Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary material

A Touch of Lavender: Gas-phase Structure and Dynamics of the Monoterpene Linalool validated by Microwave Spectroscopy

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Table S-1

The 15 most energetically favorable conformers of linalool in order of their relative energy calculated using the MP2 and B3LYP methods with various basis sets.

B3LYP/6–31++G(3df,3pd)					B3LYP6–31++G(df,pd)					B3LYP/6–31++G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6518	0.6477	0.5899	–467.170536	**I**	1.6485	0.6414	0.5849	–467.148109	**I**	1.6463	0.6408	0.5843	–467.137715
V	2.0872	0.4384	0.4316	–467.170251	V	2.0775	0.4376	0.4306	–467.1476837	V	2.0736	0.4374	0.4303	–467.137177
VII	2.0082	0.4614	0.4223	–467.170162	VII	2.0004	0.4605	0.4207	–467.147572	VII	1.9970	0.4602	0.4205	–467.13706
VIII	2.1501	0.4278	0.4228	–467.169774	VIII	2.1474	0.4250	0.4204	–467.147111	VIII	2.1471	0.4243	0.4198	–467.136618
X	2.1639	0.4245	0.4177	–467.169382	X	2.1515	0.4240	0.4170	–467.1467286	X	2.1463	0.4239	0.4167	–467.136225
XV	1.9650	0.4618	0.4205	–467.168710	XV	1.9589	0.4600	0.4185	–467.1461679	XV	1.9575	0.4592	0.4178	–467.13578
II	1.7332	0.6044	0.5566	–467.168363	II	1.7204	0.6073	0.5589	–467.1458515	II	1.7158	0.6082	0.5594	–467.135466
III	1.6808	0.6284	0.5748	–467.167973	III	1.6778	0.6241	0.5702	–467.145654	III	1.6751	0.6237	0.5697	–467.135309
VI	1.7472	0.6214	0.5698	–467.166698	VI	1.7446	0.6138	0.5665	–467.1439096	XIII	1.6720	0.5842	0.5349	–467.133446
IV	1.6945	0.6308	0.5749	–467.166408	VIII	1.6742	0.5850	0.5357	–467.1438291	XI	1.6564	0.5951	0.5315	–467.13336
XI	1.6607	0.5970	0.5343	–467.166346	XI	1.6585	0.5954	0.5319	–467.1438093	XIV	1.7661	0.5603	0.5208	–467.133351
XIV	1.7762	0.5618	0.5228	–467.166344	XIV	1.7697	0.5605	0.5212	–467.1437986	VI	1.7435	0.6127	0.5653	–467.133324
XIII	1.6767	0.5897	0.5391	–467.166306	IV	1.6871	0.6233	0.5697	–467.1437037	IV	1.6837	0.6223	0.5686	–467.133174
XII	1.7159	0.6014	0.5554	–467.166049	XII	1.7271	0.5922	0.5530	–467.1432321	XII	1.7278	0.5905	0.5519	–467.132695
IX	1.6600	0.6225	0.5722	–467.165272	IX	1.6527	0.6141	0.5632	–467.1426498	IX	1.6496	0.6133	0.5622	–467.132225

B3LYP/6–31+G(3df,3pd)					B3LYP/6–31+G(df,pd)					B3LYP/6–31+G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6518	0.6476	0.5899	–467.170277	**I**	1.6477	0.6427	0.5858	–467.147694	**I**	1.6457	0.6418	0.5850	–467.137287
V	2.0876	0.4383	0.4315	–467.169961	V	2.0780	0.4377	0.4306	–467.147244	V	2.0740	0.4374	0.4303	–467.136708
VII	2.0072	0.4617	0.4227	–467.169879	VII	1.9996	0.4609	0.4213	–467.147159	VII	1.9963	0.4606	0.4210	–467.136618
VIII	2.1509	0.4299	0.4229	–467.16952	VIII	2.1485	0.4253	0.4206	–467.146697	VIII	2.1483	0.4245	0.4199	–467.136177
X	2.1609	0.4251	0.4181	–467.169085	XV	2.1496	0.4246	0.4172	–467.146322	X	2.1449	0.4243	0.4169	–467.135795
XV	1.9638	0.4623	0.4211	–467.168398	X	1.9578	0.4605	0.4190	–467.145712	XV	1.9563	0.4596	0.4182	–467.135282
II	1.7326	0.6046	0.5568	–467.16812	II	1.7199	0.6076	0.5592	–467.145456	II	1.7154	0.6085	0.5597	–467.135047
III	1.6806	0.6284	0.5747	–467.167703	III	1.6773	0.6247	0.5708	–467.145247	III	1.6744	0.6243	0.5704	–467.13489
VI	1.7466	0.6208	0.5698	–467.166444	VI	1.7449	0.6139	0.5665	–467.14351	XIII	1.6717	0.5847	0.5353	–467.132916
IV	1.6946	0.6307	0.5749	–467.166163	XI	1.6589	0.5951	0.5316	–467.143384	XIV	1.7645	0.5609	0.5212	–467.132908
XI	1.6610	0.5967	0.5341	–467.166072	XIV	1.7679	0.5611	0.5217	–467.143376	XI	1.6570	0.5946	0.5311	–467.132903
XIV	1.7766	0.5618	0.5227	–467.166071	XIII	1.6739	0.5855	0.5360	–467.143332	VI	1.7439	0.6127	0.5653	–467.132901
XIII	1.6765	0.5902	0.5395	–467.165998	IV	1.6872	0.6234	0.5697	–467.143284	IV	1.6844	0.6220	0.5684	–467.132722
XII	1.7148	0.6021	0.5556	–467.165793	XII	1.7258	0.5932	0.5537	–467.142809	XII	1.7265	0.5914	0.5526	–467.132256
IX	1.6601	0.6224	0.5722	–467.164983	IX	1.6522	0.6146	0.5635	–467.142212	IX	1.6492	0.6136	0.5623	–467.131746

B3LYP/6–31G(3df,3pd)					B3LYP/6–31G(df,pd)					B3LYP/6–31G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6493	0.6619	0.6011	–467.158828	**I**	1.6475	0.6580	0.5990	–467.131457	**I**	1.6459	0.6572	0.5978	–467.119341
V	2.0861	0.4414	0.4341	–467.157447	V	2.0828	0.4401	0.4329	–467.129867	V	2.0789	0.4399	0.4326	–467.117617
VII	2.0012	0.4668	0.4264	–467.157352	VII	2.0048	0.4635	0.4233	–467.129761	VII	2.0015	0.4633	0.4230	–467.117506
VIII	2.1570	0.4313	0.4240	–467.156822	VIII	2.1599	0.4270	0.4221	–467.129316	VIII	2.1588	0.4261	0.4214	–467.117079
II	1.7237	0.6146	0.5635	–467.156451	X	2.1573	0.4259	0.4183	–467.12879	II	1.7122	0.6170	0.5651	–467.116595
X	2.1499	0.4297	0.4215	–467.156347	II	1.7167	0.6162	0.5646	–467.128757	X	2.1541	0.4255	0.4179	–467.11654
III	1.6671	0.6451	0.5905	–467.155751	III	1.6634	0.6417	0.5860	–467.128209	III	1.6618	0.6407	0.5850	–467.116158
XV	1.9532	0.4682	0.4258	–467.155088	XV	1.9569	0.4634	0.4214	–467.127104	XV	1.9558	0.4624	0.4206	–467.115051
VI	1.7441	0.6372	0.5816	–467.154729	IV	1.6727	0.6606	0.5944	–467.126799	IV	1.6705	0.6601	0.5937	–467.114559
IV	1.6751	0.6639	0.5976	–467.154573	VI	1.7518	0.6276	0.5745	–467.126542	VI	1.7510	0.6269	0.5737	–467.114252
XII	1.7149	0.6191	0.5724	–467.154065	XI	1.6591	0.6021	0.5376	–467.126258	XIV	1.7672	0.5660	0.5264	–467.114141
XIV	1.7632	0.5705	0.5297	–467.153966	XIV	1.7711	0.5657	0.5264	–467.126252	XI	1.6567	0.6020	0.5376	–467.114128
XI	1.6622	0.6035	0.5385	–467.153874	XII	1.7311	0.6063	0.5655	–467.126085	XII	1.7312	0.6049	0.5646	–467.113831
XIII	1.6718	0.6043	0.5516	–467.153635	XIII	1.6671	0.6012	0.5489	–467.125468	XIII	1.6649	0.6008	0.5484	–467.113454
IX	1.6593	0.6467	0.5899	–467.152518	IX	1.6553	0.6413	0.5851	–467.124114	IX	1.6516	0.6414	0.5848	–467.112072

Table S–1 continued

B3LYP/6–311++G(3df,3pd)					B3LYP/6–311++G(df,pd)					B3LYP/6–311++G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6584	0.6492	0.5913	–467.26573	**I**	1.6555	0.6480	0.5904	–467.249311	**I**	1.6500	0.6468	0.5891	–467.231273
V	2.0941	0.4401	0.4332	–467.265364	V	2.0889	0.4402	0.4332	–467.248818	V	2.0814	0.4394	0.4324	–467.230749
VII	2.0120	0.4642	0.4246	–467.265263	VII	2.0090	0.4637	0.4241	–467.248723	VII	2.0022	0.4626	0.4231	–467.230668
VIII	2.1581	0.4317	0.4247	–467.264856	VIII	2.1567	0.4308	0.4239	–467.2483	VIII	2.1527	0.4294	0.4225	–467.230201
X	2.1710	0.4263	0.4194	–467.264476	X	2.1609	0.4271	0.4197	–467.247912	XV	2.1511	0.4266	0.4189	–467.229864
XV	1.9699	0.4643	0.4228	–467.263848	XV	1.9667	0.4637	0.4222	–467.247305	X	1.9607	0.4622	0.4209	–467.229335
II	1.7338	0.6099	0.5617	–467.263465	II	1.7281	0.6109	0.5625	–467.24708	II	1.7217	0.6101	0.5616	–467.229059
III	1.6893	0.6291	0.5757	–467.263146	III	1.6847	0.6287	0.5747	–467.246725	III	1.6788	0.6273	0.5734	–467.22878
VI	1.7532	0.6224	0.5714	–467.261778	VI	1.7524	0.6200	0.5719	–467.24524	XIII	1.6743	0.5904	0.5401	–467.227141
XIII	1.6823	0.5935	0.5427	–467.261558	VIII	1.6791	0.5927	0.5421	–467.245119	VI	1.7463	0.6226	0.5714	–467.227055
XIV	1.7834	0.5639	0.5248	–467.261558	XIV	1.7781	0.5643	0.5251	–467.245057	XIV	1.7729	0.5625	0.5233	–467.227011
XI	1.6678	0.5990	0.5359	–467.261551	XI	1.6636	0.6001	0.5366	–467.245049	XI	1.6600	0.5976	0.5342	–467.226983
IV	1.6997	0.6334	0.5773	–467.261503	IV	1.6942	0.6362	0.5792	–467.244976	IV	1.6894	0.6328	0.5763	–467.226797
XII	1.7287	0.6012	0.5582	–467.261142	XII	1.7289	0.6011	0.5597	–467.24454	XII	1.7275	0.5975	0.5570	–467.226396
IX	1.6659	0.6253	0.5746	–467.260403	IX	1.6620	0.6265	0.5755	–467.243902	IX	1.6582	0.6215	0.5714	–467.225842

B3LYP/6–311+G(3df,3pd)					B3LYP/6–311+G(df,pd)					B3LYP/6–311+G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6583	0.6493	0.5914	–467.26564	**I**	1.6553	0.6482	0.5906	–467.248997	**I**	1.6497	0.6471	0.5894	–467.231044
V	2.0940	0.4401	0.4332	–467.265274	V	2.0884	0.4404	0.4334	–467.248491	V	2.0811	0.4396	0.4325	–467.230496
VII	2.0116	0.4644	0.4247	–467.265181	VII	2.0085	0.4639	0.4242	–467.248392	VII	2.0017	0.4628	0.4233	–467.23041
VIII	2.1583	0.4318	0.4248	–467.264775	VIII	2.1572	0.4308	0.4239	–467.247967	VIII	2.1532	0.4295	0.4226	–467.229943
X	2.1705	0.4264	0.4194	–467.264386	X	2.1606	0.4272	0.4198	–467.247597	X	2.1506	0.4267	0.4190	–467.229633
XV	1.9697	0.4645	0.4229	–467.263772	XV	1.9667	0.4637	0.4222	–467.246984	XV	1.9606	0.4623	0.4209	–467.229087
II	1.7334	0.6101	0.5620	–467.263374	II	1.7279	0.6110	0.5626	–467.246761	II	1.7217	0.6102	0.5617	–467.228826
III	1.6892	0.6293	0.5759	–467.263058	III	1.6846	0.6287	0.5747	–467.246398	III	1.6785	0.6275	0.5736	–467.228543
VI	1.7531	0.6228	0.5715	–467.261685	VI	1.7504	0.6242	0.5734	–467.244912	XIII	1.6743	0.5904	0.5402	–467.226896
VIII	1.6822	0.5936	0.5428	–467.261468	XIII	1.6790	0.5929	0.5423	–467.244785	VI	1.7460	0.6234	0.5718	–467.226819
XIV	1.7826	0.5643	0.5252	–467.261468	XIV	1.7773	0.5645	0.5252	–467.244738	XIV	1.7722	0.5627	0.5234	–467.226775
XI	1.6674	0.5992	0.5362	–467.261461	XI	1.6638	0.6000	0.5364	–467.244728	XI	1.6602	0.5975	0.5341	–467.226743
IV	1.6999	0.6334	0.5772	–467.261404	IV	1.6946	0.6359	0.5791	–467.244649	IV	1.6897	0.6328	0.5763	–467.226549
XII	1.7284	0.6015	0.5583	–467.261047	XII	1.7286	0.6015	0.5602	–467.244216	XII	1.7276	0.5976	0.5573	–467.226155
IX	1.6654	0.6256	0.5748	–467.260307	IX	1.6614	0.6271	0.5760	–467.24358	IX	1.6577	0.6222	0.5719	–467.225599

B3LYP/6–311G(3df,3pd)					B3LYP/6–311G(df,pd)					B3LYP/6–311G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6575	0.6524	0.5941	–467.262405	**I**	1.6546	0.6539	0.5954	–467.242495	**I**	1.6493	0.6527	0.5942	–467.225126
V	2.0951	0.4409	0.4339	–467.262093	V	2.0945	0.4410	0.4340	–467.241696	V	2.0872	0.4402	0.4332	–467.224292
VII	2.0129	0.4651	0.4250	–467.261963	VII	2.0117	0.4654	0.4255	–467.241549	VII	2.0049	0.4644	0.4247	–467.224158
VIII	2.1624	0.4317	0.4249	–467.261227	VIII	2.1666	0.4306	0.4239	–467.240987	VIII	2.1627	0.4292	0.4226	–467.223543
X	2.1704	0.4271	0.4201	–467.261157	X	2.1666	0.4275	0.4201	–467.240747	X	2.1564	0.4271	0.4193	–467.223378
II	1.7343	0.6108	0.5620	–467.260076	II	1.7239	0.6167	0.5669	–467.240126	II	1.7193	0.6149	0.5650	–467.222786
XV	1.9675	0.4649	0.4229	–467.259836	III	1.6803	0.6345	0.5800	–467.239335	III	1.6732	0.6341	0.5795	–467.222041
III	1.6856	0.6324	0.5784	–467.259457	XV	1.9631	0.4652	0.4233	–467.238898	XV	1.9569	0.4640	0.4223	–467.221637
VI	1.7589	0.6190	0.5712	–467.258738	VI	1.7583	0.6267	0.5750	–467.238215	VI	1.7545	0.6242	0.5727	–467.220726
IV	1.6975	0.6378	0.5803	–467.258215	IV	1.6733	0.6574	0.5944	–467.238095	IV	1.6689	0.6528	0.5906	–467.220609
XII	1.7329	0.6032	0.5622	–467.258196	XII	1.7424	0.5984	0.5607	–467.237664	XIV	1.7772	0.5628	0.5238	–467.220328
XIV	1.7820	0.5650	0.5256	–467.25801	XI	1.6678	0.6005	0.5366	–467.237664	XI	1.6639	0.5984	0.5346	–467.220324
XI	1.6698	0.5997	0.5361	–467.257998	XIV	1.7850	0.5638	0.5250	–467.237647	XII	1.7455	0.5921	0.5570	–467.220225
XIII	1.6825	0.5945	0.5435	–467.25776	XIII	1.6791	0.5948	0.5438	–467.236918	XIII	1.6739	0.5933	0.5424	–467.219672
IX	1.6676	0.6249	0.5746	–467.256621	IX	1.6663	0.6345	0.5815	–467.235635	IX	1.6619	0.6215	0.5718	–467.218286

Table S–1 continued

B3LYP/cc–pVDZ					B3LYP/cc–pVTZ				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	A / GHz	B / GHz	C / GHz	E Hartree
I	1.6415	0.6551	0.5959	–467.111387	**I**	1.6582	0.6502	0.5923	–467.270831
V	2.0814	0.4387	0.4317	–467.110411	V	2.0958	0.4404	0.4336	–467.270534
VII	1.9971	0.4637	0.4230	–467.110191	VII	2.0135	0.4642	0.4245	–467.270417
VIII	2.1572	0.4256	0.4212	–467.109556	VIII	2.1636	0.4288	0.4241	–467.269979
X	2.1583	0.4239	0.4171	–467.109399	X	2.1741	0.4260	0.4194	–467.26969
II	1.7203	0.6100	0.5602	–467.108827	II	1.7355	0.6090	0.5607	–467.268503
III	1.6654	0.6340	0.5788	–467.107985	XV	1.9705	0.4635	0.4219	–467.268406
XV	1.9496	0.4620	0.4199	–467.107233	III	1.6872	0.6299	0.5757	–467.267915
VI	1.7504	0.6188	0.5708	–467.107018	VI	1.7583	0.6184	0.5698	–467.266933
IV	1.6765	0.6463	0.5849	–467.106894	IV	1.6948	0.6368	0.5795	–467.26672
XII	1.7360	0.5938	0.5571	–467.106678	XI	1.6709	0.5976	0.5345	–467.266518
XIV	1.7703	0.5623	0.5232	–467.10637	XIV	1.7881	0.5619	0.5230	–467.2665
XI	1.6561	0.5986	0.5351	–467.106368	XII	1.7318	0.6005	0.5587	–467.266393
XIII	1.6658	0.5930	0.5419	–467.105422	XIII	1.6834	0.5912	0.5407	–467.266072
IX	1.6521	0.6248	0.5738	–467.104141	IX	1.6698	0.6202	0.5710	–467.26496

MP2/6–31++G(df,pd)					MP2/6–31++G(d,p)					MP2/6–31+G(df,pd)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6468	0.7043	0.6370	–465.848386	**I**	1.6368	0.6962	0.6303	–465.640812	**I**	1.6468	0.7043	0.6376	–465.846311
II	1.6770	0.6755	0.6193	–465.846536	II	1.6735	0.6634	0.6082	–465.63898	II	1.6825	0.6711	0.6154	–465.844372
V	2.0916	0.4738	0.4576	–465.844494	III	1.6439	0.6824	0.6297	–465.637682	III	1.6562	0.6899	0.6376	–465.843271
IV	1.6356	0.7532	0.6631	–465.844416	V	2.0791	0.4721	0.4552	–465.637356	V	2.0924	0.4645	0.4523	–465.842486
VII	1.9873	0.4901	0.4566	–465.844376	VII	1.9766	0.4862	0.4533	–465.637238	VII	1.9828	0.4924	0.4582	–465.84239
VI	1.7154	0.7099	0.6371	–465.844204	IV	1.6256	0.7433	0.6549	–465.636986	VI	1.7186	0.7071	0.6354	–465.842173
VIII	2.1837	0.4596	0.4411	–465.843778	VI	1.7049	0.7034	0.6312	–465.636802	IV	1.6393	0.7504	0.6613	–465.842152
X	2.0243	0.4907	0.4591	–465.84333	VIII	2.1755	0.4565	0.4382	–465.636586	VIII	2.1821	0.4520	0.4374	–465.841752
XII	1.7497	0.6755	0.6357	–465.843116	X	2.0163	0.4845	0.4545	–465.636219	X	2.0250	0.4920	0.4600	–465.841342
XI	1.6282	0.6624	0.5899	–465.843113	XI	1.6199	0.6564	0.5850	–465.635827	XII	1.7464	0.6763	0.6361	–465.841113
XIV	1.6949	0.6294	0.5816	–465.84288	XII	1.7390	0.6681	0.6285	–465.635755	XI	1.6305	0.6602	0.5882	–465.841007
IX	1.6278	0.7292	0.6504	–465.842793	XIV	1.6879	0.6228	0.5756	–465.635556	XIV	1.6989	0.6274	0.5798	–465.840819
XIII	1.6574	0.6562	0.5913	–465.84262	IX	1.6185	0.7195	0.6423	–465.635549	IX	1.6304	0.7264	0.6486	–465.840591
XV	1.9368	0.5014	0.4645	–465.842555	XV	1.9330	0.4937	0.4574	–465.635536	XV	1.9363	0.5000	0.4626	–465.840481
					XIII	1.6456	0.6539	0.5946	–465.635373	XIII	1.6705	0.6607	0.6071	–465.840403

MP2/6–31+G(d,p)					MP2/6–31G(df,pd)					MP2/6–31G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6372	0.6961	0.6305	–465.63814	**I**	1.6572	0.7102	0.6448	–465.822498	**I**	1.6481	0.6993	0.6346	–465.610716
II	1.6797	0.6586	0.6039	–465.636176	II	1.6937	0.6724	0.6148	–465.820192	II	1.6879	0.6612	0.6046	–465.608312
III	1.6448	0.6818	0.6290	–465.635069	III	1.6551	0.6957	0.6381	–465.818832	III	1.6489	0.6839	0.6270	–465.607077
V	2.0805	0.4658	0.4514	–465.634788	V	2.0859	0.5014	0.4808	–465.818308	V	2.0800	0.4899	0.4700	–465.607051
VII	1.9726	0.4879	0.4538	–465.634696	IV	1.6438	0.7603	0.6687	–465.818306	VII	1.9860	0.4869	0.4516	–465.606922
VI	1.7088	0.7002	0.6292	–465.634207	VII	1.9909	0.4947	0.4598	–465.818094	IV	1.6381	0.7454	0.6571	–465.60659
IV	1.6305	0.7396	0.6525	–465.634094	VI	1.7040	0.7350	0.6528	–465.817538	VIII	2.1862	0.4481	0.4343	–465.606244
VIII	2.1750	0.4503	0.4350	–465.633982	VIII	2.1936	0.4507	0.4371	–465.817495	X	2.0134	0.4993	0.4641	–465.605912
X	2.0166	0.4853	0.4551	–465.633654	X	2.0207	0.5081	0.4705	–465.817194	VI	1.7000	0.7214	0.6426	–465.60583
XII	1.7355	0.6688	0.6286	–465.633188	XII	1.7670	0.6746	0.6356	–465.816748	XII	1.7547	0.6662	0.6269	–465.60515
XI	1.6229	0.6536	0.5827	–465.63313	XIV	1.7073	0.6292	0.5818	–465.816549	XIV	1.7047	0.6200	0.5736	–465.605
XV	1.9332	0.4913	0.4540	–465.632894	XI	1.6524	0.6518	0.5802	–465.816493	XI	1.6421	0.6455	0.5752	–465.604982
XIV	1.6926	0.6203	0.5735	–465.632889	XIII	1.6732	0.6610	0.6047	–465.815394	XIII	1.6589	0.6524	0.5946	–465.604055
IX	1.6225	0.7161	0.6400	–465.632757	XV	1.9221	0.5129	0.4727	–465.815017	XV	1.9271	0.4981	0.4594	–465.604004
XIII	1.6544	0.6541	0.5993	–465.632596	IX	1.6397	0.7268	0.6492	–465.814947	IX	1.6336	0.7144	0.6395	–465.603603

Table S–1 continued

MP2/6–311++G(df,pd)					MP2/6–311++G(d,p)					MP2/6–311+G(df,pd)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6489	0.7061	0.6408	–465.990963	**I**	1.6378	0.7003	0.6355	–465.796119	**I**	1.6484	0.7070	0.6420	–465.98961
II	1.6758	0.6759	0.6196	–465.989103	II	1.6701	0.6670	0.6115	–465.794307	II	1.6782	0.6741	0.6182	–465.987667
III	1.6485	0.6953	0.6417	–465.987919	III	1.6364	0.6905	0.6366	–465.793107	III	1.6492	0.6947	0.6409	–465.986562
IV	1.6318	0.7603	0.6683	–465.987239	IV	1.6208	0.7540	0.6629	–465.792614	IV	1.6327	0.7601	0.6682	–465.985782
VI	1.7070	0.7185	0.6430	–465.987109	V	2.0836	0.4762	0.4567	–465.79252	VI	1.7072	0.7189	0.6432	–465.985767
V	2.0975	0.4807	0.4603	–465.986956	VI	1.6930	0.7156	0.6398	–465.792487	V	2.0968	0.4797	0.4599	–465.985547
VII	1.9747	0.4978	0.4658	–465.986904	VII	1.9671	0.4913	0.4586	–465.792437	VII	1.9728	0.4993	0.4675	–465.985505
VIII	2.1737	0.4621	0.4426	–465.986268	VIII	2.1629	0.4585	0.4395	–465.791727	VIII	2.1745	0.4601	0.4416	–465.984839
IX	1.6263	0.7327	0.6536	–465.985945	IX	1.6150	0.7276	0.6490	–465.791489	IX	1.6268	0.7320	0.6530	–465.984545
XI	1.6260	0.6628	0.5901	–465.985872	X	2.0115	0.4878	0.4562	–465.791368	XII	1.7436	0.6818	0.6415	–465.984526
X	2.0233	0.4930	0.4600	–465.985845	XI	1.6159	0.6593	0.5870	–465.791306	XI	1.6264	0.6627	0.5900	–465.984503
XIII	1.6662	0.6646	0.6105	–465.985668	XII	1.7368	0.6752	0.6357	–465.791234	X	2.0269	0.4925	0.4600	–465.984459
XIV	1.6889	0.6320	0.5843	–465.985662	XIII	1.6502	0.6589	0.6033	–465.791102	XIII	1.6701	0.6665	0.6144	–465.984299
XV	1.9252	0.5093	0.4721	–465.985468	XIV	1.6809	0.6262	0.5790	–465.791065	XV	1.9246	0.5094	0.4722	–465.984035
					XV	1.9160	0.5037	0.4667	–465.791042					

MP2/6–311+G(d,p)					MP2/6–311G(df,pd)					MP2/6–311G(d,p)				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree
I	1.6374	0.7013	0.6369	–465.794614	**I**	1.6489	0.7126	0.6458	–465.977289	**I**	1.6380	0.7064	0.6401	–465.780986
II	1.6735	0.6643	0.6093	–465.792713	II	1.6750	0.6826	0.6252	–465.975371	II	1.6718	0.6716	0.6151	–465.77913
III	1.6366	0.6900	0.6361	–465.791595	III	1.6517	0.6976	0.6434	–465.973737	V	2.0767	0.4932	0.4721	–465.77752
IV	1.6946	0.7147	0.6392	–465.791006	IV	1.6341	0.7680	0.6740	–465.97352	III	1.6408	0.6912	0.6369	–465.77748
VI	1.6219	0.7532	0.6623	–465.790993	V	2.0927	0.4966	0.4751	–465.973328	VII	1.9728	0.4926	0.4593	–465.77729
V	2.0830	0.4737	0.4553	–465.790963	VII	1.9825	0.4981	0.4647	–465.973084	IV	1.6226	0.7615	0.6685	–465.777271
VII	1.9637	0.4933	0.4607	–465.7909	VI	1.6980	0.7373	0.6548	–465.973072	VI	1.6867	0.7330	0.6508	–465.776923
VIII	2.1639	0.4556	0.4380	–465.790143	X	2.0235	0.5034	0.4675	–465.972377	X	2.0078	0.4999	0.4647	–465.776555
IX	1.6156	0.7263	0.6479	–465.789919	VIII	2.1851	0.4711	0.4504	–465.972366	VIII	2.1732	0.4655	0.4458	–465.776407
X	2.0156	0.4876	0.4563	–465.789853	XII	1.7602	0.6811	0.6428	–465.971831	XII	1.7499	0.6748	0.6368	–465.775722
XI	1.6160	0.6594	0.5870	–465.789818	XIV	1.6922	0.6340	0.5859	–465.971586	XI	1.6312	0.6515	0.5802	–465.775526
XII	1.7341	0.6768	0.6371	–465.789773	XI	1.6420	0.6552	0.5835	–465.971561	XIV	1.6876	0.6266	0.5793	–465.775501
XIV	1.6807	0.6263	0.5791	–465.789563	XIII	1.6738	0.6636	0.6100	–465.970627	XV	1.9127	0.5065	0.4687	–465.774686
XIII	1.6571	0.6619	0.6095	–465.789557	IX	1.6350	0.7319	0.6532	–465.970538	XIII	1.6588	0.6554	0.6002	–465.774613
XV	1.9157	0.5032	0.4660	–465.789475	XV	1.9225	0.5127	0.4745	–465.970461	IX	1.6262	0.7248	0.6474	–465.77444

MP2/cc–pVDZ					MP2/cc–pVTZ				
Conf	*A* / GHz	*B* / GHz	*C* / GHz	*E* Hartree	Conf	A / GHz	B / GHz	C / GHz	E Hartree
I	1.6260	0.7011	0.6350	–465.61104	**I**	1.6512	0.7082	0.6422	–466.09482
II	1.6660	0.6614	0.6052	–465.608682	II	1.6831	0.6744	0.6178	–466.092471
V	2.0605	0.4945	0.4730	–465.60767	IV	1.6380	0.7601	0.6684	–466.091188
VII	1.9647	0.4845	0.4483	–465.607473	V	2.1032	0.4818	0.4622	–466.091062
IV	1.6148	0.7506	0.6596	–465.607241	VII	1.9872	0.4928	0.4582	–466.090933
III	1.6267	0.6844	0.6290	–465.607136	X	2.0409	0.4906	0.4592	–466.09006
VI	1.6722	0.7285	0.6457	–465.606869	XI	1.6369	0.6570	0.5858	–466.089453
X	1.9863	0.5022	0.4650	–465.606656	XII	1.7524	0.6779	0.6374	–466.089408
VIII	2.1594	0.4697	0.4503	–465.606549	XIV	1.6951	0.6327	0.5846	–466.089388
XII	1.7401	0.6657	0.6269	–465.605957	XIII	1.6665	0.6619	0.6050	–466.089104
XI	1.6189	0.6449	0.5753	–465.60547	XV	1.9358	0.5037	0.4656	–466.089033
XIV	1.6814	0.6189	0.5722	–465.605351					
XIII	1.6398	0.6471	0.5879	–465.604252					
XV	1.9068	0.4950	0.4563	–465.604209					
IX	1.6211	0.7105	0.6364	–465.603974					

Table S-2

Cartesian nuclear coordinates of the five most stable conformers of linalool in the principal axes of inertia calculated at the MP2/6-311++G(d,p) level of theory.

	Conformer I			Conformer II		
	a /Å	b /Å	c /Å	a /Å	b /Å	c /Å
C1	1.057371	2.258157	–0.061052	–2.101924	2.037560	0.247937
C2	1.599941	1.133962	–0.552840	–2.161014	0.735593	0.566142
H3	0.602973	2.270270	0.924762	–1.583839	2.365475	–0.647732
H4	1.074665	3.182598	–0.630333	–2.583680	2.786869	0.868582
H5	2.068260	1.146982	–1.538982	–2.702833	0.421198	1.460346
C6	1.650321	–0.191804	0.171527	–1.540421	–0.381523	–0.240958
C7	1.117862	–1.308016	–0.747389	–0.636468	–1.241591	0.662573
C8	–0.292831	–1.070963	–1.315494	0.372282	–0.459148	1.527185
H9	1.133178	–2.243323	–0.172495	–0.106364	–1.944286	0.007208
H10	1.819270	–1.426216	–1.584070	–1.275740	–1.835788	1.329381
C11	–1.361128	–1.066001	–0.256194	1.256681	0.497326	0.761172
H12	–0.510051	–1.885069	–2.020844	0.987193	–1.185922	2.072381
H13	–0.303716	–0.142025	–1.893122	–0.178957	0.111285	2.282290
C14	–3.260060	–0.271100	1.135230	3.122591	1.199144	–0.734412
H15	–3.144674	0.507327	1.899563	4.168230	1.187026	–0.403919
H16	–3.159138	–1.247555	1.616682	2.719896	2.202968	–0.573230
H17	–4.279032	–0.181601	0.739591	3.124616	0.992734	–1.811870
H18	–1.418622	–1.978909	0.342241	1.003346	1.556373	0.828563
C19	3.094653	–0.496390	0.567486	–2.646175	–1.248975	–0.841409
H20	3.147877	–1.485801	1.032588	–2.202394	–2.109066	–1.352909
H21	3.750321	–0.476146	–0.308683	–3.327687	–1.606078	–0.062928
H22	3.438730	0.253122	1.285730	–3.213511	–0.659307	–1.567062
O23	0.926722	–0.154812	1.401499	–0.807487	0.115128	–1.362734
H24	–0.012278	–0.130257	1.169443	0.046392	0.417491	–1.024419
C25	–2.248461	–0.086635	0.031618	2.323308	0.156522	0.003354
C26	–2.344659	1.229661	–0.694105	2.783612	–1.264566	–0.189398
H27	–1.560774	1.368261	–1.438877	2.281995	–1.963912	0.482629
H28	–3.319290	1.307426	–1.192078	2.596550	–1.588628	–1.220941
H29	–2.283530	2.059647	0.020245	3.864503	–1.336885	–0.020826

Table S-2 continued

	Conformer III			**Conformer IV**		
	a /Å	b /Å	c /Å	a /Å	b /Å	c /Å
C1	–1.845204	2.095770	–0.001558	0.504588	2.237232	–0.200774
C2	–1.525445	1.006427	–0.719588	0.830805	1.056397	–0.752684
H3	–2.083570	2.038531	1.057148	0.766661	2.467601	0.827806
H4	–1.880389	3.077122	–0.464999	–0.021077	2.994126	–0.774652
H5	–1.307686	1.108072	–1.783323	0.580934	0.863284	–1.795946
C6	–1.511835	–0.422201	–0.218392	1.618467	–0.027267	–0.048090
C7	–1.077988	–0.547046	1.252929	1.150928	–1.438956	–0.450098
C8	0.282034	0.079685	1.615941	–0.244045	–1.852525	0.050610
H9	–1.058994	–1.619915	1.483604	1.887590	–2.147609	–0.051140
H10	–1.851713	–0.097027	1.887996	1.184528	–1.516054	–1.545805
C11	1.445499	–0.541943	0.892249	–1.350369	–1.058006	–0.580495
H12	0.432985	–0.065295	2.694378	–0.270289	–1.790309	1.142897
H13	0.247961	1.158080	1.446888	–0.380790	–2.914181	–0.194117
C14	3.400745	–0.735318	–0.631046	–3.161287	0.627325	–0.798031
H15	3.292060	–0.764689	–1.722253	–4.175402	0.506148	–0.398566
H16	3.437649	–1.762516	–0.258378	–3.160585	0.319628	–1.847401
H17	4.362515	–0.252945	–0.418562	–2.922201	1.698267	–0.750512
H18	1.635162	–1.591558	1.129627	–1.482234	–1.217258	–1.653395
C19	–2.905459	–1.025794	–0.396579	3.097599	0.127266	–0.408090
H20	–2.890556	–2.075054	–0.084561	3.684564	–0.635650	0.113087
H21	–3.638884	–0.474313	0.198670	3.243099	0.014017	–1.487030
H22	–3.196414	–0.978292	–1.450207	3.445421	1.118625	–0.105740
O23	–0.664052	–1.215877	–1.061861	1.565456	0.130687	1.373345
H24	0.246355	–0.959846	–0.858763	0.633519	0.192871	1.611406
C25	2.271496	0.044154	–0.004699	–2.162622	–0.157320	0.010315
C26	2.165405	1.475714	–0.463267	–2.096718	0.228031	1.463215
H27	1.310480	2.001880	–0.037548	–1.509178	–0.465486	2.070078
H28	3.080095	2.021007	–0.199474	–1.663137	1.234305	1.558435
H29	2.076109	1.513403	–1.556071	–3.103390	0.273427	1.894363

Table S-2 continued

	Conformer V		
	a /Å	b /Å	c /Å
C1	3.019601	1.602481	0.691576
C2	2.588992	0.862269	–0.341509
H3	2.805640	1.314547	1.716198
H4	3.576250	2.519554	0.526434
H5	2.797360	1.188401	–1.361682
C6	1.820542	–0.432294	–0.223883
C7	0.379951	–0.252696	–0.719902
C8	–0.436769	0.767178	0.085654
H9	–0.114101	–1.231613	–0.667199
H10	0.405671	0.042519	–1.777350
C11	–1.855532	0.838771	–0.411437
H12	0.030073	1.754757	–0.000991
H13	–0.399164	0.493429	1.143248
C14	–4.266718	0.237404	–0.567868
H15	–4.603363	–0.716234	–0.992846
H16	–4.284188	0.993938	–1.357286
H17	–4.996758	0.521112	0.200264
H18	–2.047684	1.529935	–1.234247
C19	2.525176	–1.515811	–1.045239
H20	1.970338	–2.455476	–0.965010
H21	2.588143	–1.226845	–2.099393
H22	3.545329	–1.673312	–0.675169
O23	1.703429	–0.860986	1.136543
H24	2.592333	–1.078555	1.439799
C25	–2.891576	0.096731	0.033033
C26	–2.780546	–0.921610	1.138617
H27	–1.763198	–1.028352	1.520014
H28	–3.437886	–0.650253	1.974202
H29	–3.113652	–1.902671	0.777942

Table S-3

Molecular constants of linalool obtained by a global fit using the program BELGI-C_1.

Operator[a]	Parameter[b]	BELGI-C_1 notation	Unit	Value[c]
P_a^2	A	OA	GHz	1.5884(45)
P_b^2	B	B	GHz	0.7274(30)
P_c^2	C	C	GHz	0.6256(20)
$\{P_a,P_b\}$	D_{ab}	DAB	GHz	0.1996(55)
	D_{aci}	DACI	GHz	–0.093(11)
$\{P_b,P_c\}$	D_{bci}	DBCI	GHz	–0.02238[d]
$-P^4$	Δ_J	DJ	kHz	0.0952(12)
$-P^2P_a^2$	Δ_{JK}	DJK	kHz	0.44279[e]
$-P_a^4$	Δ_K	DK	kHz	0.0[fixed]
$-2P^2(P_b^2-P_c^2)$	δ_J	ODELN	kHz	0.0[fixed]
$-[P_a^2,(P_b^2-P_c^2)]$	δ_K	ODELK	kHz	0.0779[e]
P_γ^2	F	F	GHz	157.93097[d]
$(1/2)(1-\cos 3\gamma)$	V_3	V3	cm^{-1}	399.4(17)
P_aP_γ	ρ	RHORHO	unitless	0.010236[f]
$(1-\cos 3\gamma)P^2$	F_v	FV	GHz	0.01213(95)
$\{P_a,P_b\}\ P_\gamma^2$	Δ_{ab}	DELTA	GHz	0.001285(67)

Weight / kHz	N[g]	Root mean square deviation / kHz
5	74	5.1
10	3	21.8
Not included	6	
N_{fitted}/N_{tot}	77[h]/83	6.6

[a] All constants refer to a rho-axis system. Therefore, the inertia tensor is not diagonal and the constants cannot be directly compared to those of a principal axis system. P_a, P_b, and P_c are the components of the overall rotational angular momentum. P_γ is the angular momentum of the internal rotor rotating around the internal rotor axis by an angle γ. {u,v} is the anti commutator uv + vu.

[b] The product of the parameter and operator from a given row yields the term actually used in the vibration-rotation-torsion Hamiltonian, except for F, ρ, and A, which occur in the Hamiltonian in the form $F(P\gamma-\rho P_a)^2 + AP_a$.

[c] Values of the parameters from the present fit. Statistical uncertainties are shown as one standard uncertainty in unit of the last digit.

[d] Fixed to the *ab initio* value.

[e] Fixed to the values obtained by a previous fit.

[f] Fixed to a value obtained in a fit fixing V_3

[g] Number of lines

[h] 46 A/31 E

Table S-4

Fitted frequencies ($\nu_{Obs.}$) of linalool. $\nu_{Obs.} - \nu_{Calc.}$ values obtained after a fit with the programs XIAM and BELGI-C_1. Frequencies marked with * or (10) are not included in the fit or weighted with 10 kHz, respectively.

Upper level			Lower level				$\nu_{Obs.}$	$\nu_{Obs.} - \nu_{Calc.}$	$\nu_{Obs.} - \nu_{Calc.}$
J	K_a	K_c	J	K_a	K_c		MHz	XIAM/kHz	BELGI/kHz
6	2	4	5	1	4	E	10.5208709	3.5	–2
7	1	6	6	1	5	A	9.2830431	0.0	–2
						E	9.2829370	–5.3	–14
7	2	5	6	1	5	A	11.7853567	–7.8	–7
						E	11.7853089	3.3	3
7	2	5	6	2	4	A	9.2336206	–0.3	–3
						E	9.2335150	–2.4	–4
7	3	4	6	2	4	A	13.9776961	–5.0	4
7	2	6	6	2	5	A	9.0830642	–1.1	–2
						E	9.0829959	5.3	6
7	3	5	6	2	5	A	14.1615788	–5.9	0
						E	14.1614660	1.7	–8
7	3	4	6	3	3	A	9.1374690	–2.2	–3
						E	9.1373078	0.8	3
7	3	5	6	3	4	A	9.1262905	2.0	0
						E	9.1262975	0.4	–2
7	5	2	6	5	1	A	9.1171612	–5.6	–5
						E	9.1170816	0.7	–1
8	0	8	7	0	7	A	10.1960218	–0.8	–1
						E	10.1959366	5.5	* –30
8	1	7	7	1	6	A	10.5891019	0.2	–1
						E	10.5889827	–7.6	(10) –18
8	2	6	7	1	6	A	13.0836554	–2.9	–3
						E	13.0835798	0.7	8
8	1	8	7	1	7	A	10.1035602	7.8	8
						E	10.1035341	13.0	* 45
8	2	7	7	1	7	A	14.2777137	–2.7	–2
8	2	6	7	2	5	A	10.5813368	–0.1	–2
						E	10.5812135	–2.2	–4
8	3	5	7	2	5	A	15.1992951	–1.6	8
						E	15.1992844	4.3	–5
8	2	7	7	2	6	A	10.3706706	–0.4	–1
						E	10.3705938	6.4	8
8	3	5	7	3	4	A	10.4552164	–0.2	–1
						E	10.4550938	9.2	9
8	3	6	7	3	5	A	10.4331989	–0.1	0
						E	10.4331366	6.4	5
9	0	9	8	0	8	A	11.4304905	–3.8	–5
						E	11.4303747	2.6	* –60
9	1	8	8	1	7	A	11.8855474	–1.5	0
						E	11.8854284	–1.5	–11

Table S-4 continued

Upper level			Lower level				$\nu_{Obs.}$	$\nu_{Obs.} - \nu_{Calc.}$	$\nu_{Obs.} - \nu_{Calc.}$
J	K_a	K_c	J	K_a	K_c		MHz	XIAM/kHz	BELGI/kHz
9	2	7	8	1	7	A	14.4250363	–1.7	–3
						E	14.4249375	5.8	(10) 21
9	1	9	8	1	8	A	11.3540406	–1.4	–4
9	1	8	8	2	6	A	9.3909964	4.0	4
						E	9.3908315	–9.8	* –36
9	2	7	8	2	6	A	11.9304811	–0.4	–2
						E	11.9303406	–2.5	–4
9	2	8	8	2	7	A	11.6544445	0.1	1
						E	11.6543614	7.9	12
9	3	6	8	3	5	A	11.7794825	0.8	0
						E	11.7793516	2.5	2
9	3	7	8	3	6	A	11.7400067	0.0	1
						E	11.7399110	1.8	2
9	6	3	8	6	2	A	11.7230944	–7.8	–5
						E	11.7229970	4.1	4
10	0	10	9	0	9	A	12.6620681	–2.0	–4
						E	12.6618902	–5.5	* –118
10	1	9	9	1	8	A	13.1706451	–0.1	2
						E	13.1705266	4.8	–4
10	2	8	9	1	8	A	15.8168379	1.0	0
						E	15.8166976	2.8	(10) 26
10	1	10	9	1	9	A	12.6018192	–2.3	–5
10	1	9	9	2	7	A	10.6311577	1.6	6
						E	10.6310162	–3.8	* –37
10	2	8	9	2	7	A	13.2773533	5.6	7
						E	13.2771876	–5.4	–8
10	2	9	9	2	8	A	12.9340579	–0.5	2
10	3	7	9	3	6	A	13.1116061	3.4	3
						E	13.1114579	0.3	1
10	6	4	9	6	3	A	13.0283255	–8.1	–4
						E	13.0282138	2.9	3
11	1	10	10	1	9	A	14.4430520	1.1	6
						E	14.4429312	5.8	0
11	2	9	10	2	8	A	14.6188844	6.1	9
						E	14.6187017	–6.9	–9
11	2	10	10	2	9	A	14.2092751	0.4	4
11	3	8	10	3	7	A	14.4525050	5.5	–5
						E	14.4523357	–1.0	0
11	4	8	10	4	7	A	14.3570538	–0.1	4
12	0	12	11	0	11	A	15.1242128	–0.1	–5
12	1	12	11	1	11	A	15.0906490	–1.2	–7
16	3	13	15	4	11	A	15.1992951	–1.7	–2

Table S-5

The rotational constants and angle between the internal rotor axis and the principal axes of conformer I calculated using the DFT method with two different hybrid functionals B3LYP and B3PW91and various basis sets.

	B3LYP								
Basis set	*A* / GHz	*B* / GHz	*C* / GHz	*E* / Hartree	rel. *E* kJ/mol	∠(i,*a*) / °	∠(i,*b*) / °	∠(i,*c*) / °	V_3 / cm^{-1}
6-31G	1.6344	0.6508	0.5930	–466.974325	778.5	85.31	27.19	63.29	270.3
6-31+G	1.6354	0.6319	0.5777	–466.993754	727.5	84.39	25.74	64.97	308.7
6-31++G	1.6357	0.6309	0.5771	–466.994477	725.6	84.18	25.85	64.91	305.5
6-311G	1.6408	0.6422	0.5871	–467.084786	488.5	84.31	27.19	63.50	286.6
6-311+G	1.6397	0.6368	0.5821	–467.091553	470.7	84.64	25.85	64.79	301.2
6-311++G	1.6399	0.6358	0.5816	–467.091999	469.5	84.38	26.18	64.53	300.9
6-31G(d,p)	1.6459	0.6572	0.5978	–467.119341	397.7	85.40	27.09	63.37	300.0
6-31+G(d,p)	1.6457	0.6418	0.5850	–467.137287	350.6	84.82	25.73	64.87	349.7
6-31++G(d,p)	1.6463	0.6408	0.5843	–467.137715	349.5	84.71	25.69	64.94	347.6
6-311G(d,p)	1.6493	0.6527	0.5942	–467.225126	120.0	85.46	26.01	64.45	340.0
6-311+G(d,p)	1.6497	0.6471	0.5894	–467.231044	104.5	85.39	25.14	65.34	357.7
6-311++G(d,p)	1.6500	0.6468	0.5891	–467.231273	103.9	85.36	25.14	65.35	359.3
6-31G(df,pd)	1.6475	0.6580	0.5990	–467.131457	365.9	85.14	27.24	63.27	309.3
6-31+G(df,pd)	1.6477	0.6427	0.5858	–467.147694	323.3	84.87	25.39	65.21	352.9
6-31++G(df,pd)	1.6485	0.6414	0.5849	–467.148109	322.2	84.71	25.41	65.22	351.9
6-311G(df,pd)	1.6546	0.6539	0.5954	–467.242495	74.4	85.41	25.76	64.72	341.8
6-311+G(df,pd)	1.6553	0.6482	0.5906	–467.248997	57.3	85.23	25.11	65.41	357.5
6-311++G(df,pd)	1.6555	0.6480	0.5904	–467.249311	56.5	85.21	25.12	65.40	356.5
6-31G(3df,3pd)	1.6493	0.6619	0.6011	–467.158828	294.1	86.16	25.78	64.55	296.2
6-31+G(3df,3pd)	1.6518	0.6476	0.5899	–467.170277	264.0	85.13	24.93	65.61	–
6-31++G(3df,3pd)	1.6518	0.6477	0.5899	–467.170536	263.3	85.17	24.86	65.67	–
6-311G(3df,3pd)	1.6575	0.6524	0.5941	–467.262405	22.1	85.41	25.28	65.20	355.0
6-311+G(3df,3pd)	1.6583	0.6493	0.5914	–467.265640	13.6	85.32	24.68	65.82	377.3
6-311++G(3df,3pd)	1.6584	0.6492	0.5913	–467.265730	13.4	85.32	24.67	65.83	378.6
cc-pVDZ	1.6415	0.6551	0.5959	–467.111387	418.6	85.53	26.90	63.53	326.1
cc-pVTZ	1.6582	0.6502	0.5923	–467.270831	0.0	85.21	25.27	65.25	375.1
Experiment	1.6467	0.6822	0.6188			85.04	30.01	60.49	400.2

Table S-5 continued

Basis set	*A* / GHz	*B* / GHz	*C* / GHz	*E* / Hartree	rel. *E* kJ/mol	∠(i,*a*) / °	∠(i,*b*) / °	∠(i,*c*) / °	V_3 / cm^{-1}
B3PW91									
6-31G	1.6467	0.6549	0.5972	–466.804260	740.5	84.92	27.06	63.50	269.2
6-31+G	1.6452	0.6444	0.5880	–466.819198	701.3	84.93	25.17	65.42	291.0
6-31++G	1.6451	0.6439	0.5878	–466.819854	699.6	84.81	25.26	65.36	291.0
6-311G	1.6515	0.6525	0.5957	–466.904331	477.8	84.68	26.74	63.88	–
6-311+G	1.6495	0.6494	0.5927	–466.910758	460.9	85.02	25.63	64.93	–
6-311++G	1.6493	0.6491	0.5927	–466.911294	459.5	84.86	25.92	64.67	293.8
6-31G(d,p)	1.6575	0.6621	0.6026	–466.945225	370.4	85.16	26.93	63.58	302.0
6-31+G(d,p)	1.6556	0.6529	0.5945	–466.958899	334.5	85.13	25.45	65.08	333.1
6-31++G(d,p)	1.6559	0.6524	0.5941	–466.959274	333.5	85.11	25.39	65.15	334.0
6-311G(d,p)	1.6601	0.6616	0.6020	–467.042968	113.8	85.67	25.74	64.68	341.1
6-311+G(d,p)	1.6598	0.6577	0.5986	–467.048292	99.8	85.55	25.12	65.34	352.9
6-311++G(d,p)	1.6600	0.6575	0.5984	–467.048574	99.1	85.54	25.09	65.36	353.9
6-31G(df,pd)	1.6592	0.6632	0.6039	–466.954869	345.1	84.94	27.07	63.48	308.2
6-31+G(df,pd)	1.6577	0.6536	0.5953	–466.967678	311.5	85.14	25.20	65.34	337.1
6-31++G(df,pd)	1.6581	0.6530	0.5948	–466.968070	310.4	85.07	25.18	65.38	339.4
6-311G(df,pd)	1.6648	0.6629	0.6032	–467.058486	73.0	85.62	25.50	64.93	341.9
6-311+G(df,pd)	1.6648	0.6589	0.5999	–467.064343	57.7	85.39	25.09	65.39	353.0
6-311++G(df,pd)	1.6649	0.6587	0.5997	–467.064710	56.7	85.39	25.08	65.41	351.5
6-31G(3df,3pd)	1.6607	0.6669	0.6059	–466.979482	280.5	85.92	25.53	64.84	311.5
6-31+G(3df,3pd)	1.6622	0.6565	0.5978	–466.989024	255.4	85.21	24.78	65.75	374.6
6-31++G(3df,3pd)	1.6622	0.6567	0.5979	–466.989244	254.8	85.26	24.72	65.80	372.8
6-311G(3df,3pd)	1.6678	0.6613	0.6019	–467.077793	22.3	85.51	24.96	65.50	356.6
6-311+G(3df,3pd)	1.6682	0.6591	0.6000	–467.080501	15.2	85.47	24.46	66.02	375.1
6-311++G(3df,3pd)	1.6683	0.6589	0.5999	–467.080603	15.0	85.46	24.44	66.04	376.4
cc-pVDZ	1.6525	0.6616	0.6018	–466.946295	367.6	85.59	26.69	63.73	348.9
cc-pVTZ	1.6687	0.6579	0.5991	–467.086305	0.0	85.25	24.87	65.65	377.3
Experiment	1.6467	0.6822	0.6188			85.04	30.01	60.49	400.2

Figure S-1

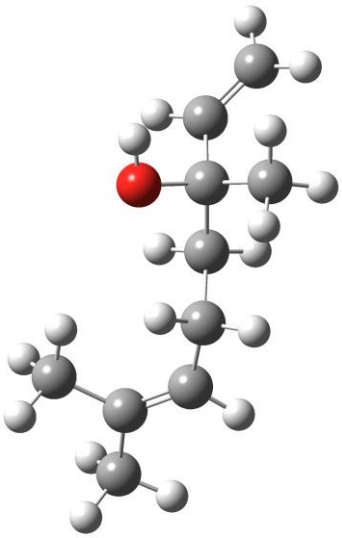

Fig. S-1 Conformer S-I of linalool (prolate shape)

Figure S-2

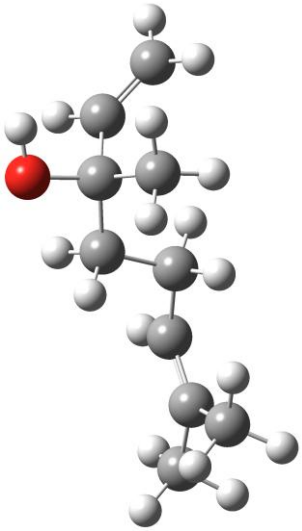

Fig. S-2 Conformer S-II of linalool (prolate shape)