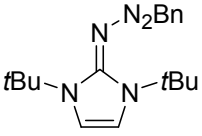
Supplementary Material (ESI) for Chemical Communications

Triazene formation via reaction of imidazol-2-ylidenes with azides

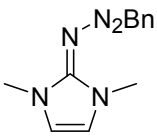
Dimitri M. Khramov and Christopher W. Bielawski*

Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712
Fax: (512) 471-8696; Tel: (512) 232-3839; E-mail: bielawski@mail.cm.utexas.edu

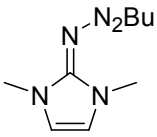
General Considerations. All reactions were performed under an atmosphere of argon at ambient temperature. Flasks were dried and cooled under atmosphere of nitrogen prior to use. Unless otherwise noted, solvents and reagents were purchased from Aldrich or Acros and used as received. Thin-layer chromatography was performed on EM 250 Kieselgel 60 F254 silica gel. The plates were developed by staining with Ceric Ammonium Nitrate (CAM) or I_2. ^{1}H-NMR and ^{13}C-NMR data was obtained on a Varian Unity Plus 300 or a Varian INOVA 400. Chemical shifts (δ) are expressed in ppm downfield from tetramethylsilane using the residual protonated solvent as an internal standard ($CDCl_3$, ^{1}H 7.24 ppm and ^{13}C 77.0 ppm; $(CD_3)_2SO$, ^{1}H 2.49 ppm and ^{13}C 39.5 ppm; C_6D_6, ^{1}H 7.15 ppm and ^{13}C 128.0 ppm). Coupling constants (*J*) are expressed in hertz. ^{13}C-NMR spectra were routinely run with broadband ^{1}H decoupling. Where appropriate, descriptions of signals include singlet (s), doublet (d), triplet (m), multiplet (m), and broad (br). HRMS (ESI, CI) were obtained with a VG analytical ZAB2-E instrument.



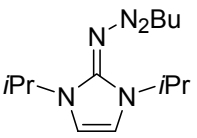
1-Benzyl-3-(1,3-di-*tert*-butylimidazol-2-ylidene)triazene (2). Benzyl azide (0.33 mmol, 44 mg) was added in one portion using a 1 mL syringe to a solution of 1,3-di-*tert*-butylimidazol-2-ylidene (0.33 mmol, 60 mg) in dry THF (1 mL). The solution was stirred overnight and solvent was removed to give pure product (102 mg, 99%) as yellow solid. ^{1}H-NMR (400 MHz, C_6D_6): δ 7.58 (d, *J* = 9.2 Hz, 2H), 7.22 (t, *J* = 9.2 Hz, 2H), 7.12-7.06 (m, 1H), 6.11 (s, 2H), 5.19 (s, 2H), 1.41 (s, 18H); ^{13}C-NMR (100 MHz, C_6D_6): δ 141.7, 129.1, 128.5, 126.6, 110.9, 65.2, 58.0, 29.7; HRMS calcd for $C_{18}H_{27}N_5$ [M+H$^+$]: 314.2345, found: 314.2340.



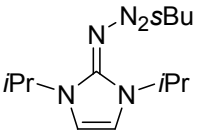
1-Benzyl-3-(1,3-dimethylimidazol-2-ylidene)triazene. Benzyl azide (1.95 mmol, 257 mg) was added in one portion using a 1 mL syringe to a slurry of methyl imidazolium iodide (0.97 mmol, 218 mg) in dry THF (4 mL). In one portion, NaH (1.07 mmol, 43 mg, 60% in mineral oil) was added to the reaction vessel and the resulting mixture was stirred for 12 h. After hexanes (1 mL) were added, the reaction mixture was filtered through Celite. Solvent was removed and pure product was obtained as a yellow solid (134 mg, 60%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.21-7.10 (m, 5H), 6.31 (s, 2H), 4.71 (s, 2H), 3.40 (s, 6H); ^{13}C-NMR (100 MHz, $CDCl_3$): δ 152.01, 138.7, 128.7, 128.1, 126.5, 115.9, 64.7, 35.4; HRMS calcd for $C_{12}H_{15}N_5$ [M+H$^+$]: 230.1406, found: 230.1408.



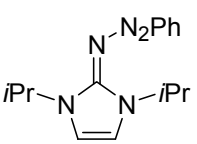
1-Butyl-3-(1,3-dimethylimidazol-2-ylidene)triazene. Butyl azide (0.95 mmol, 94 mg) was added in one portion using a 1 mL syringe to a slurry of methyl imidazolium iodide (0.79 mmol, 177 mg) in dry THF (3 mL). In one portion, KO*t*Bu (0.71 mmol, 80 mg) was added to the reaction vessel and the resulting mixture was stirred for 90 minutes. Excess hexanes (1 mL) were then added and the reaction mixture was filtered through Celite. Solvent was removed and pure product was obtained as a pale yellow solid (128 mg, 94 %). ^{1}H-NMR (400 MHz, C_6D_6): δ 5.47 (s, 2H), 3.89 (t, J = 7.2 Hz, 2H), 3.03 (s, 6H), 1.87 (pentet, J = 7.2, 2H), 1.51 (sextet, J = 7.2 Hz, 2H), 0.93 (t, J = 7.2 Hz, 3H); ^{13}C-NMR (100 MHz C_6D_6): δ 153.3, 114.9, 61.6, 34.8, 32.0, 21.2, 14.3; HRMS calcd for $C_9H_{15}N_5$ [M+H$^+$]: 196.1562, found: 196.1564.



1-Butyl-3-(1,3-di-*iso*-propylimidazol-2-ylidene)triazene. Butyl azide (0.5 mmol, 50 mg) was added in one portion using a 1 mL syringe to a slurry of isopropyl imidazolium chloride (0.5 mmol, 90 mg) in dry THF (3 mL). In one portion, KO*t*Bu (0.55 mmol, 47 mg) was added to the reaction vessel and the resulting mixture was stirred for 90 minutes. Hexanes (1 mL) were then added and the reaction mixture was filtered through Celite. Solvent was removed and pure product was obtained as white crystals (94 mg, 75 %). ^{1}H-NMR (400 MHz, C_6D_6): δ 5.98 (s, 2H), 5.08 (septet, J = 6.8 Hz, 2H), 3.94 (t, J = 6.8 Hz, 2H), 1.90 (pentet, J = 6.8 Hz, 2H), 1.52 (sextet, J = 7.2 Hz, 2H), 0.98 (d, J = 6.8 Hz, 12H), 0.92 (t, J = 7.2 Hz, 3H); ^{13}C-NMR (100 MHz C_6D_6): δ 151.5, 109.9, 61.7, 47.6, 32.2, 22.0, 21.2, 14.3; HRMS calcd for $C_{13}H_{25}N_5$ [M+H$^+$]: 252.2188, found: 252.2186.

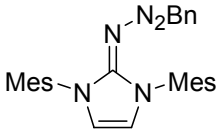


1-*sec*-Butyl-3-(1,3-di-*iso*-propylimidazol-2-ylidene)triazene. *sec*-Butyl azide (1.01 mmol, 99 mg) was added in one portion using a 1 mL syringe to a slurry of isopropyl imidazolium chloride (0.84 mmol, 158 mg) in dry THF (3 mL). In one portion, KO*t*Bu (0.75 mmol, 84 mg) was added to the reaction vessel and the resulting mixture was stirred for 180 minutes. Hexanes (1 mL) were then added and the reaction mixture was filtered through Celite. Solvent was removed and pure product was obtained as white crystals (150 mg, 81 %). ^{1}H-NMR (400 MHz, C_6D_6): δ 6.00 (s, 2H), 5.08 (septet, J = 6.8 Hz, 2H), 3.66 (sextet, J = 6.4 Hz, 1H), 2.05-1.94 (m, 1H), 1.77-1.67 (m, 1H), 1.40 (d, J = 6.4 Hz, 3H), 1.04 (t, J = 7.6 Hz, 3H), 0.98 (d, J = 6.8 Hz, 12H); ^{13}C-NMR (100 MHz C_6D_6): δ 151.6, 109.9, 67.1, 47.5, 30.1, 21.998, 21.952, 20.7, 11.6; HRMS calcd for $C_{13}H_{25}N_5$ [M+H$^+$]: 252.2188, found: 252.2188.

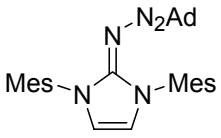


1-Phenyl-3-(1,3-di-*iso*-propylimidazol-2-ylidene)triazene. Phenyl azide (1.12 mmol, 130 mg) was added in one portion using a 1 mL syringe to a slurry of *iso*-propyl imidazolium chloride (0.93 mmol, 148 mg) in dry THF (3 mL). In one portion, KO*t*Bu (0.93 mmol, 105 mg) was added to the reaction vessel and the resulting mixture was stirred under argon for 4 hours. Hexanes (1 mL) were then added and the reaction mixture was filtered through Celite. Solvent was removed and pure product was obtained as a yellow solid (135 mg, 54%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.50 (d, J = 9.6, 2H), 7.31 (t, J = 7.6 Hz, 1H), 7.11 (t, J = 7.2 Hz), 6.65 (s, 2H), 5.17 (septet, J = 6.4 Hz, 2H), 1.40 (d,

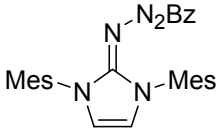
J = 6.4 Hz, 12H); ^{13}C-NMR (100 MHz $CDCl_3$): δ 152.3, 150.2, 128.7, 125.1, 120.9, 111.3, 48.0, 22.5 HRMS calcd for $C_{15}H_{21}N_5$ [M+H$^+$]: 272.1875, found: 272.1871.



1-Benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene (3). Benzyl azide (0.79 mmol, 105 mg) was added in one portion using a 1 mL syringe to a slurry of mesityl imidazolium chloride (0.53 mmol, 180 mg) in dry THF (3 mL). In one portion, KO*t*Bu (0.58 mmol, 65 mg) was added to the reaction vessel and the resulting mixture was stirred under argon for 2 hours. Excess hexanes (1 mL) were then added and the resulting mixture was filtered through Celite. After removal of solvent, the crude product was purified by flash chromatography (70% EtOAc/Hexanes) to afford product as pale yellow crystals (192 mg, 83%). Crystals suitable for X-ray analysis were grown by slow evaporation from ethyl acetate and were found to contain either the Z-isomer or the E-isomer. (Subtle factors governing the preferential formation of one geometric isomer over the other remain elusive, however the E-isomer has been found more often than the Z-isomer.) R_f = 0.33 (70% EtOAc/Hexanes); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.18-7.09 (m, 3H), 6.89 (br s, 6H), 6.44 (s, 2H), 4.04 (s, 2H), 2.28 (s, 6H), 2.14 (s, 12H); ^{13}C-NMR (100 MHz $CDCl_3$): δ 152.1, 138.5, 138.3, 135.6, 134.3, 128.9, 128.8, 127.8, 126.3, 116.0, 65.4, 21.0, 18.0; HRMS calcd for $C_{28}H_{31}N_5$ [M+H$^+$]: 438.2658, found: 438.2659.

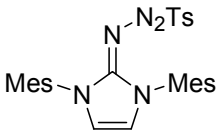


1-Adamantyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene. Mesityl imidazolium chloride (0.46 mmol, 156 mg) was added to dry toluene (3 mL) followed by addition of KO*t*Bu (0.46 mmol, 51 mg) in one portion. After stirring the slurry for 10 minutes, adamantyl azide (0.44 mmol, 77 mg) was added in one portion and the reaction mixture was stirred for 12 h. The solution was then filtered through Celite. Solvent was removed and the crude product was washed with hexanes (1 mL) to afford the product as light yellow crystals (0.125 g, 60%). R_f = 0.40 (20% EtOAc/Hexanes); ^{1}H-NMR (400 MHz, $CDCl_3$): δ 6.89 (s, 4H), 6.36 (s, 2H), 2.26 (s, 6H), 2.13 (s, 12H), 1.81 (br s, 3H), 1.54-1.50 (m, 3H), 1.42-1.39 (m, 3H), 1.17 (d, *J* = 2.4 Hz, 6H); ^{13}C-NMR (100 MHz $CDCl_3$): δ 152.4, 137.9, 135.6, 128.9, 115.9, 59.9, 40.9, 36.5, 29.4, 20.9, 18.0; HRMS calcd for $C_{31}H_{39}N_5$ [M+H$^+$]: 482.3248, found: 482.3315.

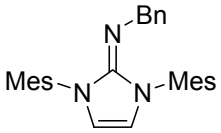


1-Benzoyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene. KO*t*Bu (0.59 mmol, 1 M in THF) was added to a slurry of mesityl imidazolium chloride (0.59 mmol, 200 mg) in dry THF (3 mL). After stirring the reaction for 15 minutes, benzoyl azide (0.59 mmol, 87 mg) was added in one portion using a 1 mL syringe and the reaction mixture was stirred for 12 h. The solution was then concentrated to approximately half the original volume and the resulting slurry was purified by flash chromatography (50% EtOAc/Hexanes gradually increasing to 80% EtOAc/Hexanes) to obtain product as orange crystals (0.197 g, 74 %). A crystal suitable for X-ray analysis was grown by slow evaporation from EtOAc. R_f = 0.20 (50% EtOAc/Hexanes); ^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 6.87 (s, 4H), 6.75 (s, 2H), 2.25 (s, 6H), 2.11 (s, 12H); ^{13}C-NMR (100 MHz $CDCl_3$): δ 178.2, 151.9, 139.1, 136.2,

134.8, 132.3, 131.2, 129.9, 129.0, 127.4, 118.5, 20.9, 17.7; HRMS calcd for $C_{28}H_{29}N_5O$ [M+H$^+$]: 452.2450, found: 452.2690.



1-Tosyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene. KO*t*Bu (0.71 mmol, 79 mg) was added to a slurry of mesityl imidazolium chloride (0.68 mmol, 230 mg) in dry THF (4 mL). After stirring the reaction mixture for 15 minutes, tosyl azide (0.74 mmol, 146 mg) was added in one portion using a 1 mL syringe. The reaction was then stirred for 12 h. Yellow precipitate formed which was collected by filtration and dried, giving pure product (310 mg, 92%) as yellow crystals. ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.11 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 7.02 (s, 4H), 6.84 (s, 2H), 2.38-2.37 (m, 9H), 2.05 (s, 12H); ^{13}C-NMR (100 MHz $CDCl_3$): δ 142.8, 140.1, 137.7, 135.3, 132.6, 129.6, 129.2, 127.8, 119.5, 21.6, 21.2, 17.8, HRMS calcd for $C_{28}H_{31}N_5O_2S$ [M+H$^+$]: 502.2277; found: 502.2520.



N-Benzyl 1,3-dimesityl-2-iminoimidazoline (4). Benzyl 1,3-dimesitylimidazol-2-ylidenetriazene (**3**) was dissolved in DMSO-d_6 and heated in an NMR tube to 120 °C for 3 hours to obtain the desired product in >95% yield. ^{1}H-NMR (400 MHz, $(CD_3)_2SO$): δ = 10.0 (s, 1H), 7.92-7.90 (m, 2H), 7.73-7.69 (m, 1H), 7.62-7.59 (m, 2H), 7.02 (s, 6H), 6.63 (s, 2H), 2.28 (s, 6H), 2.09 (s, 12H); ^{13}C-NMR (100 MHz, $(CD_3)_2SO$)): δ 192.3, 138.0, 136.4, 136.2, 134.6, 129.4, 129.2, 128.9, 113.6, 20.6, 17.4. HRMS calcd for $C_{28}H_{31}N_3$ [M+H$^+$]: 410.2596, found: 410.2595.

X-ray experimental for *(Z)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene ($C_{28}H_{31}N_5$): Crystals grew as pale yellow needles by slow evaporation from ethyl acetate. The data crystal was cut into an irregular shaped fragment that had approximate dimensions; 0.24 x 0.22 x 0.20 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 535 frames of data were collected using ω-scans with a scan range of 1° and a counting time of 142 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR97[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). There are two crystallographically unique molecules in the asymmetric unit. In one molecule, the orientation of the triaza portion is disordered about two orientations. The disorder was modeled by assigning the variable x to the site occupancy factors of one component of the disorder composed of atoms N6, N7, N8 and C9. The site occupancy factor of the alternate component, composed of atoms N6A, N7A, N8A and C9A, had a site occupancy factor of 1-x. A common isotropic displacement parameter was assigned to the relevant atoms while refining x. The variable, x, refined to 0.82(2). The geometry of the disordered moieties were restrained to be approximately equal throughout the refinement. The atoms of the minor component of the disorder were refined isotropically. The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.044*P)^2]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.137, with R(F) equal to 0.0576 and a goodness of fit, S, = 1.15. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (6.9(9)x10^{-6})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray

Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in Tables 1 through 7.

References

1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

2) SIR97. (1999). A program for crystal structure solution. Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. J. Appl. Cryst. 32, 115-119.

3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

4) $R_W(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$.
$S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for *(Z)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene.

Empirical formula	C28 H31 N5	
Formula weight	437.58	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.1191(1) Å	α= 104.680(1)°.
	b = 15.4148(2) Å	β= 92.260(1)°.
	c = 18.4677(3) Å	γ = 90.110(1)°.
Volume	2509.10(6) $Å^3$	
Z	4	
Density (calculated)	1.158 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	936	
Crystal size	0.24 x 0.22 x 0.20 mm	
Theta range for data collection	2.94 to 27.48°.	
Index ranges	-11<=h<=11, -19<=k<=20, -23<=l<=23	
Reflections collected	19912	
Independent reflections	11357 [R(int) = 0.0461]	
Completeness to theta = 27.48°	98.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11357 / 32 / 612	
Goodness-of-fit on F^2	1.152	
Final R indices [I>2sigma(I)]	R1 = 0.0576, wR2 = 0.1163	
R indices (all data)	R1 = 0.1595, wR2 = 0.1370	
Extinction coefficient	$6.9(9)x10^{-6}$	
Largest diff. peak and hole	0.298 and -0.228 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *(Z)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N1	7721(2)	3992(1)	2159(1)	40(1)
C2	6645(2)	3457(2)	1701(1)	48(1)
C3	6423(2)	3786(2)	1105(1)	51(1)
N4	7356(2)	4522(1)	1180(1)	39(1)
C5	8169(2)	4647(1)	1835(1)	37(1)
N6	9195(4)	5232(2)	2192(3)	43(1)
N7	9425(2)	5922(2)	1889(1)	45(1)
N8	10402(2)	6497(1)	2221(1)	45(1)
C9	11164(5)	6316(3)	2858(3)	61(1)
N6A	9244(17)	5257(12)	2003(10)	38(6)
N7A	10273(10)	5032(5)	2455(5)	41(2)
N8A	11155(9)	5621(5)	2816(5)	52(3)
C9A	10850(20)	6544(7)	2840(20)	108(15)
C10	12162(3)	7097(2)	3247(1)	53(1)
C11	13614(3)	6938(2)	3355(1)	64(1)
C12	14573(3)	7608(2)	3734(2)	72(1)
C13	14066(3)	8467(2)	4005(1)	65(1)
C14	12610(3)	8639(2)	3900(1)	58(1)
C15	11659(3)	7959(2)	3528(1)	52(1)
C16	8191(2)	3915(1)	2897(1)	40(1)
C17	9023(2)	3182(1)	2955(1)	41(1)
C18	9381(2)	3099(2)	3676(1)	49(1)
C19	8957(2)	3717(2)	4310(1)	56(1)
C20	8161(3)	4444(2)	4220(1)	62(1)
C21	7738(2)	4553(2)	3517(1)	51(1)
C22	9519(2)	2494(2)	2284(1)	54(1)
C23	9316(3)	3585(2)	5086(1)	86(1)
C24	6796(3)	5334(2)	3441(1)	76(1)
C25	7370(2)	5040(1)	627(1)	36(1)
C26	8043(2)	4678(1)	-43(1)	38(1)

C27	8008(2)	5182(1)	-572(1)	44(1)
C28	7332(2)	6006(2)	-443(1)	42(1)
C29	6638(2)	6324(1)	221(1)	42(1)
C30	6628(2)	5844(1)	766(1)	40(1)
C31	8767(2)	3777(1)	-209(1)	52(1)
C32	7395(3)	6548(2)	-1022(1)	63(1)
C33	5831(3)	6194(2)	1481(1)	60(1)
N1'	9055(2)	-556(1)	2377(1)	41(1)
C2'	9436(2)	-1418(2)	1998(1)	49(1)
C3'	8443(2)	-1706(2)	1436(1)	50(1)
N4'	7426(2)	-1020(1)	1460(1)	42(1)
C5'	7812(2)	-312(1)	2046(1)	37(1)
N6'	7194(2)	468(1)	2344(1)	40(1)
N7'	6244(2)	739(1)	1862(1)	48(1)
N8'	5492(2)	1431(1)	2152(1)	46(1)
C9'	5693(2)	1797(1)	2959(1)	43(1)
C10'	4797(2)	2625(1)	3245(1)	43(1)
C11'	5036(3)	3106(2)	3981(1)	60(1)
C12'	4240(3)	3876(2)	4274(2)	76(1)
C13'	3193(3)	4161(2)	3829(2)	72(1)
C14'	2939(3)	3684(2)	3103(1)	60(1)
C15'	3735(2)	2917(2)	2813(1)	48(1)
C16'	9869(2)	33(1)	2996(1)	41(1)
C17'	11130(2)	456(1)	2850(1)	44(1)
C18'	11894(2)	1011(1)	3459(1)	50(1)
C19'	11427(2)	1164(1)	4185(1)	48(1)
C20'	10144(2)	744(1)	4296(1)	49(1)
C21'	9341(2)	172(1)	3714(1)	44(1)
C22'	11626(2)	343(2)	2065(1)	62(1)
C23'	12289(3)	1777(2)	4827(1)	71(1)
C24'	7933(2)	-263(2)	3851(1)	60(1)
C25'	6062(2)	-1147(1)	1021(1)	39(1)
C26'	6058(2)	-1105(1)	278(1)	43(1)
C27'	4737(2)	-1243(1)	-133(1)	48(1)
C28'	3444(2)	-1438(1)	173(1)	47(1)
C29'	3515(2)	-1500(1)	906(1)	44(1)

C30'	4801(2)	-1350(1)	1351(1)	42(1)
C31'	7440(2)	-887(2)	-70(1)	60(1)
C32'	1999(2)	-1551(2)	-272(1)	65(1)
C33'	4810(2)	-1371(2)	2160(1)	55(1)

Table 3. Bond lengths [Å] and angles [°] for *(Z)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene.

N1-C5	1.367(2)	C11-H11	0.96
N1-C2	1.391(2)	C12-C13	1.379(3)
N1-C16	1.446(2)	C12-H12	0.96
C2-C3	1.331(3)	C13-C14	1.371(3)
C2-H2	0.96	C13-H13	0.96
C3-N4	1.393(2)	C14-C15	1.380(3)
C3-H3	0.96	C14-H14A	0.96
N4-C5	1.364(2)	C15-H15	0.96
N4-C25	1.447(2)	C16-C21	1.385(3)
C5-N6A	1.329(8)	C16-C17	1.386(3)
C5-N6	1.330(3)	C17-C18	1.395(3)
N6-N7	1.342(4)	C17-C22	1.498(3)
N7-N8	1.278(3)	C18-C19	1.379(3)
N8-C9	1.431(5)	C18-H18	0.96
N8-H9AA	1.4736	C19-C20	1.379(3)
N8-H9AB	0.5408	C19-C23	1.521(3)
C9-C10	1.517(3)	C20-C21	1.390(3)
C9-H9A	0.96	C20-H20A	0.96
C9-H9B	0.96	C21-C24	1.512(3)
C9-H9AA	1.3372	C22-H22C	0.96
C9-H9AB	1.1531	C22-H22A	0.96
N6A-N7A	1.335(11)	C22-H22B	0.96
N7A-N8A	1.250(7)	C23-H23A	0.96
N8A-C9A	1.440(10)	C23-H23B	0.96
N8A-H9A	0.6433	C23-H23C	0.96
N8A-H9B	1.2175	C24-H24C	0.96
C9A-C10	1.524(9)	C24-H24A	0.96
C9A-H9A	1.4002	C24-H24B	0.96
C9A-H9B	1.0085	C25-C30	1.384(3)
C9A-H9AA	0.96	C25-C26	1.390(3)
C9A-H9AB	0.96	C26-C27	1.392(3)
C10-C11	1.363(3)	C26-C31	1.505(3)
C10-C15	1.384(3)	C27-C28	1.382(3)
C11-C12	1.379(3)	C27-H27	0.96

C28-C29	1.380(3)	C13'-C14'	1.367(3)
C28-C32	1.516(3)	C13'-H13'	0.96
C29-C30	1.393(3)	C14'-C15'	1.388(3)
C29-H29	0.96	C14'-H14'	0.96
C30-C33	1.508(3)	C15'-H15'	0.96
C31-H31C	0.96	C16'-C17'	1.389(3)
C31-H31A	0.96	C16'-C21'	1.394(3)
C31-H31B	0.96	C17'-C18'	1.389(3)
C32-H32C	0.96	C17'-C22'	1.505(3)
C32-H32A	0.96	C18'-C19'	1.386(3)
C32-H32B	0.96	C18'-H18'	0.96
C33-H33C	0.96	C19'-C20'	1.383(3)
C33-H33A	0.96	C19'-C23'	1.508(3)
C33-H33B	0.96	C20'-C21'	1.387(3)
N1'-C5'	1.366(2)	C20'-H20'	0.96
N1'-C2'	1.387(3)	C21'-C24'	1.507(3)
N1'-C16'	1.445(2)	C22'-H22F	0.96
C2'-C3'	1.336(3)	C22'-H22D	0.96
C2'-H2'	0.96	C22'-H22E	0.96
C3'-N4'	1.400(2)	C23'-H23D	0.96
C3'-H3'	0.96	C23'-H23E	0.96
N4'-C5'	1.362(2)	C23'-H23F	0.96
N4'-C25'	1.443(2)	C24'-H24F	0.96
C5'-N6'	1.326(2)	C24'-H24D	0.96
N6'-N7'	1.359(2)	C24'-H24E	0.96
N7'-N8'	1.280(2)	C25'-C26'	1.391(3)
N8'-C9'	1.457(2)	C25'-C30'	1.393(3)
C9'-C10'	1.508(3)	C26'-C27'	1.385(3)
C9'-H9'A	0.9900	C26'-C31'	1.511(3)
C9'-H9'B	0.9901	C27'-C28'	1.391(3)
C10'-C15'	1.378(3)	C27'-H27'	0.96
C10'-C11'	1.381(3)	C28'-C29'	1.381(3)
C11'-C12'	1.392(3)	C28'-C32'	1.511(3)
C11'-H11'	0.96	C29'-C30'	1.389(3)
C12'-C13'	1.379(3)	C29'-H29'	0.96
C12'-H12'	0.96	C30'-C33'	1.503(3)

C31'-H31F	0.96	C32'-H32E	0.96
C31'-H31D	0.96	C33'-H33F	0.96
C31'-H31E	0.96	C33'-H33D	0.96
C32'-H32F	0.96	C33'-H33E	0.96
C32'-H32D	0.96		

C5-N1-C2	109.79(16)	C10-C9-H9B	108.5
C5-N1-C16	125.20(16)	H9A-C9-H9B	108.7
C2-N1-C16	124.78(16)	N8-C9-H9AA	64.2
C3-C2-N1	106.99(18)	C10-C9-H9AA	97.3
C3-C2-H2	127.2	H9A-C9-H9AA	152.2
N1-C2-H2	125.8	H9B-C9-H9AA	54.2
C2-C3-N4	108.45(18)	N8-C9-H9AB	20.8
C2-C3-H3	126.2	C10-C9-H9AB	94.0
N4-C3-H3	125.3	H9A-C9-H9AB	106.5
C5-N4-C3	108.90(15)	H9B-C9-H9AB	128.0
C5-N4-C25	128.87(15)	H9AA-C9-H9AB	77.4
C3-N4-C25	122.22(16)	C5-N6A-N7A	111.0(11)
N6A-C5-N6	15.8(9)	N8A-N7A-N6A	119.0(8)
N6A-C5-N4	120.6(6)	N7A-N8A-C9A	118.3(7)
N6-C5-N4	135.4(2)	N7A-N8A-H9A	129.2
N6A-C5-N1	133.2(6)	C9A-N8A-H9A	73.5
N6-C5-N1	118.7(2)	N7A-N8A-H9B	108.7
N4-C5-N1	105.87(16)	C9A-N8A-H9B	43.6
C5-N6-N7	114.7(3)	H9A-N8A-H9B	110.0
N8-N7-N6	116.2(2)	N8A-C9A-C10	106.9(9)
N7-N8-C9	116.4(2)	N8A-C9A-H9A	26.1
N7-N8-H9AA	101.5	C10-C9A-H9A	89.0
C9-N8-H9AA	54.8	N8A-C9A-H9B	56.4
N7-N8-H9AB	150.4	C10-C9A-H9B	105.3
C9-N8-H9AB	49.3	H9A-C9A-H9B	78.9
H9AA-N8-H9AB	89.2	N8A-C9A-H9AA	115.2
N8-C9-C10	110.8(3)	C10-C9A-H9AA	117.8
N8-C9-H9A	110.1	H9A-C9A-H9AA	141.3
C10-C9-H9A	109.7	H9B-C9A-H9AA	67.8
N8-C9-H9B	109.1	N8A-C9A-H9AB	104.0

C10-C9A-H9AB	102.4	C18-C19-C23	121.0(2)
H9A-C9A-H9AB	90.0	C19-C20-C21	122.3(2)
H9B-C9A-H9AB	149.8	C19-C20-H20A	118.6
H9AA-C9A-H9AB	109.0	C21-C20-H20A	119.0
C11-C10-C15	118.2(2)	C16-C21-C20	117.5(2)
C11-C10-C9	118.6(3)	C16-C21-C24	121.7(2)
C15-C10-C9	123.1(3)	C20-C21-C24	120.7(2)
C11-C10-C9A	135.3(8)	C17-C22-H22C	109.2
C15-C10-C9A	106.4(7)	C17-C22-H22A	110.0
C9-C10-C9A	17.4(6)	H22C-C22-H22A	109.5
C10-C11-C12	121.8(2)	C17-C22-H22B	110.2
C10-C11-H11	118.2	H22C-C22-H22B	109.5
C12-C11-H11	120.1	H22A-C22-H22B	108.3
C13-C12-C11	119.7(2)	C19-C23-H23A	110.6
C13-C12-H12	120.3	C19-C23-H23B	109.1
C11-C12-H12	120.0	H23A-C23-H23B	109.5
C14-C13-C12	119.3(2)	C19-C23-H23C	108.7
C14-C13-H13	120.5	H23A-C23-H23C	109.5
C12-C13-H13	120.2	H23B-C23-H23C	109.5
C13-C14-C15	120.4(2)	C21-C24-H24C	109.3
C13-C14-H14A	119.9	C21-C24-H24A	110.1
C15-C14-H14A	119.7	H24C-C24-H24A	109.6
C14-C15-C10	120.7(2)	C21-C24-H24B	109.9
C14-C15-H15	120.3	H24C-C24-H24B	109.6
C10-C15-H15	119.0	H24A-C24-H24B	108.3
C21-C16-C17	122.59(19)	C30-C25-C26	122.75(18)
C21-C16-N1	118.78(19)	C30-C25-N4	118.69(18)
C17-C16-N1	118.57(19)	C26-C25-N4	118.41(18)
C16-C17-C18	117.1(2)	C25-C26-C27	117.17(19)
C16-C17-C22	122.61(18)	C25-C26-C31	122.41(18)
C18-C17-C22	120.3(2)	C27-C26-C31	120.42(19)
C19-C18-C17	122.5(2)	C28-C27-C26	121.93(19)
C19-C18-H18	118.9	C28-C27-H27	119.7
C17-C18-H18	118.7	C26-C27-H27	118.4
C20-C19-C18	118.0(2)	C29-C28-C27	118.81(19)
C20-C19-C23	121.0(2)	C29-C28-C32	121.5(2)

C27-C28-C32	119.7(2)	C3'-N4'-C25'	123.13(17)
C28-C29-C30	121.6(2)	N6'-C5'-N4'	133.56(18)
C28-C29-H29	119.5	N6'-C5'-N1'	119.88(18)
C30-C29-H29	118.9	N4'-C5'-N1'	106.40(18)
C25-C30-C29	117.65(19)	C5'-N6'-N7'	113.34(17)
C25-C30-C33	121.59(18)	N8'-N7'-N6'	115.27(17)
C29-C30-C33	120.8(2)	N7'-N8'-C9'	116.48(16)
C26-C31-H31C	110.9	N8'-C9'-C10'	112.58(17)
C26-C31-H31A	108.5	N8'-C9'-H9'A	109.0
H31C-C31-H31A	110.7	C10'-C9'-H9'A	108.6
C26-C31-H31B	108.4	N8'-C9'-H9'B	109.5
H31C-C31-H31B	110.7	C10'-C9'-H9'B	109.4
H31A-C31-H31B	107.5	H9'A-C9'-H9'B	107.5
C28-C32-H32C	110.0	C15'-C10'-C11'	118.4(2)
C28-C32-H32A	108.7	C15'-C10'-C9'	123.2(2)
H32C-C32-H32A	110.1	C11'-C10'-C9'	118.3(2)
C28-C32-H32B	109.9	C10'-C11'-C12'	120.7(2)
H32C-C32-H32B	110.1	C10'-C11'-H11'	119.3
H32A-C32-H32B	108.0	C12'-C11'-H11'	120.0
C30-C33-H33C	110.3	C13'-C12'-C11'	119.9(2)
C30-C33-H33A	109.3	C13'-C12'-H12'	119.8
H33C-C33-H33A	110.3	C11'-C12'-H12'	120.3
C30-C33-H33B	108.8	C14'-C13'-C12'	119.8(2)
H33C-C33-H33B	110.3	C14'-C13'-H13'	119.8
H33A-C33-H33B	107.8	C12'-C13'-H13'	120.4
C5'-N1'-C2'	109.44(17)	C13'-C14'-C15'	120.1(2)
C5'-N1'-C16'	123.81(17)	C13'-C14'-H14'	120.2
C2'-N1'-C16'	126.65(16)	C15'-C14'-H14'	119.7
C3'-C2'-N1'	107.58(18)	C10'-C15'-C14'	121.0(2)
C3'-C2'-H2'	126.9	C10'-C15'-H15'	118.9
N1'-C2'-H2'	125.5	C14'-C15'-H15'	120.1
C2'-C3'-N4'	107.83(19)	C17'-C16'-C21'	122.50(19)
C2'-C3'-H3'	126.2	C17'-C16'-N1'	118.71(19)
N4'-C3'-H3'	125.9	C21'-C16'-N1'	118.77(17)
C5'-N4'-C3'	108.75(16)	C16'-C17'-C18'	117.3(2)
C5'-N4'-C25'	127.03(17)	C16'-C17'-C22'	121.6(2)

C18'-C17'-C22'	121.08(19)	C25'-C26'-C31'	121.37(19)
C19'-C18'-C17'	122.5(2)	C26'-C27'-C28'	121.9(2)
C19'-C18'-H18'	118.5	C26'-C27'-H27'	119.2
C17'-C18'-H18'	118.9	C28'-C27'-H27'	118.9
C20'-C19'-C18'	117.8(2)	C29'-C28'-C27'	117.84(19)
C20'-C19'-C23'	121.6(2)	C29'-C28'-C32'	120.8(2)
C18'-C19'-C23'	120.6(2)	C27'-C28'-C32'	121.4(2)
C19'-C20'-C21'	122.5(2)	C28'-C29'-C30'	122.8(2)
C19'-C20'-H20'	119.0	C28'-C29'-H29'	118.5
C21'-C20'-H20'	118.4	C30'-C29'-H29'	118.7
C20'-C21'-C16'	117.36(19)	C29'-C30'-C25'	117.17(19)
C20'-C21'-C24'	121.2(2)	C29'-C30'-C33'	121.10(19)
C16'-C21'-C24'	121.39(19)	C25'-C30'-C33'	121.69(18)
C17'-C22'-H22F	109.2	C26'-C31'-H31F	109.7
C17'-C22'-H22D	110.6	C26'-C31'-H31D	110.2
H22F-C22'-H22D	108.7	H31F-C31'-H31D	109.3
C17'-C22'-H22E	110.6	C26'-C31'-H31E	109.9
H22F-C22'-H22E	108.7	H31F-C31'-H31E	109.3
H22D-C22'-H22E	108.9	H31D-C31'-H31E	108.5
C19'-C23'-H23D	109.4	C28'-C32'-H32F	110.3
C19'-C23'-H23E	108.9	C28'-C32'-H32D	109.0
H23D-C23'-H23E	109.5	H32F-C32'-H32D	110.2
C19'-C23'-H23F	110.0	C28'-C32'-H32E	109.2
H23D-C23'-H23F	109.5	H32F-C32'-H32E	110.2
H23E-C23'-H23F	109.5	H32D-C32'-H32E	107.9
C21'-C24'-H24F	109.8	C30'-C33'-H33F	109.5
C21'-C24'-H24D	110.0	C30'-C33'-H33D	109.7
H24F-C24'-H24D	109.2	H33F-C33'-H33D	109.6
C21'-C24'-H24E	110.1	C30'-C33'-H33E	110.1
H24F-C24'-H24E	109.2	H33F-C33'-H33E	109.6
H24D-C24'-H24E	108.5	H33D-C33'-H33E	108.3
C26'-C25'-C30'	122.19(18)		
C26'-C25'-N4'	119.32(18)		
C30'-C25'-N4'	118.43(18)		
C27'-C26'-C25'	118.03(19)		
C27'-C26'-C31'	120.6(2)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *(Z)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N1	39(1)	47(1)	40(1)	21(1)	-4(1)	-6(1)
C2	40(1)	54(2)	57(2)	30(1)	-7(1)	-10(1)
C3	45(1)	54(2)	56(2)	23(1)	-18(1)	-17(1)
N4	38(1)	44(1)	39(1)	20(1)	-6(1)	-5(1)
C5	36(1)	41(1)	36(1)	13(1)	-2(1)	1(1)
N6	52(2)	40(2)	41(2)	18(2)	-4(2)	-5(1)
N7	49(1)	48(2)	41(1)	17(1)	-3(1)	-2(1)
N8	55(1)	43(1)	39(1)	15(1)	-10(1)	-9(1)
C9	64(2)	55(2)	62(3)	15(2)	-20(2)	-16(2)
C10	58(2)	61(2)	42(1)	19(1)	-11(1)	-13(1)
C11	70(2)	53(2)	63(2)	5(1)	-13(1)	5(1)
C12	54(2)	76(2)	79(2)	12(2)	-19(1)	6(2)
C13	61(2)	66(2)	65(2)	12(2)	-21(1)	-13(1)
C14	69(2)	50(2)	52(2)	11(1)	-8(1)	1(1)
C15	51(1)	56(2)	52(2)	19(1)	-4(1)	0(1)
C16	40(1)	47(1)	37(1)	21(1)	0(1)	-4(1)
C17	40(1)	44(1)	43(1)	18(1)	-2(1)	-5(1)
C18	50(1)	53(2)	50(2)	24(1)	-4(1)	4(1)
C19	63(2)	68(2)	43(2)	24(1)	2(1)	12(1)
C20	75(2)	70(2)	44(2)	21(1)	13(1)	19(1)
C21	54(1)	57(2)	48(2)	23(1)	9(1)	11(1)
C22	60(2)	51(2)	49(2)	13(1)	-4(1)	4(1)
C23	112(2)	106(2)	48(2)	36(2)	-2(2)	27(2)
C24	92(2)	81(2)	63(2)	30(2)	20(1)	41(2)
C25	35(1)	40(1)	37(1)	16(1)	-6(1)	-3(1)
C26	39(1)	37(1)	37(1)	10(1)	-2(1)	-1(1)
C27	49(1)	48(2)	35(1)	11(1)	-1(1)	-2(1)
C28	42(1)	46(2)	43(1)	20(1)	-10(1)	-7(1)
C29	44(1)	38(1)	46(1)	14(1)	-8(1)	2(1)
C30	43(1)	41(1)	36(1)	8(1)	-3(1)	0(1)

C31	62(2)	42(2)	53(2)	12(1)	3(1)	3(1)
C32	65(2)	71(2)	64(2)	41(1)	-1(1)	2(1)
C33	69(2)	61(2)	52(2)	14(1)	8(1)	17(1)
N1'	40(1)	41(1)	44(1)	13(1)	-5(1)	4(1)
C2'	46(1)	43(2)	58(2)	12(1)	-2(1)	12(1)
C3'	52(1)	38(1)	56(2)	7(1)	-2(1)	12(1)
N4'	44(1)	39(1)	41(1)	9(1)	-4(1)	5(1)
C5'	42(1)	33(1)	38(1)	11(1)	0(1)	1(1)
N6'	39(1)	39(1)	43(1)	15(1)	-7(1)	3(1)
N7'	55(1)	44(1)	44(1)	10(1)	-8(1)	3(1)
N8'	55(1)	40(1)	40(1)	6(1)	-5(1)	4(1)
C9'	42(1)	45(1)	42(1)	13(1)	1(1)	-1(1)
C10'	46(1)	41(1)	42(1)	10(1)	11(1)	-4(1)
C11'	66(2)	58(2)	50(2)	7(1)	6(1)	2(1)
C12'	96(2)	67(2)	56(2)	-1(2)	13(2)	7(2)
C13'	88(2)	58(2)	71(2)	13(2)	30(2)	22(2)
C14'	67(2)	56(2)	60(2)	17(1)	18(1)	15(1)
C15'	51(1)	46(2)	47(1)	14(1)	8(1)	5(1)
C16'	40(1)	36(1)	47(1)	13(1)	-9(1)	3(1)
C17'	38(1)	42(1)	55(2)	20(1)	3(1)	6(1)
C18'	38(1)	47(2)	71(2)	26(1)	-6(1)	-5(1)
C19'	48(1)	43(1)	56(2)	22(1)	-17(1)	-3(1)
C20'	52(1)	54(2)	45(1)	22(1)	-9(1)	-1(1)
C21'	39(1)	51(1)	46(1)	23(1)	-8(1)	-3(1)
C22'	58(2)	57(2)	71(2)	15(1)	18(1)	4(1)
C23'	75(2)	56(2)	82(2)	21(2)	-32(1)	-16(1)
C24'	51(1)	80(2)	54(2)	29(1)	-5(1)	-12(1)
C25'	44(1)	31(1)	40(1)	7(1)	-6(1)	5(1)
C26'	54(1)	33(1)	41(1)	10(1)	1(1)	4(1)
C27'	64(2)	39(1)	39(1)	9(1)	-8(1)	3(1)
C28'	55(2)	31(1)	48(2)	1(1)	-13(1)	3(1)
C29'	43(1)	34(1)	50(2)	1(1)	2(1)	4(1)
C30'	51(1)	33(1)	39(1)	5(1)	1(1)	5(1)
C31'	73(2)	54(2)	55(2)	15(1)	7(1)	-2(1)
C32'	66(2)	51(2)	72(2)	7(1)	-25(1)	-1(1)
C33'	60(2)	57(2)	47(2)	12(1)	3(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *(Z)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene.

	x	y	z	U(eq)
H2	6160	2950	1803	57
H3	5731	3562	695	61
H9A	11733	5781	2705	73
H9B	10462	6225	3206	73
H9AA	9889	6742	2993	129
H9AB	10957	6578	2331	129
H11	13964	6341	3158	77
H12	15590	7477	3803	86
H13	14726	8937	4269	78
H14A	12247	9235	4084	69
H15	10637	8079	3460	63
H18	9932	2588	3731	59
H20A	7861	4878	4658	74
H22C	10035	2789	1969	80
H22A	8686	2173	2009	80
H22B	10154	2072	2438	80
H23A	9892	3057	5053	129
H23B	9854	4099	5378	129
H23C	8414	3525	5322	129
H24C	6508	5661	3928	114
H24A	5938	5119	3128	114
H24B	7337	5722	3213	114
H27	8464	4942	-1039	53
H29	6136	6886	309	51
H31C	9292	3690	228	78
H31A	9418	3740	-611	78
H31B	8022	3322	-380	78
H32C	6778	7062	-885	94
H32A	7072	6173	-1501	94
H32B	8388	6733	-1060	94

H33C	5255	6704	1450	91
H33A	6533	6353	1895	91
H33B	5213	5724	1559	91
H2'	10256	-1746	2128	59
H3'	8440	-2274	1071	60
H9'A	6743	1951	3084	51
H9'B	5425	1335	3220	51
H11'	5757	2902	4291	71
H12'	4432	4217	4781	91
H13'	2622	4683	4031	87
H14'	2219	3884	2790	72
H15'	3545	2576	2306	57
H18'	12778	1304	3374	60
H20'	9793	849	4793	59
H22F	12472	719	2076	93
H22D	10864	513	1756	93
H22E	11885	-268	1848	93
H23D	13143	2000	4642	107
H23E	11682	2271	5057	107
H23F	12585	1457	5191	107
H24F	7116	-12	3634	90
H24D	7812	-165	4379	90
H24E	7956	-898	3631	90
H27'	4712	-1213	-646	57
H29'	2637	-1657	1117	53
H31F	8112	-1375	-121	90
H31D	7896	-351	239	90
H31E	7205	-791	-555	90
H32F	1655	-2161	-371	98
H32D	2130	-1388	-733	98
H32E	1293	-1153	6	98
H33F	5628	-1716	2268	82
H33D	3912	-1637	2259	82
H33E	4885	-772	2477	82

Table 6. Torsion angles [°] for (*Z*)-1,3-dimesityl-2-imidazolylidene-(1-benzyl)triazene.

C5-N1-C2-C3	-0.6(2)
C16-N1-C2-C3	174.09(19)
N1-C2-C3-N4	0.3(2)
C2-C3-N4-C5	0.1(2)
C2-C3-N4-C25	-179.11(18)
C3-N4-C5-N6A	173.6(12)
C25-N4-C5-N6A	-7.3(12)
C3-N4-C5-N6	-179.3(4)
C25-N4-C5-N6	-0.1(5)
C3-N4-C5-N1	-0.5(2)
C25-N4-C5-N1	178.67(18)
C2-N1-C5-N6A	-172.3(14)
C16-N1-C5-N6A	13.0(15)
C2-N1-C5-N6	179.7(3)
C16-N1-C5-N6	5.0(4)
C2-N1-C5-N4	0.7(2)
C16-N1-C5-N4	-174.01(17)
N4-C5-N6-N7	7.5(6)
N1-C5-N6-N7	-171.2(3)
C5-N6-N7-N8	179.8(3)
N6-N7-N8-C9	2.3(5)
N7-N8-C9-C10	-173.7(3)
N4-C5-N6A-N7A	-152.9(10)
N1-C5-N6A-N7A	19(2)
C5-N6A-N7A-N8A	-162.2(13)
N6A-N7A-N8A-C9A	12(3)
N7A-N8A-C9A-C10	-174.7(15)
N8-C9-C10-C11	-124.8(4)
N8-C9-C10-C15	58.1(5)
N8-C9-C10-C9A	41(6)
N8A-C9A-C10-C11	26(4)
N8A-C9A-C10-C15	-156.8(19)
N8A-C9A-C10-C9	8(3)
C15-C10-C11-C12	0.2(4)

C9-C10-C11-C12	-177.0(3)
C9A-C10-C11-C12	177(2)
C10-C11-C12-C13	-1.0(4)
C11-C12-C13-C14	0.8(4)
C12-C13-C14-C15	0.1(4)
C13-C14-C15-C10	-0.9(3)
C11-C10-C15-C14	0.8(3)
C9-C10-C15-C14	177.9(3)
C9A-C10-C15-C14	-176.7(16)
C5-N1-C16-C21	68.7(3)
C2-N1-C16-C21	-105.2(2)
C5-N1-C16-C17	-114.1(2)
C2-N1-C16-C17	72.0(3)
C21-C16-C17-C18	0.9(3)
N1-C16-C17-C18	-176.13(17)
C21-C16-C17-C22	-179.71(19)
N1-C16-C17-C22	3.3(3)
C16-C17-C18-C19	-0.9(3)
C22-C17-C18-C19	179.7(2)
C17-C18-C19-C20	-0.6(3)
C17-C18-C19-C23	177.6(2)
C18-C19-C20-C21	2.2(4)
C23-C19-C20-C21	-175.9(2)
C17-C16-C21-C20	0.6(3)
N1-C16-C21-C20	177.65(18)
C17-C16-C21-C24	-178.3(2)
N1-C16-C21-C24	-1.2(3)
C19-C20-C21-C16	-2.3(3)
C19-C20-C21-C24	176.6(2)
C5-N4-C25-C30	-78.9(2)
C3-N4-C25-C30	100.1(2)
C5-N4-C25-C26	105.4(2)
C3-N4-C25-C26	-75.6(2)
C30-C25-C26-C27	3.0(3)
N4-C25-C26-C27	178.48(16)
C30-C25-C26-C31	-176.12(18)

N4-C25-C26-C31	-0.7(3)
C25-C26-C27-C28	-0.2(3)
C31-C26-C27-C28	178.94(18)
C26-C27-C28-C29	-1.8(3)
C26-C27-C28-C32	176.81(18)
C27-C28-C29-C30	1.2(3)
C32-C28-C29-C30	-177.42(18)
C26-C25-C30-C29	-3.6(3)
N4-C25-C30-C29	-179.08(16)
C26-C25-C30-C33	176.30(19)
N4-C25-C30-C33	0.8(3)
C28-C29-C30-C25	1.5(3)
C28-C29-C30-C33	-178.46(19)
C5'-N1'-C2'-C3'	0.2(2)
C16'-N1'-C2'-C3'	-176.09(18)
N1'-C2'-C3'-N4'	0.0(2)
C2'-C3'-N4'-C5'	-0.1(2)
C2'-C3'-N4'-C25'	-168.94(18)
C3'-N4'-C5'-N6'	-175.0(2)
C25'-N4'-C5'-N6'	-6.8(3)
C3'-N4'-C5'-N1'	0.2(2)
C25'-N4'-C5'-N1'	168.48(17)
C2'-N1'-C5'-N6'	175.79(17)
C16'-N1'-C5'-N6'	-7.8(3)
C2'-N1'-C5'-N4'	-0.2(2)
C16'-N1'-C5'-N4'	176.14(16)
N4'-C5'-N6'-N7'	-22.8(3)
N1'-C5'-N6'-N7'	162.40(16)
C5'-N6'-N7'-N8'	171.92(16)
N6'-N7'-N8'-C9'	-3.5(2)
N7'-N8'-C9'-C10'	178.32(16)
N8'-C9'-C10'-C15'	9.7(3)
N8'-C9'-C10'-C11'	-171.43(17)
C15'-C10'-C11'-C12'	-1.1(3)
C9'-C10'-C11'-C12'	180.0(2)
C10'-C11'-C12'-C13'	0.5(4)

C11'-C12'-C13'-C14'	0.2(4)
C12'-C13'-C14'-C15'	-0.2(4)
C11'-C10'-C15'-C14'	1.1(3)
C9'-C10'-C15'-C14'	179.96(19)
C13'-C14'-C15'-C10'	-0.4(3)
C5'-N1'-C16'-C17'	-100.1(2)
C2'-N1'-C16'-C17'	75.6(3)
C5'-N1'-C16'-C21'	78.3(2)
C2'-N1'-C16'-C21'	-105.9(2)
C21'-C16'-C17'-C18'	2.2(3)
N1'-C16'-C17'-C18'	-179.44(17)
C21'-C16'-C17'-C22'	-175.94(19)
N1'-C16'-C17'-C22'	2.5(3)
C16'-C17'-C18'-C19'	-1.3(3)
C22'-C17'-C18'-C19'	176.82(19)
C17'-C18'-C19'-C20'	-0.4(3)
C17'-C18'-C19'-C23'	-179.59(19)
C18'-C19'-C20'-C21'	1.3(3)
C23'-C19'-C20'-C21'	-179.5(2)
C19'-C20'-C21'-C16'	-0.5(3)
C19'-C20'-C21'-C24'	-178.93(19)
C17'-C16'-C21'-C20'	-1.3(3)
N1'-C16'-C21'-C20'	-179.72(17)
C17'-C16'-C21'-C24'	177.14(19)
N1'-C16'-C21'-C24'	-1.2(3)
C5'-N4'-C25'-C26'	111.1(2)
C3'-N4'-C25'-C26'	-82.2(2)
C5'-N4'-C25'-C30'	-71.8(3)
C3'-N4'-C25'-C30'	94.9(2)
C30'-C25'-C26'-C27'	2.0(3)
N4'-C25'-C26'-C27'	178.98(17)
C30'-C25'-C26'-C31'	-179.79(19)
N4'-C25'-C26'-C31'	-2.8(3)
C25'-C26'-C27'-C28'	-1.2(3)
C31'-C26'-C27'-C28'	-179.46(19)
C26'-C27'-C28'-C29'	-0.8(3)

C26'-C27'-C28'-C32'	177.55(19)
C27'-C28'-C29'-C30'	2.2(3)
C32'-C28'-C29'-C30'	-176.2(2)
C28'-C29'-C30'-C25'	-1.4(3)
C28'-C29'-C30'-C33'	176.31(19)
C26'-C25'-C30'-C29'	-0.7(3)
N4'-C25'-C30'-C29'	-177.73(17)
C26'-C25'-C30'-C33'	-178.43(19)
N4'-C25'-C30'-C33'	4.5(3)

X-ray experimental for *(E)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene ($C_{28}H_{31}N_5$): Crystals grew as pale yellow prisms by slow evaporation from ethyl acetate. The data crystal was a long lathe that had approximate dimensions; 0.24 x 0.21 x 0.08 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 306 frames of data were collected using ω-scans with a scan range of 1° and a counting time of 249 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR97[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). There are two crystallographically unique molecules in the asymmetric unit. These two molecules differ only slightly in conformation (Figure 3). The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.042*P)^2]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.119, with R(F) equal to 0.0525 and a goodness of fit, S, = 1.00. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (2.5(3)x10^{-6})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in Tables 1 through 7.

References

1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

2) SIR97. (1999). A program for crystal structure solution. Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. J. Appl. Cryst. 32, 115-119.

3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

4) $R_W(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$.
$S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for *(E)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene.

Empirical formula	C28 H31 N5	
Formula weight	437.58	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 14.6396(3) Å	α= 90°.
	b = 12.1965(2) Å	β= 90.634(1)°.
	c = 28.0462(5) Å	γ = 90°.
Volume	5007.40(16) $Å^3$	
Z	8	
Density (calculated)	1.161 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	1872	
Crystal size	0.24 x 0.21 x 0.08 mm	
Theta range for data collection	3.07 to 25.00°.	
Index ranges	-17<=h<=17, -14<=k<=14, -33<=l<=33	
Reflections collected	16441	
Independent reflections	8809 [R(int) = 0.0682]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8809 / 0 / 596	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0525, wR2 = 0.0974	
R indices (all data)	R1 = 0.1441, wR2 = 0.1187	
Extinction coefficient	$2.5(3)x10^{-6}$	
Largest diff. peak and hole	0.173 and -0.201 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *(E)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N1	90(1)	786(2)	1847(1)	34(1)
C2	230(2)	1723(2)	2128(1)	41(1)
C3	-79(2)	1514(2)	2563(1)	39(1)
N4	-411(1)	442(2)	2562(1)	34(1)
C5	-307(1)	-10(2)	2122(1)	31(1)
N6	-518(1)	-1056(2)	2026(1)	34(1)
N7	-515(1)	-1217(2)	1543(1)	35(1)
N8	-513(1)	-2221(2)	1435(1)	40(1)
C9	-522(2)	-2345(2)	915(1)	46(1)
C10	298(2)	-2950(2)	730(1)	40(1)
C11	265(2)	-3443(2)	281(1)	56(1)
C12	1030(2)	-3949(2)	95(1)	68(1)
C13	1831(2)	-3982(2)	350(1)	66(1)
C14	1871(2)	-3521(2)	798(1)	56(1)
C15	1108(2)	-3007(2)	984(1)	46(1)
C16	492(2)	626(2)	1387(1)	32(1)
C17	54(2)	1049(2)	984(1)	36(1)
C18	464(2)	879(2)	545(1)	44(1)
C19	1268(2)	289(2)	504(1)	42(1)
C20	1676(2)	-132(2)	915(1)	39(1)
C21	1310(2)	47(2)	1361(1)	35(1)
C22	-858(2)	1614(2)	1023(1)	48(1)
C23	1700(2)	110(3)	25(1)	71(1)
C24	1761(2)	-417(2)	1804(1)	45(1)
C25	-813(2)	-103(2)	2964(1)	32(1)
C26	-1751(2)	-236(2)	2976(1)	38(1)
C27	-2116(2)	-777(2)	3368(1)	43(1)
C28	-1575(2)	-1150(2)	3739(1)	41(1)
C29	-645(2)	-968(2)	3720(1)	39(1)
C30	-241(2)	-447(2)	3334(1)	35(1)

C31	-2365(2)	198(2)	2583(1)	55(1)
C32	-1995(2)	-1742(2)	4156(1)	64(1)
C33	774(2)	-280(2)	3315(1)	52(1)
N1'	5174(1)	1621(2)	1775(1)	34(1)
C2'	5302(2)	656(2)	2041(1)	41(1)
C3'	5022(2)	843(2)	2483(1)	39(1)
N4'	4717(1)	1926(2)	2501(1)	32(1)
C5'	4811(1)	2403(2)	2064(1)	30(1)
N6'	4598(1)	3455(2)	1993(1)	33(1)
N7'	4633(1)	3700(2)	1519(1)	34(1)
N8'	4559(1)	4714(2)	1440(1)	40(1)
C9'	4598(2)	4931(2)	930(1)	43(1)
C10'	5482(2)	5451(2)	775(1)	34(1)
C11'	6280(2)	5343(2)	1043(1)	47(1)
C12'	7095(2)	5775(2)	879(1)	54(1)
C13'	7127(2)	6312(2)	447(1)	52(1)
C14'	6333(2)	6433(2)	186(1)	48(1)
C15'	5523(2)	6013(2)	347(1)	39(1)
C16'	5445(2)	1716(2)	1284(1)	32(1)
C17'	4848(2)	1339(2)	930(1)	37(1)
C18'	5130(2)	1401(2)	462(1)	43(1)
C19'	5976(2)	1819(2)	340(1)	43(1)
C20'	6542(2)	2204(2)	701(1)	42(1)
C21'	6296(2)	2147(2)	1178(1)	35(1)
C22'	3911(2)	927(2)	1056(1)	53(1)
C23'	6269(2)	1861(2)	-176(1)	62(1)
C24'	6922(2)	2558(2)	1572(1)	49(1)
C25'	4333(2)	2448(2)	2914(1)	30(1)
C26'	4918(2)	2777(2)	3280(1)	33(1)
C27'	4529(2)	3279(2)	3673(1)	40(1)
C28'	3602(2)	3458(2)	3703(1)	41(1)
C29'	3046(2)	3096(2)	3338(1)	44(1)
C30'	3396(2)	2573(2)	2937(1)	37(1)
C31'	5932(2)	2608(2)	3249(1)	51(1)
C32'	3201(2)	4051(2)	4127(1)	63(1)
C33'	2764(2)	2150(2)	2548(1)	55(1)

Table 3. Bond lengths [Å] and angles [°] for *(E)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene.

N1-C5	1.373(3)	C19-C23	1.507(3)
N1-C2	1.401(3)	C20-C21	1.384(3)
N1-C16	1.438(2)	C20-H20A	0.96
C2-C3	1.330(3)	C21-C24	1.511(3)
C2-H2	0.96	C22-H22A	0.98
C3-N4	1.394(3)	C22-H22B	0.98
C3-H3	0.96	C22-H22C	0.98
N4-C5	1.362(2)	C23-H23A	0.98
N4-C25	1.439(3)	C23-H23B	0.98
C5-N6	1.339(3)	C23-H23C	0.98
N6-N7	1.370(2)	C24-H24A	0.98
N7-N8	1.261(2)	C24-H24B	0.98
N8-C9	1.468(2)	C24-H24C	0.98
C9-C10	1.506(3)	C25-C26	1.383(3)
C9-H9A	0.96	C25-C30	1.392(3)
C9-H9B	0.96	C26-C27	1.392(3)
C10-C15	1.378(3)	C26-C31	1.512(3)
C10-C11	1.395(3)	C27-C28	1.380(3)
C11-C12	1.387(3)	C27-H27	0.96
C11-H11	0.96	C28-C29	1.381(3)
C12-C13	1.368(4)	C28-C32	1.510(3)
C12-H12	0.96	C29-C30	1.392(3)
C13-C14	1.378(3)	C29-H29	0.96
C13-H13	0.96	C30-C33	1.501(3)
C14-C15	1.387(3)	C31-H31A	0.98
C14-H14	0.96	C31-H31B	0.98
C15-H15	0.96	C31-H31C	0.98
C16-C17	1.392(3)	C32-H32A	0.98
C16-C21	1.394(3)	C32-H32B	0.98
C17-C18	1.389(3)	C32-H32C	0.98
C17-C22	1.507(3)	C33-H33A	0.98
C18-C19	1.387(3)	C33-H33B	0.98
C18-H18	0.96	C33-H33C	0.98
C19-C20	1.388(3)	N1'-C5'	1.364(3)

N1'-C2'	1.406(3)	C19'-C23'	1.516(3)
N1'-C16'	1.441(2)	C20'-C21'	1.392(3)
C2'-C3'	1.329(3)	C20'-H20'	0.96
C2'-H2'	0.96	C21'-C24'	1.511(3)
C3'-N4'	1.395(3)	C22'-H22D	0.98
C3'-H3'	0.96	C22'-H22E	0.98
N4'-C5'	1.366(2)	C22'-H22F	0.98
N4'-C25'	1.440(2)	C23'-H23D	0.98
C5'-N6'	1.335(3)	C23'-H23E	0.98
N6'-N7'	1.364(2)	C23'-H23F	0.98
N7'-N8'	1.260(2)	C24'-H24D	0.98
N8'-C9'	1.458(2)	C24'-H24E	0.98
C9'-C10'	1.509(3)	C24'-H24F	0.98
C9'-H9'A	0.96	C25'-C30'	1.382(3)
C9'-H9'B	0.96	C25'-C26'	1.389(3)
C10'-C15'	1.384(3)	C26'-C27'	1.388(3)
C10'-C11'	1.388(3)	C26'-C31'	1.502(3)
C11'-C12'	1.386(3)	C27'-C28'	1.378(3)
C11'-H11'	0.96	C27'-H27'	0.96
C12'-C13'	1.378(3)	C28'-C29'	1.376(3)
C12'-H12'	0.96	C28'-C32'	1.515(3)
C13'-C14'	1.374(3)	C29'-C30'	1.394(3)
C13'-H13'	0.96	C29'-H29'	0.96
C14'-C15'	1.374(3)	C30'-C33'	1.512(3)
C14'-H14'	0.96	C31'-H31D	0.98
C15'-H15'	0.96	C31'-H31E	0.98
C16'-C21'	1.387(3)	C31'-H31F	0.98
C16'-C17'	1.393(3)	C32'-H32D	0.98
C17'-C18'	1.383(3)	C32'-H32E	0.98
C17'-C22'	1.505(3)	C32'-H32F	0.98
C18'-C19'	1.386(3)	C33'-H33D	0.98
C18'-H18'	0.96	C33'-H33E	0.98
C19'-C20'	1.383(3)	C33'-H33F	0.98

C5-N1-C2	108.74(17)	C2-N1-C16	123.83(19)
C5-N1-C16	126.00(18)	C3-C2-N1	108.1(2)

C3-C2-H2	126.5	C10-C15-H15	118.7
N1-C2-H2	125.4	C14-C15-H15	120.0
C2-C3-N4	107.5(2)	C17-C16-C21	122.3(2)
C2-C3-H3	126.9	C17-C16-N1	119.3(2)
N4-C3-H3	125.7	C21-C16-N1	118.40(19)
C5-N4-C3	109.79(18)	C18-C17-C16	117.7(2)
C5-N4-C25	124.95(18)	C18-C17-C22	121.6(2)
C3-N4-C25	125.26(18)	C16-C17-C22	120.7(2)
N6-C5-N4	122.63(19)	C19-C18-C17	121.7(2)
N6-C5-N1	131.29(19)	C19-C18-H18	119.6
N4-C5-N1	105.94(18)	C17-C18-H18	118.6
C5-N6-N7	109.35(17)	C18-C19-C20	118.8(2)
N8-N7-N6	112.12(17)	C18-C19-C23	120.9(2)
N7-N8-C9	109.84(18)	C20-C19-C23	120.3(2)
N8-C9-C10	113.21(19)	C21-C20-C19	121.6(2)
N8-C9-H9A	107.9	C21-C20-H20A	118.9
C10-C9-H9A	107.9	C19-C20-H20A	119.5
N8-C9-H9B	109.6	C20-C21-C16	117.9(2)
C10-C9-H9B	109.9	C20-C21-C24	121.0(2)
H9A-C9-H9B	108.2	C16-C21-C24	121.0(2)
C15-C10-C11	117.8(2)	C17-C22-H22A	109.5
C15-C10-C9	122.1(2)	C17-C22-H22B	109.4
C11-C10-C9	120.0(2)	H22A-C22-H22B	109.5
C12-C11-C10	120.7(3)	C17-C22-H22C	109.5
C12-C11-H11	120.6	H22A-C22-H22C	109.5
C10-C11-H11	118.6	H22B-C22-H22C	109.5
C13-C12-C11	120.6(3)	C19-C23-H23A	109.6
C13-C12-H12	120.1	C19-C23-H23B	109.5
C11-C12-H12	119.3	H23A-C23-H23B	109.5
C12-C13-C14	119.5(3)	C19-C23-H23C	109.4
C12-C13-H13	120.0	H23A-C23-H23C	109.5
C14-C13-H13	120.5	H23B-C23-H23C	109.5
C13-C14-C15	120.1(3)	C21-C24-H24A	109.5
C13-C14-H14	119.8	C21-C24-H24B	109.5
C15-C14-H14	120.0	H24A-C24-H24B	109.5
C10-C15-C14	121.3(2)	C21-C24-H24C	109.4

H24A-C24-H24C	109.5	H33A-C33-H33C	109.5
H24B-C24-H24C	109.5	H33B-C33-H33C	109.5
C26-C25-C30	122.3(2)	C5'-N1'-C2'	108.68(17)
C26-C25-N4	119.29(19)	C5'-N1'-C16'	128.66(18)
C30-C25-N4	118.4(2)	C2'-N1'-C16'	122.58(18)
C25-C26-C27	117.8(2)	C3'-C2'-N1'	108.1(2)
C25-C26-C31	121.5(2)	C3'-C2'-H2'	126.6
C27-C26-C31	120.7(2)	N1'-C2'-H2'	125.2
C28-C27-C26	121.9(2)	C2'-C3'-N4'	107.4(2)
C28-C27-H27	118.6	C2'-C3'-H3'	126.9
C26-C27-H27	119.5	N4'-C3'-H3'	125.7
C27-C28-C29	118.3(2)	C5'-N4'-C3'	109.57(17)
C27-C28-C32	120.4(2)	C5'-N4'-C25'	125.26(18)
C29-C28-C32	121.2(2)	C3'-N4'-C25'	125.14(18)
C28-C29-C30	122.2(2)	N6'-C5'-N1'	132.53(19)
C28-C29-H29	118.6	N6'-C5'-N4'	121.17(19)
C30-C29-H29	119.3	N1'-C5'-N4'	106.24(19)
C25-C30-C29	117.4(2)	C5'-N6'-N7'	110.14(17)
C25-C30-C33	121.3(2)	N8'-N7'-N6'	112.37(17)
C29-C30-C33	121.2(2)	N7'-N8'-C9'	110.25(18)
C26-C31-H31A	109.5	N8'-C9'-C10'	113.64(18)
C26-C31-H31B	109.5	N8'-C9'-H9'A	109.6
H31A-C31-H31B	109.5	C10'-C9'-H9'A	108.9
C26-C31-H31C	109.4	N8'-C9'-H9'B	108.2
H31A-C31-H31C	109.5	C10'-C9'-H9'B	108.3
H31B-C31-H31C	109.5	H9'A-C9'-H9'B	108.0
C28-C32-H32A	109.5	C15'-C10'-C11'	118.2(2)
C28-C32-H32B	109.5	C15'-C10'-C9'	120.1(2)
H32A-C32-H32B	109.5	C11'-C10'-C9'	121.7(2)
C28-C32-H32C	109.5	C10'-C11'-C12'	120.4(2)
H32A-C32-H32C	109.5	C10'-C11'-H11'	119.2
H32B-C32-H32C	109.5	C12'-C11'-H11'	120.4
C30-C33-H33A	109.5	C13'-C12'-C11'	120.7(2)
C30-C33-H33B	109.4	C13'-C12'-H12'	119.6
H33A-C33-H33B	109.5	C11'-C12'-H12'	119.7
C30-C33-H33C	109.5	C14'-C13'-C12'	118.8(2)

C14'-C13'-H13'	120.1	H23D-C23'-H23F	109.5
C12'-C13'-H13'	121.0	H23E-C23'-H23F	109.5
C15'-C14'-C13'	120.8(2)	C21'-C24'-H24D	109.6
C15'-C14'-H14'	119.1	C21'-C24'-H24E	109.4
C13'-C14'-H14'	120.1	H24D-C24'-H24E	109.5
C14'-C15'-C10'	121.0(2)	C21'-C24'-H24F	109.4
C14'-C15'-H15'	120.5	H24D-C24'-H24F	109.5
C10'-C15'-H15'	118.5	H24E-C24'-H24F	109.5
C21'-C16'-C17'	122.05(19)	C30'-C25'-C26'	122.5(2)
C21'-C16'-N1'	119.45(19)	C30'-C25'-N4'	118.93(19)
C17'-C16'-N1'	118.5(2)	C26'-C25'-N4'	118.6(2)
C18'-C17'-C16'	117.8(2)	C27'-C26'-C25'	117.3(2)
C18'-C17'-C22'	121.5(2)	C27'-C26'-C31'	121.3(2)
C16'-C17'-C22'	120.6(2)	C25'-C26'-C31'	121.33(19)
C17'-C18'-C19'	122.1(2)	C28'-C27'-C26'	122.2(2)
C17'-C18'-H18'	119.1	C28'-C27'-H27'	118.6
C19'-C18'-H18'	118.8	C26'-C27'-H27'	119.2
C20'-C19'-C18'	118.3(2)	C29'-C28'-C27'	118.5(2)
C20'-C19'-C23'	121.0(2)	C29'-C28'-C32'	120.4(2)
C18'-C19'-C23'	120.7(2)	C27'-C28'-C32'	121.0(2)
C19'-C20'-C21'	121.8(2)	C28'-C29'-C30'	121.9(2)
C19'-C20'-H20'	118.9	C28'-C29'-H29'	118.5
C21'-C20'-H20'	119.2	C30'-C29'-H29'	119.6
C16'-C21'-C20'	117.9(2)	C25'-C30'-C29'	117.6(2)
C16'-C21'-C24'	120.6(2)	C25'-C30'-C33'	121.8(2)
C20'-C21'-C24'	121.6(2)	C29'-C30'-C33'	120.6(2)
C17'-C22'-H22D	109.4	C26'-C31'-H31D	109.5
C17'-C22'-H22E	109.5	C26'-C31'-H31E	109.5
H22D-C22'-H22E	109.5	H31D-C31'-H31E	109.5
C17'-C22'-H22F	109.4	C26'-C31'-H31F	109.4
H22D-C22'-H22F	109.5	H31D-C31'-H31F	109.5
H22E-C22'-H22F	109.5	H31E-C31'-H31F	109.5
C19'-C23'-H23D	109.6	C28'-C32'-H32D	109.4
C19'-C23'-H23E	109.4	C28'-C32'-H32E	109.6
H23D-C23'-H23E	109.5	H32D-C32'-H32E	109.5
C19'-C23'-H23F	109.4	C28'-C32'-H32F	109.4

H32D-C32'-H32F	109.5	H33D-C33'-H33E	109.5
H32E-C32'-H32F	109.5	C30'-C33'-H33F	109.4
C30'-C33'-H33D	109.4	H33D-C33'-H33F	109.5
C30'-C33'-H33E	109.6	H33E-C33'-H33F	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *(E)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N1	43(1)	28(1)	32(1)	1(1)	6(1)	-2(1)
C2	52(2)	28(2)	41(2)	-4(1)	2(1)	-5(1)
C3	48(2)	30(2)	39(2)	-6(1)	2(1)	-3(1)
N4	45(1)	29(1)	28(1)	-2(1)	3(1)	-2(1)
C5	33(2)	28(2)	32(1)	-1(1)	0(1)	1(1)
N6	43(1)	31(1)	28(1)	-4(1)	2(1)	-1(1)
N7	37(1)	36(1)	31(1)	-3(1)	0(1)	-3(1)
N8	54(1)	34(1)	32(1)	-5(1)	1(1)	-4(1)
C9	56(2)	48(2)	34(1)	-8(1)	-4(1)	-4(1)
C10	54(2)	31(2)	35(2)	0(1)	4(1)	-5(1)
C11	78(2)	49(2)	42(2)	-8(1)	-2(1)	3(2)
C12	102(3)	55(2)	48(2)	-14(2)	17(2)	8(2)
C13	74(2)	50(2)	74(2)	-3(2)	28(2)	5(2)
C14	60(2)	48(2)	61(2)	-1(2)	10(2)	-4(2)
C15	57(2)	37(2)	43(2)	-2(1)	8(2)	-5(1)
C16	35(2)	31(1)	31(1)	1(1)	6(1)	-6(1)
C17	38(2)	32(2)	38(2)	6(1)	2(1)	-3(1)
C18	46(2)	51(2)	35(2)	9(1)	1(1)	-7(1)
C19	37(2)	55(2)	35(2)	0(1)	9(1)	-4(1)
C20	33(2)	42(2)	41(2)	0(1)	6(1)	0(1)
C21	35(2)	32(2)	36(1)	3(1)	0(1)	-4(1)
C22	47(2)	49(2)	48(2)	4(1)	-2(1)	8(1)
C23	55(2)	115(3)	41(2)	3(2)	12(1)	2(2)
C24	45(2)	47(2)	44(2)	2(1)	-2(1)	4(1)
C25	39(2)	29(1)	28(1)	-5(1)	4(1)	0(1)
C26	38(2)	40(2)	34(1)	-3(1)	1(1)	3(1)
C27	40(2)	49(2)	41(2)	-6(1)	10(1)	-4(1)
C28	51(2)	37(2)	36(2)	-5(1)	12(1)	2(1)
C29	52(2)	36(2)	29(1)	-2(1)	-1(1)	7(1)
C30	36(2)	34(2)	33(1)	-2(1)	0(1)	3(1)

C31	43(2)	69(2)	51(2)	1(2)	-6(1)	5(2)
C32	81(2)	60(2)	50(2)	8(2)	26(2)	3(2)
C33	48(2)	51(2)	56(2)	4(1)	-8(1)	1(1)
N1'	44(1)	27(1)	31(1)	-2(1)	5(1)	4(1)
C2'	52(2)	28(2)	42(2)	1(1)	5(1)	8(1)
C3'	49(2)	31(2)	38(2)	3(1)	2(1)	4(1)
N4'	44(1)	26(1)	27(1)	0(1)	2(1)	3(1)
C5'	30(1)	30(2)	29(1)	-1(1)	1(1)	-1(1)
N6'	44(1)	28(1)	27(1)	4(1)	4(1)	1(1)
N7'	36(1)	35(1)	31(1)	3(1)	3(1)	1(1)
N8'	56(1)	32(1)	32(1)	7(1)	3(1)	1(1)
C9'	50(2)	46(2)	34(1)	9(1)	0(1)	0(1)
C10'	43(2)	28(1)	31(1)	-2(1)	3(1)	2(1)
C11'	51(2)	47(2)	43(2)	4(1)	-3(1)	2(1)
C12'	43(2)	62(2)	57(2)	-2(2)	-7(1)	4(2)
C13'	47(2)	64(2)	45(2)	-11(2)	10(1)	-10(2)
C14'	60(2)	50(2)	34(1)	-3(1)	3(1)	-9(2)
C15'	45(2)	38(2)	33(1)	0(1)	2(1)	-1(1)
C16'	39(2)	30(1)	27(1)	-2(1)	5(1)	5(1)
C17'	37(2)	37(2)	37(2)	-6(1)	2(1)	1(1)
C18'	51(2)	43(2)	34(2)	-7(1)	-7(1)	2(1)
C19'	54(2)	44(2)	30(2)	-2(1)	5(1)	13(1)
C20'	41(2)	40(2)	44(2)	5(1)	11(1)	5(1)
C21'	33(2)	34(2)	39(2)	0(1)	-1(1)	4(1)
C22'	45(2)	57(2)	56(2)	-9(1)	-3(1)	-7(2)
C23'	76(2)	71(2)	40(2)	2(1)	9(1)	19(2)
C24'	43(2)	55(2)	50(2)	-2(1)	-7(1)	-4(1)
C25'	38(2)	24(1)	27(1)	4(1)	5(1)	-2(1)
C26'	39(2)	28(1)	32(1)	3(1)	2(1)	-1(1)
C27'	58(2)	32(2)	30(1)	1(1)	0(1)	-4(1)
C28'	62(2)	29(2)	33(2)	5(1)	15(1)	-1(1)
C29'	41(2)	40(2)	50(2)	9(1)	14(1)	5(1)
C30'	39(2)	35(2)	35(1)	4(1)	1(1)	0(1)
C31'	46(2)	55(2)	54(2)	-6(1)	-6(1)	-2(1)
C32'	93(2)	47(2)	49(2)	-4(1)	32(2)	-3(2)
C33'	45(2)	62(2)	58(2)	-2(2)	-9(1)	-3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *(E)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene.

	x	y	z	U(eq)
H2	498	2396	2021	49
H3	-73	2002	2831	47
H9A	-524	-1625	776	55
H9B	-1072	-2713	815	55
H11	-302	-3432	105	68
H12	996	-4264	-218	82
H13	2360	-4327	216	79
H14	2426	-3564	983	67
H15	1138	-2682	1295	55
H18	177	1181	265	52
H20A	2224	-559	890	47
H22A	-1013	1966	719	72
H22B	-824	2170	1275	72
H22C	-1328	1073	1102	72
H23A	2273	522	9	106
H23B	1282	363	-227	106
H23C	1824	-673	-18	106
H24A	1779	146	2054	67
H24B	2385	-648	1731	67
H24C	1410	-1050	1916	67
H27	-2762	-912	3378	52
H29	-267	-1223	3978	47
H31A	-3005	67	2665	82
H31B	-2225	-179	2283	82
H31C	-2262	987	2544	82
H32A	-2653	-1596	4161	95
H32B	-1714	-1482	4454	95
H32C	-1891	-2532	4123	95
H33A	1009	-595	3019	78

H33B	1064	-642	3589	78
H33C	910	507	3325	78
H2'	5542	-20	1920	49
H3'	5036	338	2745	47
H9'A	4100	5400	838	52
H9'B	4527	4248	764	52
H11'	6260	4976	1345	57
H12'	7642	5698	1067	65
H13'	7692	6592	327	62
H14'	6340	6813	-114	58
H15'	4969	6108	165	46
H18'	4728	1145	213	51
H20'	7120	2521	619	50
H22D	3969	254	1244	79
H22E	3563	774	763	79
H22F	3592	1486	1242	79
H23D	6249	1121	-313	93
H23E	6893	2148	-194	93
H23F	5854	2341	-356	93
H24D	6595	3088	1769	74
H24E	7456	2912	1431	74
H24F	7122	1938	1769	74
H27'	4916	3505	3933	48
H29'	2399	3208	3362	52
H31D	6233	2946	3526	77
H31E	6158	2947	2956	77
H31F	6065	1821	3245	77
H32D	3353	4832	4108	94
H32E	3455	3743	4423	94
H32F	2536	3961	4123	94
H33D	2877	2552	2252	82
H33E	2128	2256	2643	82
H33F	2879	1367	2498	82

Table 6. Torsion angles [°] for *(E)*-1-benzyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene.

C5-N1-C2-C3	-0.5(3)	C21-C16-C17-C22	176.4(2)
C16-N1-C2-C3	-167.53(19)	N1-C16-C17-C22	-3.5(3)
N1-C2-C3-N4	0.4(3)	C16-C17-C18-C19	1.5(3)
C2-C3-N4-C5	-0.1(3)	C22-C17-C18-C19	-175.1(2)
C2-C3-N4-C25	-179.48(19)	C17-C18-C19-C20	-0.7(4)
C3-N4-C5-N6	176.0(2)	C17-C18-C19-C23	179.7(2)
C25-N4-C5-N6	-4.7(3)	C18-C19-C20-C21	-1.5(4)
C3-N4-C5-N1	-0.2(2)	C23-C19-C20-C21	178.1(2)
C25-N4-C5-N1	179.17(18)	C19-C20-C21-C16	2.7(3)
C2-N1-C5-N6	-175.3(2)	C19-C20-C21-C24	179.9(2)
C16-N1-C5-N6	-8.6(4)	C17-C16-C21-C20	-1.8(3)
C2-N1-C5-N4	0.4(2)	N1-C16-C21-C20	178.04(19)
C16-N1-C5-N4	167.09(19)	C17-C16-C21-C24	-179.1(2)
N4-C5-N6-N7	168.22(18)	N1-C16-C21-C24	0.8(3)
N1-C5-N6-N7	-16.7(3)	C5-N4-C25-C26	-75.2(3)
C5-N6-N7-N8	165.69(19)	C3-N4-C25-C26	104.1(3)
N6-N7-N8-C9	179.24(16)	C5-N4-C25-C30	106.9(2)
N7-N8-C9-C10	119.6(2)	C3-N4-C25-C30	-73.8(3)
N8-C9-C10-C15	-22.9(3)	C30-C25-C26-C27	-2.8(3)
N8-C9-C10-C11	159.3(2)	N4-C25-C26-C27	179.35(19)
C15-C10-C11-C12	-1.6(4)	C30-C25-C26-C31	176.6(2)
C9-C10-C11-C12	176.3(2)	N4-C25-C26-C31	-1.2(3)
C10-C11-C12-C13	0.6(4)	C25-C26-C27-C28	1.6(3)
C11-C12-C13-C14	0.9(4)	C31-C26-C27-C28	-177.9(2)
C12-C13-C14-C15	-1.4(4)	C26-C27-C28-C29	0.5(4)
C11-C10-C15-C14	1.1(4)	C26-C27-C28-C32	-179.5(2)
C9-C10-C15-C14	-176.8(2)	C27-C28-C29-C30	-1.5(3)
C13-C14-C15-C10	0.4(4)	C32-C28-C29-C30	178.4(2)
C5-N1-C16-C17	109.6(2)	C26-C25-C30-C29	1.8(3)
C2-N1-C16-C17	-85.6(3)	N4-C25-C30-C29	179.71(19)
C5-N1-C16-C21	-70.3(3)	C26-C25-C30-C33	-179.1(2)
C2-N1-C16-C21	94.5(3)	N4-C25-C30-C33	-1.3(3)
C21-C16-C17-C18	-0.2(3)	C28-C29-C30-C25	0.4(3)
N1-C16-C17-C18	179.9(2)	C28-C29-C30-C33	-178.7(2)

C5'-N1'-C2'-C3'	0.1(2)	C21'-C16'-C17'-C22'	-177.0(2)
C16'-N1'-C2'-C3'	177.22(19)	N1'-C16'-C17'-C22'	4.8(3)
N1'-C2'-C3'-N4'	-0.1(3)	C16'-C17'-C18'-C19'	0.0(4)
C2'-C3'-N4'-C5'	0.1(3)	C22'-C17'-C18'-C19'	177.3(2)
C2'-C3'-N4'-C25'	178.15(19)	C17'-C18'-C19'-C20'	-1.2(4)
C2'-N1'-C5'-N6'	176.9(2)	C17'-C18'-C19'-C23'	179.2(2)
C16'-N1'-C5'-N6'	0.0(4)	C18'-C19'-C20'-C21'	2.1(4)
C2'-N1'-C5'-N4'	-0.1(2)	C23'-C19'-C20'-C21'	-178.3(2)
C16'-N1'-C5'-N4'	-176.94(19)	C17'-C16'-C21'-C20'	0.4(3)
C3'-N4'-C5'-N6'	-177.39(19)	N1'-C16'-C21'-C20'	178.60(19)
C25'-N4'-C5'-N6'	4.5(3)	C17'-C16'-C21'-C24'	179.4(2)
C3'-N4'-C5'-N1'	0.0(2)	N1'-C16'-C21'-C24'	-2.4(3)
C25'-N4'-C5'-N1'	-178.08(18)	C19'-C20'-C21'-C16'	-1.7(3)
N1'-C5'-N6'-N7'	11.5(3)	C19'-C20'-C21'-C24'	179.3(2)
N4'-C5'-N6'-N7'	-171.95(17)	C5'-N4'-C25'-C30'	76.0(3)
C5'-N6'-N7'-N8'	-171.01(18)	C3'-N4'-C25'-C30'	-101.8(2)
N6'-N7'-N8'-C9'	-179.85(16)	C5'-N4'-C25'-C26'	-105.9(2)
N7'-N8'-C9'-C10'	-107.0(2)	C3'-N4'-C25'-C26'	76.3(3)
N8'-C9'-C10'-C15'	-159.8(2)	C30'-C25'-C26'-C27'	-2.0(3)
N8'-C9'-C10'-C11'	23.2(3)	N4'-C25'-C26'-C27'	179.94(18)
C15'-C10'-C11'-C12'	-1.0(3)	C30'-C25'-C26'-C31'	178.6(2)
C9'-C10'-C11'-C12'	176.2(2)	N4'-C25'-C26'-C31'	0.6(3)
C10'-C11'-C12'-C13'	-0.4(4)	C25'-C26'-C27'-C28'	-0.5(3)
C11'-C12'-C13'-C14'	1.4(4)	C31'-C26'-C27'-C28'	178.8(2)
C12'-C13'-C14'-C15'	-1.0(4)	C26'-C27'-C28'-C29'	2.0(3)
C13'-C14'-C15'-C10'	-0.3(4)	C26'-C27'-C28'-C32'	-177.4(2)
C11'-C10'-C15'-C14'	1.3(3)	C27'-C28'-C29'-C30'	-1.1(3)
C9'-C10'-C15'-C14'	-175.9(2)	C32'-C28'-C29'-C30'	178.3(2)
C5'-N1'-C16'-C21'	82.5(3)	C26'-C25'-C30'-C29'	2.9(3)
C2'-N1'-C16'-C21'	-94.0(3)	N4'-C25'-C30'-C29'	-179.06(19)
C5'-N1'-C16'-C17'	-99.3(3)	C26'-C25'-C30'-C33'	-176.3(2)
C2'-N1'-C16'-C17'	84.2(3)	N4'-C25'-C30'-C33'	1.7(3)
C21'-C16'-C17'-C18'	0.4(3)	C28'-C29'-C30'-C25'	-1.3(3)
N1'-C16'-C17'-C18'	-177.81(19)	C28'-C29'-C30'-C33'	177.9(2)

X-ray experimental for (*E*)-1-benzoyl-3-(1,3-dimesitylimidazol-2-ylidene)triazene ($C_{28}H_{29}N_5O$): Crystals grew as large, orange prisms by slow evaporation from ethyl acetate. The data crystal was cut from a much larger crystal and had approximate dimensions; 0.37 x 0.32 x 0.20 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 226 frames of data were collected using ω-scans with a scan range of 1° and a counting time of 65 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR97[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.044*P)^2 + (0.1*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.114, with R(F) equal to 0.0511 and a goodness of fit, S, = 1.19. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (1.2(2)x10^{-5})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in Tables 1 through 7.

References

1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

2) SIR97. (1999). A program for crystal structure solution. Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. J. Appl. Cryst. 32, 115-119.

3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

4) $R_W(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$.
$S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for *(E)*-1-benzoyl-(1,3-dimesitylimidazol-2-ylidene)triazene.

Empirical formula	C28 H29 N5 O	
Formula weight	451.56	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 14.0109(3) Å	α= 90°.
	b = 14.0230(3) Å	β= 90°.
	c = 12.6469(2) Å	γ = 90°.
Volume	2484.80(8) $Å^3$	
Z	4	
Density (calculated)	1.207 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	960	
Crystal size	0.37 x 0.32 x 0.20 mm	
Theta range for data collection	3.22 to 27.48°.	
Index ranges	-18<=h<=18, -17<=k<=18, -15<=l<=16	
Reflections collected	5434	
Independent reflections	5434 [R(int) = 0.0000]	
Completeness to theta = 27.48°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5434 / 0 / 308	
Goodness-of-fit on F^2	1.191	
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.1018	
R indices (all data)	R1 = 0.1036, wR2 = 0.1135	
Absolute structure parameter	1.5(17)	
Extinction coefficient	$1.20(15)x10^{-5}$	
Largest diff. peak and hole	0.222 and -0.190 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *(E)*-1-benzoyl-(1,3-dimesitylimidazol-2-ylidene)triazene. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N1	2219(1)	3572(1)	993(1)	33(1)
C2	2536(2)	4039(2)	84(2)	37(1)
C3	2626(2)	4958(2)	311(2)	38(1)
N4	2361(1)	5081(1)	1368(1)	32(1)
C5	2123(2)	4222(2)	1782(2)	30(1)
N6	1822(1)	4137(1)	2796(1)	30(1)
N7	1839(1)	3229(1)	3095(1)	29(1)
N8	1456(1)	3103(1)	4017(1)	30(1)
C9	1589(2)	2152(2)	4358(2)	30(1)
O10	2292(1)	1678(1)	4158(1)	45(1)
C11	802(2)	1779(2)	5028(2)	26(1)
C12	939(2)	929(2)	5564(2)	37(1)
C13	207(2)	543(2)	6155(2)	43(1)
C14	-668(2)	994(2)	6202(2)	43(1)
C15	-817(2)	1836(2)	5670(2)	38(1)
C16	-77(2)	2236(2)	5087(2)	31(1)
C17	1882(2)	2594(2)	971(2)	33(1)
C18	980(2)	2433(2)	549(2)	40(1)
C19	660(2)	1492(2)	476(2)	47(1)
C20	1233(2)	736(2)	802(2)	48(1)
C21	2113(2)	939(2)	1235(2)	42(1)
C22	2465(2)	1860(2)	1325(2)	35(1)
C23	348(2)	3248(2)	215(2)	58(1)
C24	891(2)	-289(2)	677(2)	64(1)
C25	3420(2)	2049(2)	1818(2)	46(1)
C26	2340(2)	5985(2)	1914(2)	34(1)
C27	3198(2)	6459(2)	2071(2)	42(1)
C28	3155(2)	7366(2)	2547(2)	51(1)
C29	2302(3)	7779(2)	2831(2)	55(1)
C30	1463(2)	7274(2)	2654(2)	47(1)

C31	1460(2)	6372(2)	2195(2)	38(1)
C32	4132(2)	6037(2)	1743(2)	51(1)
C33	2287(3)	8762(2)	3329(2)	79(1)
C34	543(2)	5849(2)	2032(2)	43(1)

Table 3. Bond lengths [Å] and angles [°] for *(E)*-1-benzoyl-(1,3-dimesitylimidazol-2-ylidene)triazene.

N1-C5	1.358(3)	C20-C24	1.523(3)
N1-C2	1.396(3)	C21-C22	1.387(3)
N1-C17	1.451(3)	C21-H21	0.96
C2-C3	1.327(3)	C22-C25	1.500(3)
C2-H2	0.96	C23-H23C	0.96
C3-N4	1.398(3)	C23-H23A	0.96
C3-H3	0.96	C23-H23B	0.96
N4-C5	1.355(3)	C24-H24A	0.96
N4-C26	1.444(3)	C24-H24B	0.96
C5-N6	1.355(3)	C24-H24C	0.96
N6-N7	1.328(2)	C25-H25A	0.96
N7-N8	1.295(2)	C25-H25B	0.96
N8-C9	1.414(3)	C25-H25C	0.96
C9-O10	1.215(2)	C26-C27	1.387(3)
C9-C11	1.486(3)	C26-C31	1.393(3)
C11-C12	1.385(3)	C27-C28	1.408(3)
C11-C16	1.391(3)	C27-C32	1.495(4)
C12-C13	1.380(3)	C28-C29	1.376(4)
C12-H12	0.96	C28-H28	0.96
C13-C14	1.380(3)	C29-C30	1.391(4)
C13-H13	0.96	C29-C33	1.516(3)
C14-C15	1.375(3)	C30-C31	1.392(3)
C14-H14	0.96	C30-H30	0.96
C15-C16	1.390(3)	C31-C34	1.495(3)
C15-H15	0.96	C32-H32C	0.96
C16-H16	0.96	C32-H32A	0.96
C17-C22	1.388(3)	C32-H32B	0.96
C17-C18	1.390(3)	C33-H33A	0.96
C18-C19	1.396(3)	C33-H33B	0.96
C18-C23	1.506(4)	C33-H33C	0.96
C19-C20	1.393(4)	C34-H34C	0.96
C19-H19	0.96	C34-H34A	0.96
C20-C21	1.378(4)	C34-H34B	0.96

C5-N1-C2	108.77(17)	C15-C16-C11	120.2(2)
C5-N1-C17	128.03(18)	C15-C16-H16	120.5
C2-N1-C17	122.10(18)	C11-C16-H16	119.3
C3-C2-N1	107.92(19)	C22-C17-C18	122.6(2)
C3-C2-H2	126.4	C22-C17-N1	120.2(2)
N1-C2-H2	125.6	C18-C17-N1	117.2(2)
C2-C3-N4	107.6(2)	C17-C18-C19	118.1(2)
C2-C3-H3	126.5	C17-C18-C23	121.3(2)
N4-C3-H3	125.9	C19-C18-C23	120.6(2)
C5-N4-C3	108.96(18)	C20-C19-C18	121.0(2)
C5-N4-C26	126.20(16)	C20-C19-H19	119.5
C3-N4-C26	124.83(18)	C18-C19-H19	119.5
N6-C5-N4	121.37(19)	C21-C20-C19	118.4(2)
N6-C5-N1	131.8(2)	C21-C20-C24	121.1(2)
N4-C5-N1	106.78(17)	C19-C20-C24	120.4(2)
N7-N6-C5	110.43(17)	C20-C21-C22	122.9(2)
N8-N7-N6	112.34(16)	C20-C21-H21	118.7
N7-N8-C9	110.40(17)	C22-C21-H21	118.5
O10-C9-N8	124.0(2)	C21-C22-C17	117.0(2)
O10-C9-C11	121.90(19)	C21-C22-C25	121.0(2)
N8-C9-C11	114.07(19)	C17-C22-C25	121.9(2)
C12-C11-C16	119.5(2)	C18-C23-H23C	109.5
C12-C11-C9	118.7(2)	C18-C23-H23A	110.5
C16-C11-C9	121.75(19)	H23C-C23-H23A	109.5
C13-C12-C11	120.0(2)	C18-C23-H23B	109.5
C13-C12-H12	120.4	H23C-C23-H23B	109.5
C11-C12-H12	119.6	H23A-C23-H23B	108.4
C12-C13-C14	120.2(2)	C20-C24-H24A	109.2
C12-C13-H13	119.6	C20-C24-H24B	108.8
C14-C13-H13	120.2	H24A-C24-H24B	109.5
C15-C14-C13	120.5(2)	C20-C24-H24C	110.4
C15-C14-H14	120.2	H24A-C24-H24C	109.5
C13-C14-H14	119.3	H24B-C24-H24C	109.5
C14-C15-C16	119.5(2)	C22-C25-H25A	108.9
C14-C15-H15	120.3	C22-C25-H25B	110.3
C16-C15-H15	120.2	H25A-C25-H25B	109.5

C22-C25-H25C	109.2	C31-C34-H34B	111.2
H25A-C25-H25C	109.5	H34C-C34-H34B	108.3
H25B-C25-H25C	109.5	H34A-C34-H34B	109.2
C27-C26-C31	122.9(2)		
C27-C26-N4	118.1(2)		
C31-C26-N4	118.8(2)		
C26-C27-C28	117.2(2)		
C26-C27-C32	122.0(2)		
C28-C27-C32	120.8(2)		
C29-C28-C27	121.9(3)		
C29-C28-H28	118.8		
C27-C28-H28	119.4		
C28-C29-C30	118.6(2)		
C28-C29-C33	120.3(3)		
C30-C29-C33	121.2(3)		
C29-C30-C31	122.1(3)		
C29-C30-H30	119.3		
C31-C30-H30	118.6		
C30-C31-C26	117.3(2)		
C30-C31-C34	120.4(2)		
C26-C31-C34	122.4(2)		
C27-C32-H32C	109.4		
C27-C32-H32A	110.3		
H32C-C32-H32A	109.5		
C27-C32-H32B	109.8		
H32C-C32-H32B	109.5		
H32A-C32-H32B	108.4		
C29-C33-H33A	108.9		
C29-C33-H33B	109.8		
H33A-C33-H33B	109.5		
C29-C33-H33C	109.7		
H33A-C33-H33C	109.5		
H33B-C33-H33C	109.5		
C31-C34-H34C	108.3		
C31-C34-H34A	111.5		
H34C-C34-H34A	108.3		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *(E)*-1-benzoyl-(1,3-dimesitylimidazol-2-ylidene)triazene. The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N1	42(1)	28(1)	28(1)	0(1)	0(1)	-4(1)
C2	51(2)	36(1)	25(1)	6(1)	5(1)	-4(1)
C3	44(2)	37(1)	31(1)	6(1)	2(1)	-7(1)
N4	43(1)	27(1)	26(1)	5(1)	0(1)	-6(1)
C5	35(1)	28(1)	26(1)	5(1)	-2(1)	-3(1)
N6	36(1)	29(1)	25(1)	4(1)	0(1)	-4(1)
N7	34(1)	26(1)	28(1)	5(1)	-1(1)	-4(1)
N8	38(1)	26(1)	27(1)	4(1)	3(1)	-5(1)
C9	32(1)	28(1)	29(1)	-1(1)	-3(1)	0(1)
O10	39(1)	39(1)	57(1)	15(1)	11(1)	8(1)
C11	30(1)	22(1)	27(1)	1(1)	-1(1)	-3(1)
C12	35(1)	36(1)	41(1)	11(1)	1(1)	6(1)
C13	46(2)	32(1)	52(2)	16(1)	7(1)	4(1)
C14	45(2)	37(2)	47(1)	7(1)	12(1)	-3(1)
C15	33(1)	39(2)	42(1)	-3(1)	6(1)	3(1)
C16	36(1)	26(1)	30(1)	0(1)	-3(1)	0(1)
C17	45(2)	28(1)	27(1)	-2(1)	4(1)	-5(1)
C18	50(2)	36(2)	34(1)	0(1)	-4(1)	-5(1)
C19	55(2)	45(2)	39(1)	-3(1)	-5(1)	-14(1)
C20	67(2)	35(2)	40(2)	-6(1)	7(1)	-10(1)
C21	59(2)	31(1)	37(1)	-2(1)	14(1)	3(1)
C22	41(2)	34(1)	29(1)	-3(1)	6(1)	2(1)
C23	59(2)	50(2)	65(2)	11(2)	-25(2)	-2(2)
C24	86(2)	38(2)	68(2)	-7(2)	7(2)	-19(2)
C25	40(2)	50(2)	47(1)	-4(1)	6(1)	8(1)
C26	53(2)	24(1)	26(1)	5(1)	-4(1)	-6(1)
C27	61(2)	37(2)	29(1)	13(1)	-11(1)	-17(1)
C28	80(2)	39(2)	35(2)	13(1)	-18(1)	-25(2)
C29	101(3)	34(2)	30(1)	5(1)	-9(2)	-15(2)
C30	80(2)	30(1)	29(1)	4(1)	0(1)	5(2)

C31	60(2)	27(1)	26(1)	6(1)	-7(1)	-1(1)
C32	49(2)	52(2)	52(2)	20(1)	-13(1)	-18(1)
C33	157(3)	37(2)	43(2)	-5(1)	-13(2)	-12(2)
C34	50(2)	45(2)	34(1)	8(1)	-3(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *(E)*-1-benzoyl-(1,3-dimesitylimidazol-2-ylidene)triazene.

	x	y	z	U(eq)
H2	2671	3741	-583	44
H3	2834	5452	-162	45
H12	1548	618	5533	45
H13	307	-44	6530	52
H14	-1171	716	6615	52
H15	-1428	2145	5699	45
H16	-168	2827	4717	37
H19	38	1365	190	56
H21	2498	421	1488	51
H23C	280	3688	791	87
H23A	-270	3016	9	87
H23B	628	3568	-380	87
H24A	1374	-714	938	96
H24B	317	-371	1080	96
H24C	766	-428	-54	96
H25A	3539	2723	1808	68
H25B	3429	1824	2534	68
H25C	3904	1726	1418	68
H28	3737	7708	2678	61
H30	864	7552	2858	56
H32C	4144	5964	989	77
H32A	4222	5427	2073	77
H32B	4644	6449	1958	77
H33A	1637	8935	3476	118
H33B	2645	8756	3976	118
H33C	2561	9217	2851	118
H34C	26	6279	2176	64
H34A	488	5314	2503	64
H34B	483	5630	1316	64

Table 6. Torsion angles [°] for *(E)*-1-benzoyl-(1,3-dimesitylimidazol-2-ylidene)triazene.

C5-N1-C2-C3	-0.4(3)
C17-N1-C2-C3	168.5(2)
N1-C2-C3-N4	-0.3(3)
C2-C3-N4-C5	0.9(3)
C2-C3-N4-C26	-178.6(2)
C3-N4-C5-N6	-178.9(2)
C26-N4-C5-N6	0.6(3)
C3-N4-C5-N1	-1.1(2)
C26-N4-C5-N1	178.3(2)
C2-N1-C5-N6	178.4(2)
C17-N1-C5-N6	10.3(4)
C2-N1-C5-N4	0.9(2)
C17-N1-C5-N4	-167.1(2)
N4-C5-N6-N7	-165.96(19)
N1-C5-N6-N7	16.9(3)
C5-N6-N7-N8	-172.77(17)
N6-N7-N8-C9	-173.10(17)
N7-N8-C9-O10	34.1(3)
N7-N8-C9-C11	-148.09(17)
O10-C9-C11-C12	9.7(3)
N8-C9-C11-C12	-168.11(18)
O10-C9-C11-C16	-167.0(2)
N8-C9-C11-C16	15.2(3)
C16-C11-C12-C13	-0.3(3)
C9-C11-C12-C13	-177.1(2)
C11-C12-C13-C14	1.0(4)
C12-C13-C14-C15	-0.6(4)
C13-C14-C15-C16	-0.5(3)
C14-C15-C16-C11	1.2(3)
C12-C11-C16-C15	-0.8(3)
C9-C11-C16-C15	175.93(19)
C5-N1-C17-C22	-90.8(3)
C2-N1-C17-C22	102.5(3)
C5-N1-C17-C18	91.6(3)

C2-N1-C17-C18	-75.1(3)
C22-C17-C18-C19	-0.5(3)
N1-C17-C18-C19	177.0(2)
C22-C17-C18-C23	177.4(2)
N1-C17-C18-C23	-5.0(3)
C17-C18-C19-C20	-0.8(4)
C23-C18-C19-C20	-178.8(2)
C18-C19-C20-C21	2.2(4)
C18-C19-C20-C24	-177.6(2)
C19-C20-C21-C22	-2.3(3)
C24-C20-C21-C22	177.4(2)
C20-C21-C22-C17	1.1(3)
C20-C21-C22-C25	179.0(2)
C18-C17-C22-C21	0.4(3)
N1-C17-C22-C21	-177.06(19)
C18-C17-C22-C25	-177.5(2)
N1-C17-C22-C25	5.0(3)
C5-N4-C26-C27	115.4(2)
C3-N4-C26-C27	-65.2(3)
C5-N4-C26-C31	-68.9(3)
C3-N4-C26-C31	110.5(2)
C31-C26-C27-C28	0.7(3)
N4-C26-C27-C28	176.18(17)
C31-C26-C27-C32	-178.7(2)
N4-C26-C27-C32	-3.2(3)
C26-C27-C28-C29	-1.1(3)
C32-C27-C28-C29	178.4(2)
C27-C28-C29-C30	0.9(3)
C27-C28-C29-C33	-179.2(2)
C28-C29-C30-C31	-0.4(3)
C33-C29-C30-C31	179.8(2)
C29-C30-C31-C26	0.0(3)
C29-C30-C31-C34	179.2(2)
C27-C26-C31-C30	-0.2(3)
N4-C26-C31-C30	-175.64(17)
C27-C26-C31-C34	-179.3(2)

N4-C26-C31-C34 5.2(3)
