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Research Article

The dimerization of α-phellandrene: Implications for *Boswellia* chemotaxonomy

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Abstract

Frankincense oleogum resin essential oils, rich in α-phellandrene, often contain small amounts of several α-phellandrene dimers. The desert habitats of frankincense (*Boswellia* spp.) trees expose the resins to both heat and sunlight, which could promote the dimerization reactions of α-phellandrene. We hypothesized that thermally and/or photochemically-allowed cycloaddition reactions account for the formation of α-phellandrene dimers. In this study, the profiles of α-phellandrene dimers from several *Boswellia* species were analyzed by GC-MS and compared. In addition, both thermal and photochemical reactions of α-phellandrene were carried out and the reaction mixtures were also analyzed by GC-MS. These results, coupled with density functional theory (DFT) calculations (ωB97X-D/6-31G*), suggest that photochemically allowed [2 + 2] cycloaddition reactions are important contributors to the formation of α-phellandrene dimers in frankincense essential oils. These results also contribute to the body of *Boswellia* chemotaxonomic markers, particularly between *B. sacra* and *B. carteri*.

1. Introduction

Dimers of α-phellandrene are conspicuous, albeit minor, components of frankincense (*Boswellia* Roxb. ex Colebr. species) oleogum resin essential oils [1–9]. Indeed, at least eight different α-phellandrene dimers have been detected in *Boswellia* volatiles [5]. The desert geographical locations of *Boswellia* species expose the resins to both heat and sunlight, both of which might alter resin chemistry. We hypothesize that either thermally or photochemically allowed (or both) cycloaddition reactions account for the α-phellandrene dimers found in frankincense essential oils. In order to shed some light on the dimers of α-phellandrene, both thermal and photochemical dimerization reactions of α-phellandrene were carried out. Based on the presence of α-phellandrene dimers in several *Boswellia* essential oils, the purpose of this study is to examine the distribution of α-phellandrene dimers and to carry out quantum chemical calculations (ωB97X-D/6-31G*) on the possible cycloaddition dimerization reactions. It has been

Table 1. α-Phellandrene dimers (relative distributions within the total detected dimer fraction) from *Boswellia* oleogum resin essential oils and thermal and photochemical reactions of α-phellandrene.

RI	*B. carteri* (n = 12)	*B. frereana* (n = 10)	*B. rivae* (n = 8)	*B. sacra* (n = 13)	Thermal	Photochemical
1726	0.0	0.0	0.8 ± 1.3	0.2 ± 0.6	1.4	0.0
1735	0.2 ± 0.8	2.3 ± 0.3	0.3 ± 0.9	0.0	2.6	2.1
1740	0.0	0.1 ± 0.1	0.0	2.8 ± 3.0	0.8	0.0
1749	0.0	0.0 ± 0.1	0.0	0.1 ± 0.3	1.7	0.7
1761	0.0	0.0	0.7 ± 1.2	0.0	0.0	0.0
1766	0.0	0.2 ± 0.4	0.0	0.0	38.3	0.0
1774	0.0	0.1 ± 0.3	0.0	0.0	2.9	0.0
1781	0.0	0.2 ± 0.3	0.0	0.0	4.1	0.0
1794	**46.0 ± 11.0**	**66.0 ± 1.5**	**70.8 ± 5.5**	**63.6 ± 9.0**	3.7	63.3
1797	**8.8 ± 5.1**	**0.1 ± 0.2**	**0.0**	**0.0**	0.0	0.0
1801	**5.3 ± 5.0**	**10.1 ± 1.9**	**10.5 ± 1.7**	**10.6 ± 2.1**	4.2	6.1
1806	0.0	0.2 ± 0.3	0.0	0.0	17.0	0.0
1813	3.0 ± 5.5	1.6 ± 0.5	1.0 ± 0.8	2.4 ± 1.2	3.1	1.4
1825	1.0 ± 2.6	1.6 ± 0.3	1.1 ± 1.0	1.9 ± 0.8	0.0	1.4
1829	**1.0 ± 2.6**	**9.3 ± 0.6**	**9.9 ± 0.6**	**8.9 ± 1.3**	0.0	7.7
1832	0.0	0.7 ± 0.3	0.6 ± 0.5	0.3 ± 0.4	0.0	0.0
1839	0.0	0.8 ± 0.3	1.3 ± 2.0	0.9 ± 0.5	8.6	1.1
1864	**4.5 ± 5.7**	**0.0**	**0.0**	**0.0**	0.0	0.9
1868	3.4 ± 4.7	0.0	0.0	1.1 ± 1.2	0.0	0.0
1904	**15.0 ± 6.2**	**0.0**	**0.0**	**4.5 ± 5.5**	4.5	6.8
1906	1.0 ± 3.6	2.3 ± 1.6	0.2 ± 0.4	0.0	0.0	0.0
1912	**8.8 ± 7.7**	**2.3 ± 1.0**	**2.2 ± 3.7**	**3.8 ± 3.0**	2.2	5.3

RI = Experimentally determined retention index using the arithmetic formula of van den Dool and Kratz [14]. The α-phellandrene dimers used in the ANOVA comparison are highlighted in bold. The *Boswellia* sample data taken from previously published studies (*B. frereana*, *B. rivae*, *B. sacra*) or newly generated in the present study (*B. carteri*, *B. sacra*).

pointed out that density functional theory (DFT) calculations generally perform better than post Hartree-Fock methods for pericyclic reactions [10, 11]. Additionally, we provide commentary on the chemotaxonomic applications of α-phellandrene dimers to distinguish between closely related species.

2. Materials and methods

2.1. Thermal reaction of α-phellandrene

α-Phellandrene (63.8%, Sigma-Aldrich, St. Louis, MO, USA), 2 mL, was sealed in an NMR tube (Norell NRS5600HWIPV7 heavy-wall glass NMR tube, Sigma-Aldrich, St. Louis, MO, USA) and heated to 140-150 °C in a sand bath for 16 h. After the reaction, the NMR tube was opened and the reaction mixture analyzed by GC-MS (Table 1).

2.2. Photochemical reaction of α-phellandrene

α-Phellandrene (63.8%, Sigma-Aldrich, St. Louis, MO, USA), 2 mL, was sealed in a quartz NMR tube (Wilmad Z562890 quartz NMR tube, Sigma-Aldrich, St. Louis, MO, USA) and exposed to UV radiation (365 nm, 72 h) using a FisherBiotech UV lamp, model FBUVLS-80, (FisherBiotech, Pittsburgh, PA, USA). After the reaction, the NMR tube was opened and the reaction mixture analyzed by GC-MS (Table 1).

2.3. Hydrodistillation of Boswellia oleogum resins

The oleogum resins of *Boswellia* species were hydrodistilled as previously described [8,9,12,13].

2.4. Gas chromatography – mass spectrometry (GC-MS)

The oleogum resins of *Boswellia* species were analyzed by GC-MS. Instrument: Shimadzu GC-MS-QP2010 Ultra (Shimadzu Scientific Instruments, Columbia, MD, USA). GC Column: Zebron ZB-5ms fused silica capillary column (60 m × 0.25 mm × 0.25 µm film thickness) (Phenomenex, Torrance, CA, USA). MS detector conditions: Electron impact (EI) mode, electron energy = 70 eV, scan range = 40–400 atomic mass units, scan rate = 3.0 scans/second. Carrier gas,

conditions: Helium, column head pressure = 208.3 kPa, flow rate = 2.00 mL/min. Injector, detector temperatures: Injector temperature = 260 °C, interface temperature = 260 °C, ion source temperature = 260 °C. GC oven temperature program: Initial temperature = 50 °C, ramp 2 °C/min to 260 °C, hold 260 °C for 5 min. Sample concentration, volume injected: 5% (in dichloromethane), 0.1 µL volume. Split mode: 24.5 : 1.0. Retention index values were calculated using the van den Dool and Kratz method [14]. Percentages of the essential oil components were calculated based on peak integration without standardization.

2.5. Statistical analysis

Analysis of variance was conducted by one-way ANOVA, followed by Tukey's post hoc test using Minitab® 18 (Minitab Inc., State College, PA, USA). Differences at $p < 0.05$ were considered to be statistically significant.

2.6. Computational methods

All calculations were carried out using Spartan '24 for Windows, v. 1.3.1 (Wavefunction, Inc., Irvine, CA, USA). Initial conformational analyses were carried out on α-phellandrene and each of the dimeric products using a Monte-Carlo molecular mechanics conformational search using the MMFF force field [15]. For each compound, the lowest-energy conformations from the MMFF conformational analysis were then modeled using density functional theory with the ωB97X-D functional [16] and the 6-31G* basis set [17] for the optimization of the structures in the gas phase as well as transition-state structures. Frequency calculations were used to characterize stationary points as minima or first-order saddle points. Considered to be one of the best hybrid generalized gradient approximation (GGA) functionals [18], the ωB97X-D functional was selected for this study.

3. Results and discussion

Commercial α-phellandrene was analyzed by GC-MS and was found to be composed of 63.8% α-phellandrene, 35.9% other monoterpenoids and an unidentified diterpenoid (0.3%). The GC-MS data for commercial α-phellandrene are presented in Table 2. There were no α-phellandrene dimers detected in commercial α-phellandrene.

Table 2. Chemical composition of commercial (Sigma-Aldrich, St. Louis, MO, USA) α-phellandrene.

RI_{calc}	RI_{db}	Compounds	Composition (%)
932	933	α-Pinene	0.6
972	972	Sabinene	0.4
977	978	β-Pinene	2.6
989	989	Myrcene	6.2
1000	1000	δ-2-Carene	0.6
1008	1007	α-Phellandrene	63.8
1017	1017	α-Terpinene	2.3
1025	1025	*p*-Cymene	8.6
1029	1030	Limonene	1.5
1033	1032	1,8-Cineole	10.8
1173	1173	Borneol	0.5
1203	1202	*cis*-Sabinol	1.5
1247	---	Unidentified monoterpenoid	0.3
1826	---	Unidentified diterpenoid	0.3

RI_{calc} = Retention index calculated with respect to a homologous series of *n*-alkanes on a ZB-5ms column. RI_{db} = Reference retention index from the databases.

Dimerization reactions of α-phellandrene led to a total of 17 compounds with mass spectra (Fig. 1) consistent with dimers of α-phellandrene (Table 1). Treatment of commercial α-phellandrene, 140-150 °C for 16 h, resulted in the formation of small amounts of α-phellandrene dimers (2.9% of the total composition) (Table 1). The major α-phellandrene dimers from the thermal treatment had RI values of 1766 (38.3%), 1806(17.1%), and 1829 (8.6%). Conversely, the photochemical reaction of α-phellandrene under UV light gave a very different profile of α-phellandrene dimers with RI 1794 (63.3%) dominating along with RI 1801 (6.1%), RI 1829 (7.7%), RI 1904 (6.8%), and RI 1912 (5.3%) (Table 1). The yield of α-phellandrene dimers after UV treatment of α-phellandrene was 3.1%.

Most of these dimers were also observed in *Boswellia* oleo-gum resin essential oils, including *B. frereana* Birdw. from Somaliland [7], *B. rivae* Engl. from Ethiopia [8], *B. sacra* Flück. from Oman [9], and *B. carteri* Birdw. from Somaliland. Although World Flora Online [20] considers *B. carteri* to be a synonym of *B. sacra*, we use *B. carteri* here to refer to the Somalia populations of *B. sacra* due to the distinct chemistry, research history, and market positioning. Not surprisingly, there are several *Boswellia* species that did not show the presence of α-phellandrene dimers,

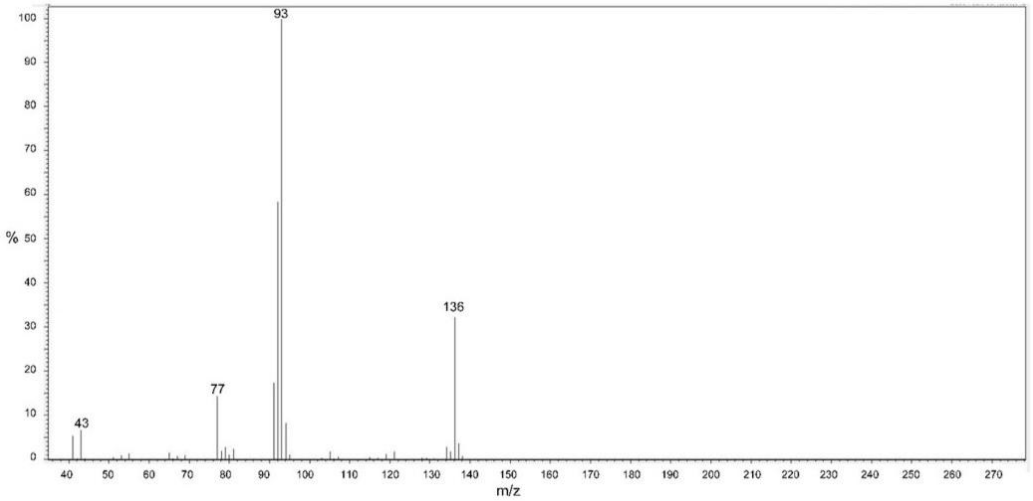

Figure 1. Mass spectrum of α-phellandrene dimer from the photochemical reaction (RI 1794). Note: Mass spectra of all α-phellandrene dimers are similar: MS(EI): 136(35%), 93(100%), 92(60%), 77(15%), 43(7%). A molecular ion at m/z 272 was not observed; each dimer undergoes retro-cycloaddition under MS conditions to give a spectrum that looks like α-phellandrene. This phenomenon is sometimes observed for retro-pericyclic reactions [19].

including *B. dalzielii* Hutch. [13, 21], *B. occulta* Thulin, DeCarlo, & S.P. Johnson [22, 23], *B. ogadensis* Vollesen [24], and *B. papyrifera* (Delile) Hochst. [25], which can be attributed to the low concentrations (only trace amounts) of α-phellandrene.

The major α-phellandrene dimers in the *Boswellia* (*B. carteri*, *B. frereana*, *B. rivae*, *B. sacra*) essential oils were RI 1794, RI 1797, RI 1801, RI 1829, RI 1864, RI 1904, and RI 1912, which are summarized in Table 1. The distributions of the α-phellandrene dimers were similar for *B. frereana*, *B. rivae*, and *B. sacra*, but *B. carteri* showed a significantly different profile (Fig. 2 shows the ANOVA (Tukey) comparison between the distributions of α-phellandrene dimers in *Boswellia* oleogum essential oils). The distributions of α-phellandrene dimers in the resin essential oils of *Boswellia* species do not correspond to the distribution from the thermal reaction. However, the photochemical reaction of α-phellandrene does show some similarities (Table 1).

It has long been debated whether *B. sacra* (growing in southern Arabia) and *B. carteri* (growing in Somalia and Somaliland) are the same or are different species. It is generally recognized botanically as one variable species under the name *B. sacra*, but chemists in particular continue to dispute this classification given the often-pronounced differences in oleo-gum resin essential oil composition and chirality [26, 27]. These results follow the same pattern, with RI 1794, RI 1797, RI 1801, RI 1829, and RI 1864 in particular being useful for distinguishing between the two "species". While this doesn't prove speciation, it contributes to the growing set of chemical markers differentiating their oleo-gum resins.

The energies of the [4 + 2] and [2 + 2] cycloaddition dimerization reactions for α-phellandrene were calculated using density functional theory (DFT) at the ωB97X-D/6-31G* level. There are eight possible [4 + 2] cycloaddition dimerization reactions for α-phellandrene. The products from these eight [4 + 2] cycloadditions are shown in Fig. 3. Based on the thermodynamic stabilities and the transition-state energies for the [4 + 2] cycloaddition reactions, there are four major [4 + 2] cycloaddition dimers (A, B, C, and D). Based on both the transition-state energies and the relative energies of the final dimeric products, formation of dimer D is the lowest-energy path for the thermal [4 + 2] dimerization of α-phellandrene. The reaction profile for dimer D is shown in Fig. 4.

In the doctoral dissertation of Simla Basar [1], an α-phellandrene dimer from *Boswellia frereana* was isolated and characterized by ^{1}H and ^{13}C NMR spectroscopy. The NMR data were consistent with a [2 + 2] dimer of α-phellandrene. There are 4 possible [2 + 2] cycloadducts of α-phellandrene (Fig. 5). All of these have either mirror-plane or 2-fold symmetry,

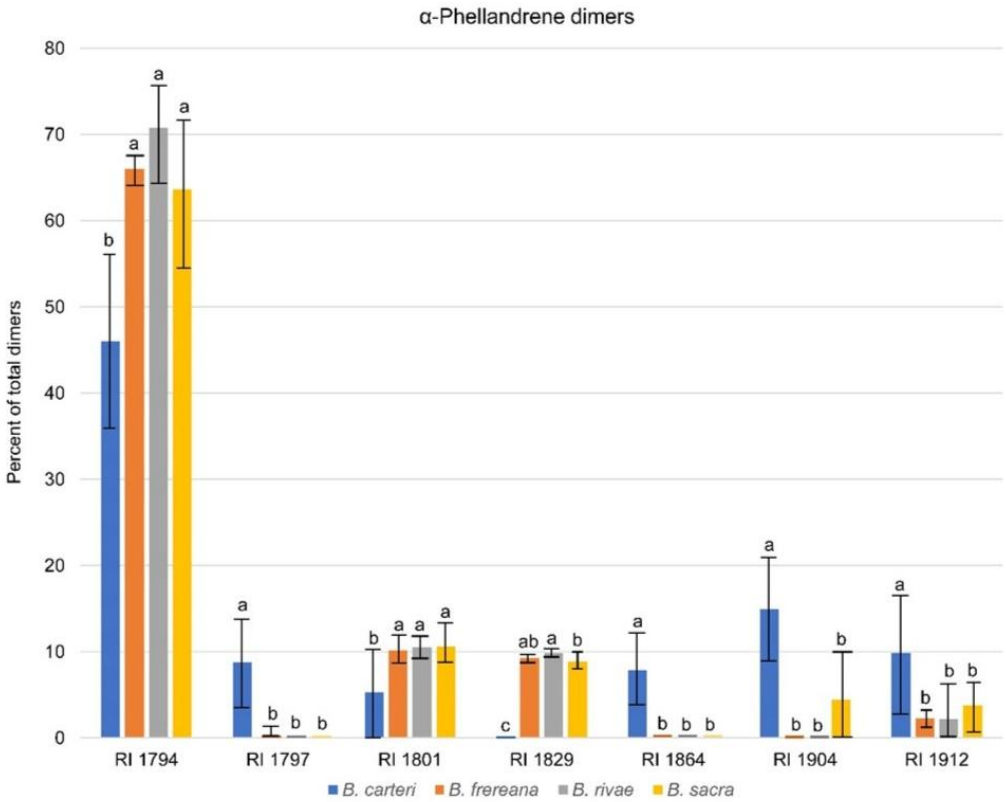

Figure 2. Distributions of major α-phellandrene dimers in *Boswellia* oleogum resin essential oils. Compounds with the same letter for each dimer are not significantly different ($p > 0.05$, ANOVA, Tukey).

which is consistent with the NMR data.

The dimeric structure shown in Basar's dissertation [1] and re-iterated by Mertens and co-authors [3], however, is the highest-energy ground-state structure of the four possible cycloadducts (dimer I in Fig. 5). Based on the calculated thermodynamic characteristics, it is more likely that dimer L is the thermal [2 + 2] cycloadduct described by Basar. The transition-state energies shown in Fig. 5 are for the ground-state (thermal) cycloaddition. Thermal [2 + 2] cycloadditions are symmetry disallowed, which accounts for the relatively high transition-state energies compared to those for [4 + 2] cycloadditions. It does not rule out, however, a sequential rather than concerted dimerization mechanism.

The [2 + 2] cyclization is photochemically allowed. The calculated relative energies (relative to the energies of the ground-state monomers) of the singlet excited states for the four [2 + 2] dimers are 82.6 kcal/mol, 79.2 kcal/mol, 81.7 kcal/mol, and 103.4 kcal/mol for dimers I, J, K, and L (Fig. 6), respectively, which predicts a Boltzmann distribution of 98.3% for dimer J, even though the ground state energy of dimer L is lower (Fig. 5). Interestingly, however, the transition-state energies favor formation of [2 + 2] dimer I. The relative transition-state energies ($\Delta E^{\ddagger}$, relative to the ground state monomers) are 106.6, 114.2, 126.8, and 123.9 kcal/mol for dimers I, J, K, and L, respectively. Dimer I is the dimer proposed by Basar [1]. Therefore, under kinetic control and photochemical conditions, dimer I is predicted to be the major product, but under thermodynamic control, dimer J should be preferred. The reaction profile for the photochemical [2 + 2] cycloaddition reaction of α-phellandrene forming dimers I and J is shown in Fig. 7.

Based on the general agreement of the distribution of α-phellandrene dimers from the photochemical reaction with those found in *Boswellia* oleogum resin essential oils, we can conclude that the results suggest that the major dimer in the essential oils is likely dimer I, the dimeric structure proposed by Basar [1], and results from exposure of the resin to sunlight.

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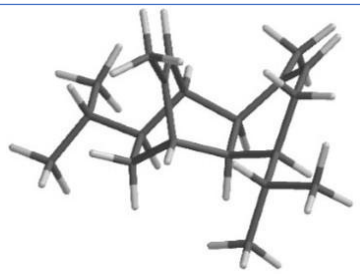
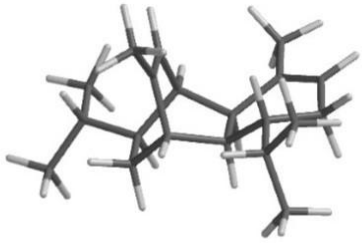


Dimer A

ΔE –41.3 kcal/mol, Boltzmann distribution 15.4%

ΔE‡ 19.7 kcal/mol, Boltzmann distribution 14.3%



Dimer B

ΔE –41.3 kcal/mol, Boltzmann distribution 15.2%

ΔE‡ 21.2 kcal/mol, Boltzmann distribution 1.2%

Dimer C

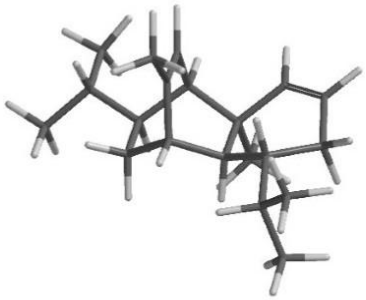
ΔE –41.1 kcal/mol, Boltzmann distribution 10.4%

ΔE‡ 20.5 kcal/mol, Boltzmann distribution 3.7%

Dimer D

ΔE –42.1 kcal/mol, Boltzmann distribution 55.5%

ΔE‡ 18.6 kcal/mol, Boltzmann distribution 80.6%



Dimer E

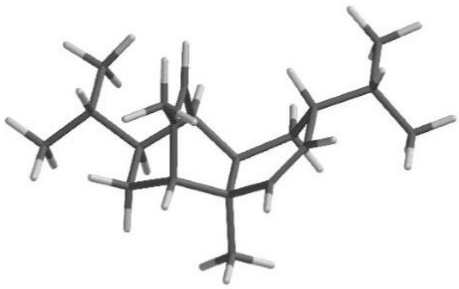
ΔE –37.9 kcal/mol, Boltzmann distribution 0.1%

ΔE‡ 24.2 kcal/mol, Boltzmann distribution 0.0%

Dimer F

ΔE –38.7 kcal/mol, Boltzmann distribution 0.2%

ΔE‡ 23.9 kcal/mol, Boltzmann distribution 0.0%



Dimer G

ΔE –40.4 kcal/mol, Boltzmann distribution 3.0%

ΔE‡ 22.1 kcal/mol, Boltzmann distribution 0.2%

Dimer H

ΔE –39.0 kcal/mol, Boltzmann distribution 0.3%

ΔE‡ 24.1 kcal/mol, Boltzmann distribution 0.0%

Figure 3. α-Phellandrene dimers from [4 + 2] cycloaddition reactions of α-phellandrene. ΔE = Electronic energies (kcal/mol, ωB97X-D/6-31G*) relative to two monomeric α-phellandrenes and Boltzmann distribution based on ΔE (298.15 K). ΔE‡ = Transition-state energies (kcal/mol) and the corresponding Boltzmann distributions.

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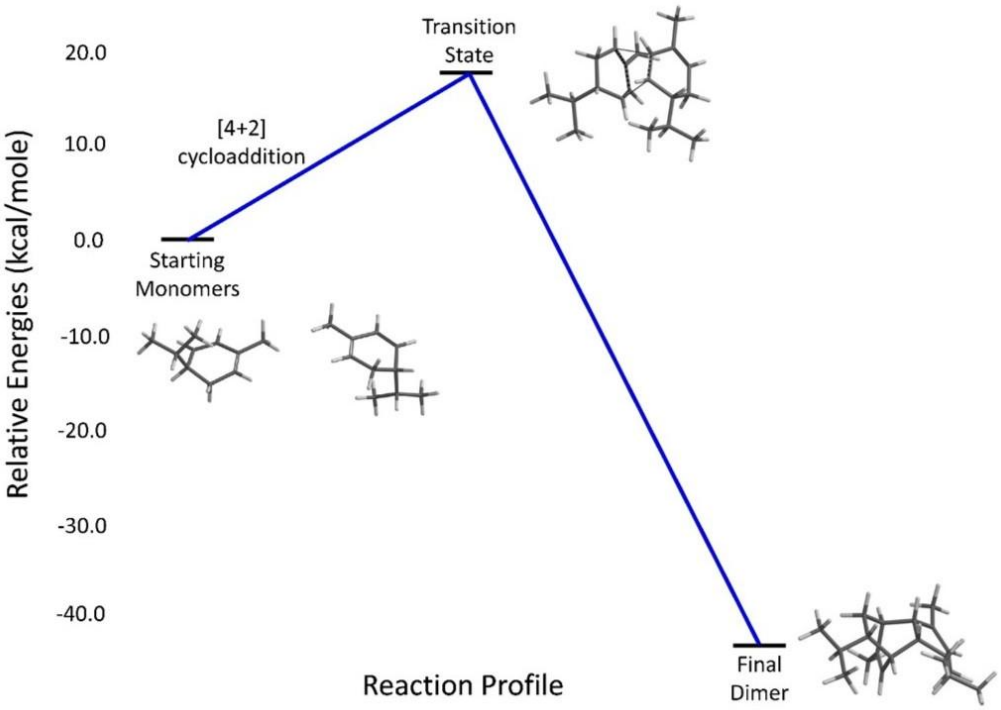

Figure 4. Reaction profile (ωB97X-D/6-31G*) for the thermally-allowed [4 + 2] cycloaddition reaction leading to formation of dimer D.

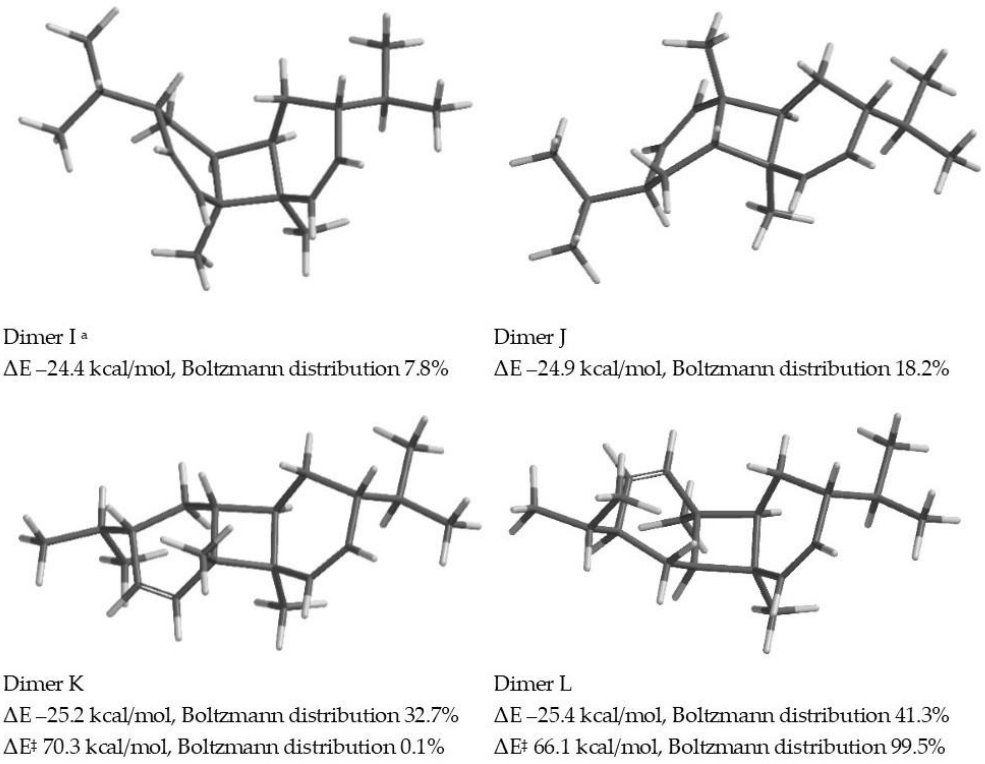

Figure 5. α-Phellandrene dimers from thermal [2 + 2] cycloaddition reactions of α-phellandrene. ΔE = Electronic energies (kcal/mol, ωB97X-D/6-31G*) relative to two monomeric α-phellandrenes and Boltzmann distribution based on ΔE (298.15 K). ΔE‡ = Transition-state energies (kcal/mol, ωB97X-D/6-31G*) and the corresponding Boltzmann distributions. [a] This is the structure proposed by Basar [1].

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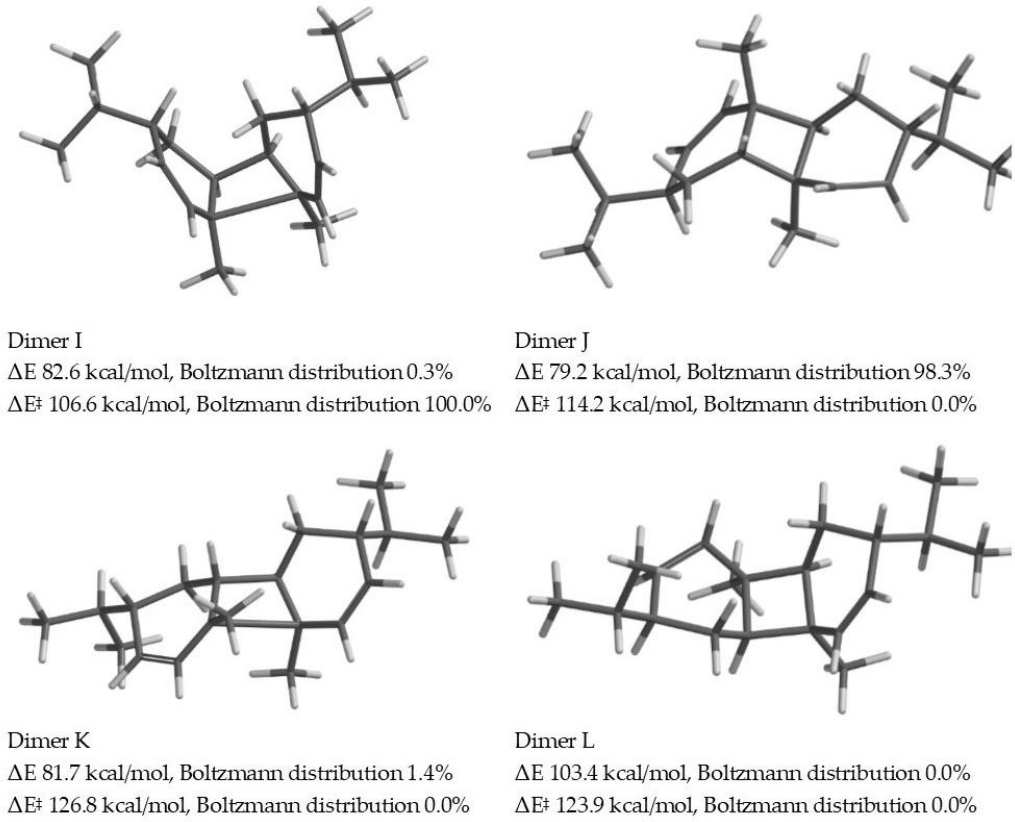

Figure 6. α-Phellandrene dimers from photochemical [2 + 2] cycloaddition reactions of α-phellandrene. ΔE = Electronic energies (kcal/mol, ωB97X-D/6-31G*) relative to two monomeric α-phellandrenes and Boltzmann distribution based on ΔE (298.15 K). ΔE‡ = Transition-state energies (kcal/mol, ωB97X-D/6-31G*) and the corresponding Boltzmann distributions.

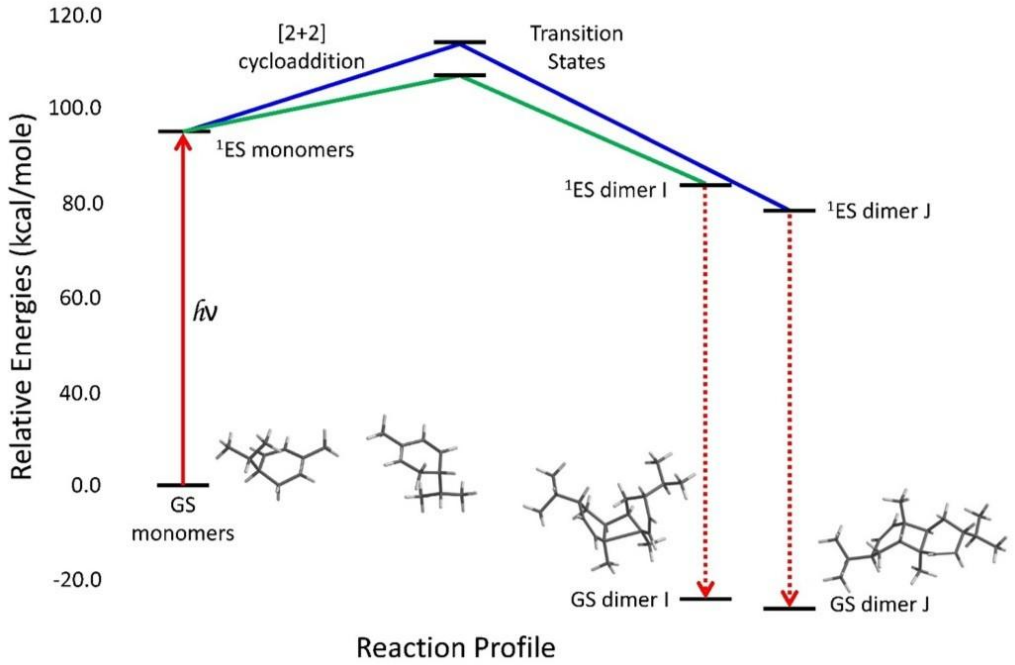

Figure 7. Reaction profile (ωB97X-D/6-31G*) for the photochemically-allowed [2 + 2] cycloaddition reaction leading to formation of dimers I and J. GS = ground state, hν = photochemical excitation, ¹ES = singlet excited state.

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4. Conclusions

Frankincense essential oils rich in α-phellandrene often contain small amounts of α-phellandrene dimers. The results of this study are consistent with the formation of several α-phellandrene dimers via photochemically-allowed [2 + 2] cycloaddition reactions; thermally-allowed [4 + 2] cycloaddition reactions appear less important. In addition, the [2 + 2] dimer proposed by Basar is consistent with the singlet excited-state [2 + 2] dimerization. There are several limitations to the present study. The computations were carried out in the gas phase (i.e., no solvent effects). The oleogum resin matrix may affect the reaction enthalpies. In addition to pericyclic cycloaddition mechanisms, other mechanisms for the dimerization may be possible. For example, it may be possible that other components in the *Boswellia* resins can act as triplet sensitizers, leading to diradical intermediates, which would further complicate the dimerization scenario. Future research should be carried out using higher-purity α-phellandrene for the dimerization, and to assign each α-phellandrene dimer to its corresponding RI value. Quantitative structure-retention relationship calculations may be useful.

Disclaimer (artificial intelligence)

Authors hereby state that no generative AI tools such as Large Language Models (ChatGPT, Copilot, etc.) and text-to-image generators were utilized in the preparation or editing of this manuscript.

Authors' contributions

Conceptualization, W.N.S.; methodology, P.S., W.N.S.; validation, P.S., W.N.S.; formal analysis, P.S., W.N.S.; investigation, P.S., S.J., A.D., W.N.S.; resources, P.S., S.J., W.N.S.; data curation, W.N.S.; writing—original draft preparation, S.J., W.N.S.; writing—review and editing, P.S., S.J., A.D., W.N.S.; visualization, W.N.S.; supervision, P.S., S.J., W.N.S.; project administration, S.J., W.N.S.

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Availability of data and materials

All data will be made available on request according to the journal policy.

Conflicts of interest

The authors declare no conflicts of interest.

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