(6*S*)-6-Isopropyl-3-methyl-9-oxo-2*E*,
4*E*-decadienoic Acid from Turkish
Nicotiana tabacum L., Assignment
of Absolute Configuration[†]

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A large number of the organoleptically important volatile constituents present in tobacco leaves and tobacco smoke have carbon skeletons reminiscent of those of the thunberganoid diterpenoids which appear to be generally present in tobacco.^{1,2)} The previously advanced hypothesis that the thunberganoids are the precursors of these volatiles has recently been supported by the fact that both the precursors and four of the postulated degradation products possess the same absolute configuration at the carbon atom carrying the isopropyl group.³⁻⁶⁾

Recently one of us (T. Chuman)⁷⁾ reported the isolation from Turkish tobacco and the structure elucidation of (–)-6-isopropyl-3-methyl-9-oxo-2*E*,4*E*-decadienoic acid (**1**, R=H). Since its carbon framework suggested a relationship with the thunberganoids, we have subjected the corresponding methyl ester (**1**, R=CH₃) to ozonolytic degradation to establish the chirality of the carbon atom carrying the isopropyl group. The methyl ester (**1**, R=CH₃, 10 mg) was treated with excess ozone at –60°C and the ozonide reduced with zinc/acetic acid as previously described³⁾ furnishing (2*S*)-2-isopropyl-5-oxohexanal (**2**, 2 mg). This exhibited spectral data (NMR,

IR, (GC)MS, [α]²⁰ +40° (589 nm), +46° (578), +50° (546), +126° (436), +330° (365), (c=0.1, CHCl₃); lit.³⁾ +43.7° (589 nm), +45.9° (578), +55.6° (546), +133.3° (436), +364.8° (365)) identical with those reported for the corresponding ketoaldehyde prepared similarly from solanone,⁸⁾ which has been correlated

with (2*S*)-2-isopropyl-5-oxohexanoic acid⁸⁾ by Fukuzumi and co-workers.⁴⁾ Hence, (6*S*)-6-isopropyl-3-methyl-9-oxo-2*E*,4*E*-decadienoic acid (**1**, R=H) can be allotted to the series of compounds which has the same chirality as their presumed thunberganoid precursors. The absolute configurations of the following thunberganoid degradation products have been previously established: (2*S*)-2-isopropyl-5-oxohexanoic acid,⁴⁾ solanone ((5*S*)-5-isopropyl-2-methyl-1,3*E*-nonadien-8-one),^{3,4)} nor-solanadione ((5*S*)-5-isopropyl-3*E*-nonen-2,8-dione)⁵⁾ and (7*S*)-7-isopropyl-4*ε*-methyl-10-oxo-5*E*-undecen-4-olide.³⁾

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