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Supporting information for article:

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Unanticipated Formation of a Novel Octaazacyclodecane Ring Upon Oxidation of a 1,1-bis-Urazole

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Supporting Information

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S1. Computational Details

S1.1. Compound *trans*-5

RB3LYP/6-311G(d,p) E = –1590.06498508 Hartrees
Number of Imaginary Frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.427849
2	7	0	-0.785081	-0.859157	0.500480
3	7	0	-0.354399	-0.585902	-0.851544
4	7	0	0.785081	0.859157	0.500480
5	7	0	0.354399	0.585902	-0.851544
6	6	0	-1.124692	0.747253	2.227034
7	6	0	1.124692	-0.747253	2.227034
8	6	0	-1.749003	-0.008852	3.370352
9	1	0	-1.776092	-1.083309	3.175309
10	1	0	-1.159454	0.161117	4.277078
11	1	0	-2.753391	0.376924	3.539966
12	6	0	1.749003	0.008852	3.370352
13	1	0	2.753391	-0.376924	3.539966
14	1	0	1.776092	1.083309	3.175309
15	1	0	1.159454	-0.161117	4.277078
16	8	0	-1.498247	1.825540	1.847283
17	8	0	1.498247	-1.825540	1.847283
18	6	0	-0.197454	1.779799	-1.398114
19	6	0	0.792199	2.279101	0.638148
20	6	0	0.197454	-1.779799	-1.398114
21	6	0	-0.792199	-2.279101	0.638148
22	7	0	0.303995	2.792413	-0.564814
23	8	0	1.213571	2.874130	1.591205
24	8	0	-0.845704	1.869934	-2.396140
25	8	0	-1.213571	-2.874130	1.591205
26	8	0	0.845704	-1.869934	-2.396140
27	7	0	-0.303995	-2.792413	-0.564814
28	6	0	0.192745	4.194078	-0.843877
29	6	0	1.292694	5.021646	-0.620721
30	6	0	-1.003795	4.712985	-1.336169
31	6	0	1.187752	6.382478	-0.889207
32	1	0	2.212114	4.606466	-0.230305
33	6	0	-1.090068	6.074061	-1.614958
34	1	0	-1.847147	4.059445	-1.507996
35	6	0	0.000000	6.911134	-1.390273
36	1	0	2.039668	7.028048	-0.710767
37	1	0	-2.017173	6.478773	-2.003595
38	1	0	-0.075359	7.970954	-1.604149
39	6	0	-0.192745	-4.194078	-0.843877
40	6	0	-1.292694	-5.021646	-0.620721
41	6	0	1.003795	-4.712985	-1.336169
42	6	0	-1.187752	-6.382478	-0.889207
43	1	0	-2.212114	-4.606466	-0.230305

44	6	0	1.090068	-6.074061	-1.614958
45	1	0	1.847147	-4.059445	-1.507996
46	6	0	0.000000	-6.911134	-1.390273
47	1	0	-2.039668	-7.028048	-0.710767
48	1	0	2.017173	-6.478773	-2.003595
49	1	0	0.075359	-7.970954	-1.604149

S1.2. Compound *cis*–5

RB3LYP/6-311G(d,p) E = –1590.05385385 Hartrees
Number of Imaginary Frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.216955	2.146935	-0.044735
2	7	0	1.000461	1.419441	-0.354351
3	7	0	0.819776	0.676205	-1.567865
4	7	0	-1.216368	1.455914	-0.972456
5	7	0	-0.557680	0.327300	-1.573716
6	6	0	-0.532933	1.953389	1.497595
7	6	0	-0.212168	3.624963	-0.542564
8	6	0	-0.225799	3.063991	2.454613
9	1	0	0.757539	3.493311	2.253255
10	1	0	-0.968925	3.854873	2.329450
11	1	0	-0.258143	2.663435	3.466199
12	6	0	0.746601	3.986015	-1.646409
13	1	0	0.506450	4.983932	-2.008945
14	1	0	1.771874	3.969835	-1.264308
15	1	0	0.698363	3.259442	-2.460477
16	8	0	-0.981569	0.885790	1.826107
17	8	0	-0.997160	4.397518	-0.054575
18	6	0	-1.087243	-0.860798	-0.977801
19	6	0	-2.421532	0.928380	-0.395984
20	6	0	1.795612	-0.399165	-1.531657
21	6	0	1.929867	0.798183	0.470927
22	7	0	-2.352342	-0.461928	-0.536703
23	8	0	-3.293030	1.586323	0.088956
24	8	0	-0.589219	-1.949141	-0.976657
25	8	0	2.259497	1.142074	1.575594
26	8	0	2.001282	-1.173472	-2.413349
27	7	0	2.462214	-0.244980	-0.313599
28	6	0	3.531662	-1.098517	0.116276
29	6	0	4.691474	-0.538063	0.648243
30	6	0	3.392252	-2.480143	-0.006867
31	6	0	5.722074	-1.375600	1.063800
32	1	0	4.779208	0.535539	0.748731
33	6	0	4.436440	-3.305216	0.399090
34	1	0	2.483063	-2.896485	-0.419556
35	6	0	5.599681	-2.757466	0.935707
36	1	0	6.623177	-0.944599	1.483959

37	1	0	4.334714	-4.379459	0.300163
38	1	0	6.407607	-3.405510	1.254954
39	6	0	-3.349150	-1.375968	-0.062227
40	6	0	-3.898796	-1.211641	1.207875
41	6	0	-3.748183	-2.426219	-0.886992
42	6	0	-4.869986	-2.107327	1.645646
43	1	0	-3.569490	-0.395700	1.835783
44	6	0	-4.708422	-3.323826	-0.431408
45	1	0	-3.306564	-2.541420	-1.868779
46	6	0	-5.274446	-3.163185	0.831620
47	1	0	-5.304827	-1.981260	2.630200
48	1	0	-5.017469	-4.144761	-1.067662
49	1	0	-6.027717	-3.859919	1.180769

S1.3. Compound 9

B3LYP/6-311G(d,p) E = –3180.17690821 Hartrees
Number of Imaginary Frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.246552	0.208701	-3.249045
2	6	0	-2.160168	1.720756	0.998989
3	6	0	-0.101960	1.665656	2.024293
4	6	0	-4.373414	-0.833734	-4.163728
5	6	0	-1.307271	-1.857094	-0.046228
6	8	0	-1.218771	-2.225129	-2.415531
7	6	0	2.106327	-2.084115	3.467881
8	6	0	2.160168	-1.720756	0.998989
9	7	0	1.474644	-1.853387	2.196516
10	8	0	3.340552	-1.739116	0.793000
11	6	0	4.246552	-0.208701	-3.249045
12	6	0	3.191002	0.943256	-1.304005
13	8	0	3.896618	1.916915	-1.259213
14	7	0	3.264940	-0.112885	-2.207488
15	6	0	1.307271	1.857094	-0.046228
16	8	0	1.218771	2.225129	-2.415531
17	6	0	-2.106327	2.084115	3.467881
18	8	0	0.752260	1.712436	2.873242
19	7	0	-1.474644	1.853387	2.196516
20	7	0	-3.264940	0.112885	-2.207488
21	8	0	-2.056147	2.064932	-2.572039
22	6	0	-2.250049	1.026410	-2.012488
23	6	0	-5.330165	-0.737524	-5.169746
24	6	0	-0.887417	-2.679135	-1.353497
25	8	0	-1.814742	-3.930022	1.050851
26	6	0	2.095449	-1.079099	4.431563
27	6	0	0.101960	-1.665656	2.024293
28	8	0	-0.752260	-1.712436	2.873242
29	7	0	1.163056	-1.498108	0.001769

30	6	0	5.050913	-1.342318	-3.328645
31	8	0	2.056147	-2.064932	-2.572039
32	6	0	2.250049	-1.026410	-2.012488
33	7	0	1.439804	-0.496792	-0.935954
34	6	0	2.188338	2.794594	0.917017
35	8	0	1.814742	3.930022	1.050851
36	6	0	-2.095449	1.079099	4.431563
37	8	0	-3.340552	1.739116	0.793000
38	7	0	0.101960	1.429970	0.661214
39	7	0	-1.439804	0.496792	-0.935954
40	8	0	-3.896618	-1.916915	-1.259213
41	6	0	-3.191002	-0.943256	-1.304005
42	6	0	-6.137889	0.394121	-5.264996
43	6	0	-2.188338	-2.794594	0.917017
44	6	0	2.712325	-1.315450	5.657335
45	7	0	-0.101960	-1.429970	0.661214
46	6	0	5.994734	-1.433044	-4.347479
47	7	0	2.112092	0.672047	-0.435702
48	6	0	0.887417	2.679135	-1.353497
49	6	0	-2.712325	1.315450	5.657335
50	7	0	-1.163056	1.498108	0.001769
51	7	0	-2.112092	-0.672047	-0.435702
52	6	0	-5.994734	1.433044	-4.347479
53	6	0	-0.147137	-3.984038	-1.228220
54	6	0	3.340552	-2.534099	5.905720
55	6	0	6.137889	-0.394121	-5.264996
56	6	0	3.411306	2.256429	1.613715
57	6	0	-3.340552	2.534099	5.905720
58	6	0	-5.050913	1.342318	-3.328645
59	6	0	-3.411306	-2.256429	1.613715
60	6	0	3.351003	-3.527025	4.928128
61	6	0	5.330165	0.737524	-5.169746
62	6	0	0.147137	3.984038	-1.228220
63	6	0	-2.727260	3.307396	3.703641
64	6	0	4.373414	0.833734	-4.163728
65	6	0	2.727260	-3.307396	3.703641
66	6	0	-3.351003	3.527025	4.928128
67	1	0	-6.877701	0.466678	-6.053916
68	1	0	-3.434027	-1.171617	1.671957
69	1	0	-4.291772	-2.593272	1.064052
70	1	0	0.316827	-4.132709	-0.258626
71	1	0	0.592998	-4.011920	-2.026359
72	1	0	-0.872381	-4.789056	-1.376948
73	1	0	0.872381	4.789056	-1.376948
74	1	0	-0.316827	4.132709	-0.258626
75	1	0	4.291772	2.593272	1.064052
76	1	0	-3.823721	2.709747	6.859893
77	1	0	-2.707599	0.540481	6.414700
78	1	0	-3.423616	-2.691695	2.612366
79	1	0	-0.592998	4.011920	-2.026359
80	1	0	3.434027	1.171617	1.671957
81	1	0	3.423616	2.691695	2.612366
82	1	0	3.731813	1.701106	-4.080906
83	1	0	5.438236	1.545910	-5.883284
84	1	0	6.877701	-0.466678	-6.053916

85	1	0	6.621355	-2.314246	-4.419473
86	1	0	2.722388	-4.073279	2.938003
87	1	0	3.840117	-4.475022	5.117984
88	1	0	3.823721	-2.709747	6.859893
89	1	0	2.707599	-0.540481	6.414700
90	1	0	-2.722388	4.073279	2.938003
91	1	0	-3.840117	4.475022	5.117984
92	1	0	-4.932466	2.138091	-2.604768
93	1	0	-6.621355	2.314246	-4.419473
94	1	0	-5.438236	-1.545910	-5.883284
95	1	0	-1.620509	0.129231	4.219137
96	1	0	4.932466	-2.138091	-2.604768
97	1	0	1.620509	-0.129231	4.219137
98	1	0	-3.731813	-1.701106	-4.080906

S1.4. Compound 12

B3LYP/6-311G(d,p) E = –822.51368972 Hartrees
Number of Imaginary Frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.825461
2	7	0	-0.465827	1.044842	0.914258
3	7	0	0.000000	0.773628	-0.410018
4	7	0	0.465827	-1.044842	0.914258
5	7	0	0.000000	-0.773628	-0.410018
6	6	0	1.077784	-1.240974	-1.290452
7	6	0	1.816902	-1.427225	0.893283
8	6	0	-1.077784	1.240974	-1.290452
9	6	0	-1.816902	1.427225	0.893283
10	7	0	2.079165	-1.687039	-0.450134
11	8	0	2.546771	-1.548119	1.838124
12	8	0	1.041171	-1.229377	-2.480209
13	8	0	-2.546771	1.548119	1.838124
14	8	0	-1.041171	1.229377	-2.480209
15	7	0	-2.079165	1.687039	-0.450134
16	1	0	-0.837269	-0.317847	2.447202
17	1	0	0.837269	0.317847	2.447202
18	1	0	-2.967448	2.030020	-0.782639
19	1	0	2.967448	-2.030020	-0.782639

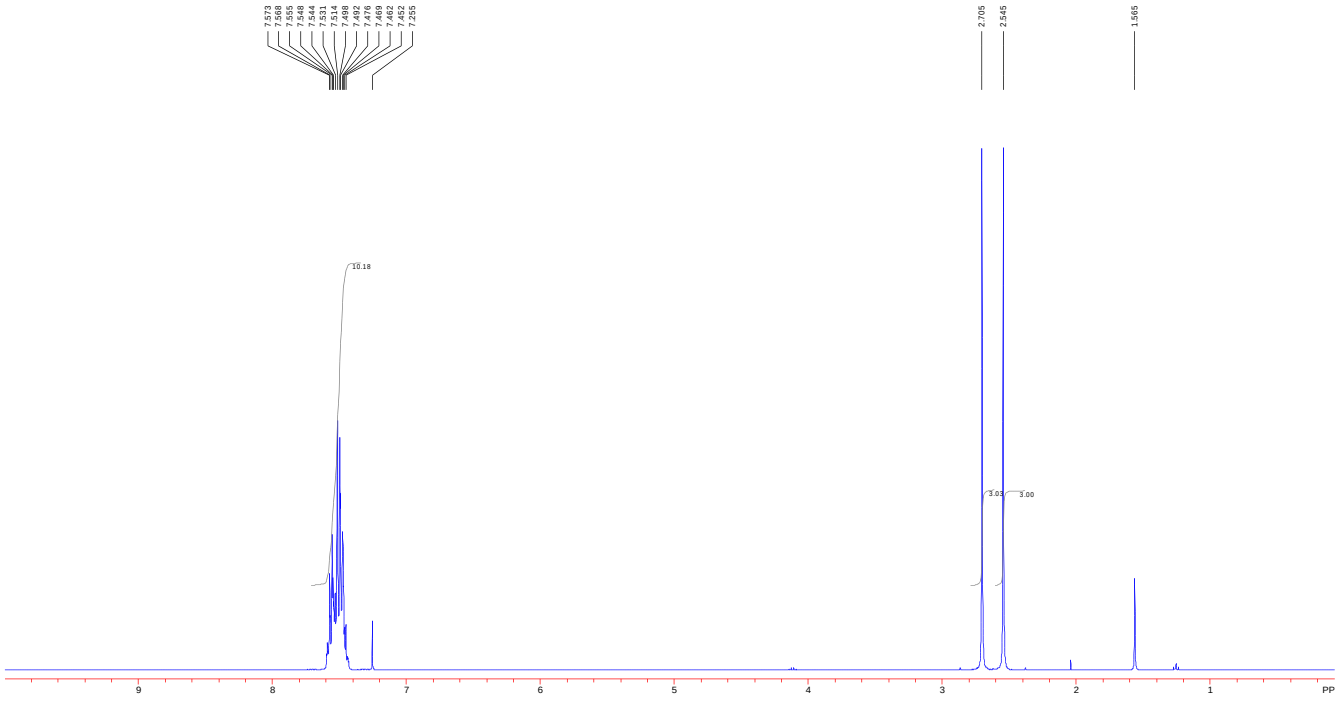
S1.5. Transition State Structure for N–N Bond Cleavage of Compound 12

CASSCF/6-31G(d) E = –817.79051920 Hartrees
Single Point Energy Calculation UB3LYP/6-311G(d,p)// CASSCF/6-31G(d) E = –822.50010650 Hartrees
Number of Imaginary Frequencies = 1 (–94.7 cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.784582	0.000000
2	7	0	-1.068534	-0.916239	0.465292
3	7	0	-0.639411	0.294918	0.895495
4	7	0	1.068534	-0.916239	-0.465292
5	7	0	0.639411	0.294918	-0.895495
6	6	0	1.714644	1.202029	-0.623552
7	6	0	2.251303	-0.801499	0.280414
8	6	0	-1.714643	1.202029	0.623552
9	6	0	-2.251303	-0.801499	-0.280414
10	7	0	2.659310	0.487269	0.068106
11	8	0	2.766028	-1.652439	0.918542
12	8	0	1.741932	2.328574	-0.957925
13	8	0	-2.766028	-1.652439	-0.918542
14	8	0	-1.741932	2.328575	0.957925
15	7	0	-2.659310	0.487269	-0.068106
16	1	0	-0.393187	-2.397703	-0.792835
17	1	0	0.393187	-2.397703	0.792835
18	1	0	-3.493951	0.877549	-0.446347
19	1	0	3.493951	0.877549	0.446347

S2. NMR Spectra of Relevant Compounds

S2.1. ^{1}H NMR Spectrum for Compound 9 (400 MHz, $CDCl_3$)



S2.2. ^{13}C NMR Spectrum for Compound 9 (100 MHz, $CDCl_3$)

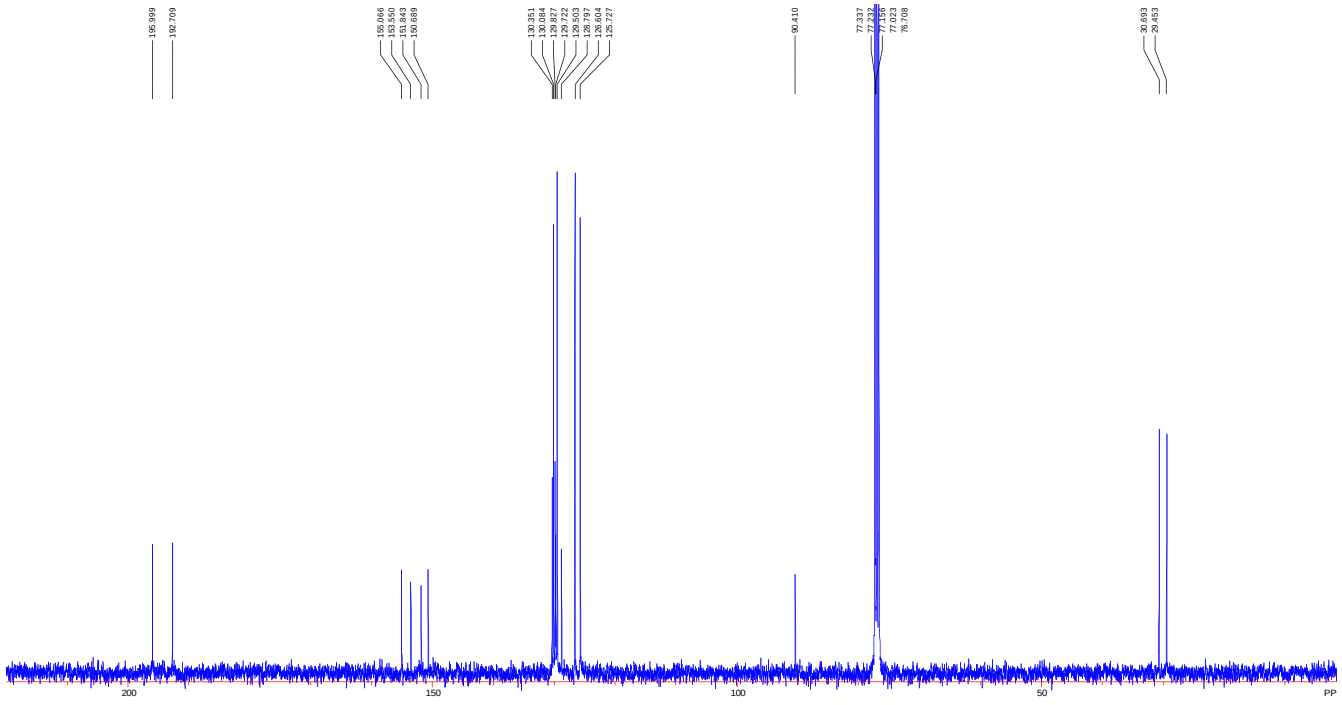


Table S1 Crystal parameters and refinement metrics for **9**.

Computing details
Data collection: *APEX2* v2014.11 (Bruker, 2014); cell refinement: *SAINT* V8.34A (Bruker AXS Inc., 2013); data reduction: *SAINT* V8.34A (Bruker AXS Inc., 2013); program(s) used to solve structure: *SHELXS* SHELXTL Version 2013/1 (Bruker AXS Inc., 2013); program(s) used to refine structure: *SHELXL-2017/1* (Sheldrick, 2017); molecular graphics: *ShelXle* (Hübschle, Sheldrick, and Dittrich, 2011); software used to prepare material for publication: *SHELXL-2017/1* (Sheldrick, 2017) via *ShelXle* (Hübschle, Sheldrick, and Dittrich, 2011)

7,7,18,18-tetraacetyl-4,10,15,21-tetraphenyl-1,2,4,6,8,10,12,13,15,17,19,21-dodecaaza-pentacyclo[17.3.0.02,6.08,12.013,17]docosan-3,5,9,11,14,16,20,22-octone

Crystal data

$C_{42}H_{32}N_{12}O_{12}$	$F(000) = 928$
$M_r = 896.79$	$D_x = 1.436$ Mg m^{-3}
Triclinic, *P*-1	Mo Kα radiation, $\lambda = 0.71073$ Å
$a = 11.4603$ (12) Å	Cell parameters from 9916 reflections
$b = 11.6052$ (13) Å	$\theta = 2.29 – 31.11°$
$c = 16.3587$ (18) Å	$\mu = 0.11$ mm^{-1}
$V = 2074.1$ (7) Å^3	$T = 90$ K
$Z = 2$	Block, colourless
	0.489 × 0.624 × 0.709 mm

Data collection

APEX-II CCD (Bruker, 2014)	39079 measured reflections
Graphite monochromator	13178 independent reflections
ϕ and ω scans	10248 reflections with $I > 2\sigma(I)$
Absorption correction: Multi-Scan, *SADABS* V2014/5 (Bruker-AXS)	$R_{int} = 0.0384$
	$\theta_{max} = 31.06°$, $\theta_{min} = 1.30°$
$T_{min} = 0.6543$, $T_{max} = 0.7462$	$h = -16 \rightarrow 16$, $k = -16 \rightarrow 16$, $l = -23 \rightarrow 23$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters fully refined
$R[F^2 > 2\sigma(F^2)] = 0.0548$	$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 1.4448P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.1269$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.029$	$\Delta\rho_{max} = 0.483$ e Å^{-3}
13178 reflections	$\Delta\rho_{min} = -0.283$ e Å^{-3}
723 parameters	
0 restraints	

Special details
Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry.

An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates, isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}* / U_{eq}
C1	0.24608 (12)	0.39858 (12)	0.39427 (9)	0.0130 (2)
N1	0.31131 (10)	0.43400 (10)	0.33208 (7)	0.0130 (2)
O1	0.37537 (10)	0.49611 (10)	0.52499 (7)	0.0190 (2)
C4	0.28114 (12)	0.27649 (12)	0.42394 (9)	0.0140 (2)
O4	0.53906 (10)	0.37334 (10)	0.24205 (7)	0.0208 (2)
N4	0.29468 (11)	0.27230 (10)	0.23218 (7)	0.0133 (2)
C3	0.19691 (15)	0.58488 (15)	0.47717 (12)	0.0241 (3)
H3A	0.247 (2)	0.660 (2)	0.4924 (14)	0.031 (6)*
H3B	0.135 (2)	0.588 (2)	0.4250 (16)	0.041 (7)*
H3C	0.159 (3)	0.570 (2)	0.5222 (18)	0.052 (8)*
N3	0.37290 (10)	0.35171 (10)	0.29934 (8)	0.0136 (2)
O3	0.35598 (10)	0.63195 (9)	0.36913 (7)	0.0163 (2)
C2	0.28000 (13)	0.49659 (13)	0.47208 (9)	0.0158 (3)
N2	0.47231 (11)	0.53250 (10)	0.29990 (8)	0.0140 (2)
O2	0.20036 (10)	0.19420 (9)	0.40480 (7)	0.0187 (2)
C5	0.40888 (13)	0.26733 (14)	0.47423 (10)	0.0180 (3)
H5A	0.431 (2)	0.193 (2)	0.4555 (14)	0.032 (6)*
H5B	0.4695 (19)	0.3310 (19)	0.4695 (13)	0.024 (5)*
H5C	0.408 (2)	0.2675 (19)	0.5346 (15)	0.030 (6)*
N5	0.35635 (12)	0.14249 (11)	0.15121 (8)	0.0160 (2)
O5	0.37973 (10)	0.11364 (9)	0.29333 (7)	0.0186 (2)
C6	0.37786 (12)	0.54449 (12)	0.33755 (8)	0.0125 (2)
O6	0.28976 (11)	0.21950 (10)	0.02152 (7)	0.0213 (2)
N6	0.28172 (11)	0.31233 (11)	0.14880 (7)	0.0147 (2)
C7	0.56356 (13)	0.62976 (13)	0.29845 (9)	0.0160 (3)
N7	0.13708 (11)	0.43388 (10)	0.17176 (8)	0.0133 (2)
O7	0.09704 (11)	0.44105 (10)	-0.02179 (7)	0.0221 (2)
C8	0.52530 (15)	0.73599 (14)	0.27799 (10)	0.0199 (3)
H8	0.436 (2)	0.739 (2)	0.2593 (14)	0.032 (6)*
N8	0.06491 (11)	0.59341 (10)	0.20767 (8)	0.0144 (2)
O8	0.08330 (11)	0.15582 (9)	0.09693 (7)	0.0211 (2)
C9	0.61298 (17)	0.83326 (15)	0.28526 (11)	0.0250 (3)
H9	0.586 (2)	0.909 (2)	0.2718 (16)	0.039 (6)*
N9	0.03532 (11)	0.39687 (10)	0.20407 (8)	0.0145 (2)
O9	0.22320 (10)	0.61325 (9)	0.14225 (7)	0.0180 (2)
C10	0.73652 (17)	0.82374 (16)	0.31052 (11)	0.0278 (4)
H10	0.798 (2)	0.891 (2)	0.3163 (14)	0.032 (6)*
N10	0.06315 (11)	0.32378 (10)	0.27181 (7)	0.0132 (2)
O10	-0.08712 (10)	0.50155 (10)	0.26342 (8)	0.0221 (2)

Fractional atomic coordinates, isotropic or equivalent isotropic displacement parameters (Å²)
(continued)

	x	*y*	*z*	U_{iso}* / U_{eq}
C11	0.77312 (16)	0.71606 (17)	0.32720 (11)	0.0265 (3)
H11	0.859 (2)	0.7088 (19)	0.3431 (14)	0.030 (6)*
N11	-0.05242 (11)	0.25801 (11)	0.35741 (8)	0.0146 (2)
O11	-0.11892 (10)	0.19426 (10)	0.21348 (7)	0.0191 (2)
C12	0.68704 (14)	0.61756 (15)	0.32163 (10)	0.0200 (3)
H12	0.7112 (19)	0.5402 (19)	0.3330 (13)	0.024 (5)*
N12	0.11224 (10)	0.38634 (11)	0.35481 (8)	0.0136 (2)
O12	0.07152 (10)	0.35539 (10)	0.48427 (7)	0.0199 (2)
C13	0.47374 (13)	0.41727 (13)	0.27664 (9)	0.0147 (3)
C14	0.34883 (13)	0.16658 (12)	0.23253 (9)	0.0142 (2)
C15	0.40963 (13)	0.04569 (13)	0.12586 (9)	0.0162 (3)
C16	0.53077 (14)	0.06568 (15)	0.12328 (10)	0.0200 (3)
H16	0.5784 (19)	0.1423 (19)	0.1369 (13)	0.023 (5)*
C17	0.58237 (16)	-0.02754 (17)	0.09866 (11)	0.0253 (3)
H17	0.664 (2)	-0.015 (2)	0.0957 (14)	0.032 (6)*
C18	0.51398 (18)	-0.13774 (16)	0.07846 (11)	0.0263 (4)
H18	0.552 (2)	-0.2016 (19)	0.0600 (14)	0.029 (5)*
C19	0.39377 (18)	-0.15623 (15)	0.08272 (11)	0.0254 (3)
H19	0.346 (2)	-0.234 (2)	0.0691 (14)	0.032 (6)*
C20	0.34025 (15)	-0.06375 (14)	0.10626 (10)	0.0206 (3)
H20	0.257 (2)	-0.0734 (19)	0.1074 (14)	0.027 (5)*
C21	0.30814 (13)	0.22312 (13)	0.09749 (9)	0.0160 (3)
C22	0.16640 (13)	0.35719 (12)	0.10931 (9)	0.0142 (2)
C23	0.18716 (15)	0.42737 (13)	0.03221 (9)	0.0177 (3)
C24	0.31380 (17)	0.47431 (16)	0.02730 (12)	0.0246 (3)
H24A	0.311 (2)	0.551 (2)	0.0054 (15)	0.037 (6)*
H24B	0.371 (2)	0.484 (2)	0.0805 (16)	0.039 (6)*
H24C	0.339 (2)	0.424 (2)	-0.0108 (17)	0.045 (7)*
C25	0.05842 (14)	0.25055 (13)	0.07876 (9)	0.0164 (3)
C26	-0.06640 (15)	0.26985 (15)	0.02957 (10)	0.0213 (3)
H26A	-0.125 (2)	0.217 (2)	0.0483 (14)	0.030 (6)*
H26B	-0.079 (2)	0.351 (2)	0.0376 (15)	0.034 (6)*
H26C	-0.075 (2)	0.250 (2)	-0.0277 (15)	0.032 (6)*
C27	0.15076 (13)	0.55470 (12)	0.17043 (8)	0.0135 (2)
C28	0.05292 (14)	0.71531 (12)	0.21756 (9)	0.0166 (3)
C29	0.15085 (16)	0.79129 (14)	0.26863 (11)	0.0228 (3)
H29	0.224 (2)	0.7626 (19)	0.3002 (14)	0.029 (5)*
C30	0.14256 (19)	0.91030 (15)	0.27420 (13)	0.0295 (4)
H30	0.211 (2)	0.963 (2)	0.3068 (16)	0.042 (7)*
C31	0.0379 (2)	0.95040 (15)	0.22947 (13)	0.0324 (4)
H31	0.037 (2)	1.033 (2)	0.2318 (16)	0.046 (7)*

Fractional atomic coordinates, isotropic or equivalent isotropic displacement parameters (Å²)
(continued)

	x	*y*	*z*	U_{iso}* / U_{eq}
C32	-0.0603 (2)	0.87235 (17)	0.18003 (12)	0.0326 (4)
H32	-0.131 (2)	0.899 (2)	0.1495 (16)	0.039 (6)*
C33	-0.05403 (16)	0.75345 (15)	0.17386 (10)	0.0234 (3)
H33	-0.118 (2)	0.6981 (19)	0.1422 (14)	0.026 (5)*
C34	-0.00721 (13)	0.50172 (13)	0.22881 (9)	0.0158 (3)
C35	-0.04846 (12)	0.25021 (12)	0.27377 (9)	0.0138 (2)
C36	-0.13569 (12)	0.18572 (12)	0.39226 (9)	0.0150 (3)
C37	-0.26087 (13)	0.17956 (14)	0.35755 (10)	0.0194 (3)
H37	-0.2920 (19)	0.2238 (18)	0.3088 (13)	0.024 (5)*
C38	-0.33902 (15)	0.11269 (16)	0.39501 (12)	0.0275 (4)
H38	-0.423 (2)	0.106 (2)	0.3730 (15)	0.036 (6)*
C39	-0.29274 (17)	0.05439 (16)	0.46554 (13)	0.0299 (4)
H39	-0.352 (2)	0.011 (2)	0.4934 (17)	0.048 (7)*
C40	-0.16729 (17)	0.06081 (15)	0.49883 (12)	0.0267 (3)
H40	-0.136 (2)	0.020 (2)	0.5486 (15)	0.032 (6)*
C41	-0.08785 (14)	0.12622 (14)	0.46216 (10)	0.0204 (3)
H41	-0.0021 (19)	0.1302 (18)	0.4844 (13)	0.024 (5)*
C42	0.04521 (12)	0.33534 (13)	0.40814 (9)	0.0149 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0110 (5)	0.0135 (6)	0.0132 (6)	0.0005 (5)	0.0022 (5)	-0.0014 (5)
N1	0.0137 (5)	0.0111 (5)	0.0139 (5)	0.0022 (4)	0.0040 (4)	-0.0026 (4)
O1	0.0214 (5)	0.0195 (5)	0.0127 (5)	-0.0031 (4)	0.0022 (4)	-0.0017 (4)
C4	0.0148 (6)	0.0152 (6)	0.0117 (6)	0.0027 (5)	0.0030 (5)	-0.0003 (5)
O4	0.0185 (5)	0.0218 (5)	0.0240 (5)	0.0056 (4)	0.0085 (4)	-0.0020 (4)
N4	0.0163 (5)	0.0115 (5)	0.0109 (5)	0.0046 (4)	0.0007 (4)	-0.0012 (4)
C3	0.0207 (7)	0.0190 (7)	0.0323 (9)	-0.0004 (6)	0.0104 (7)	-0.0107 (6)
N3	0.0134 (5)	0.0119 (5)	0.0148 (5)	0.0030 (4)	0.0031 (4)	-0.0036 (4)
O3	0.0201 (5)	0.0130 (5)	0.0154 (5)	0.0041 (4)	0.0037 (4)	-0.0008 (4)
C2	0.0179 (6)	0.0140 (6)	0.0153 (6)	-0.0019 (5)	0.0069 (5)	-0.0036 (5)
N2	0.0146 (5)	0.0124 (5)	0.0149 (5)	0.0020 (4)	0.0042 (4)	0.0008 (4)
O2	0.0171 (5)	0.0152 (5)	0.0219 (5)	0.0004 (4)	0.0027 (4)	0.0014 (4)
C5	0.0155 (6)	0.0206 (7)	0.0161 (7)	0.0035 (5)	0.0006 (5)	0.0006 (5)
N5	0.0218 (6)	0.0136 (5)	0.0134 (5)	0.0091 (5)	0.0033 (4)	-0.0005 (4)
O5	0.0227 (5)	0.0164 (5)	0.0160 (5)	0.0061 (4)	0.0023 (4)	0.0019 (4)
C6	0.0126 (5)	0.0132 (6)	0.0103 (6)	0.0023 (5)	0.0004 (4)	0.0016 (5)
O6	0.0291 (6)	0.0237 (6)	0.0131 (5)	0.0115 (5)	0.0059 (4)	0.0008 (4)

Atomic displacement parameters (Å^2) (continued)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N6	0.0176 (5)	0.0154 (6)	0.0115 (5)	0.0071 (4)	0.0025 (4)	0.0011 (4)
C7	0.0188 (6)	0.0164 (6)	0.0122 (6)	-0.0016 (5)	0.0051 (5)	0.0004 (5)
N7	0.0160 (5)	0.0112 (5)	0.0140 (5)	0.0044 (4)	0.0049 (4)	0.0015 (4)
O7	0.0326 (6)	0.0198 (5)	0.0146 (5)	0.0096 (5)	0.0044 (4)	0.0035 (4)
C8	0.0251 (7)	0.0187 (7)	0.0146 (6)	0.0012 (6)	0.0039 (6)	0.0036 (5)
N8	0.0179 (5)	0.0109 (5)	0.0148 (5)	0.0058 (4)	0.0033 (4)	0.0003 (4)
O8	0.0264 (6)	0.0135 (5)	0.0215 (5)	0.0047 (4)	0.0027 (4)	0.0003 (4)
C9	0.0372 (9)	0.0179 (7)	0.0191 (7)	-0.0020 (6)	0.0087 (7)	0.0028 (6)
N9	0.0163 (5)	0.0123 (5)	0.0164 (6)	0.0062 (4)	0.0047 (4)	0.0035 (4)
O9	0.0224 (5)	0.0147 (5)	0.0171 (5)	0.0029 (4)	0.0057 (4)	0.0021 (4)
C10	0.0338 (9)	0.0243 (8)	0.0234 (8)	-0.0099 (7)	0.0119 (7)	-0.0003 (6)
N10	0.0146 (5)	0.0120 (5)	0.0110 (5)	0.0017 (4)	0.0005 (4)	0.0002 (4)
O10	0.0202 (5)	0.0200 (5)	0.0304 (6)	0.0082 (4)	0.0114 (5)	0.0039 (5)
C11	0.0214 (7)	0.0324 (9)	0.0251 (8)	-0.0039 (6)	0.0094 (6)	0.0004 (7)
N11	0.0129 (5)	0.0147 (5)	0.0149 (5)	0.0006 (4)	0.0024 (4)	-0.0004 (4)
O11	0.0187 (5)	0.0177 (5)	0.0172 (5)	0.0000 (4)	0.0004 (4)	-0.0022 (4)
C12	0.0189 (7)	0.0232 (8)	0.0191 (7)	0.0011 (6)	0.0081 (6)	0.0019 (6)
N12	0.0120 (5)	0.0145 (5)	0.0129 (5)	0.0017 (4)	0.0018 (4)	-0.0027 (4)
O12	0.0175 (5)	0.0251 (6)	0.0155 (5)	-0.0008 (4)	0.0041 (4)	-0.0032 (4)
C13	0.0148 (6)	0.0147 (6)	0.0138 (6)	0.0036 (5)	0.0018 (5)	0.0000 (5)
C14	0.0150 (6)	0.0116 (6)	0.0149 (6)	0.0032 (5)	0.0022 (5)	-0.0022 (5)
C15	0.0208 (6)	0.0153 (6)	0.0137 (6)	0.0100 (5)	0.0036 (5)	0.0006 (5)
C16	0.0201 (7)	0.0229 (8)	0.0184 (7)	0.0078 (6)	0.0050 (6)	0.0035 (6)
C17	0.0251 (8)	0.0350 (9)	0.0225 (8)	0.0178 (7)	0.0103 (6)	0.0089 (7)
C18	0.0415 (9)	0.0260 (8)	0.0202 (7)	0.0234 (7)	0.0137 (7)	0.0067 (6)
C19	0.0385 (9)	0.0166 (7)	0.0230 (8)	0.0093 (7)	0.0093 (7)	0.0000 (6)
C20	0.0235 (7)	0.0178 (7)	0.0210 (7)	0.0052 (6)	0.0063 (6)	-0.0010 (6)
C21	0.0183 (6)	0.0146 (6)	0.0160 (6)	0.0068 (5)	0.0044 (5)	0.0008 (5)
C22	0.0179 (6)	0.0126 (6)	0.0123 (6)	0.0062 (5)	0.0024 (5)	0.0011 (5)
C23	0.0281 (7)	0.0125 (6)	0.0157 (6)	0.0073 (5)	0.0091 (6)	0.0014 (5)
C24	0.0292 (8)	0.0220 (8)	0.0281 (8)	0.0076 (6)	0.0149 (7)	0.0060 (7)
C25	0.0211 (6)	0.0145 (6)	0.0125 (6)	0.0040 (5)	0.0024 (5)	0.0004 (5)
C26	0.0202 (7)	0.0218 (8)	0.0177 (7)	0.0033 (6)	-0.0021 (6)	0.0024 (6)
C27	0.0167 (6)	0.0123 (6)	0.0098 (6)	0.0048 (5)	-0.0004 (5)	0.0005 (5)
C28	0.0252 (7)	0.0120 (6)	0.0159 (6)	0.0088 (5)	0.0081 (5)	0.0035 (5)
C29	0.0259 (8)	0.0154 (7)	0.0273 (8)	0.0055 (6)	0.0064 (6)	0.0011 (6)
C30	0.0412 (10)	0.0146 (7)	0.0371 (10)	0.0035 (7)	0.0188 (8)	0.0009 (7)
C31	0.0574 (12)	0.0152 (7)	0.0370 (10)	0.0179 (8)	0.0272 (9)	0.0097 (7)
C32	0.0492 (11)	0.0293 (9)	0.0287 (9)	0.0288 (9)	0.0144 (8)	0.0101 (7)
C33	0.0302 (8)	0.0229 (8)	0.0190 (7)	0.0154 (7)	0.0046 (6)	0.0011 (6)
C34	0.0159 (6)	0.0144 (6)	0.0163 (6)	0.0059 (5)	0.0014 (5)	0.0011 (5)
C35	0.0134 (6)	0.0117 (6)	0.0156 (6)	0.0035 (5)	0.0022 (5)	0.0011 (5)

Atomic displacement parameters (Å^2) (continued)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C36	0.0127 (6)	0.0137 (6)	0.0184 (6)	0.0005 (5)	0.0051 (5)	-0.0011(5)
C37	0.0141 (6)	0.0198 (7)	0.0216 (7)	0.0017 (5)	0.0014 (5)	-0.0041(6)
C38	0.0148 (7)	0.0294 (9)	0.0361 (9)	-0.0034 (6)	0.0082 (6)	-0.0076(7)
C39	0.0294 (9)	0.0253 (8)	0.0373 (10)	-0.0057 (7)	0.0191 (8)	-0.0028(7)
C40	0.0328 (9)	0.0216 (8)	0.0284 (8)	0.0026 (7)	0.0130 (7)	0.0063(7)
C41	0.0185 (7)	0.0212 (7)	0.0219 (7)	0.0044 (6)	0.0050 (6)	0.0047(6)
C42	0.0126 (6)	0.0150 (6)	0.0169 (6)	0.0025 (5)	0.0038 (5)	-0.0005(5)

Geometric parameters (Å, º)

O1—C2	1.2047 (18)	N11—C35	1.3797 (18)
O2—C4	1.2063 (18)	N11—C36	1.4362 (18)
O3—C6	1.2007 (17)	N11—C42	1.3871 (18)
O4—C13	1.1970 (17)	N12—C1	1.4853 (17)
O5—C14	1.1942 (18)	N12—C42	1.4087 (18)
O6—C21	1.2027 (18)	C1—C2	1.5958 (19)
O7—C23	1.2050 (19)	C1—C4	1.587 (2)
O8—C25	1.2034 (18)	C2—C3	1.500 (2)
O9—C27	1.2032 (18)	C4—C5	1.500 (2)
O10—C34	1.1957 (18)	C7—C8	1.389 (2)
O11—C35	1.1956 (17)	C7—C12	1.394 (2)
O12—C42	1.2052 (18)	C8—C9	1.388 (2)
N1—N3	1.4211 (15)	C9—C10	1.388 (3)
N1—C1	1.4567 (18)	C10—C11	1.387 (3)
N1—C6	1.3898 (18)	C11—C12	1.392 (2)
N2—C6	1.3964 (18)	C15—C16	1.389 (2)
N2—C7	1.4407 (19)	C15—C20	1.382 (2)
N2—C13	1.3753 (18)	C16—C17	1.389 (2)
N3—N4	1.4243 (16)	C17—C18	1.386 (3)
N3—C13	1.4407 (18)	C18—C19	1.387 (3)
N4—N6	1.4400 (17)	C19—C20	1.389 (2)
N4—C14	1.4450 (17)	C22—C23	1.587 (2)
N5—C14	1.3727 (18)	C22—C25	1.590 (2)
N5—C15	1.4393 (17)	C23—C24	1.506 (2)
N5—C21	1.3843 (18)	C25—C26	1.498 (2)
N6—C21	1.4127 (18)	C28—C29	1.383 (2)
N6—C22	1.4839 (18)	C28—C33	1.387 (2)
N7—N9	1.4276 (17)	C29—C30	1.397 (2)
N7—C22	1.4544 (18)	C30—C31	1.383 (3)
N7—C27	1.3923 (18)	C31—C32	1.387 (3)
N8—C27	1.3936 (18)	C32—C33	1.391 (2)

Geometric parameters (Å, º) (continued)

N8—C28	1.4443 (18)	C36—C37	1.389 (2)
N8—C34	1.3754 (19)	C36—C41	1.391 (2)
N9—C34	1.4460 (18)	C37—C38	1.390 (2)
N9—N10	1.4244 (16)	C38—C39	1.386 (3)
N10—N12	1.4432 (16)	C39—C40	1.389 (3)
N10—C35	1.4509 (18)	C40—C41	1.384 (2)
N3—N1—C1	118.57 (11)	C11—C12—C7	118.43 (16)
N3—N1—C6	108.56 (11)	O4—C13—N2	130.56 (14)
C1—N1—C6	122.53 (11)	O4—C13—N3	123.25 (13)
C6—N2—C7	121.75 (12)	N2—C13—N3	106.15 (11)
C6—N2—C13	111.18 (12)	O5—C14—N4	124.81 (13)
C7—N2—C13	126.53 (12)	O5—C14—N5	128.81 (13)
N1—N3—N4	113.56 (10)	N4—C14—N5	106.38 (12)
N1—N3—C13	106.89 (11)	N5—C15— C16	118.34 (14)
N4—N3—C13	113.91 (11)	N5—C15—C20	119.50 (13)
N3—N4—N6	114.20 (11)	C16—C15—C20	122.16 (14)
N3—N4—C14	107.29 (10)	C15—C16—C17	118.46 (16)
N6—N4—C14	106.58 (10)	C16—C17—C18	120.13 (16)
C14—N5—C15	123.64 (12)	C17—C18—C19	120.51 (15)
C14—N5—C21	111.83 (12)	C18—C19—C20	120.14 (16)
C15—N5—C21	124.52 (12)	C15—C20—C19	118.59 (15)
N4—N6— C21	107.30 (11)	O6—C21—N5	127.80 (13)
N4—N6—C22	116.81 (11)	O6—C21—N6	125.31 (13)
C21—N6—C22	113.81 (11)	N5—C21—N6	106.88 (12)
N9—N7—C22	119.50 (11)	N6—C22—N7	109.55 (11)
N9—N7—C27	108.79 (11)	N6—C22—C23	107.60 (11)
C22—N7— C27	122.97 (12)	N6—C22—C25	109.21 (11)
C27—N8— C34	111.51 (11)	N7—C22—C23	110.15 (11)
C28—N8—C34	126.11 (12)	N7—C22—C25	108.53 (11)
C27—N8—C28	122.31 (12)	C23—C22—C25	111.78 (11)
N7—N9—N10	113.37 (10)	O7—C23—C22	116.81 (14)
N7—N9—C34	106.46 (11)	O7—C23—C24	121.94 (14)
N10—N9—C34	112.45 (11)	C22—C23—C24	121.24 (13)
N9—N10—N12	114.16 (11)	O8—C25—C22	116.44 (13)
N9—N10—C35	108.69 (10)	O8—C25—C26	123.05 (14)
N12—N10—C35	106.83 (10)	C22—C25—C26	120.51 (12)
C35—N11—C36	125.71 (12)	O9—C27—N7	125.96 (13)
C35—N11—C42	111.54 (12)	O9—C27—N8	127.25 (13)
C36—N11—C42	122.28 (12)	N7—C27—N8	106.79 (12)
N10—N12—C1	118.25 (10)	N8—C28—C29	118.50 (13)
N10—N12—C42	106.92 (11)	N8—C28—C33	119.49 (14)
C1—N12—C42	111.71 (11)	C29—C28—C33	121.98 (14)
N1—C1—N12	109.66 (11)	C28—C29—C30	118.72 (16)

Geometric parameters (Å, º) (continued)

N1—C1—C2	109.67 (11)	C29—C30—C31	120.17 (18)
N1—C1—C4	108.38 (10)	C30—C31—C32	120.13 (16)
N12—C1—C2	107.77 (11)	C31—C32—C33	120.59 (17)
N12—C1—C4	109.43 (11)	C28—C33—C32	118.37 (17)
C2—C1—C4	111.92 (11)	O10—C34—N8	130.25 (14)
O1—C2—C1	116.51 (13)	O10—C34—N9	123.45 (14)
O1—C2—C3	122.61 (14)	N8—C34—N9	106.25 (12)
C1—C2—C3	120.88 (13)	O11—C35—N10	124.93 (13)
O2—C4—C1	116.67 (12)	O11—C35—N11	129.09 (14)
O2—C4—C5	122.98 (13)	N10—C35—N11	105.97 (11)
C1—C4—C5	120.34 (12)	N11—C36—C37	119.75 (13)
O3—C6—N1	125.23 (13)	N11—C36—C41	118.49 (13)
O3—C6—N2	127.93 (13)	C37—C36—C41	121.73 (14)
N1—C6—N2	106.84 (11)	C36—C37—C38	118.31 (16)
N2—C7—C8	118.22 (13)	C37—C38—C39	120.65 (16)
N2—C7—C12	120.05 (13)	C38—C39—C40	120.16 (16)
C8—C7—C12	121.64 (14)	C39—C40—C41	120.15 (17)
C7—C8—C9	118.75 (15)	C36—C41—C40	119.00 (15)
C8—C9—C10	120.51 (16)	O12—C42—N11	127.40 (14)
C9—C10—C11	120.00 (16)	O12—C42—N12	124.91 (13)
C10—C11—C12	120.58 (16)	N11—C42—N12	107.68 (12)

C1—N1—N3—N4	81.82 (14)	C34—N9—N10—N12	-34.05 (15)
C1—N1—N3—C13	-151.71 (11)	C34—N9—N10—C35	85.08 (13)
C6—N1—N3—N4	-132.21 (12)	N7—N9—C34—O10	-175.18 (14)
C6—N1—N3—C13	-5.74 (14)	N7—N9—C34—N8	2.42 (14)
C6—N1—C1—N12	109.95 (13)	N10—N9—C34—O10	-50.45 (19)
C6—N1—C1—C4	-130.65 (12)	N10—N9—C34—N8	127.15 (12)
C6—N1—C1—C2	-8.20 (17)	N9—N10—N12—C1	-102.20 (13)
N3—N1—C1—N12	-109.05 (13)	N9—N10—N12—C42	130.77 (12)
N3—N1—C1—C4	10.35 (15)	C35—N10—N12—C1	137.63 (12)
N3—N1—C1—C2	132.80 (12)	C35—N10—N12—C42	10.59 (13)
N3—N1—C6—O3	-173.61 (13)	N9—N10—C35—O11	49.19 (18)
N3—N1—C6—N2	6.34 (14)	N9—N10—C35—N11	-131.89 (11)
C1—N1—C6—O3	-29.3 (2)	N12—N10—C35—O11	172.81 (13)
C1—N1—C6—N2	150.68 (12)	N12—N10—C35—N11	-8.26 (14)
N1—N3—N4—N6	88.78 (13)	C36—N11—C35—O11	9.6 (2)
N1—N3—N4—C14	-153.35 (11)	C36—N11—C35—N10	-169.29 (12)
C13—N3—N4—N6	-33.90 (15)	C42—N11—C35—O11	-178.26 (14)
C13—N3—N4—C14	83.96 (13)	C42—N11—C35—N10	2.88 (15)
C7—N2—C6—O3	3.3 (2)	C35—N11—C36—C37	-56.6 (2)
C7—N2—C6—N1	-176.68 (12)	C35—N11—C36—C41	125.31 (16)
C13—N2—C6—O3	175.31 (14)	C42—N11—C36—C37	131.99 (15)
C13—N2—C6—N1	-4.64 (15)	C42—N11—C36—C41	-46.07 (19)

Geometric parameters (Å, º) (continued)

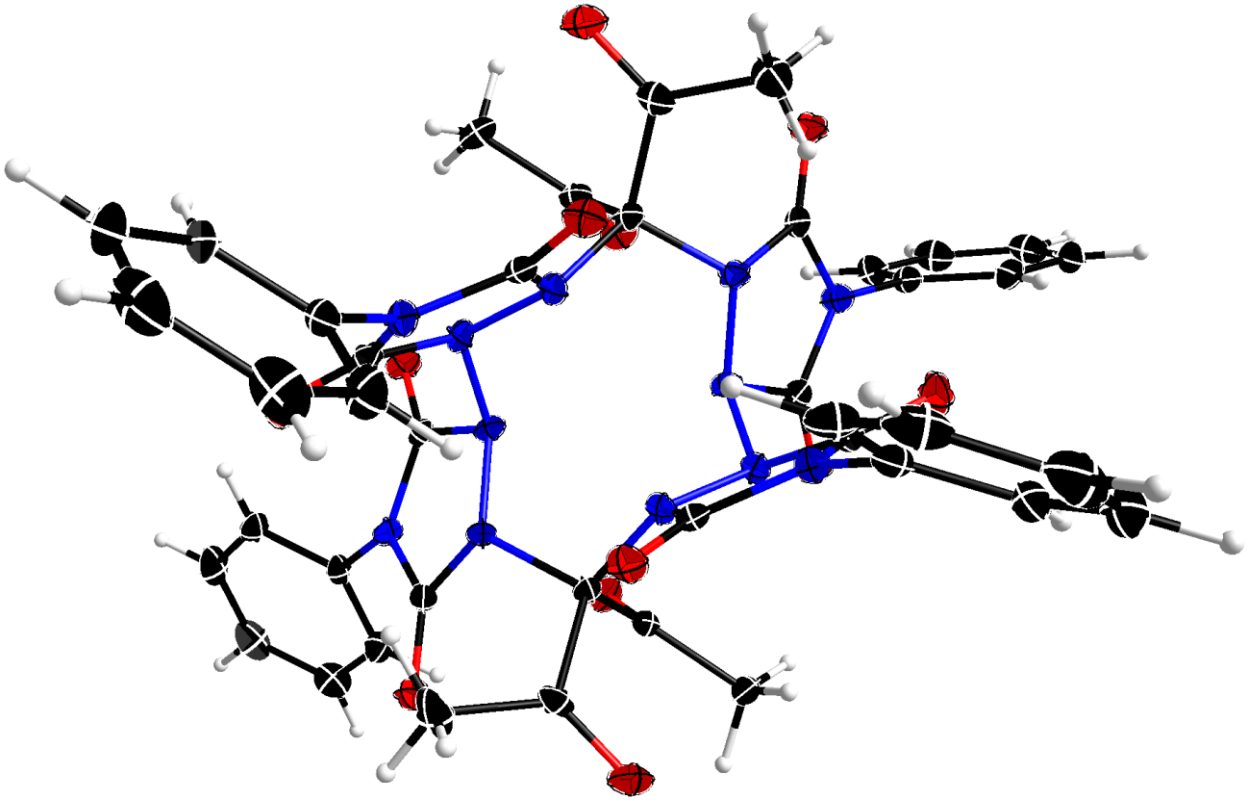
C6—N2—C7—C8	-44.03 (19)	C35—N11—C42—O12	-174.88 (14)
C6—N2—C7—C12	132.58 (14)	C35—N11—C42—N12	3.81 (16)
C13—N2—C7—C8	145.21 (14)	C36—N11—C42—O12	-2.4 (2)
C13—N2—C7—C12	-38.2 (2)	C36—N11—C42—N12	176.29 (12)
C6—N2—C13—O4	178.80 (15)	C42—N12—C1—N1	171.01 (11)
C6—N2—C13—N3	1.06 (15)	C42—N12—C1—C4	52.26 (14)
C7—N2—C13—O4	-9.6 (2)	C42—N12—C1—C2	-69.66 (14)
C7—N2—C13—N3	172.64 (12)	N10—N12—C1—N1	46.30 (15)
N1—N3—C13—O4	-175.09 (13)	N10—N12—C1—C4	-72.45 (14)
N1—N3—C13—N2	2.85 (14)	N10—N12—C1—C2	165.63 (11)
N4—N3—C13—O4	-48.83 (18)	N10—N12—C42—O12	169.82 (14)
N4—N3—C13—N2	129.11 (12)	N10—N12—C42—N11	-8.91 (14)
N3—N4—N6—C21	127.63 (12)	C1—N12—C42—O12	39.01 (19)
N3—N4—N6—C22	-103.24 (13)	C1—N12—C42—N11	-139.72 (11)
C14—N4—N6—C21	9.36 (14)	N1—C1—C2—O1	-80.54 (16)
C14—N4—N6—C22	138.49 (12)	N1—C1—C2—C3	98.66 (15)
N3—N4—C14—O5	52.31 (18)	N12— C1—C2—O1	160.14 (13)
N3—N4—C14—N5	-127.59 (12)	N12—C1—C2—C3	-20.66 (18)
N6—N4—C14—O5	175.04 (14)	C4—C1—C2—O1	39.78 (17)
N6—N4—C14—N5	-4.86 (15)	C4—C1—C2—C3	-141.03 (14)
C15—N5—C14—O5	-2.2 (2)	N1—C1—C4—O2	-113.81 (14)
C15—N5—C14—N4	177.66 (13)	N1—C1—C4—C5	66.98 (15)
C21—N5—C14—O5	178.54 (15)	N12—C1—C4—O2	5.74 (17)
C21—N5—C14—N4	-1.57 (16)	N12—C1—C4—C5	-173.47 (12)
C14—N5—C15—C16	-96.40 (18)	C2—C1—C4—O2	125.13 (13)
C14—N5—C15—C20	82.60 (19)	C2—C1—C4—C5	-54.08 (16)
C21—N5—C15—C16	82.73 (19)	N2—C7—C8—C9	173.14 (14)
C21—N5—C15—C20	-98.28 (18)	C12—C7—C8—C9	-3.4 (2)
C14—N5—C21—O6	-171.63 (16)	N2—C7—C12—C11	-174.04 (14)
C14—N5—C21—N6	7.49 (17)	C8—C7—C12—C11	2.5 (2)
C15—N5—C21—O6	9.2 (3)	C7—C8—C9—C10	1.6 (2)
C15—N5—C21—N6	-171.72 (13)	C8—C9—C10—C11	1.2 (3)
N4—N6—C21—O6	168.88 (15)	C9—C10—C11—C12	-2.2 (3)
N4—N6—C21—N5	-10.27 (15)	C10—C11—C12—C7	0.4 (2)
C22—N6—C21—O6	38.1 (2)	N5—C15—C16—C17	-179.87 (13)
C22—N6—C21—N5	-141.09 (12)	C20—C15—C16—C17	1.2 (2)
N4—N6—C22—N7	44.72 (16)	N5—C15—C20—C19	-179.39 (14)
N4—N6—C22—C23	164.47 (11)	C16—C15—C20—C19	-0.4 (2)
N4—N6—C22—C25	-74.02 (14)	C15—C16—C17—C18	-0.9 (2)
C21—N6—C22—N7	170.67 (12)	C16—C17—C18—C19	-0.1 (3)
C21—N6—C22—C23	-69.58 (15)	C17—C18—C19—C20	0.9 (3)
C21—N6—C22—C25	51.93 (15)	C18—C19—C20—C15	-0.6 (2)
C22—N7—N9—N10	82.96 (14)	N6—C22—C23—O7	159.04 (13)
C22—N7—N9—C34	-152.88 (12)	N6—C22—C23—C24	-20.97 (18)

Geometric parameters (Å, º) (continued)

C27—N7—N9—N10	-128.51 (12)	N7—C22—C23—O7	-81.60 (16)
C27—N7—N9—C34	-4.36 (14)	N7—C22—C23—C24	98.40 (15)
N9—N7—C22—N6	-109.87 (13)	C25—C22—C23—O7	39.15 (17)
N9—N7—C22—C23	131.96 (12)	C25—C22—C23—C24	-140.86 (14)
N9—N7—C22—C25	9.29 (16)	N6—C22—C25—O8	5.07 (17)
C27—N7—C22—N6	106.23 (14)	N6—C22—C25—C26	-174.52 (13)
C27—N7—C22—C23	-11.94 (18)	N7—C22—C25—O8	-114.30 (14)
C27—N7—C22—C25	-134.61 (13)	N7—C22—C25—C26	66.11 (16)
N9—N7—C27—O9	-175.40 (13)	C23—C22—C25—O8	124.02 (14)
N9—N7—C27—N8	4.56 (14)	C23—C22—C25—C26	-55.58 (17)
C22—N7—C27—O9	-28.2 (2)	N8—C28—C29—C30	176.06 (15)
C22—N7—C27—N8	151.76 (12)	C33—C28—C29—C30	-1.8 (2)
C28—N8—C27—O9	-0.3 (2)	N8—C28—C33—C32	-175.83 (15)
C28—N8—C27—N7	179.74 (12)	C29—C28—C33—C32	2.1 (2)
C34—N8—C27—O9	176.88 (14)	C28—C29—C30—C31	0.2 (3)
C34—N8—C27—N7	-3.08 (15)	C29—C30—C31—C32	1.1 (3)
C27—N8—C28—C29	-62.87 (19)	C30—C31—C32—C33	-0.9 (3)
C27—N8—C28—C33	115.09 (16)	C31—C32—C33—C28	-0.6 (3)
C34—N8—C28—C29	120.37 (16)	N11—C36—C37—C38	-177.33 (14)
C34—N8—C28—C33	-61.7 (2)	C41—C36—C37—C38	0.7 (2)
C27—N8—C34—O10	177.74 (15)	N11—C36—C41—C40	176.90 (14)
C27—N8—C34—N9	0.36 (15)	C37—C36—C41—C40	-1.1 (2)
C28—N8—C34—O10	-5.2 (2)	C36—C37—C38—C39	0.4 (2)
C28—N8—C34—N9	177.42 (12)	C37—C38—C39—C40	-1.0 (3)
N7—N9—N10—N12	86.78 (13)	C38—C39—C40—C41	0.5 (3)
N7—N9—N10—C35	-154.09 (11)	C39—C40—C41—C36	0.5 (3)

S3. ORTEP diagrams of heterocycle 9 (50% probability thermal elipsoids)

S3.1. Top view



S3.2. Side view