Refinement of the disordered structures

(*Z*)-2-(9-anthrylmethylene)-1-indanone (*cis*-1)

The molecular structures of the irradiated *cis*-**1** crystal, which contains *cis*- and *trans*-**1,** were refined as follows. Only carbonyl oxygen and methylene hydrogen atoms of the two forms were refined at separate positions in the disorder model. H atoms were refined according to the riding model. All the C and O atoms were refined anisotropically.

Populations of the cis- and trans-forms were determined from the same refinement as above except that the disordered O atoms were refined isotropically using a common temperature factor. These O atoms were then refined anisotropically using a common temperature factor with the fixed populations.

(*E*)-2-(9-anthrylmethylene)-6-methyl-1-indanone (*trans*-2)

The molecular structures of the irradiated *trans*-**2** crystal, which contains *trans*- and *cis*-**2**, were refined as follows. All the C and O atoms of the product (*cis*-**1**) were refined as a rigid body, where the structures of the anthracene ring and the 2-methylene-1-indanone moiety were taken from those of *trans*-**2** before irradiation. H atoms were refined according to the riding model. All the C and O atoms were refined anisotropically. Each pair of the corresponding non-H atoms of *trans*- and *cis*-**2** were refined using a common temperature factor.

Populations of the trans- and cis-forms were determined from the same refinement as above except that all atoms were refined isotropically using a common temperature factor for all the C atoms and another temperature factor for the O atoms. The populations were held constant during the subsequent anisotropic refinement.

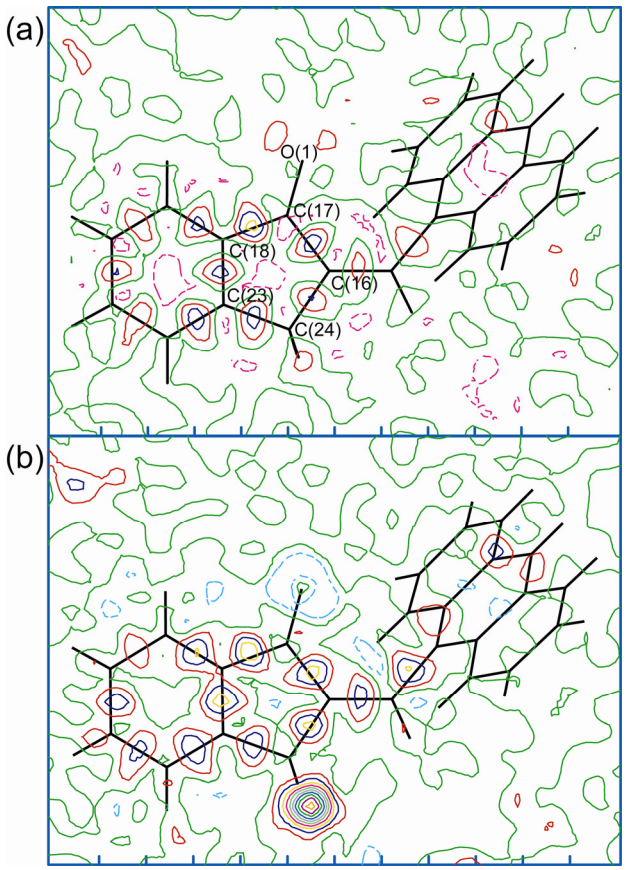

Fig. S1 Difference electron density maps of (*Z*)-2-(9-anthrylmethylene)-1-indanone (*cis*-**1**). The section of each map is the least-squares mean plane of five carbon atoms (C(16), C(17), C(18), C(23) and C(24)). The contour lines are at 0.1 eÅ^{-3} intervals. Negative contours are indicated by broken lines. (a) Before irradiation; (b) after 20 hr irradiation.

Table S1 Crystal data and structure refinements for compounds *cis*-**1** and *trans*-**2**

Compound	*cis*-**1**				*trans*-**2**	
Chemical formula	$C_{24}H_{16}O$				$C_{25}H_{18}O$	
Formula weight	320.37				334.39	
Crystal system	Monoclinic				Monoclinic	
Space group	$P2_1/a$				$C2/c$	
Irradiation time/hr	30	40	50	70	0	16
Temperature	Room temperature				Room temperature	
a/Å	11.6272(8)	11.6561(8)	11.7174(10)	11.8493(9)	18.769(2)	18.7933(11)
b/Å	13.9254(10)	13.9147(10)	13.8685(12)	13.8243(11)	10.7865(12)	10.8304(7)
c/Å	10.4577(8)	10.5076(8)	10.5133(9)	10.4921(8)	18.524(2)	18.5389(11)
β/°	102.408(1)	102.099(1)	101.625(2)	101.018(2)	108.689(2)	108.858(1)
V/Å^3	1653.7(2)	1666.4(2)	1673.4(2)	1687.0(2)	3552.4(7)	3570.8(4)
Z	4				8	
Reflections collected	25652	25641	25403	25739	26763	26883
Independent reflections	4837	4875	4909	4953	5215	5238
R_{int}	0.0301	0.0330	0.0448	0.0605	0.0316	0.0296
Data/restraints/parameters	4837/0/229	4875/0/229	4909/0/229	4953/0/229	5215/0/296	5238/0/243
Goodness-of-fit on F^2	1.033	1.032	1.027	1.026	1.042	1.031
$R[F^2 > 2\sigma(F^2)]$	0.0530	0.0602	0.0667	0.0664	0.0494	0.0545
$wR(F^2)$ (all data)	0.1601	0.1840	0.1897	0.1821	0.1426	0.1548
ρ_{min} (e Å^{-3})	0.259	0.300	0.267	0.239	0.278	0.261
ρ_{max} (e Å^{-3})	-0.163	-0.223	-0.217	-0.161	-0.224	-0.331