Table S1 Crystal data and structure refinement for compound **1** in orthorhombic form at room temperature after heating

Chemical formula	$C_{18}H_{16}$
Formula weight	232.31
Crystal system	Orthorhombic
Space group	*Pbca*
Temperature/K	Room temperature
a/Å	7.7439(5)
b/Å	9.8691(7)
c/Å	18.1365(12)
α/°	90.0
β/°	90.0
γ/°	90.0
V/Å^3	1386.09(16)
Z	4
Reflections collected	19949
Independent reflections	2022
R_{int}	0.0256
Data/parameters	2022/115
Goodness-of-fit on F^2	0.994
$R[F^2 > 2\sigma(F^2)]$	0.0398
$wR(F^2)$ (all data)	0.1130
ρ_{min} (e Å^{-3})	0.107
ρ_{max} (e Å^{-3})	-0.100

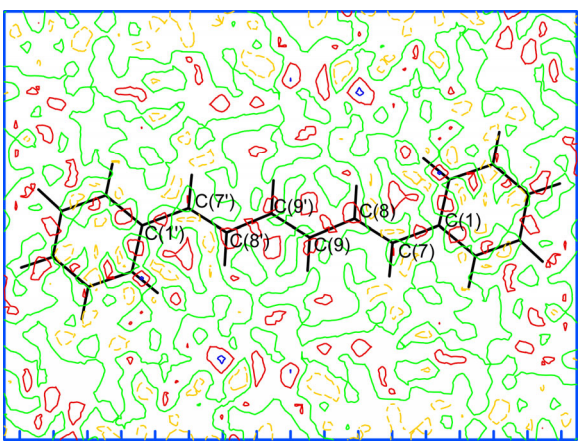

Fig. S1 A difference electron density map of orthorhombic crystal of *all-trans*-1,6-diphenyl-1,3,5-hexatriene (**1**) at room temperature after heating. The section of the map is the least-squares mean plane of eight central carbon atoms (C(1), C(7), C(8), C(9), C(9'), C(8'), C(7') and C(1')). The contour lines are at 0.05 e^{-3} intervals. Negative contours are indicated by broken lines.