020461575,2.2844384551\H,-9.1797
 492804,1.7784686821,2.1930736365\H,-6.2858832941,-0.8672251478,-0.1738
 096403\H,-8.662768568,-0.9321462462,-2.0531395839\H,-8.8326974845,-2.1
 863316367,-3.296892109\H,-9.8494570868,-2.2226676969,-1.8424676413\H,-
 5.5810285806,-3.0459386812,-1.6267807398\H,-6.3999778566,-2.951016405,
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 [X(C40H55)]\@

15Z,12Z

l (bet_car_12_15_c9m)

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 ,0.5527444946\C,-2.8416177207,3.2958624644,0.43028249\C,-2.2516322378,
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J]\\@

15,15'-cis (15Z)

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15Z,13Z

l (bet_car_13_15_c9m)

1\1\GINC-S3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\17-May-2016\0\#P

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 765733891\H,-11.5537183347,0.868207892,3.3414954619\H,-10.1191287992,-
 0.0241580941,2.7883983357\H,-10.1737235733,1.7425789128,2.694933282\H,
 -14.0051497394,2.4111708697,-0.4143380222\H,-12.3297451262,2.531817486
 6,-0.9367573898\H,-13.5424380828,0.6145850189,-2.0777091325\H,13.69792
 25815,-3.016473854,0.9753069033\H,12.5894476314,-2.9438424324,-1.17246
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 2-1=0.\\S2A=0.770112\\RMSD=7.576e-09\\RMSF=4.077e-06\\Dipole=0.2254613,0.1
 729654,-0.0534019\\Quadrupole=10.9033322,1.473872,-12.3772042,-3.605599
 6,-0.9173372,-3.0511001\\PG=C01 [X(C40H55)]\\@

15Z,10Z

1 (car_H_021_cis)

1\\GINC-R1\\FOpt\\UB3LYP\\6-31G(d)\\C40H55(2)\\SANDHIYA\\05-Dec-2016\\0\\#P
 UB3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\
 0,2\\C,7.8933679565,-4.5210037487,-0.1671882384\\C,7.5548838598,-3.05276
 28894,-0.3496554855\\C,8.1458458494,-2.0679306731,0.3767603368\\C,9.2761
 574456,-2.3541167903,1.3973720617\\C,9.3135216262,-3.8523282991,1.77661
 0364\\C,9.2111323472,-4.775048184,0.5651151205\\C,6.5101680801,-2.815310
 0941,-1.4161614196\\C,7.8096158531,-0.6415805999,0.2321184165\\C,6.56684
 45643,-0.098126453,0.1598178393\\C,6.25363354,1.3109833195,0.0411227919
 \\C,4.9279716488,1.68229727,-0.0000116785\\C,4.3798411181,2.9909183231,-
 0.110250023\\C,3.0222654857,3.2341913407,-0.1532452347\\C,2.3894139761,4

.5030789438,-0.258854828\C,0.9905451649,4.5453290222,-0.2951959245\C,0
.168731583,5.6733372529,-0.386129593\C,-1.244808195,5.6883358654,-0.43
21092937\C,-2.0995039341,4.5978686455,-0.4263234892\C,-3.5265716982,4.
6483161163,-0.4696276178\C,-4.2224335898,3.4524787519,-0.4783774031\C,
-5.6414165185,3.2714548826,-0.4513999167\C,-6.330651859,2.0957673914,-
0.5536331418\C,9.0449440089,-1.5548091542,2.7002520899\C,10.6395756132
,-1.9316751322,0.796205252\C,-5.8274649403,0.7457412757,-0.8433441092\
C,7.3905961486,2.3008169395,-0.0327760523\C,3.2451224929,5.7465582541,
-0.3281585396\C,-4.209924789,5.9971634828,-0.5192354559\C,-6.583772262
1,-0.3568168605,-0.2070912133\C,-4.7781274945,0.5034840815,-1.66392003
1\C,-6.7639557119,-1.5829999205,-0.7365966172\C,-7.5155513507,-2.69825
55917,-0.1253422417\C,-8.5267975476,-3.3968789179,-1.0659704336\C,-9.0
792378412,-4.6934542437,-0.4289426777\C,-9.4325591955,-4.5243220151,1.
0463774804\C,-8.1725659473,-4.1546045758,1.8265464186\C,-7.3381187517,
-3.0749339938,1.1657942964\C,-6.2777054058,-2.5163843265,2.086715556\C
,-7.8566677635,-3.7954294744,-2.4030630372\C,-9.6883334531,-2.42308024
87,-1.3781611375\H,7.9069686114,-5.0108248634,-1.1507058872\H,7.066252
4632,-5.0029292988,0.3813866648\H,8.4745738307,-4.0666026907,2.4544715
825\H,10.2315794072,-4.0528223903,2.3450914162\H,10.0519563706,-4.5972
848745,-0.1174499039\H,9.2776184049,-5.8257930939,0.8734588345\H,6.466
649703,-1.7756657888,-1.7447651141\H,6.7163661494,-3.4460221164,-2.291
0000085\H,5.5057032318,-3.096674704,-1.0664329054\H,8.657228545,0.0422
103665,0.2541695811\H,5.7074288922,-0.7639465341,0.2180450109\H,4.1971
02765,0.8741338234,0.0572539255\H,5.0606556674,3.836054591,-0.16307469
97\H,2.3600287833,2.3688629472,-0.1012919768\H,0.4954466997,3.57624995
08,-0.2428328763\H,0.6447720718,6.6499178076,-0.4230872134\H,-1.695421
4445,6.6774098851,-0.4812110909\H,-1.6655264503,3.6000208703,-0.389576
2652\H,-3.6244901042,2.5437145264,-0.4716833686\H,-6.2504847419,4.1559
537746,-0.2763417653\H,-7.4043085747,2.1490009762,-0.3747733439\H,9.80
55062972,-1.8226685274,3.444532278\H,9.1029999866,-0.4734924565,2.5405
934591\H,8.0601491659,-1.7753952995,3.127523459\H,11.4427889336,-2.084
1085241,1.528380993\H,10.8832295764,-2.5085699132,-0.1017572715\H,10.6
491793325,-0.872126442,0.5170928796\H,8.013830361,2.2499102671,0.86967
55655\H,8.0468111946,2.079774298,-0.8841272976\H,7.0465258044,3.331051
365,-0.1382621784\H,3.9156905253,5.7126358211,-1.1962126718\H,2.654851
7371,6.6607770812,-0.4054887934\H,3.8794717654,5.8363934093,0.56272285
5\H,-5.2970888749,5.915953791,-0.5589433677\H,-3.9504159874,6.60216621
14,0.3581627124\H,-3.8924242091,6.5630497964,-1.4037953907\H,-7.060221
9427,-0.1198444818,0.74335739\H,-4.2969975905,1.2964305927,-2.22557765

68\H,-4.4004932218,-0.5038131126,-1.8114930441\H,-6.3734784294,-1.7503
 287254,-1.7396545253\H,-8.3219842312,-5.4860844782,-0.518549927\H,-9.9
 504577205,-5.0288550356,-1.0068847479\H,-9.8729960408,-5.445325449,1.4
 47713214\H,-10.1884216043,-3.7375835833,1.1670367104\H,-7.5431932464,-
 5.0490902932,1.9685947062\H,-8.4325688898,-3.8248339099,2.843275685\H,
 -6.7154575206,-1.8566188803,2.8494868893\H,-5.7956383606,-3.338201549,
 2.6346993344\H,-5.5066162779,-1.951731029,1.5601744878\H,-8.5470824883
 ,-4.4138154174,-2.9896639707\H,-7.5985890172,-2.9284063755,-3.01954381
 9\H,-6.9448026128,-4.3801485884,-2.2329531987\H,-10.2567537993,-2.1699
 24448,-0.4766628017\H,-9.3103983008,-1.4862589458,-1.8015898189\H,-10.
 3807527079,-2.8687903045,-2.1036239242\\Version=ES64L-G09RevD.01\State
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 RMSF=2.114e-06\Dipole=0.1604844,-0.1455296,0.1336996\Quadrupole=5.6187
 893,6.2133676,-11.832157,2.240691,-2.3418353,-0.9541642\PG=C01 [X(C40H
 55)]\\@

15Z,7Z

l (bet_car_7_15_c9m)

l\1\GINC-Q1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\ROOT\16-May-2016\0\#P Beck
 e3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\0
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 941,0.0336030709\C,9.8763638445,-2.4240051633,2.1789522582\C,11.684954
 4462,-1.2234907912,0.9233498583\C,5.0672364349,2.6790612349,0.17572578
 91\C,3.6928464882,2.7403573895,0.0925354732\C,2.8840626415,3.906217810
 4,0.2134005656\C,3.5525188505,5.2400347958,0.4527462509\C,1.4981660898
 ,3.7638729513,0.1051107382\C,0.5219700136,4.7664098714,0.1836141637\C,
 11.2074750489,-3.6017830163,0.3707885703\C,10.1971311086,-4.6213947288
 ,-0.1478097243\C,9.509040069,-4.0594801173,-1.3903967418\C,9.064465802
 6,-2.6178419437,-1.2466599522\C,8.1491174997,-2.1807760376,-2.36712593
 19\C,9.4903361056,-1.8116858845,-0.239262755\C,8.9772362847,-0.4436920
 103,-0.0474901606\C,7.6732202839,-0.0668822645,-0.0956375702\C,7.15968
 99249,1.2742139904,0.0951521851\C,8.1394652553,2.3940552448,0.34795405
 12\C,-0.8742916512,4.5937863537,0.0825742221\C,-1.5668082109,3.4029519
 695,-0.0970790108\C,-2.9803182481,3.2617198969,-0.1875771898\C,-3.5035
 843915,1.9883233758,-0.358582778\C,-3.8526365607,4.4942853376,-0.09304
 28366\C,-4.8699471252,1.6019646665,-0.4636217575\C,-5.2696088005,0.303
 5915874,-0.6115875115\C,-6.6440700539,-0.1873048466,-0.7349941314\C,-6

.7931894286,-1.642009339,-0.4934471357\C,-7.6720504458,0.616611292,-1.
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,-2.010626808,0.2688203655\C,-10.3417260019,-2.731458587,-0.5370910619
\C,-9.5041977383,-1.1561705609,1.2832364591\C,-10.3664216198,-2.183999
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16792874\C,-8.4501889702,-0.513937474,2.1492823594\C,-11.9601027797,-1
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3867319956,-1.49257823,2.4831421777\H,9.1112408162,-3.2078114874,2.170
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6328431573,1.5442409121\H,12.1098875422,-0.9734129495,-0.0559938969\H,
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.1394448723,5.2229869563,1.3797942232\H,1.14758592,2.7458786678,-0.060
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790967056,-0.4766417418\H,7.651087223,3.3629883188,0.4643162596\H,-1.4
617474437,5.5061969329,0.1610301944\H,-0.9946886634,2.4797045644,-0.17
25956525\H,-2.7810322754,1.1732704205,-0.4165692418\H,-3.6048484693,5.
2115767323,-0.8850091394\H,-4.9154187297,4.2634018441,-0.1793905843\H,
-3.7027999626,5.008278279,0.8643150294\H,-5.6336030076,2.3739201394,-0
.405160491\H,-4.4926732263,-0.4615482845,-0.6081010112\H,-5.8694042187
,-2.1969851064,-0.6640217423\H,-7.5134114696,1.6615982134,-1.349480439
5\H,-8.6847341738,0.2419512103,-1.1806539332\H,-7.6507227132,-3.460546
7023,-0.0731048874\H,-9.376991273,-2.2568552879,-2.4489534491\H,-11.07
25057989,-2.7561653713,-2.5998798435\H,-10.6703022058,-1.1317980951,-2
.0165360117\H,-9.9198474408,-4.6791116643,0.391263429\H,-10.9398321034
,-4.7586631583,-1.055424868\H,-9.2027624479,-4.4970933368,-1.223269204
5\H,-11.8042248493,-3.2138970963,0.9904158776\H,-10.9277126219,0.33032
17597,1.8649146309\H,-11.1740499912,-1.2264013394,2.6219981734\H,-8.76
85406415,-0.5243153913,3.2006709351\H,-7.4800565495,-1.0083876148,2.07
39836262\H,-8.3071636556,0.5401970148,1.8721638442\H,-12.9714492914,-0
.9979956743,1.0163478695\H,-11.8880838598,-0.4093816182,-0.238148482\H

, -12.5051261293, -2.8480016764, -0.582811905\H, 10.6913968671, -5.57216232
 99, -0.3825991431\H, 10.1844617297, -4.1356875197, -2.2590963738\\Version=
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 66\Quadrupole=9.4319521, 3.825074, -13.2570261, -1.236697, -1.6277405, 2.51
 26638\PG=C01 [X(C40H55)]\@

15Z,11Z

1 (bet_car_11_15_c9m)

1\1\GINC-R1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\16-May-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
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 233429\C, 3.7187212446, 2.0493019528, -0.2695180423\C, 2.6809183304, 3.0245
 675925, -0.3586384488\C, 3.0483895334, 4.4535844199, -0.6837750806\C, 1.367
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 5452\C, 12.4875511692, -2.3039294411, 0.6142376885\C, 11.6825208747, -3.596
 792168, 0.7137328045\C, 10.7382732643, -3.6921806759, -0.4830251683\C, 9.98
 98306909, -2.4071542004, -0.7754958386\C, 8.8652423091, -2.6044554017, -1.7
 659035837\C, 10.3362742511, -1.212449204, -0.229364472\C, 9.5404263347, 0.0
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 780479\C, -1.1148524675, 2.9613311726, 0.0559131971\C, -1.5365327504, 1.658
 4797689, 0.3179787076\C, -2.8630365611, 1.2078872654, 0.5432387424\C, -3.04
 92446082, -0.1623608849, 0.7365684127\C, -4.015823888, 2.1832914443, 0.5892
 648305\C, -4.224496924, -0.9435688158, 0.944006109\C, -5.5493263107, -0.603
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 , 0.7865159896\C, -10.4985961893, 0.2230601127, 2.4511409764\C, -12.7436586
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 2\H,3.7267686747,4.8661446586,0.0738057793\H,1.2431230682,1.5530872911
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 20841,-0.3315948268\H,9.2010565763,-3.2675382905,-2.5755610383\H,8.000
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 2825809\H,10.1006451258,0.9273882744,-0.6026427493\H,7.6251330392,-0.7
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 6795511676,2.4931360587,-1.7789601054\H,7.4279357082,3.4395586253,-0.9
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 5816272\H,-4.680052541,1.955529726,1.4296693364\H,-4.0093750691,-1.980
 0789064,1.2019500442\H,-5.8123862344,0.3989423026,0.520265238\H,-8.060
 7071417,0.214934384,0.9626878327\H,-5.6389415934,-3.2633992078,1.64445
 37064\H,-7.479474076,-3.3617990062,1.7053722531\H,-9.0253578956,-2.563
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 6878055985,-0.9246023382,-3.3109916063\H,-10.3067268399,0.4777524917,-
 2.2920302204\H,-11.5763134494,-3.2978902139,-0.5392757015\H,-11.723227
 2673,-3.024885094,-2.2840453077\H,-10.1262874709,-3.2021059342,-1.5598
 779869\H,-13.198153556,-1.449175826,-0.6620471101\H,-12.2545884757,1.6
 933632017,1.1548288959\H,-13.1298251056,0.2001624089,1.3988808383\H,-1
 1.3224654845,0.1782404299,3.1773883545\H,-9.7232572049,-0.4783985357,2
 .7630800352\H,-10.0832294982,1.2384558298,2.5242276607\H,-13.782255521
 2,0.9833393915,-0.7974733968\H,-12.1233127264,1.3583089364,-1.24804529
 96\H,-12.9208930571,-0.8200115872,-2.283111599\H,12.3491426218,-4.4674
 427356,0.7443623034\H,11.3034638981,-3.9861360373,-1.3834753083\\Versi
 on=ES64L-G09RevD.01\State=2-A\HF=-1557.253502\S2=0.911561\S2-1=0.\S2A=
 0.76985\RMSD=5.732e-09\RMSF=4.552e-06\Dipole=0.1992535,0.2746922,-0.11
 24474\Quadrupole=11.8327773,1.9606332,-13.7934105,-3.7691082,-0.652988
 7,-1.4257565\PG=C01 [X(C40H55)]\@

Structure of the 15E isomer and rotamers of C7 radical

15E,7Z

1 (Car_H_021)

I\1\GINC-LXA66\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\05-Dec-2016\0\#\n
p opt freq ub3lyp/6-31g(d) scf=tight\bet_car-rad\0,2\C,-13.786709839
5,0.5930865569,-1.0225185487\C,-12.3683117395,0.0868243499,-0.98369271
28\C,-11.7863582445,-0.4590330593,0.1814529234\C,-12.5936526656,-0.603
8141337,1.5059652075\C,-13.8795276356,0.254221114,1.4555988008\C,-14.6
510983577,0.1085224228,0.1444840517\C,-11.5942949622,0.2355958084,-2.2
627450976\C,-10.5059696734,-0.9131178648,0.188392254\C,-9.3069344573,-
1.463342014,0.205211031\C,-8.0409915789,-0.7933181477,0.5256536525\C,-
6.8934683653,-1.5312565478,0.5072154535\C,-5.555155748,-1.0943481652,0
.7958856631\C,-4.4763354068,-1.9271006674,0.7521383038\C,-3.1039972365
,-1.57591997,1.0322065196\C,-2.1487366704,-2.5585582827,0.9447382321\C
,-0.7429398765,-2.452114491,1.1799052069\C,0.1239962194,-3.5047622376,
1.0661611527\C,1.5290096823,-3.4016576775,1.3058699453\C,2.4816067504,
-4.3876692119,1.2202650884\C,3.8517474098,-4.04524588,1.516410478\C,4.
9259642187,-4.8862990865,1.4823135773\C,6.2604823878,-4.4642082187,1.7
984994685\C,-11.7490678172,-0.1332759651,2.7066957129\C,-12.9493661528
,-2.0942507095,1.7077410562\C,7.4075595938,-5.2107436177,1.8014994864\
C,-8.1056919834,0.6742718415,0.8605926853\C,-2.7898202542,-0.147521813
1,1.4087393054\C,2.1641366435,-5.8128250794,0.8334576587\C,8.654231606
1,-4.5572498208,2.1670480087\C,7.4447144711,-6.6780077487,1.4492743609
\C,9.8726254802,-5.1446479052,2.2469921512\C,11.1305827493,-4.48217086
69,2.6423454379\C,11.9700155521,-5.2468891142,3.6952757126\C,13.370823
6669,-4.6129210821,3.8630228524\C,13.3283017226,-3.0877645854,3.914611
0025\C,12.7619188482,-2.5562489668,2.5993838489\C,11.5222593229,-3.289
2599562,2.1265933842\C,10.8178635734,-2.5702995063,0.9990772749\C,12.1
850437968,-6.7194419368,3.2703214897\C,11.2198465264,-5.2381874844,5.0
488535536\H,-14.245199051,0.3121981796,-1.9827093353\H,-13.7714612591,
1.6984218377,-1.0290366042\H,-13.609181919,1.3120062279,1.5889067534\H
,-14.5123068668,-0.0146904569,2.3116946459\H,-14.934353217,-0.93990503
92,-0.0130891436\H,-15.5856637648,0.6812909432,0.1840525055\H,-10.5481
726241,-0.0609319574,-2.1556394547\H,-12.0384254262,-0.3731322389,-3.0
649989492\H,-11.6222612461,1.2764606474,-2.6191445229\H,-9.2153612976,
-2.5276536194,-0.0446516186\H,-6.9925341218,-2.5861873619,0.2464909503
\H,-5.403830368,-0.0525488371,1.0652519218\H,-4.6527877214,-2.96916805
11,0.4819498237\H,-2.49814526,-3.5528702806,0.6626827742\H,-0.33140445

71,-1.4861471468,1.4673656006\H,-0.2884110607,-4.4702192187,0.77837166
 11\H,1.8799353147,-2.4096333225,1.5940419972\H,4.0313959144,-3.0063267
 288,1.7964007032\H,4.7676880841,-5.9247363879,1.2048262611\H,6.3611874
 51,-3.4126406427,2.0713896081\H,-12.3319888591,-0.21298192,3.632824185
 6\H,-10.8452230867,-0.7395564104,2.8231127526\H,-11.4441185699,0.91297
 0429,2.5883185779\H,-13.5069511449,-2.2329937991,2.6426688728\H,-13.55
 97312633,-2.4845746985,0.8864777534\H,-12.0399278985,-2.7023047019,1.7
 615129285\H,-8.5920709287,1.2316733794,0.0503976935\H,-8.7130762752,0.
 839450687,1.7594434644\H,-7.1214600167,1.1146774437,1.0316985819\H,-3.
 3331954014,0.1464950945,2.315824876\H,-1.7267577653,0.0160077558,1.592
 6948852\H,-3.0995515753,0.5425043845,0.6136068671\H,2.456806691,-6.508
 169325,1.630445742\H,1.103154845,-5.9686773808,0.6319413011\H,2.719396
 6353,-6.1067670595,-0.0663879897\H,8.5727368277,-3.4999516738,2.416055
 5073\H,7.8268621992,-7.2719414114,2.2897520279\H,6.4628571566,-7.07404
 60582,1.184607944\H,8.1174319111,-6.8596811337,0.6014477593\H,9.931609
 7071,-6.2147278727,2.0606885387\H,14.0038333242,-4.9163211696,3.016296
 7685\H,13.8403323711,-5.0246011145,4.766224324\H,14.3300083324,-2.6774
 910047,4.092453149\H,12.7003783548,-2.7547159657,4.751071367\H,13.5298
 36244,-2.6154343576,1.8098415579\H,12.5259185102,-1.4852430517,2.68738
 00304\H,10.2706554523,-1.6881034532,1.3616887237\H,11.5602221034,-2.19
 42792918,0.2809498869\H,10.1103631174,-3.2056134783,0.4633528222\H,12.
 9005109753,-7.19726372,3.9506835374\H,11.2626583813,-7.3076804826,3.30
 91983593\H,12.5926538987,-6.7857269636,2.2546159849\H,11.1131421482,-4
 .225223652,5.4450609953\H,10.2124706873,-5.6542987915,4.9411044578\H,
 11.7587127114,-5.838979394,5.7926705553\\Version=AS64L-G09RevD.01\Stat
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 \RMSF=2.372e-06\Dipole=-0.3776616,0.1972797,-0.0590535\Quadrupole=15.9
 262046,-0.8840484,-15.0421562,-6.8176782,3.4990183,1.6925191\PG=C01 [X
 (C40H55)]\@

all-trans

1 (bet_car_030_004)

I\1\GINC-S3\FOpt\UB3LYP/6-31G(d)\C40H55(2)\SANDHIYA\13-Nov-2016\0\#P
 UB3LYP/6-31G(d) scf=tight opt freq scf=tight\Beta_Carotene (-30) opti
 mization\0,2\C,12.7403447376,-0.2847910469,-0.875788404\C,6.855777649
 7,-0.441877342,0.5409980203\C,12.112124496,-0.634486595,-2.2463617904\
 C,13.2049396358,-1.6007159663,-0.2064054502\C,5.6075761382,-1.08028528

22,0.8473658839\C,4.3963076637,-0.5172094397,0.5677357377\C,3.09894450
09,-1.0904695544,0.8331970367\C,3.0335451167,-2.4466366887,1.495046443
4\C,1.983249575,-0.3778315626,0.4667378086\C,0.6097798304,-0.742039210
9,0.6192958187\C,13.9982544968,0.5915676118,-1.0780165256\C,13.6613198
042,2.048870566,-1.3829879783\C,12.8958116247,2.6461348846,-0.20378758
54\C,11.791262387,1.7525984955,0.3252124028\C,10.8695586322,2.47176454
73,1.2831168236\C,11.6863506372,0.4398196991,-0.0029919031\C,10.557082
9641,-0.4017221107,0.4383403426\C,9.2443510173,-0.0796995429,0.3467629
932\C,8.1233641057,-0.9114002482,0.754817856\C,8.4176028055,-2.2512332
411,1.384551467\C,-0.4313988757,0.0429198044,0.2041934884\C,-1.8050134
902,-0.3254170288,0.3473668007\C,-2.9192823192,0.3754799916,-0.0437751
753\C,-4.2173256494,-0.2103276148,0.1950174423\C,-2.852884352,1.725953
6786,-0.7168411383\C,-5.4257028472,0.3261508295,-0.1384856477\C,-6.675
5745669,-0.3321436299,0.1258204646\C,-7.9332811364,0.1014884255,-0.177
2463151\C,-9.072346421,-0.7510913592,0.1838914602\C,-8.2419723463,1.40
61625837,-0.8651333026\C,-10.3456455735,-0.5044120198,-0.0576942282\C,
-11.6773767467,-0.3179436884,-0.2473449011\C,-12.4687703713,0.37823939
13,0.8997267822\C,-12.3221661489,-0.769485991,-1.4206458234\C,-12.6346
061822,-0.6250132815,2.0636346832\C,-11.6988278999,1.6089610545,1.4175
611495\C,-13.851098345,0.8516615295,0.3933935104\C,-13.7943088412,-0.5
67476879,-1.6685908266\C,-11.5679514431,-1.4401484659,-2.5337736408\C,
-14.5956623432,-0.2113217922,-0.4135246346\H,6.7706805944,0.5406992944
,0.0743870158\H,11.2013655724,-1.2293865055,-2.1190385768\H,11.8383054
754,0.2658067587,-2.8071572296\H,12.8157958927,-1.2149330492,-2.856692
6725\H,14.0472200433,-2.0220596426,-0.7687372958\H,13.5422516155,-1.42
69466222,0.8224065873\H,12.4187591969,-2.3622651991,-0.1859087626\H,5.
6326095215,-2.058394296,1.3197542382\H,4.3927716712,0.4639088196,0.090
8864934\H,3.5370951046,-2.4304402521,2.4699736685\H,2.0097581723,-2.78
72109709,1.6576469712\H,3.5426592391,-3.203928109,0.8852733723\H,2.157
5371167,0.589862442,-0.0060267244\H,0.3695538418,-1.6955377817,1.08627
81961\H,14.6107219036,0.1531541539,-1.8769339095\H,14.6080232304,0.557
8541443,-0.1631818847\H,13.0516565607,2.1138609535,-2.2933283498\H,12.
4607408808,3.6180097848,-0.4806863838\H,11.4621260016,3.0967689738,1.9
661147529\H,10.1913611222,3.157098478,0.7542852386\H,10.2589670947,1.7
914538961,1.8792626909\H,10.8130343865,-1.3897936799,0.8147770295\H,8.
9787275403,0.8813372949,-0.0921156684\H,8.9769668597,-2.8942812479,0.6
924709378\H,9.0401863774,-2.1334086466,2.2804326414\H,7.5135013021,-2.
7883203923,1.676197337\H,-0.1909304092,0.9956143061,-0.2643523976\H,-1
.9797928234,-1.2910677671,0.824079627\H,-4.2145420871,-1.1834406261,0.

6880215524\H,-1.829939971,2.0838213436,-0.8435723535\H,-3.3184688311,1.6912881174,-1.7100998168\H,-3.3987291364,2.4791815882,-0.1346564757\H,-5.4520141903,1.2942913832,-0.6311387354\H,-6.5964214214,-1.2985699242,0.6262356846\H,-8.806314004,-1.6850757179,0.6939901045\H,-7.3450487856,1.942178454,-1.1817019821\H,-8.8667944752,1.2349988599,-1.7503059208\H,-8.8158676254,2.0666137536,-0.2025875932\H,-11.6557207079,-0.9439349828,2.437636354\H,-13.182783137,-0.1637653407,2.8949555618\H,-13.1779968528,-1.5240683871,1.7547966845\H,-11.5255238308,2.3327549662,0.6128337568\H,-12.2744099929,2.1104586503,2.2055802223\H,-10.7275099273,1.3269917366,1.8358561297\H,-13.7137719222,1.7413994866,-0.2383935725\H,-14.2085529085,-1.4683241044,-2.1460534087\H,-13.921006512,0.23385272,-2.4195809323\H,-11.7191776803,-0.9090579028,-3.4859944867\H,-10.4939966996,-1.4926657328,-2.3401279669\H,-11.9341360175,-2.4653032017,-2.6954727085\H,-15.5924404565,0.1500774528,-0.6944024743\H,-14.7514077112,-1.1098739629,0.1968647386\H,-14.4483756303,1.1731552664,1.2570028424\H,14.5743275323,2.6254564483,-1.5764723533\H,13.5936419772,2.8704240075,0.6204400614\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2433388\S2=0.784886\S2-1=0.\S2A=0.750718\RMSD=7.093e-09\RMSF=2.953e-06\Dipole=-0.4177507,0.0803551,-0.1096927\Quadrupole=17.7150265,-4.489207,-13.2258195,-1.5789893,3.7319395,-4.9558811\PG=C01 [X(C40H55)]\\@

15E,9Z

l (bet_car_9_c7_c2)

1\1\GINC-HP1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\11-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizati
on\0,2\C,-12.5780312748,0.4688528518,0.5576878119\C,-6.6762006652,-0.8322423821,-0.0804710933\C,-12.0577000279,0.876132319,1.9569145516\C,-13.1532496915,-0.9649883218,0.6530418964\C,-5.4905292861,-1.6186529474,0.1060597923\C,-4.2325052351,-1.0926278704,0.0504909148\C,-2.9919053567,-1.8085053831,0.2261198315\C,-3.0512774139,-3.2909003783,0.509442399\C,-1.8143341506,-1.1085645398,0.1252227571\C,-0.4786392334,-1.599407734,0.2576294366\C,-13.7414965153,1.3963161347,0.1349939556\C,-13.2635414063,2.7589450782,-0.3595842784\C,-12.3884264251,2.5645226775,-1.5962512489\C,-11.3643571052,1.4563804899,-1.4531932009\C,-10.3325330221,1.4752462914,-2.5574339551\C,-11.411900773,0.5327153213,-0.4592606548\C,-10.357981728,-0.4807341384,-0.2634686201\C,-9.0219166749,-0.2538605042,-0.2713095626\C,-7.9806581624,-1.2459418165,-0.0571000498\C,-8.3936

974746,-2.6781818001,0.1810763802\C,0.6338887054,-0.8134712595,0.12850
387\C,1.9688089906,-1.3084067349,0.2579915322\C,3.1491110979,-0.617357
582,0.139389238\C,4.3873692667,-1.3419170819,0.3085856861\C,3.21678492
33,0.8608013473,-0.1619094743\C,5.6482481199,-0.8331933056,0.217654151
8\C,6.829081073,-1.6359843976,0.3979349596\C,8.1365030566,-1.250970082
3,0.3197037991\C,8.5427907932,0.1261033178,0.0158015189\C,9.2361635743
, -2.2587032864,0.5428715657\C,9.7856166029,0.5584643677,-0.081815288\C
,11.0273612206,1.0990686746,-0.1751711737\C,11.6292677692,1.7237771459
,1.118762521\C,11.7276743149,1.124103311,-1.4023539136\C,10.9201098171
,3.0695001475,1.3933435716\C,11.4015002466,0.7934569602,2.3264140797\C
,13.1517092129,1.9395680081,0.9557690487\C,13.111193007,1.7050316064,-
1.5371644384\C,11.1568117598,0.5222779333,-2.6550966787\C,13.528554964
1,2.6022094367,-0.3687753139\H,-6.5036805416,0.229253934,-0.2644674721
\H,-11.2139582083,0.2464458743,2.2591931406\H,-11.7118433145,1.9153855
609,1.9724391762\H,-12.8493282744,0.7692381772,2.7096227179\H,-14.0646
694776,-0.9545643053,1.2631632221\H,-13.4166274646,-1.3552191151,-0.33
71725419\H,-12.4589203896,-1.6672930779,1.1252693276\H,-5.6044272701,-
2.6816214674,0.2999222737\H,-4.1396966924,-0.0238378372,-0.1472551842\
H,-3.5561108722,-3.8244874078,-0.3059681369\H,-2.0631000402,-3.7366411
383,0.6336398695\H,-3.6234332856,-3.4910516907,1.4242289736\H,-1.89889
11351,-0.0413267315,-0.0848125153\H,-0.3284569218,-2.6562456525,0.4711
124814\H,-14.4340345259,1.5044959445,0.9802754677\H,-14.3093419764,0.9
118057186,-0.672895847\H,-12.6897011869,3.2672448417,0.4259958438\H,-1
1.8634912542,3.4985359937,-1.8465648708\H,-10.8256828736,1.6754439221,
-3.5191542845\H,-9.6022008069,2.2850140525,-2.4154491896\H,-9.77993366
17,0.5378231319,-2.6415321847\H,-10.6979848395,-1.4886553421,-0.036583
1124\H,-8.6710386896,0.7647447588,-0.4312474857\H,-9.0323226813,-2.758
0537103,1.0704376582\H,-8.9788520524,-3.0618872,-0.6643367896\H,-7.541
9451241,-3.344968264,0.3251059117\H,0.4853703581,0.2433034971,-0.08666
63212\H,2.0491118986,-2.3742426539,0.4766210264\H,4.287196363,-2.40568
00413,0.5289502718\H,2.2304450342,1.31523511,-0.2685394206\H,3.7458993
151,1.3977975261,0.635617979\H,3.769869974,1.0449144379,-1.0917860594\
H,5.7722704753,0.2237899398,-0.00238142\H,6.6411558812,-2.6863106279,0
.6233508462\H,7.7366582268,0.8459439128,-0.1537129671\H,8.8300101149,-
3.2555352348,0.7389117633\H,9.8981687493,-2.3216291331,-0.3304719104\H
,9.8699769797,-1.972832515,1.3921532803\H,9.844616876,2.9152183417,1.5
323231686\H,11.3174421705,3.5346119274,2.3044044014\H,11.0480824992,3.
7763781315,0.5668562595\H,11.8649873082,-0.1862609217,2.1627174412\H,1
1.8461298695,1.2313091736,3.2288148906\H,10.3350928441,0.6368592109,2.

5168928107\H,13.6585547743,0.9656372746,1.0197835297\H,13.1823490017,2.2549283957,-2.4878455053\H,13.8361552607,0.8762710469,-1.6356944773\H,11.8418013083,-0.2290515338,-3.0767560762\H,10.1888770103,0.0440679687,-2.4873787812\H,11.026210493,1.2871902243,-3.4355457182\H,14.6080125271,2.7924718881,-0.4082238433\H,13.0372278531,3.5795839462,-0.455655456\H,13.5128598423,2.5347966236,1.8048417613\H,-14.1165844237,3.4076989108,-0.5936622188\H,-13.0219789183,2.3495783296,-2.4732250296\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2421949\S2=0.783392\S2-1=0.\S2A=0.750621\RMSD=8.806e-09\RMSF=9.699e-06\Dipole=0.4179386,0.1573134,-0.1117481\Quadrupole=17.4138185,-2.5337398,-14.8800787,4.2934093,-1.1921896,-3.1777773\PG=C01 [X(C40H55)]\@

15E,13Z

1 (bet_car_13_c7_c2)

I\I\GINC-T4FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\10-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
n\\0,2\C,-11.1895108862,-1.6009397222,-0.5004264317\C,-5.9395781813,1.3501985383,0.2223391831\C,-10.588996203,-1.7402000466,-1.9200263525\C,-12.1608148129,-0.3960019019,-0.5032761709\C,-5.0469998567,2.4666633224,0.0921092463\C,-3.6893050708,2.3342189068,0.0643882865\C,-2.723281439,3.3980670855,-0.071810551\C,-3.2285403525,4.8161747914,-0.1957935198\C,-1.3896433208,3.071644831,-0.0857339259\C,-0.2655026994,3.9455715591,-0.219666931\C,-12.0229826637,-2.8563416794,-0.1516296917\C,-11.1578938111,-4.0505317008,0.2428104556\C,-10.3502726835,-3.6982453937,1.4908265781\C,-9.7026078203,-2.3289793994,1.4363396631\C,-8.6882193341,-2.123072549,2.5378414751\C,-10.0427398894,-1.3889047369,0.5183168855\C,-9.3445464847,-0.0934624373,0.4105077231\C,-8.0019654442,0.0877167998,0.3882834938\C,-7.3075366756,1.3588049504,0.2590063788\C,-8.1322940951,2.6196121579,0.1673636691\C,1.0321867954,3.5157280627,-0.2218077317\C,2.1531090285,4.3950946928,-0.3666885003\C,3.4901091454,4.0787220482,-0.3839667744\C,3.9752219974,2.7265097276,-0.2349110023\C,4.5004615534,5.1892607757,-0.5645315797\C,5.2826043333,2.3408971248,-0.2507750342\C,5.70093071,0.9751058764,-0.087938264\C,6.9728750493,0.482168772,-0.0911926405\C,7.1635672219,-0.9608394072,0.100891167\C,8.2115686328,1.3194005017,-0.2793870044\C,8.3152372224,-1.6037291718,0.1244026074\C,9.4492673255,-2.3509173029,0.1297749007\C,9.8926169469,-2.9773491267,-1.2258642735\C,10.1725370489,-2.5808344026,1.3212798575\C,8.946603996,-4.15

40154717,-1.557129339\C,9.7982974733,-1.9375655138,-2.3599324705\C,11.
 3563824934,-3.4690205471,-1.142171772\C,11.4380661059,-3.3972207132,1.
 3595365267\C,9.7535066111,-1.9794560114,2.6328929163\C,11.6519505119,-
 4.2740201534,0.1227932363\H,-5.4544068115,0.375937751,0.2985090908\H,-
 9.9684429817,-0.8724601474,-2.1681784533\H,-9.9561034461,-2.6300762319
 ,-2.0061849672\H,-11.3859591916,-1.8146812318,-2.6709674903\H,-13.0366
 314336,-0.6314051409,-1.1203151875\H,-12.5156359767,-0.1667663956,0.50
 86110809\H,-11.7075807133,0.5087345298,-0.9211584223\H,-5.4771348323,3
 .4610135429,0.0084287991\H,-3.2776375824,1.3275927335,0.1491107427\H,-
 3.8340864191,5.0921818045,0.6767699407\H,-2.4210232282,5.5449711258,-0
 .2810033558\H,-3.8713473101,4.9268538733,-1.078417573\H,-1.145739317,2
 .0129439212,0.0139120595\H,-0.4436974349,5.0138361386,-0.3303451688\H,
 -12.6678167842,-3.1026554398,-1.0055752457\H,-12.6934774972,-2.6177479
 606,0.6870617051\H,-10.4781258444,-4.3128470658,-0.5780695812\H,-9.567
 5523997,-4.4512310507,1.6667986211\H,-9.080491969,-2.5286800483,3.4811
 251785\H,-7.7555054466,-2.6694192686,2.3358081412\H,-8.4332807717,-1.0
 732287708,2.6927179339\H,-9.9768616202,0.7822020334,0.2815435462\H,-7.
 3613286326,-0.7910765773,0.4505540141\H,-8.7943585732,2.5915134816,-0.
 7079960832\H,-8.7770621847,2.7294209262,1.0485497543\H,-7.5196760209,3
 .5193305009,0.0897844927\H,1.2118396194,2.4476720757,-0.1113283364\H,1
 .8978382678,5.4489790586,-0.4806938662\H,3.2306632828,1.9452344995,-0.
 0948722734\H,4.0082356316,6.1613743025,-0.6582249354\H,5.1941010559,5.
 2432005227,0.284747003\H,5.1107472724,5.033854,-1.463952647\H,6.050812
 5538,3.0959958856,-0.3922608061\H,4.8946377867,0.254213214,0.056282226
 1\H,6.2393674176,-1.533372613,0.2468893733\H,7.9967886097,2.387917055,
 -0.3417917262\H,8.9117705197,1.1598636495,0.5497620946\H,8.7414381555,
 1.0256771964,-1.1944017211\H,7.9123320477,-3.8031407813,-1.6405045318\
 H,9.2273295694,-4.6163272223,-2.5119666534\H,8.9706317423,-4.928775600
 9,-0.7836842266\H,10.4329293385,-1.068099987,-2.1525464353\H,10.131226
 8552,-2.3805637587,-3.3067736255\H,8.7712141236,-1.5843343825,-2.49523
 73665\H,12.0274910842,-2.5980343136,-1.1701767589\H,11.4450089586,-4.0
 121343069,2.272157933\H,12.2990585686,-2.7131973987,1.4732865923\H,10.
 5677633286,-1.3798232012,3.0677169031\H,8.8728508472,-1.3397908693,2.5
 380082009\H,9.5254714171,-2.763666092,3.3705155525\H,12.6811822168,-4.
 6525946061,0.1038162067\H,10.997743781,-5.1535532882,0.1728800136\H,11
 .5781024986,-4.0608466125,-2.0401069706\H,-11.7796572049,-4.9351427069
 ,0.4280783566\H,-10.9979914011,-3.7469178873,2.3822785628\\Version=ES6
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 46\RMSD=5.738e-09\RMSF=1.194e-05\Dipole=0.487532,-0.1369497,0.0545387\

Quadrupole=14.9169745,0.393339,-15.3103136,-4.0570831,0.3599325,-2.373
2168\PG=C01 [X(C40H55)]\@

15E,8Z

l (bet_car_8_c7)

l\1\GINC-R2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\10-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizatio
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368583146,-0.4450790957\C,-11.3737687729,-1.3293216122,2.0347324384\C,
-12.178218742,-2.5079832819,-0.0272980124\C,-4.6565905817,-0.887983864
,-0.6277607219\C,-3.5703012458,-0.1102225702,-0.348912592\C,-2.1837198
555,-0.4827244151,-0.4904655988\C,-1.8584860368,-1.8661990181,-1.00230
06373\C,-1.2228896673,0.4376003178,-0.1483830475\C,0.1981737058,0.2937
27567,-0.1914189475\C,-13.3188578753,-0.415312056,0.6915728613\C,-13.2
020265012,1.0852230237,0.9455716115\C,-12.4501012774,1.7329917579,-0.2
153495714\C,-11.2014780301,0.9804653425,-0.6292944068\C,-10.3264243333
,1.7810058839,-1.5662974307\C,-10.9371524555,-0.2879391116,-0.22365719
87\C,-9.6692140066,-0.9741119585,-0.5372374224\C,-8.4283633108,-0.4467
037071,-0.4011663006\C,-7.1696879273,-1.1189434433,-0.6793953815\C,-7.
2118749747,-2.533134385,-1.2051573368\C,1.0691853527,1.2816015859,0.18
06686527\C,2.4906364913,1.1379572488,0.1465572382\C,3.4475787337,2.057
4580547,0.5005981042\C,4.8369229106,1.682435622,0.3854289533\C,3.11610
43355,3.4416478868,1.0065105381\C,5.916902839,2.4560186677,0.694648313
\C,7.2722771932,2.0019181943,0.5538451495\C,8.4159489979,2.6860557167,
0.8365850051\C,9.7464513832,2.0716682948,0.641113827\C,8.4531013183,4.
0997736627,1.3645510641\C,10.021345953,0.854110146,0.2190590772\C,10.3
688442794,-0.3986025635,-0.1725937734\C,10.5539432375,-1.4610892657,0.
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10.6126021237,-2.8834633481,0.3464701137\C,10.9961023905,-2.0842562225
,-1.9946687803\C,10.3911604815,0.3082439419,-2.6197731962\C,11.5267249
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2849\H,-10.3844727342,-1.7975830179,1.9946732211\H,-11.2658498195,-0.3
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,-1.084802019\H,-11.3009875309,-3.1588940012,0.0451320467\H,-4.4965499
007,-1.8962050401,-1.0000620649\H,-3.7542018646,0.897894193,0.02524415

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2308,-1.0842235404\H,-2.2730499075,-2.6363092498,-0.3392553454\H,-1.58
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1486257\H,-13.9207556154,-0.9016317644,1.4706899769\H,-13.8541428933,-
0.5682213681,-0.2570089011\H,-12.6650911278,1.2697299538,1.8850910201\H,
-12.1702022692,2.7666921255,0.0371050877\H,-10.9543850393,2.29350926
35,-2.3087359734\H,-9.7786999299,2.5717441299,-1.0333510991\H,-9.59561
22194,1.1678414936,-2.0966121509\H,-9.7475571389,-2.0140682221,-0.8466
343695\H,-8.3401991703,0.5722110195,-0.0263598471\H,-7.7148606567,-3.2
010263271,-0.4935709805\H,-7.7796570499,-2.5843875964,-2.142882314\H,-
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507\H,5.7490505094,3.4631231049,1.0671866767\H,7.3918567447,0.98648077
64,0.1747448226\H,10.5885018873,2.7322919372,0.8823002524\H,7.46096250
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,9.0123472237,4.7546926971,0.6823767191\H,11.8112599346,-0.1487553181,
2.1638139676\H,12.0119180921,-1.874157679,2.5274952137\H,12.7352484464
,-1.177654786,1.0638240777\H,8.4217538351,-1.5964048204,1.4303870764\H
,9.4973178345,-2.1640171626,2.7217138913\H,9.3023576458,-0.4259382552,
2.4263036516\H,9.5980631468,-3.1887485686,0.051579854\H,11.7429035464,
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\H,9.7126974891,-0.074895059,-3.3965943531\H,9.9815317313,1.2486555813
,-2.2432426014\H,11.3417391539,0.5318877311,-3.1278540302\H,11.5882027
615,-4.0215179865,-1.2228992119\H,12.548229884,-2.683023844,-0.6084500
926\H,10.9322078327,-3.582722936,1.1303770071\H,-14.1947293547,1.53838
31813,1.0580098847\H,-13.1165427348,1.8234340276,-1.0896093966\\Versio
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.750784\RMSD=6.107e-09\RMSF=1.844e-06\Dipole=0.4120789,-0.1280038,-0.0
965809\Quadrupole=10.4490273,1.4559004,-11.9049277,-2.4224999,-1.31019
68,5.2545806\PG=C01 [X(C40H55)]\#@

15E,12Z

1 (Bet_car_032)

(Enter /lrz/sys/applications/gaussian/g09.D.01/amd64_sse4/exe/19999.exe)

1\1\GINC-LXA35\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\03-Dec-2016\0\#

pub3lyp/6-31g(d) opt freq scf=tight\\Beta_Carotene (-30) optimization
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 048277833,1.0162882923\\C,-12.3672408158,-1.6965801372,-1.6674327622\\C,
 -10.221968556,-0.6154256041,-2.3634365863\\C,-5.1424911311,1.7721631922
 ,1.072123067\\C,-4.3912617432,2.855099949,1.4176243398\\C,-2.9438418047,
 2.9609104949,1.4934074149\\C,-2.434407145,4.1862408109,2.2216259898\\C,-
 2.1101444393,2.024003641,0.9397864418\\C,-0.6812963436,1.9957124379,0.9
 773419853\\C,-12.1283376956,0.8305467815,-1.6139049888\\C,-13.4211777166
 ,-1.892178455,-0.5785514229\\C,-12.7385582232,-2.2274665704,0.750120918
 \\C,-11.5522543267,-1.3542866965,1.0666918545\\C,-11.0702114429,-1.41103
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 225383\\C,-7.4300545467,0.7909625582,0.6881090727\\C,-6.995622201,-0.600
 9947844,0.3093373641\\C,0.0772103325,1.0279944375,0.3763396439\\C,1.5057
 112928,1.0135458287,0.4124158242\\C,2.3656529341,0.103828221,-0.1531839
 975\\C,3.7841526533,0.3139716317,0.0056431341\\C,1.8986275732,-1.0996740
 29,-0.9370549247\\C,4.787006932,-0.4689005023,-0.4883190904\\C,6.1765220
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 ,-0.9438935934\\H,-12.842102327,-1.5330435983,-2.6438773749\\H,-10.58607
 68504,-0.6067984856,-3.3983470111\\H,-9.5303387779,0.224238735,-2.24203
 77059\\H,-9.660171851,-1.5443131844,-2.211081522\\H,-4.6428008968,0.8354
 706037,0.8376372269\\H,-4.9352257939,3.7597085767,1.6948959026\\H,-2.635
 9444758,4.1157996809,3.2992752195\\H,-1.3629264254,4.3501360696,2.09300
 10662\\H,-2.9515757563,5.0854627992,1.863433939\\H,-2.5723987296,1.20330
 11115,0.3920524826\\H,-0.158083037,2.7841495139,1.5153917892\\H,-12.4899
 309327,0.9015626826,-2.6475567487\\H,-11.4445644061,1.6673499533,-1.434
 9131266\\H,-14.115453971,-2.6941356004,-0.857491017\\H,-12.4095648477,-3
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 ,2.6477783545\\H,-9.146419995,2.0839933269,0.992896971\\H,-7.4590404334,

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H,-5.9132129472,-0.7356830311,0.3549206128\H,-0.4425101789,0.234058420
6,-0.1572360625\H,1.9636116444,1.8404251972,0.9574120994\H,4.07016919,
1.1972952857,0.5783575087\H,0.8110222072,-1.1757494407,-0.9835993859\H
,2.2742140302,-1.0657143952,-1.9678208328\H,2.2773485739,-2.0275855334
,-0.4899628462\H,4.5269987596,-1.3539719832,-1.0625477328\H,6.37628531
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485\H,12.2706678419,-2.6614171907,1.9485718355\H,11.6251524844,-1.0401
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965356678,-3.3155866196,-0.4122058687\H,11.2665440655,-3.2525307242,-0
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\H,11.1720364879,2.561075035,-1.9561001646\H,9.7473281227,1.5050230426
,-1.8414157715\H,10.1214001053,2.6587518868,-0.5514303929\H,14.5799139
857,0.9580355326,0.915509637\H,13.0972540375,0.6247717189,1.8027941331
\H,14.1478029111,-1.4942897228,0.8737974095\H,-14.0246655321,-0.982343
6495,-0.4683366312\H,-13.4608632456,-2.1712208753,1.5783964711\\Versio
n=AS64L-G09RevD.01\State=2-A\HF=-1557.2381144\S2=0.785721\S2-1=0.\S2A=
0.75077\RMSD=5.216e-09\RMSF=2.741e-06\Dipole=-0.5442916,-0.2656717,-0.
0712342\Quadrupole=14.5005604,-2.8334689,-11.6670915,5.7220637,0.02159
14,5.3916253\PG=C01 [X(C40H55)]\@

15E,10Z

1 (bet_car_10_c7)

1\I\GINC-HP1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\17-May-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizati
on\0,2\C,-12.2361778982,-1.2799602933,0.4148021659\C,-6.2949829223,-0
.2931489723,-0.3898071093\C,-11.688644396,-1.8126249487,1.7603099388\C
,-12.4397683756,-2.4843522205,-0.5357416043\C,-4.9376988882,-0.6509199
947,-0.6876770258\C,-3.8665474649,0.0605878052,-0.2305731807\C,-2.4738
95019,-0.2175636009,-0.4853994962\C,-2.1235273252,-1.4077676284,-1.346
983664\C,-1.531245973,0.6147341442,0.0673371832\C,-0.1085802633,0.5442
811864,-0.0486461865\C,-13.6233978082,-0.6294619333,0.628393647\C,-13.
5336833683,0.7705727517,1.2302558727\C,-12.7674959995,1.6807452245,0.2

720641235\C,-11.5018229256,1.0585131686,-0.2822672924\C,-10.6223774931
 ,2.0657410004,-0.9870784276\C,-11.2281587969,-0.2676141602,-0.18267500
 84\C,-9.9483431624,-0.8484993658,-0.6309982825\C,-8.7160806857,-0.3551
 821871,-0.358327604\C,-7.4459773735,-0.9196297053,-0.7848031735\C,-7.4
 638741933,-2.1632374575,-1.6398518931\C,0.7431779926,1.4300716715,0.55
 32622378\C,2.1662863283,1.363943552,0.4355206011\C,3.1070986288,2.1913
 197759,0.9978862083\C,4.5027004636,1.9200651277,0.7301266588\C,2.75042
 1832,3.364301008,1.8796453763\C,5.556325302,2.6559931129,1.1900598501\
 C,6.9733767625,2.4657812893,0.9791270522\C,7.6770602572,1.3812123991,0.
 5385264406\C,9.1357428531,1.5138415264,0.4219702464\C,7.0573471098,0.
 0554440183,0.1792546436\C,9.9922955322,0.5829336347,0.0476670921\C,10.
 9643627104,-0.3043319306,-0.2891601067\C,11.6232309766,-1.1062738087,0.
 8728354938\C,11.3821547663,-0.4656862776,-1.6287327035\C,12.550579850
 6,-0.1560191428,1.6644383497\C,10.5467506464,-1.6524905896,1.831441021
 6\C,12.427212649,-2.3041540736,0.3164154411\C,12.4594961924,-1.4388994
 261,-2.0320987495\C,10.7460145788,0.2973248154,-2.7558405353\C,13.3204
 762378,-1.9323703013,-0.8666032724\H,-6.412155195,0.597205656,0.229836
 8056\H,-10.6919593369,-2.2483077838,1.6319719432\H,-11.6038839581,-1.0
 146183028,2.5058432703\H,-12.3499296345,-2.5889681282,2.1659837345\H,-
 13.260920821,-3.1100650593,-0.165170598\H,-12.7002029774,-2.1537496548
 ,-1.5482149816\H,-11.5531625181,-3.1232579389,-0.6010416845\H,-4.75929
 44135,-1.5259070732,-1.3067948128\H,-4.069165477,0.9334992302,0.391564
 7808\H,-2.5804340152,-1.318695298,-2.3407237467\H,-1.0476795642,-1.524
 6021711,-1.4867369449\H,-2.5034996443,-2.3367511864,-0.9030265731\H,-1
 .9070553844,1.4398157233,0.6741963474\H,0.3297648378,-0.2528088024,-0.
 6466398049\H,-14.2322909294,-1.29126864,1.2585291453\H,-14.13879469,-0
 .5607686733,-0.3408097944\H,-13.0193093559,0.7340841634,2.1993559657\H
 ,-12.5060565051,2.6275418559,0.7678799749\H,-11.2454023256,2.737246181
 4,-1.59457055\H,-10.0893902129,2.70902518,-0.2719807635\H,-9.878624775
 ,1.6021135001,-1.6375856631\H,-10.0108680298,-1.7838656917,-1.18285448
 77\H,-8.6452421819,0.5439492262,0.2523662565\H,-7.9587792397,-2.991105
 6618,-1.1153996766\H,-8.0275406326,-1.9931936281,-2.5659511739\H,-6.46
 30684829,-2.4993238195,-1.9165205402\H,0.3035210459,2.2257378759,1.152
 1025372\H,2.5427233187,0.5472897638,-0.1822969494\H,4.6906843178,1.067
 1923764,0.0850907672\H,1.6746065111,3.4644987046,2.0314483113\H,3.2183
 676666,3.26760827,2.8672739737\H,3.1132915956,4.3049205925,1.445895809
 6\H,5.3211998807,3.5386808899,1.7827695073\H,7.5744312996,3.3352771289
 ,1.2471604918\H,9.5262273963,2.5079011856,0.6722352191\H,6.2666882132,
 -0.2191945329,0.8857768428\H,6.606250198,0.0800192575,-0.822257196\H,7

.8120832883,-0.7361115206,0.1748637828\H,11.9791768798,0.6831333165,2.0756814202\H,13.0228155931,-0.687862954,2.5001541346\H,13.3439191098,0.2618850147,1.0357199138\H,9.8476717121,-2.3123966062,1.3047115741\H,11.0172451107,-2.2321717428,2.6353686343\H,9.9693974018,-0.8438125567,2.2900930286\H,11.7253006839,-3.0875693768,-0.0047339563\H,13.0899555153,-0.9793761872,-2.808327653\H,11.9874801254,-2.3064369164,-2.5285380914\H,10.377271562,-0.3883013951,-3.5336807272\H,9.9098315029,0.9164523572,-2.4224307855\H,11.4783370604,0.9536473902,-3.2501081608\H,13.919616445,-2.7956449075,-1.1809446333\H,14.0315829243,-1.1503826881,-0.5719044902\H,13.021962909,-2.7352513846,1.1325687337\H,-14.5350248894,1.1752835119,1.4225516555\H,-13.4181582541,1.9703167362,-0.5702014519\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.236543\S2=0.784739\S2-1=0.\S2A=0.750709\RMSD=7.139e-09\RMSF=1.909e-06\Dipole=0.315898,-0.2580417,-0.1963351\Quadrupole=13.6109633,-3.7647672,-9.8461961,-5.1487014,-3.1054216,6.5014591\PG=C01 [X(C40H55)]\\@

15E,14Z

l (bet_car_14_c7_c1)

1\1\GINC-HP1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\10-Jun-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizati
 on\0,2\C,-12.6021093125,-0.5324425264,0.8948508586\C,-6.6297906393,-0.2063425085,-0.1505300193\C,-12.1264678094,0.087078041,2.230807634\C,-12.7380605855,-2.0613973222,1.0926525552\C,-5.2628939758,-0.6358566972,-0.0677007743\C,-4.2059251471,0.2183153413,-0.1903145373\C,-2.806404852,-0.1308029787,-0.1344458903\C,-2.4358061461,-1.5800637066,0.0758096857\C,-1.8774505483,0.8703692266,-0.2763650775\C,-0.4502395102,0.7609638932,-0.271068318\C,-14.0052856689,0.0057725633,0.529699207\C,-13.9671361524,1.421141957,-0.0416090138\C,-13.1436943667,1.4241389374,-1.3287952825\C,-11.8442615323,0.6503207027,-1.2306203572\C,-10.9305435515,0.901985203,-2.4081147724\C,-11.57089221,-0.2049452948,-0.2126325482\C,-10.2692453072,-0.8867926587,-0.0779450268\C,-9.0516058974,-0.3008548463,-0.1767517025\C,-7.7643479337,-0.9637231181,-0.0415336791\C,-7.7487193939,-2.4522497773,0.2089541377\C,0.3698764221,1.8448808975,-0.440710639\C,1.8052734859,1.9206723147,-0.479205358\C,2.769712968,1.0451239365,-0.0398968112\C,4.1515529014,1.3877847212,-0.2913720706\C,2.444613879,-0.2291037379,0.7016818708\C,5.2549051557,0.6347776183,-0.0190397245\C,6.5910031606,1.0661631808,-0.3268517148\C,7.7585521322,0.390544404

4,-0.1215432082\C,9.0175455944,1.0342722373,-0.5164823176\C,7.85222947
71,-0.9846135434,0.4870213731\C,10.2285037967,0.5227573174,-0.40529378
61\C,11.5053274675,0.0732272716,-0.2975107271\C,12.2810060559,0.440913
7523,1.0023819172\C,12.1151139888,-0.6646637931,-1.3369421281\C,12.672
4787732,1.9345344957,0.9376768213\C,11.3937400293,0.2197486665,2.24352
40857\C,13.5413090391,-0.4428030273,1.1482352641\C,13.5219728332,-1.19
46767525,-1.2408512248\C,11.3768778582,-1.020806759,-2.5960954974\C,14
.3609624118,-0.5434240122,-0.1379102964\H,-6.7697423344,0.8610123811,-
0.327970661\H,-11.1203157955,-0.2621806069,2.4863737802\H,-12.08995210
67,1.1804034499,2.178705354\H,-12.8023503594,-0.1930401327,3.048906756
5\H,-13.572278044,-2.2713587701,1.7731430545\H,-12.9437836648,-2.57005
64195,0.1432463948\H,-11.8420366342,-2.5088669374,1.5346033144\H,-5.06
52607972,-1.6916539024,0.0959005843\H,-4.4252769182,1.274686896,-0.351
3283999\H,-2.8416112672,-2.20831757,-0.7272934006\H,-1.3568137403,-1.7
393450151,0.1074535502\H,-2.8538831604,-1.9570271968,1.0178835476\H,-2
.2662618068,1.8803914064,-0.4143274592\H,-0.0136218785,-0.2256082801,-
0.1665315852\H,-14.6463187783,-0.0416899824,1.4199821788\H,-14.4595074
687,-0.6612215095,-0.2176548827\H,-13.5222402675,2.1114613435,0.686652
2123\H,-12.916755585,2.4558470048,-1.6365357246\H,-11.5193261198,0.912
148638,-3.3361973433\H,-10.4484781189,1.8881568924,-2.3421805596\H,-10
.1437413078,0.1520793577,-2.5061521212\H,-10.3044692014,-1.9448213581,
0.1722230389\H,-9.0088940686,0.7718702976,-0.3611288821\H,-8.279349713
6,-2.6970200717,1.1383175113\H,-8.2605845313,-2.9903456976,-0.59897538
64\H,-6.7382570819,-2.8562613371,0.2903440123\H,-0.1308626788,2.798079
4861,-0.6191046218\H,2.1813114501,2.8425588142,-0.9236197353\H,4.31246
49732,2.3517149999,-0.7761256574\H,1.5353814454,-0.1127177147,1.298478
6519\H,2.2858879057,-1.0741129186,0.0174212413\H,3.2535499218,-0.50971
64957,1.3823087275\H,5.1298152132,-0.3411457487,0.4415004096\H,6.66900
61454,2.0550625304,-0.7813208393\H,8.9079749033,2.0352457224,-0.951449
6142\H,6.8752987753,-1.4229325506,0.6999519091\H,8.3911297831,-1.66500
51895,-0.1839307853\H,8.4231821528,-0.9549149159,1.4235809858\H,11.778
1292111,2.5613333122,0.854242902\H,13.2127457871,2.2303307436,1.845961
691\H,13.3106643191,2.1541372078,0.0754740799\H,11.0601691526,-0.82235
28327,2.3095963172\H,11.9567634539,0.4528514909,3.1558969251\H,10.5061
280258,0.8597800766,2.2221183245\H,13.2342432225,-1.4548194425,1.45026
12838\H,14.0185796888,-1.0841065366,-2.2167032928\H,13.4788612822,-2.2
857555878,-1.0680699522\H,11.3731828019,-2.1100611191,-2.7549515352\H,
10.3406201486,-0.6748360795,-2.585690169\H,11.8712032788,-0.5861280726
,-3.478010333\H,15.2731378789,-1.1274997091,0.0345828683\H,14.68665935

59,0.4543865661,-0.4580693426\H,14.1535790137,-0.0461754786,1.96909197
 24\H,-14.9825070889,1.7870638496,-0.2380293972\H,-13.7408876622,1.0054
 080929,-2.1562558059\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2358
 798\S2=0.784596\S2-1=0.\S2A=0.750698\RMSD=4.483e-09\RMSF=3.584e-06\Dip
 ole=0.4050225,-0.4263567,0.01613\Quadrupole=17.7909925,-3.9550404,-13.
 8359521,-4.3596715,0.6279987,-3.2124583\PG=C01 [X(C40H55)]\@

15E,11Z

1 (bet_car_11_c7)

1\1\GINC-T1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\14-May-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
 n\\0,2\C,-11.7302915312,1.3240021462,1.2820866974\C,-6.2193916361,-0.0
 04644733,-0.2466009784\C,-11.4268733723,2.7190645311,1.8739387747\C,-1
 1.1415714199,0.2527277957,2.2212021467\C,-5.2175056456,-1.0343324919,-
 0.281190278\C,-3.8796911962,-0.7706311026,-0.2866983586\C,-2.810510849
 5,-1.7402834581,-0.32277863\C,-3.1708851442,-3.206467876,-0.3614973193
 \C,-1.5150153232,-1.2842169326,-0.3201787039\C,-0.3078345062,-2.048229
 4423,-0.3560995045\C,-13.2573513229,1.0978399398,1.190554887\C,-13.919
 0398372,1.8960977456,0.0678509174\C,-13.3546986225,1.4558984627,-1.285
 5063025\C,-11.8548795032,1.315616352,-1.3081340867\C,-11.236373151,1.2
 214980422,-2.6741548517\C,-11.0793591358,1.2298357216,-0.1303299594\C,
 -9.7288154788,1.0963520042,-0.1809927385\C,-8.4103271053,1.0541010965,
 -0.1968115099\C,-7.5757344232,-0.1528181223,-0.2334088861\C,-8.2881859
 04,-1.4804682456,-0.2511068382\C,0.9425359053,-1.4916024398,-0.3410705
 451\C,2.1458072047,-2.2612762038,-0.378210741\C,3.4491148482,-1.820336
 0948,-0.3601005915\C,4.4815986494,-2.8334274745,-0.4067386718\C,3.7957
 86198,-0.3522925349,-0.2998109271\C,5.8506311219,-2.7760279779,-0.3829
 583576\C,6.7385961588,-1.6516476147,-0.2785586548\C,8.1094151249,-1.68
 35480912,-0.2689010992\C,8.8202782529,-0.4215497163,-0.1364549697\C,8.
 9250062938,-2.9482869776,-0.3840581983\C,10.1644633329,-0.2588417979,-
 0.0796643773\C,10.87628076,1.0234938658,0.0798769245\C,11.9946760069,1
 .0214282956,1.151091813\C,10.5721908096,2.1255271524,-0.6519909274\C,1
 1.35538773,0.8886637042,2.5542249485\C,12.9590681331,-0.1713303322,0.9
 443002473\C,12.844413099,2.311855961,1.0762737934\C,11.2307779642,3.47
 14259889,-0.4243273169\C,9.5925198701,2.1464744869,-1.8028124476\C,11.
 9971621766,3.5684276198,0.8935693396\H,-5.8368239696,1.0170989876,-0.2
 283467207\H,-10.3456799637,2.8742851837,1.9553042803\H,-11.8304388579,

3.5244608702,1.2513013988\H,-11.8609255219,2.813554752,2.8774013627\H,
 -11.6235108304,0.3072431256,3.2052952844\H,-11.3042806324,-0.754684305
 9,1.8208081046\H,-10.0653747266,0.3919623486,2.3640582008\H,-5.5486278
 385,-2.0691089294,-0.3034641122\H,-3.5703204085,0.2751499985,-0.261875
 2969\H,-3.7703197149,-3.4387955196,-1.2509769198\H,-2.2942211059,-3.85
 59516811,-0.3742914984\H,-3.7756052783,-3.4823117172,0.511697943\H,-1.
 3796556001,-0.2021726213,-0.286869945\H,-0.3769851422,-3.1338521996,-0
 .3980725059\H,-13.7062110627,1.3466762754,2.1613673423\H,-13.45074495,
 0.0280966352,1.0234313113\H,-13.7431243607,2.9695056908,0.2128750611\H
 ,-13.6652664051,2.1548675551,-2.0767951165\H,-11.6925617772,0.40632729
 94,-3.2564798512\H,-11.4120156191,2.1425677683,-3.2502435709\H,-10.158
 1827848,1.0492325156,-2.6345135502\H,-7.8546542775,1.9998624224,-0.190
 5790304\H,-8.8753441189,-1.6162407231,0.6659794523\H,-8.9999752441,-1.
 5236044286,-1.0847716335\H,-7.6054935307,-2.3273336536,-0.3436293938\H
 ,1.0112337973,-0.4062380316,-0.2960441172\H,1.9983144101,-3.3410065413
 ,-0.4243919501\H,4.0792183314,-3.843886178,-0.4757491876\H,2.909440195
 7,0.2841687295,-0.3214446561\H,4.3495963514,-0.1133112288,0.6163943733
 \H,4.4291287236,-0.0634756773,-1.1468968934\H,6.3324526361,-3.74902506
 61,-0.4458954611\H,6.2917721881,-0.6675729608,-0.1906512463\H,8.190807
 0128,0.4637179911,-0.0550953452\H,8.3107104536,-3.8424660012,-0.496943
 7592\H,9.6006053587,-2.8975162327,-1.2472652139\H,9.5555376072,-3.0880
 064061,0.5037159084\H,10.7847323795,-1.1520869384,-0.0943713498\H,10.7
 22267094,-0.0031899439,2.6127449553\H,12.1314687637,0.8064336173,3.32
 59134883\H,10.7265121487,1.7525913956,2.7951397637\H,13.3388614416,-0.
 203740016,-0.0838016107\H,13.8195715524,-0.0690289017,1.6167419063\H,1
 2.4902201554,-1.1351108738,1.1675575269\H,13.5400758458,2.2324874022,0
 .2280169107\H,10.459678783,4.2543774083,-0.4789208859\H,11.9093045525,
 3.6801763174,-1.2684868195\H,10.0189789138,2.7177081925,-2.6394604936\H
 ,9.3343098691,1.148767645,-2.1620084675\H,8.6583380718,2.6582940133,-
 1.5296031512\H,12.6276088528,4.4661079437,0.9032693375\H,11.2909701729
 ,3.6730950641,1.7273543186\H,13.4629036664,2.382055504,1.9808078972\H,
 -15.0064423003,1.7537291006,0.0860473132\H,-13.8067194543,0.4881027721
 ,-1.5704864058\\Version=ES64L-G09RevD.01\\State=2-A\\HF=-1557.2356458\\S2
 =0.785145\\S2-1=0.\\S2A=0.750735\\RMSD=7.703e-09\\RMSF=1.245e-06\\Dipole=-0
 .4364394,0.0927053,-0.0438125\\Quadrupole=18.7312416,-2.9035371,-15.827
 7045,2.2341385,1.1642502,0.1834737\\PG=C01 [X(C40H55)]\\@

Structure of *15Z* isomer and rotamers of C7 radical

15,15'-cis (15Z)

l (bet_car_trans)

l\1\GINC-S3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\13-Nov-2016\0\#P
UB3LYP/6-31G(d) scf=tight opt freq\Beta_Carotene (-30) optimization\
0,2\C,10.2665799546,-2.2779431547,1.1031120444\C,5.7507080624,1.603725
1832,-0.0797013675\C,9.6451893891,-2.1351985057,2.5129567916\C,11.4786
352729,-1.3201348886,1.0072878543\C,5.0980171482,2.8820697654,-0.09288
18672\C,3.7408669793,3.0195197108,-0.1158984776\C,2.9963660945,4.25663
09054,-0.1278140777\C,3.7663773739,5.5560064337,-0.1162194101\C,1.6246
479728,4.1875157651,-0.1482431262\C,0.6928137845,5.273812,-0.158548936
\C,10.8051147605,-3.7147160211,0.9069342151\C,9.6998575504,-4.72245571
85,0.6009577901\C,9.0151952737,-4.3327639698,-0.7075352796\C,8.6805904
55,-2.857654535,-0.8058530365\C,7.7552085517,-2.5478185734,-1.95982829
39\C,9.2002612914,-1.9276958639,0.0359049895\C,8.7890486171,-0.5110892
599,0.0062687044\C,7.5132496952,-0.0571651234,-0.0426266158\C,7.092150
9361,1.334486292,-0.0526845283\C,8.1544355855,2.4063514574,-0.03017421
07\C,-0.6766832824,5.1811613619,-0.1779755261\C,-1.4553767457,3.980102
6453,-0.1985650759\C,-2.8238725993,3.8671922397,-0.208879947\C,-3.4000
465783,2.5422147535,-0.2323160757\C,-3.7592225822,5.0530033601,-0.1961
960468\C,-4.7268763699,2.2298736753,-0.237277825\C,-5.2117203676,0.876
9531752,-0.2651291224\C,-6.506740791,0.4479276241,-0.2653230768\C,-6.7
633359881,-0.9969848929,-0.300053332\C,-7.7067880097,1.3585729244,-0.2
309477494\C,-7.9438466208,-1.5858675317,-0.3029874314\C,-9.1084351282,
-2.2843584479,-0.27720075\C,-9.6382006309,-2.7275237713,1.1191215625\C
,-9.7882283106,-2.6247114409,-1.467708203\C,-8.7546207375,-3.885367961
,1.6363676994\C,-9.5565720666,-1.5609237391,2.1234962626\C,-11.1143856
889,-3.1782444702,1.0214770311\C,-11.0833572723,-3.3942865092,-1.47238
67538\C,-9.2866053217,-2.1982062223,-2.8182834314\C,-11.3830175618,-4.
1153396133,-0.1554798473\H,5.0802589592,0.7430778536,-0.0928414057\H,9
.2329675772,-1.1312227845,2.6604744984\H,8.829391229,-2.8494894081,2.6
680981857\H,10.402460523,-2.3096417887,3.2880179762\H,12.2805587949,-1
.6740465302,1.6667572396\H,11.8762559902,-1.2822169889,-0.0138162025\H
,11.2338189722,-0.2996331146,1.3185181936\H,5.7159785186,3.7757811584,
-0.0831023432\H,3.1424979315,2.1074415483,-0.124835669\H,4.4283403947,
5.6245186645,-0.9888104404\H,3.1168615125,6.4324595061,-0.1247979876\H
,4.4041785681,5.6234583134,0.7742690213\H,1.2015399905,3.184581688,-0.

1552500361\H,1.1019053785,6.280930586,-0.1475980192\H,11.3691496143,-4.0073344147,1.8024132344\H,11.521305256,-3.717446287,0.0722617579\H,10.108738426,-5.7379708136,0.5308478376\H,9.6556104411,-4.6091125083,-1.5619963147\H,8.0710471067,-3.1140553339,-2.8474400123\H,6.7235343471,-2.8642049265,-1.7482018979\H,7.7336611106,-1.4872794216,-2.2163684603\H,9.5867972364,0.2238326029,0.088602985\H,6.7061422888,-0.7884125296,-0.0574530664\H,8.7786454455,2.3188979733,0.868667956\H,8.8260771804,2.3101680063,-0.8927488069\H,7.7364060043,3.4143266307,-0.0451315082\H,-1.2173312006,6.1242343069,-0.1778161866\H,-0.902857818,3.0421492804,-0.2076658223\H,-2.687096591,1.7166427054,-0.2468035932\H,-3.2320867828,6.0081140716,-0.1921966814\H,-4.4167515573,5.0394892076,-1.0746049919\H,-4.4083184774,5.0278155621,0.6884061599\H,-5.4567497129,3.0347906243,-0.2189402163\H,-4.4393625619,0.1065515071,-0.2889323859\H,-5.8642585514,-1.6245578064,-0.3355546713\H,-7.4387449563,2.4159793844,-0.2753058586\H,-8.3779010948,1.1413143205,-1.0710985518\H,-8.2907660606,1.1944173867,0.6835684764\H,-7.711965683,-3.56189948,1.7259663385\H,-9.0945063415,-4.2166829157,2.6258285739\H,-8.7755195272,-4.7485206685,0.962810876\H,-10.1418038375,-0.7008764072,1.7777964585\H,-9.9555699595,-1.8720913757,3.0969612802\H,-8.52332967,-1.231608222,2.2716719356\H,-11.3980363065,-3.653759534,1.96972728\H,-11.0768667444,-4.109131981,-2.3090163014\H,-11.9108669524,-2.6980573917,-1.7017531831\H,-10.0571000703,-1.6301202688,-3.3615786045\H,-8.388275911,-1.579592579,-2.7550369274\H,-9.0536370558,-3.0720351156,-3.4454406386\H,-10.7587550396,-5.0140570715,-0.0735475403\H,8.9643129014,-4.7357482652,1.4155754152\H,8.0905003512,-4.912888082,-0.8453193599\H,-12.4249894622,-4.4576183684,-0.1425616168\H,-11.7531702196,-2.2890075648,0.9163990979\\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2394484\S2=0.784294\S2-1=0.\S2A=0.750674\RMSD=7.498e-09\RMSF=1.242e-06\Dipole=-0.4006629,-0.1202949,-0.0621821\Quadrupole=13.9664356,1.3481021,-15.3145376,3.4196191,1.3416309,0.8189437\PG=C01 [X(C40H55)]\\@

15Z,7Z

1 (Car_H_021_cis)

I\1\GINC-LXA105\FOpt\UB3LYP\6-31G(d)\C40H55(2)\DI49BOQ\03-Dec-2016\0\\#p ub3lyp/6-31g(d) opt freq scf=tight\\Beta_Carotene (-30) optimization\\0,2\C,9.0016364258,-4.5312594655,-0.5470205151\C,8.583698421,-3.0831000366,-0.72514748\C,9.1578328803,-2.064587815,-0.0345553018\C,10.344

922928,-2.2838381843,0.9367525652\C,10.4724600258,-3.7746105456,1.3260
823973\C,10.3617104053,-4.7127213252,0.1271946488\C,7.4814709284,-2.90
81687545,-1.7448475113\C,8.7445235943,-0.6562125926,-0.1776287459\C,7.
4769675002,-0.1787241005,-0.1642279606\C,7.0783520138,1.2148213476,-0.
283116815\C,5.743650379,1.5120013015,-0.2306641183\C,5.1120715422,2.79
7568544,-0.3251650666\C,3.7586933965,2.9628057989,-0.2776208376\C,3.03
59213881,4.2095322178,-0.3687574215\C,1.663858163,4.1692492239,-0.3176
95068\C,0.7522064438,5.2699111277,-0.3944426831\C,-0.6185139774,5.2062
981632,-0.3568883908\C,-1.4206224838,4.0269097987,-0.2339930294\C,-2.7
909991239,3.9439746434,-0.2057061489\C,-3.3949409905,2.6375968706,-0.0
758712227\C,-4.7283394649,2.3571287823,-0.0373704245\C,-5.2445271733,1
.0224133911,0.0980359108\C,10.1325238123,-1.4823605026,2.2411171968\C,
11.6579246845,-1.8023287167,0.2709935378\C,-6.5495678798,0.6275850964,
0.1454972695\C,8.1548406942,2.2576615909,-0.4605714035\C,3.8281744707,
5.4867530514,-0.5191697501\C,-3.7017669564,5.1448472314,-0.3044024211\
C,-6.8413482133,-0.8030253384,0.2975242186\C,-7.7263794458,1.564345128
8,0.0563227391\C,-8.0356886756,-1.3584146434,0.3737407089\C,-9.2209903
603,-2.0188148337,0.442208604\C,-9.8385855443,-2.5154891125,-0.8997112
655\C,-10.9835413235,-3.5196353183,-0.6284842853\C,-11.9512587518,-3.0
522187439,0.4580128384\C,-11.2071564807,-2.9160613146,1.7889087638\C,-
9.8786438999,-2.2153941554,1.6769928234\C,-9.2750248747,-1.7687473565,
2.9785029637\C,-8.7634960011,-3.2265104862,-1.7456468467\C,-10.3695661
458,-1.3019257449,-1.6949777979\H,8.9960933497,-5.0295483056,-1.526384
3433\H,8.2245989029,-5.0479255793,0.0415360464\H,9.6758391199,-4.02252
67767,2.0424609255\H,11.4234920404,-3.9243313423,1.8546804838\H,11.161
8708105,-4.5006301007,-0.5933932226\H,10.4940240258,-5.7559605353,0.43
99858138\H,7.3573554981,-1.8721325901,-2.0638065779\H,7.6900454802,-3.
5209215148,-2.6320121754\H,6.5132760956,-3.2554328126,-1.3544437058\H,
9.5581899364,0.0660424214,-0.2335949122\H,6.6597283191,-0.8862235701,-
0.0325084235\H,5.060672546,0.6706189396,-0.1040398626\H,5.7436021346,3
.6740578076,-0.441755073\H,3.1456075645,2.0678913995,-0.1625107639\H,1
.2230594338,3.1798770516,-0.2090085907\H,1.1797916832,6.2642006604,-0.
4958383048\H,-1.1406669735,6.15677151,-0.431638311\H,-0.8869997043,3.0
812578143,-0.1554201823\H,-2.7000012053,1.7998592363,-0.0028559495\H,-
5.4395341109,3.1754086515,-0.1120821914\H,-4.4906806993,0.2370952194,0
.1726534122\H,10.9390179134,-1.7017221263,2.952195758\H,10.1260889462,
-0.4015747438,2.0678857619\H,9.1810142959,-1.7485957159,2.7152893985\H
,12.5006549129,-1.9144632146,0.9651267482\H,11.8853386367,-2.372101841
5,-0.6357359311\H,11.6060589103,-0.7447036745,-0.010731738\H,8.8439428

878,2.2595870585,0.394126561\H,8.7577527344,2.0486443378,-1.3533527117
 \H,7.751125158,3.2664854324,-0.5616457943\H,4.438861754,5.4619802013,-
 1.4307022805\H,3.1950886343,6.3737164038,-0.5699421653\H,4.5182675028,
 5.6185313032,0.3237831388\H,-4.3488668313,5.2161321529,0.5789908229\H,
 -3.1552598193,6.0850187123,-0.3908394803\H,-4.3618177043,5.0624602009,
 -1.1773031195\H,-5.957327947,-1.4490803,0.3649667103\H,-8.3969695173,1
 .4206920877,0.9122948951\H,-7.4316706708,2.6151529926,0.0279645361\H,-
 8.3209299829,1.3553229464,-0.8423111276\H,-10.5498188855,-4.482763265,
 -0.3221625667\H,-11.5158922907,-3.7047465962,-1.5708665919\H,-12.78247
 18042,-3.7602111146,0.5621525861\H,-12.3958333101,-2.0881786663,0.1799
 756329\H,-11.0456037966,-3.9210778161,2.2197585793\H,-11.8321424013,-2
 .3908520685,2.5272407119\H,-9.9076993733,-1.0126599225,3.4680939533\H,
 -9.203233575,-2.6094225523,3.6850746146\H,-8.2760257561,-1.3446855204,
 2.8532510205\H,-9.2019816581,-3.5985387017,-2.6800137686\H,-7.94348849
 77,-2.5483928124,-2.0019141679\H,-8.339347885,-4.0813859322,-1.2064563
 588\H,-11.1360676812,-0.750764531,-1.1399438124\H,-9.5566751493,-0.603
 090168,-1.9191140512\H,-10.8069363276,-1.6286143527,-2.6469055302\\Ver
 sion=AS64L-G09RevD.01\State=2-A\HF=-1557.2386978\S2=0.784356\S2-1=0.\S
 2A=0.750678\RMSD=7.802e-09\RMSF=1.294e-06\Dipole=-0.3620638,-0.1126494
 ,0.0374805\Quadrupole=14.5366553,0.9417122,-15.4783675,2.5462289,-1.85
 16188,-1.7702423\PG=C01 [X(C40H55)]\@

15Z,9Z

1 (bet_car_9_15_c7)

1\1\GINC-T1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\17-May-2016\0\#P
 Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
 n\\0,2\C,10.9789161313,-1.6437861541,0.9682533649\C,5.9265908147,1.447
 1447218,-0.4096779092\C,10.5037769939,-1.2613561819,2.3903171596\C,12.
 0529207921,-0.62157353,0.5241156185\C,5.1279805729,2.6235562731,-0.605
 7339824\C,3.7660595662,2.6154003923,-0.52555873\C,2.8820299201,3.74205
 73187,-0.7101168182\C,3.4936000637,5.0895560462,-1.0127127299\C,1.5290
 71884,3.5295840874,-0.6047225568\C,0.4784764095,4.4907334494,-0.751026
 2851\C,11.6577593385,-3.0332871888,0.9932839345\C,10.6529974598,-4.181
 1822643,1.0434502344\C,9.7876463419,-4.1437709786,-0.214621475\C,9.274
 341672,-2.7606453542,-0.5619527159\C,8.2007095991,-2.7922868571,-1.625
 4259775\C,9.7680767539,-1.6284708887,0.0022456739\C,9.1899344612,-0.29
 59925725,-0.254437737\C,7.8702394179,0.011699314,-0.2410637694\C,7.287

8069719,1.3230188009,-0.4759846499\C,8.2138120759,2.4752113337,-0.7811
 883862\C,-0.8705568331,4.2560587923,-0.6568625393\C,-1.5080763677,3.00
 08441506,-0.3957576796\C,-2.854344648,2.7462179562,-0.3085928965\C,-3.
 2781634379,1.390272246,-0.0408799011\C,-3.9165509054,3.8059241431,-0.4
 810369137\C,-4.5605460497,0.9439839205,0.0684022567\C,-4.89105835,-0.4
 320958882,0.3321938148\C,-6.1279497293,-0.9970018543,0.4522211226\C,-7
 .3695612701,-0.2245330352,0.3268460282\C,-6.2634508344,-2.4739543165,0
 .7245713261\C,-8.5926422769,-0.7132941884,0.4067477512\C,-9.8903188703
 ,-1.1125389058,0.4323921189\C,-10.54448205,-1.4778573364,-0.9337758163
 \C,-10.6220597412,-1.1610525635,1.6397632259\C,-10.8015384137,-0.17392
 58773,-1.7227776674\C,-9.6035214991,-2.3757970667,-1.7611854782\C,-11.
 8699091951,-2.2434384486,-0.7116538058\C,-12.0616945773,-1.6014153575,
 1.6997602786\C,-9.9960983988,-0.8179203471,2.9617875931\C,-12.76934452
 2,-1.5994124255,0.3423891017\H,5.3645069264,0.5401563747,-0.1821121092
 \H,9.9914649717,-0.2932806474,2.385263668\H,9.8026013615,-1.9999960232
 ,2.7935990113\H,11.3571229414,-1.1915949286,3.0770337221\H,12.95629713
 ,-0.7498877629,1.1329680924\H,12.3324057989,-0.7684638978,-0.525890740
 5\H,11.7256044274,0.4154239267,0.6501677834\H,5.634834061,3.5581815475
 ,-0.830067207\H,3.2802492932,1.6646737127,-0.3016321318\H,4.0819653788
 ,5.0515709234,-1.9383300217\H,2.7470036695,5.8765390726,-1.1284276549\H,
 4.1781338573,5.3958675668,-0.2116485025\H,1.2258741616,2.5070207815,
 -0.3865518994\H,0.7690498168,5.5170981085,-0.9603579594\H,12.347880323
 5,-3.0753542763,1.8462407464\H,12.2725270187,-3.1467696055,0.088391630
 3\H,10.0180656126,-4.0897991984,1.9341827693\H,8.9273326215,-4.8217720
 715,-0.110229963\H,8.4800476081,-3.5117284718,-2.4081097585\H,7.239095
 4037,-3.1405011612,-1.2212767451\H,8.0339331289,-1.8204636068,-2.09339
 62942\H,9.8982588903,0.5144620062,-0.4119378783\H,7.1580894537,-0.7815
 269453,-0.0178734801\H,8.9251318318,2.6324183715,0.0400114793\H,8.8085
 891685,2.2712361707,-1.6806796667\H,7.6808112348,3.4140363469,-0.94086
 61458\H,-1.5143886345,5.1201435903,-0.8002742728\H,-0.8530584664,2.143
 3358915,-0.2519208884\H,-2.4774296213,0.6593475603,0.0804711252\H,-3.4
 996269673,4.7954593512,-0.6734558772\H,-4.5829071143,3.558011474,-1.31
 70539055\H,-4.5440530634,3.8786646921,0.4162835692\H,-5.3744913236,1.6
 538315511,-0.0518692293\H,-4.0349590552,-1.0982153958,0.444776959\H,-7
 .2596964915,0.8510097891,0.1596324516\H,-5.2850395006,-2.9550030119,0.
 8156880726\H,-6.8245255294,-2.6552375773,1.6504654978\H,-6.8195680724,
 -2.9750054564,-0.078075734\H,-9.8619232113,0.3615743,-1.8966516212\H,-
 11.2505433048,-0.3972881731,-2.6988009093\H,-11.4736822593,0.504074463
 8,-1.1862675125\H,-9.3688709861,-3.3019641548,-1.2238090682\H,-10.0804

92364,-2.6477664949,-2.7110557104\H,-8.6614893267,-1.8675562458,-1.989
6230074\H,-11.6396584219,-3.2719376063,-0.3974516929\H,-12.6048439692,
-0.9678591129,2.4171809268\H,-12.105682199,-2.6185060629,2.130722743\H
,-10.1129351964,-1.6462761871,3.6768927781\H,-8.9310373653,-0.59038773
84,2.8743120464\H,-10.4920241163,0.0517120199,3.4190297446\H,-13.72186
6116,-2.1384297109,0.4141814032\H,-13.0150362949,-0.5700497252,0.05234
04226\H,-12.3929604534,-2.3220335412,-1.6738360869\H,11.1690960009,-5.
1458293556,1.1238456338\H,10.3577120613,-4.5363758106,-1.0733987851\\V
ersion=ES64L-G09RevD.01\State=2-A\HF=-1557.2381508\S2=0.783021\S2-1=0.
\S2A=0.750591\RMSD=4.259e-09\RMSF=1.846e-06\Dipole=-0.4570874,-0.08587
3,0.0064846\Quadrupole=16.1036537,-0.8551903,-15.2484634,2.3087358,-2.
1876507,-2.7290864\PG=C01 [X(C40H55)]\\@

15Z,13Z

1 (bet_car_13_15_c7)

I\1\GINC-S1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\16-May-2016\0\\#P
Becke3LYP/6-31G(d) opt freq scf=tight\\Beta_Carotene (-30) optimizatio
n\\0,2\C,12.2144218203,-0.2168704104,0.8010191639\C,6.3805760599,0.881
4916402,-0.4921335368\C,11.6838919763,0.1343196071,2.2117003375\C,12.8
605644971,1.0531573174,0.1965838727\C,5.235192003,1.7124227437,-0.7339
866183\C,3.9540359347,1.2873150933,-0.5379010778\C,2.7483395748,2.0535
247123,-0.7533215069\C,2.8843342933,3.4760551477,-1.2426785991\C,1.541
1561988,1.4492197248,-0.5032480934\C,0.2332229231,2.0152278864,-0.6470
386154\C,13.3270547818,-1.2861150209,0.9054800209\C,12.7776887865,-2.6
924652845,1.1298849504\C,11.9048055459,-3.0855192023,-0.0603490228\C,1
0.9387797363,-2.0015069467,-0.4950076935\C,9.8998816983,-2.5083097008,
-1.468774009\C,11.0398340626,-0.7136524969,-0.0773566712\C,10.03910927
89,0.3146928138,-0.4203972108\C,8.6937125899,0.1756236375,-0.338283948
9\C,7.7031764757,1.192457034,-0.6545963682\C,8.1868496995,2.5363785443
,-1.1430814587\C,-0.9641592254,1.3960785625,-0.3955733372\C,-1.1571456
578,0.051312124,0.0644936156\C,-2.3471936534,-0.5871401355,0.318411179
3\C,-3.6339243457,0.0479563241,0.1466869554\C,-2.3155243941,-2.0208928
368,0.7991747824\C,-4.8475121081,-0.5284231498,0.3753092863\C,-6.09233
986,0.1647462226,0.1799416284\C,-7.3564844783,-0.3105503173,0.37059627
95\C,-8.4873490666,0.583571424,0.0935257929\C,-7.6811023777,-1.7041582
75,0.8430249676\C,-9.7683574066,0.2920401329,0.2127657563\C,-11.111178
625,0.0912093046,0.2595510443\C,-11.7983486812,-0.3959587097,-1.050882

6189\C,-11.8533170939,0.3454794457,1.4337132082\C,-11.8431883771,0.780
 7310226,-2.0517738047\C,-10.9954136317,-1.5495743164,-1.6844209286\C,-
 13.2275948059,-0.9085081153,-0.757259018\C,-13.3432319639,0.1363975267
 ,1.5141261219\C,-11.1964684218,0.8063453226,2.7039123294\C,-14.0294185
 506,0.0237225042,0.1502648598\H,6.1554430331,-0.1240272929,-0.13348832
 27\H,10.8739387356,0.8694463614,2.1537146564\H,11.2878796672,-0.748343
 7539,2.7255113546\H,12.4848826405,0.5580784315,2.8310126576\H,13.77419
 89977,1.2992826226,0.7512950293\H,13.1365225871,0.8989138507,-0.853282
 8152\H,12.2044593148,1.9275302295,0.2541965295\H,5.4016789002,2.725615
 5973,-1.0890639819\H,3.8093918259,0.2662157091,-0.1822284003\H,3.40193
 30614,3.5076168801,-2.2098785562\H,1.922354983,3.9754012681,-1.3666706
 581\H,3.4808287007,4.0737074044,-0.5418526943\H,1.590096188,0.41868545
 5,-0.1559071956\H,0.1729410971,3.0442833856,-0.9920721499\H,14.0192094
 717,-1.0005686928,1.7087053719\H,13.9125158511,-1.284582387,-0.0256624
 167\H,12.1839630946,-2.724217518,2.052578912\H,11.3317310791,-3.996709
 2405,0.1675155345\H,10.3763211375,-3.1737805082,-2.202511315\H,9.13199
 66887,-3.1121500453,-0.9638050861\H,9.3930319005,-1.7063478483,-2.0083
 060393\H,10.430050463,1.2873261093,-0.7103827526\H,8.2925781687,-0.773
 2701722,0.0152293049\H,8.8404623527,3.0102180304,-0.3992002312\H,8.778
 0080567,2.429008136,-2.0614408064\H,7.3696224394,3.2284052548,-1.35305
 72993\H,-1.8535612298,1.9971341937,-0.5668490348\H,-0.25631248,-0.5351
 280126,0.2320273273\H,-3.6364048338,1.0801043048,-0.1973692543\H,-1.28
 8399473,-2.3851613431,0.8906026961\H,-2.7986801905,-2.1261256392,1.779
 3815636\H,-2.8485736753,-2.6877367645,0.1088355208\H,-4.8855532093,-1.
 5590020662,0.7171960176\H,-6.001782208,1.1954402758,-0.1665841965\H,-8
 .2080353116,1.590614451,-0.2401758876\H,-6.7929390192,-2.2769735266,1.
 1167703192\H,-8.345639531,-1.6677815632,1.7148874838\H,-8.2186104911,-
 2.2617708307,0.0654436837\H,-10.8306305176,1.1343267791,-2.2738826307\H,
 -12.308515995,0.4662313787,-2.9945759815\H,-12.4109040361,1.63081096
 89,-1.6591318424\H,-10.9069222941,-2.3950543878,-0.9923945529\H,-11.49
 9214882,-1.9061613336,-2.5914765874\H,-9.9858159276,-1.2306473972,-1.9
 620526688\H,-13.1618679904,-1.8957004107,-0.2768685993\H,-13.791480852
 9,0.9503242347,2.1037539991\H,-13.543750973,-0.7800029287,2.0989322925
 \H,-11.4399443218,0.1311961996,3.5383030363\H,-10.1088260489,0.8621441
 402,2.6162778127\H,-11.5643877272,1.8006344692,2.9991520399\H,-15.0532
 190683,-0.3497707712,0.2740608283\H,-14.1137453882,1.0177745656,-0.307
 0075926\H,-13.7460469528,-1.0620209845,-1.7129734932\H,13.5951458381,-
 3.4125818803,1.2584414222\H,12.5419181428,-3.3566092888,-0.9189603657\H,
 \Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2378659\S2=0.783479\S2-1=

0.\S2A=0.750617\RMSD=6.636e-09\RMSF=2.762e-06\Dipole=-0.5046136,-0.119
5224,0.05078\Quadrupole=18.6123088,-3.5399277,-15.0723811,1.6357322,-2
.822262,-3.9317866\PG=C01 [X(C40H55)]\@

15Z,8Z

1 (bet_car_8_15_c7)

1\1\GINC-S2\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\11-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq=scf=tight\Beta_Carotene (-30) optimizatio
n\0,2\C,8.8477717269,-2.7738123919,0.8702282318\C,4.5673054169,1.4435
680421,-0.0740184231\C,8.382394852,-2.5441345808,2.328109496\C,10.1147
126643,-1.9185447026,0.6266610658\C,4.0293637783,2.774076026,-0.095716
5194\C,2.6911011235,3.0352038583,-0.0474867736\C,2.0648297507,4.336105
347,-0.0713717634\C,2.9534547924,5.5558138772,-0.1405321685\C,0.693004
6144,4.3980733615,-0.0353903152\C,-0.1304955672,5.5683743526,-0.056705
6962\C,9.2542300464,-4.2526521683,0.6708292572\C,8.052450968,-5.180320
4184,0.5162178978\C,7.2627007565,-4.7747645839,-0.726909293\C,7.035792
5224,-3.2808954201,-0.8479018137\C,6.0238147849,-2.9343004276,-1.91572
26727\C,7.7097781283,-2.3699846258,-0.0995859777\C,7.4122862219,-0.926
0673369,-0.1463616904\C,6.1794858146,-0.3649849151,-0.1038805494\C,5.8
787087651,1.0571662566,-0.1367970541\C,7.0269447442,2.0312589599,-0.24
21819661\C,-1.502524885,5.6105632041,-0.0412957998\C,-2.3979298314,4.4
946356358,-0.0014868151\C,-3.7711222948,4.5211821106,-0.0028869822\C,-
4.480733284,3.2632264477,0.0366883774\C,-4.580451304,5.7959536402,-0.0
475990071\C,-5.8333354588,3.090759158,0.0272436121\C,-6.4578369509,1.7
975726731,0.0686964709\C,-7.7897192952,1.5123566644,0.0575194664\C,-8.
2767692055,0.1171575287,0.1091406259\C,-8.8820961449,2.5525247852,-0.0
038453521\C,-7.5608384006,-0.9877995873,0.1588847929\C,-6.873646947,-2
.1584791929,0.1830567534\C,-6.5649349419,-2.8250760613,-1.1901557449\C
,-6.4912164477,-2.7600586642,1.4025406864\C,-7.8751795475,-3.412616335
3,-1.7619238416\C,-6.0200025863,-1.7785874144,-2.1823227652\C,-5.50304
21452,-3.9373905418,-1.0251783349\C,-5.741519043,-4.0650263747,1.46327
99508\C,-6.7740431811,-2.1130593648,2.7287608266\C,-5.7795332118,-4.86
44639641,0.1580428549\H,3.8258857238,0.6462652152,-0.0029352609\H,8.06
50069292,-1.5067042457,2.4786992064\H,7.5339652847,-3.1864781595,2.587
7419568\H,9.1980478896,-2.7562292345,3.0312433975\H,10.9478373083,-2.3
213584726,1.2155585075\H,10.4107239816,-1.9359104753,-0.4289389742\H,9
.983514034,-0.8746670883,0.9292527844\H,4.7227933022,3.6081837771,-0.1

573841007\H,2.0120745981,2.1833807698,0.0107814142\H,3.5732435067,5.53
 59197665,-1.0460090071\H,2.3902989528,6.4900644191,-0.1470767191\H,3.6
 396086167,5.587308965,0.7152627104\H,0.1768856623,3.4406781458,0.01043
 03227\H,0.3737628967,6.530638655,-0.0924719531\H,9.8862043882,-4.56347
 7371,1.5132133782\H,9.8763906133,-4.3329524102,-0.2326319241\H,7.40855
 79163,-5.1162444836,1.4027836774\H,6.2861089137,-5.2814146082,-0.74433
 65347\H,6.1958969617,-3.5600403879,-2.802842591\H,4.9968988231,-3.1492
 647131,-1.5861590187\H,6.0646897549,-1.8866356674,-2.2189187063\H,8.27
 157609,-0.2595226968,-0.1622158029\H,5.3153383988,-1.0227521109,-0.021
 1518739\H,7.7133775921,1.9206316972,0.6073516914\H,7.6145448132,1.8463
 017536,-1.1504085902\H,6.6966582871,3.0710507917,-0.2667794786\H,-1.94
 64426904,6.6024598598,-0.0660491535\H,-1.9433966754,3.5059193488,0.029
 9916713\H,-3.857873849,2.3685833142,0.0754992815\H,-3.9591746552,6.692
 4634149,-0.0655142005\H,-5.2222066007,5.8187424833,-0.9375621828\H,-5.
 2423688591,5.8674023488,0.8246914974\H,-6.4724180049,3.9688458971,-0.0
 143240488\H,-5.7762978073,0.9476941083,0.1165590175\H,-9.3695235387,0.
 0201932314,0.1116910434\H,-8.5009649206,3.5749345522,-0.0306083353\H,-
 9.5087126228,2.4060168843,-0.8942772983\H,-9.5487560828,2.4667178453,0.
 .865084927\H,-8.6229807816,-2.6236150831,-1.8966524005\H,-7.6933842278
 ,-3.8788764525,-2.7385221559\H,-8.3092106973,-4.168957905,-1.099382226
 3\H,-5.1005521713,-1.3176330017,-1.8038538394\H,-5.7891537821,-2.25394
 33027,-3.143852001\H,-6.7467653153,-0.9807401228,-2.3645732016\H,-4.51
 66782845,-3.4717559193,-0.8844804182\H,-6.1328253236,-4.6689394334,2.2
 959716215\H,-4.6894476849,-3.8593901789,1.7330714627\H,-5.8526654401,-
 2.0215567527,3.3231219352\H,-7.2125660668,-1.1178318547,2.6242599673\H
 ,-7.4641351512,-2.7266856869,3.327888527\H,-5.0403165248,-5.6739936816
 ,0.191176516\H,-6.7605331104,-5.3424969792,0.0426340835\H,-5.446455319
 6,-4.5075310098,-1.9618311354\H,8.3760592292,-6.2256607606,0.439047404
 5\H,7.7832319219,-5.128061851,-1.6329559165\\Version=ES64L-G09RevD.01\
 State=2-A\HF=-1557.2351718\S2=0.784922\S2-1=0.\S2A=0.750729\RMSD=5.321
 e-09\RMSF=1.554e-06\Dipole=-0.1663156,-0.2677941,0.0112571\Quadrupole=
 6.1708289,5.9476073,-12.1184362,0.3413511,-0.7455215,-0.6487053\PG=C01
 [X(C40H55)]\@

15Z,12Z

1 (bet_car_12_15_c7)

I\1\GINC-T1\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\12-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizatio
n\0,2\C,-7.9449955021,-3.0755676571,-1.0393326019\C,-4.308749552,1.66
32374351,0.0753785436\C,-7.3580798305,-2.8421472095,-2.4520437087\C,-9
.3248849862,-2.3783561001,-0.9658546019\C,-3.9334653113,3.0482849047,0
.0489218703\C,-2.6367404023,3.4684627437,0.1070659826\C,-2.1713189116,
4.8351857101,0.0801003587\C,-3.1979958892,5.9373824068,-0.035317433\C,
-0.8194373209,5.0642094411,0.1624290486\C,-0.1438238348,6.3259974841,0
.1499119103\C,-8.1882284123,-4.5860927631,-0.8107955885\C,-6.90715189,
-5.3479943734,-0.4836083926\C,-6.3175201316,-4.801715385,0.8153294515\
C,-6.2833857917,-3.2877293814,0.8810972657\C,-5.4412500538,-2.77592063
3,2.0270442815\C,-6.974313783,-2.4973418402,0.0200393834\C,-6.85277205
46,-1.0271643458,0.0162972521\C,-5.6955483988,-0.3238000775,0.06651746
7\C,-5.5660585869,1.1242046308,0.0369061523\C,-6.8241377739,1.95506428
35,-0.0368497362\C,1.2085946272,6.5370512565,0.2513631289\C,2.22852467
83,5.5420306779,0.3968895156\C,3.5756283719,5.7578727498,0.5281714685\
C,4.5260019205,4.6601350689,0.6155759144\C,4.1891640522,7.1396543817,0
.6033807841\C,4.3414185272,3.3629984002,0.243744859\C,5.348795344,2.35
07979714,0.4044450307\C,5.2749271955,1.0323514965,0.0610150244\C,6.433
0248252,0.1734479103,0.3371761485\C,4.074871193,0.3840907417,-0.579238
939\C,6.5358586558,-1.1148551995,0.0725013285\C,6.7150486086,-2.445321
0324,-0.1325661636\C,6.324445631,-3.4011088522,1.0338724804\C,7.264386
0006,-2.9363930634,-1.3379003819\C,7.3883304702,-3.2820309527,2.148778
2111\C,4.954151821,-3.0067774254,1.6194289837\C,6.2323482112,-4.860048
8028,0.5296247021\C,7.470510292,-4.4058363173,-1.5980956045\C,7.639098
7256,-2.0219932605,-2.4697251092\C,7.4200627962,-5.2744549651,-0.33806
65336\H,-3.4770067955,0.9594863549,0.1331100697\H,-7.1514075751,-1.779
6517064,-2.6194750596\H,-6.4169754101,-3.3848182506,-2.5929658563\H,-8
.0631095893,-3.1773069825,-3.2235296762\H,-10.0356281737,-2.901235094,
-1.6174625499\H,-9.7275159124,-2.3984754571,0.0538174514\H,-9.28958473
92,-1.3365278886,-1.3004730101\H,-4.7213832271,3.7929465862,-0.0221096
905\H,-1.8610806744,2.7049389558,0.181492808\H,-3.9050090428,5.9005108
607,0.8032063119\H,-2.7512380121,6.9325282903,-0.0457843426\H,-3.78716
97569,5.8273023146,-0.9545813939\H,-0.1933451447,4.1777117526,0.248694
2117\H,-0.7572868805,7.2173569042,0.0465499404\H,-8.6800901701,-5.0043
720223,-1.6989051095\H,-8.8926138742,-4.7124031555,0.0245043008\H,-6.1
806515291,-5.23342311,-1.2983118647\H,-5.2964492341,-5.1833731989,0.96

50208458\H,-5.6360912773,-3.3790500705,2.9250833337\H,-4.3665194732,-2.8794786033,1.8182720603\H,-5.6358494916,-1.7287697236,2.2652375614\H,-7.7797688295,-0.4694941896,-0.0963003799\H,-4.7576298439,-0.8755993321,0.1123366703\H,-7.3941196313,1.7225577001,-0.9458839877\H,-7.4834550237,1.7410829071,0.8138784705\H,-6.6221952641,3.0274995964,-0.038340514\H,1.5320086317,7.5740661412,0.2106000044\H,1.8968180849,4.5069898741,0.4200383779\H,5.5106619838,4.9265476314,1.0037829398\H,3.4574337187,7.9257800703,0.7993127644\H,4.939261621,7.1797934479,1.4030558282\H,4.7111135984,7.3913750322,-0.3300075792\H,3.3942081939,3.0752651315,-0.2060264159\H,6.2799277308,2.6884802042,0.8621334082\H,7.2838493722,0.6824442814,0.8065306216\H,3.2921859526,1.100271848,-0.8367303539\H,4.3679978062,-0.1432638082,-1.4951828001\H,3.6397226237,-0.3705212125,0.088324523\H,7.4409162252,-2.2530312793,2.5205336349\H,7.1355359948,-3.9358920652,2.9931042936\H,8.3872220574,-3.5559929886,1.7934347913\H,4.1722146951,-3.0418225388,0.8520948914\H,4.6725173434,-3.7004700142,2.4214629851\H,4.9735793953,-1.9959813745,2.0388797487\H,5.3096749263,-4.9780158378,-0.0572981138\H,8.4252045318,-4.5497961759,-2.1262787371\H,6.698765598,-4.7525737652,-2.3095829313\H,7.1292024717,-2.3186480495,-3.3988834143\H,7.3919704806,-0.9778586951,-2.2636308132\H,8.7174069325,-2.0798435834,-2.6821797191\H,7.3421976572,-6.3331001958,-0.6139938996\H,8.3556643421,-5.1670320494,0.2251264285\H,6.1348798031,-5.52475283,1.3981978419\H,-7.1071410693,-6.4225930587,-0.3905242671\H,-6.8929156567,-5.1813436354,1.6764516082\Version=ES64L-G09RevD.01\State=2-A\HF=-1557.2340839\S2=0.784335\S2-1=0\S2A=0.750679\RMSD=8.108e-09\RMSF=1.478e-06\Dipole=0.1662712,-0.4223517,-0.1102727\Quadrupole=4.5493661,6.5781878,-11.127554,-4.2093226,0.1698474,0.5568251\PG=C01 [X(C40H55)]\@

15Z,10Z

l (bet_car_10_15_c7)

l\1\GINC-HP3\FOpt\UB3LYP\6-31G(d)\C40H55(2)\SANDHIYA\12-Jun-2016\0\#P
Becke3LYP/6-31G(d) opt freq scf=tight\Beta_Carotene (-30) optimizati
on\0,2\C,8.6504679491,-2.9069732759,1.1209045488\C,4.7389195326,1.5164321491,-0.2630655879\C,8.0669932032,-2.5940661694,2.5196562196\C,9.98

45063846,-2.1373541012,0.9692343708\C,4.2837107455,2.8738344204,-0.365
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15Z,11Z

1 (bet_car_11_15_c7)

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