Table 1: calculated D_0 vibrational frequencies (B3-LYP/6-311++G(d,p))for 2-methylindenyl radical (2MIR), inden-2-ylmethyl radical (I2MR), *trans*-1-phenylallyl radical (*t*-1PAR), and *cis*-1-phenylallyl radical (*c*-1PAR).

2MIR			**I2MR**			***c*-1PAR**			***t*-1PAR**		
ν	Γ	ω	ν	Γ	ω	ν	Γ	ω	ν	Γ	ω
34	a'	268	34	a'	251	48	a	63	33	a'	160
33	a'	450	33	a'	448	47	a	153	32	a'	361
32	a'	488	32	a'	484	46	a	172	31	a'	414
31	a'	600	31	a'	573	45	a	299	30	a'	624
30	a'	667	30	a'	653	44	a	328	29	a'	631
29	a'	806	29	a'	823	43	a	412	28	a'	835
28	a'	874	28	a'	870	42	a	466	27	a'	991
27	a'	888	27	a'	961	41	a	498	26	a'	1008
26	a'	981	26	a'	974	40	a	562	25	a'	1045
25	a'	1036	25	a'	1032	39	a	629	24	a'	1100
24	a'	1117	24	a'	1088	38	a	669	23	a'	1178
23	a'	1169	23	a'	1155	37	a	698	22	a'	1188
22	a'	1189	22	a'	1171	36	a	742	21	a'	1210
21	a'	1195	21	a'	1181	35	a	802	20	a'	1223
20	a'	1223	20	a'	1212	34	a	817	19	a'	1303
19	a'	1277	19	a'	1219	33	a	843	18	a'	1320
18	a'	1325	18	a'	1287	32	a	850	17	a'	1354
17	a'	1344	17	a'	1337	31	a	923	16	a'	1375
16	a'	1383	16	a'	1400	30	a	982	15	a'	1462
15	a'	1409	15	a'	1423	29	a	990	14	a'	1502
14	a'	1451	14	a'	1480	28	a	995	13	a'	1511
13	a'	1476	13	a'	1486	27	a	1004	12	a'	1542
12	a'	1500	12	a'	1496	26	a	1023	11	a'	1593
11	a'	1535	11	a'	1534	25	a	1047	10	a'	1618
10	a'	1602	10	a'	1614	24	a	1110	9	a'	3132
9	a'	1621	9	a'	1625	23	a	1122	8	a'	3138
8	a'	3030	8	a'	3021	22	a	1180	7	a'	3147
7	a'	3138	7	a'	3098	21	a	1198	6	a'	3158
6	a'	3157	6	a'	3159	20	a	1236	5	a'	3164
5	a'	3163	5	a'	3164	19	a	1281	4	a'	3175
4	a'	3175	4	a'	3175	18	a	1331	3	a'	3186
3	a'	3187	3	a'	3188	17	a	1354	2	a'	3193
2	a'	3198	2	a'	3197	16	a	1437	1	a'	3231
1	a'	3227	1	a'	3200	15	a	1453	48	a''	91
51	a''	106	51	a''	47	14	a	1491	47	a''	137
50	a''	197	50	a''	127	13	a	1508	46	a''	255
49	a''	273	49	a''	238	12	a	1556	45	a''	411
48	a''	422	48	a''	310	11	a	1596	44	a''	499
47	a''	463	47	a''	422	10	a	1620	43	a''	599
46	a''	541	46	a''	537	9	a	3120	42	a''	692
45	a''	592	45	a''	559	8	a	3146	41	a''	759
44	a''	719	44	a''	740	7	a	3154	40	a''	819
43	a''	751	43	a''	743	6	a	3159	39	a''	839
42	a''	791	42	a''	788	5	a	3166	38	a''	856
41	a''	817	41	a''	800	4	a	3176	37	a''	914
40	a''	865	40	a''	884	3	a	3189	36	a''	973
39	a''	930	39	a''	942	2	a	3212	35	a''	987
38	a''	962	38	a''	974	1	a	3243	34	a''	999
37	a''	980	37	a''	1055						
36	a''	1165	36	a''	1487						
35	a''	3058	35	a''	3066						

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Table 2: Optimized geometries for 2-methyl-indenyl radical (2MIR), inden-2-ylmethyl radical (I2MR).

2MIR

C	0.763194	-1.436407	0.000000
C	-0.433958	-0.611229	0.000000
C	-1.785716	-0.914811	0.000000
C	-2.719748	0.139018	0.000000
C	-2.297531	1.464628	0.000000
C	-0.926944	1.781920	0.000000
C	0.000000	0.749520	0.000000
C	1.448886	0.730672	0.000000
C	1.890733	-0.608453	0.000000
C	3.323397	-1.061144	0.000000
H	0.777494	-2.519078	0.000000
H	-2.127962	-1.944553	0.000000
H	-3.779989	-0.087354	0.000000
H	-3.031345	2.262608	0.000000
H	-0.608213	2.819177	0.000000
H	2.086115	1.606294	0.000000
H	3.859299	-0.694148	0.881160
H	3.391417	-2.151075	0.000000
H	3.859299	-0.694148	-0.881160

I2MR

C	3.285589	-1.002305	0.000000
C	1.977535	-0.603212	0.000000
C	0.832116	-1.433442	0.000000
C	-0.358185	-0.641051	0.000000
C	-1.714065	-1.013072	0.000000
C	-2.684201	-0.016292	0.000000
C	-2.324130	1.336882	0.000000
C	-0.974328	1.715732	0.000000
C	0.000000	0.733349	0.000000
C	1.505869	0.850453	0.000000
H	3.549434	-2.053408	0.000000
H	4.098271	-0.285763	0.000000
H	0.859902	-2.515838	0.000000
H	-1.998736	-2.059650	0.000000
H	-3.733998	-0.288410	0.000000
H	-3.096510	2.097581	0.000000
H	-0.705134	2.767173	0.000000
H	1.874779	1.388038	0.880130
H	1.874779	1.388038	-0.880130

Table 3: Optimized geometries for *trans*-1-phenylallyl radical (*t*-1PAR), and *cis*-1-phenylallyl radical (*c*-1PAR).

t-1PAR

C	-1.712257	-1.509950	0.000000
C	-2.722644	-0.543430	0.000000
C	-2.375847	0.809672	0.000000
C	-1.041562	1.188845	0.000000
C	0.000000	0.228952	0.000000
C	-0.376630	-1.136871	0.000000
C	1.363945	0.677812	0.000000
C	2.521724	-0.121020	0.000000
C	3.797364	0.371731	0.000000
H	4.657032	-0.286223	0.000000
H	3.989180	1.439544	0.000000
H	2.402286	-1.201257	0.000000
H	1.512021	1.755167	0.000000
H	-0.781117	2.242227	0.000000
H	-3.150768	1.568265	0.000000
H	-3.764548	-0.842009	0.000000
H	-1.973180	-2.562669	0.000000
H	0.384538	-1.907481	0.000000

c-1PAR

C	-1.512988	1.422474	-0.138841
C	-2.571946	0.539691	0.081634
C	-2.311521	-0.828568	0.188558
C	-1.011314	-1.300755	0.088682
C	0.083181	-0.423027	-0.103995
C	-0.208273	0.955344	-0.232069
C	1.405926	-0.990658	-0.195482
C	2.675283	-0.384024	-0.084833
C	3.014819	0.873788	0.338125
H	4.055718	1.171111	0.373198
H	2.291993	1.592365	0.699408
H	3.505412	-1.041578	-0.335981
H	1.422479	-2.064606	-0.359748
H	-0.818547	-2.365446	0.170765
H	-3.126934	-1.525767	0.346546
H	-3.587537	0.911173	0.155654
H	-1.708959	2.483346	-0.250418
H	0.587377	1.653824	-0.450098