STRUCTURAL CHEMISTRY

Volume 73 (2017)

Supporting information for article:

Computational, ^{1}H NMR, and X-ray structural studies on 1-aryl-urazole tetrazane dimers

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S1. Computing details

Data collection: *APEX2* v2014.11 (Bruker, 2014); cell refinement: *SAINT* V8.37A (Bruker AXS Inc., 2015); data reduction: *SAINT* V8.37A (Bruker AXS Inc., 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL-2017/1* (Sheldrick, 2017); molecular graphics: *ShelXle* (Hübschle, Sheldrick, and Dittrich, 2011) and *VESTA* (Momma and Izumi, 2011); software used to prepare material for publication: *SHELXL-2017/1* (Sheldrick, 2017) via *ShelXle* (Hübschle, Sheldrick, and Dittrich, 2011)

S2. 4-Methyl-1-[4-methyl-3,5-dioxo-2-(2,4,6-trimethylphenyl)-1,2,4-triazolidin-1-yl]-2-(2,4,6-trimethylphenyl)-1,2,4-triazolidine-3,5-dione

Crystal data

$C_{24}H_{28}N_6O_4$
M_r = 464.52
Orthorhombic, *Pccn*
a = 9.1077 (7) Å
b = 13.5893 (11) Å
c = 19.4760 (16) Å
V = 2410.5 (3) Å^3
Z = 4

F(000) = 984
D_x = 1.280 Mg m^{-3}
Mo Kα radiation, λ = 0.71073 Å
Cell parameters from 9977 reflections
θ = 2.57 – 30.68°
μ = 0.090 mm^{-1}
T = 100 K
Block, colourless
0.842 × 0.503 × 0.341 mm

Data collection

APEX-II CCD (Bruker, 2014)
Graphite monochromator
ϕ and ω scans
Absorption correction: Multi-Scan, *SADABS* (Bruker-AXS, 2008)
T_{min} = 0.6611, T_{max} = 0.7461

22618 measured reflections
3721 independent reflections
3323 reflections with $I > 2\sigma(I)$
R_{int} = 0.0248
θ_{max} = 30.68°, θ_{min} = 2.57°
h = -10 → 13, *k* = -19 → 19, *l* = -25 → 27

Refinement

Refinement on F^2
Least-squares matrix: full
R [$F^2 > 2\sigma(F^2)$] = 0.0446
$wR(F^2)$ = 0.1195
S = 1.036
3721 reflections
223 parameters
72 restraints

Hydrogen site location: difference Fourier map
Aryl H-atom parameters fully refined
Methyl H-atom parameters restrained
$w = 1/[\sigma^2(F_o^2) + (0.0749P)^2 + 0.8555P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.015
$\Delta\rho_{max}$ = 0.473 e Å^{-3}
$\Delta\rho_{max}$ = -0.218 e Å^{-3}

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 (Å^2), and occupancy factors

	x	*y*	*z*	U_{iso}* / U_{eq}	*Occupancy*
O1	0.14248 (8)	0.15831 (5)	0.25907 (4)	0.01958 (16)	1
O2	0.56911 (8)	0.04859 (5)	0.35811 (4)	0.02095 (16)	1
N1	0.26561 (8)	0.20011 (5)	0.35988 (4)	0.01305 (16)	1
N2	0.35286 (8)	0.07732 (5)	0.29746 (4)	0.01640 (16)	1
N3	0.41174 (8)	0.17803 (5)	0.38272 (4)	0.01289 (15)	1
C1	0.24245 (10)	0.14570 (6)	0.29872 (4)	0.01453 (17)	1
C2	0.36322 (13)	-0.00245 (8)	0.24773 (6)	0.0268 (2)	1
H2A	0.2665 (17)	-0.0188 (14)	0.2306 (11)	0.018 (7)*	0.59 (4)
H2B	0.421 (3)	0.0219 (16)	0.2080 (9)	0.052 (11)*	0.59 (4)
H2C	0.412 (3)	-0.0587 (12)	0.2677 (10)	0.027 (8)*	0.59 (4)
H2D	0.308 (3)	0.0144 (17)	0.2066 (10)	0.021 (10)*	0.41 (4)
H2E	0.4647 (18)	-0.0156 (19)	0.2365 (13)	0.017 (10)*	0.41 (4)
H2F	0.321 (4)	-0.0626 (13)	0.2681 (12)	0.037 (12)*	0.41 (4)
C3	0.45849 (10)	0.09596 (6)	0.34806 (5)	0.01476 (17)	1
C4	0.45249 (9)	0.20492 (6)	0.45127 (4)	0.01326 (16)	1
C5	0.54272 (11)	0.28700 (7)	0.45977 (5)	0.01975 (19)	1
C6	0.59948 (14)	0.34619 (9)	0.40023 (6)	0.0310 (3)	1
H6A	0.5857 (19)	0.3145 (12)	0.3563 (7)	0.052 (6)*	1
H6B	0.7012 (14)	0.3635 (11)	0.4040 (8)	0.040 (4)*	1
H6C	0.546 (2)	0.4099 (12)	0.3951 (10)	0.086 (8)*	1
C7	0.57694 (15)	0.31505 (8)	0.52693 (6)	0.0300 (3)	1
H7	0.6382 (19)	0.3702 (13)	0.5328 (9)	0.039 (4)*	1
C8	0.52312 (15)	0.26429 (8)	0.58352 (5)	0.0284 (2)	1
C9	0.5563 (3)	0.29835 (13)	0.65532 (7)	0.0595 (6)	1
H9A	0.592 (2)	0.2490 (16)	0.6836 (9)	0.089 (8)*	1
H9B	0.618 (2)	0.3521 (13)	0.6560 (9)	0.059 (6)*	1
H9C	0.468 (2)	0.3191 (18)	0.6777 (11)	0.132 (13)*	1
C10	0.43458 (12)	0.18197 (7)	0.57286 (5)	0.0213 (2)	1
H10	0.3980 (18)	0.1460 (12)	0.6115 (8)	0.032 (4)*	1
C11	0.39823 (10)	0.15077 (6)	0.50710 (5)	0.01638 (18)	1
C12	0.30343 (13)	0.06119 (8)	0.49601 (6)	0.0260 (2)	1
H12A	0.2787 (17)	0.0309 (11)	0.5393 (7)	0.045 (5)*	1
H12B	0.3582 (18)	0.0119 (11)	0.4697 (8)	0.056 (6)*	1
H12C	0.2162 (16)	0.0770 (12)	0.4718 (8)	0.052 (5)*	1

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0168 (3)	0.0192 (3)	0.0228 (3)	0.0009 (2)	-0.0055 (2)	-0.0024 (2)
O2	0.0162 (3)	0.0188 (3)	0.0279 (4)	0.0057 (2)	-0.0029 (3)	-0.0039 (3)
N1	0.0119 (3)	0.0094 (3)	0.0178 (3)	0.0016 (2)	-0.0024 (2)	-0.0012 (2)
N2	0.0143 (3)	0.0139 (3)	0.0210 (4)	0.0019 (2)	-0.0021 (3)	-0.0053 (3)

N3	0.0113 (3)	0.0124 (3)	0.0150 (3)	0.0021 (2)	-0.0019 (2)	-0.0013 (2)
C1	0.0140 (4)	0.0116 (3)	0.0180 (4)	-0.0008 (3)	0.0000 (3)	-0.0014 (3)
C2	0.0242 (5)	0.0231 (4)	0.0330 (5)	0.0041 (4)	-0.0034 (4)	-0.0161 (4)
C3	0.0135 (4)	0.0123 (3)	0.0185 (4)	-0.0002 (3)	0.0001 (3)	-0.0010 (3)
C4	0.0135 (4)	0.0122 (3)	0.0141 (4)	-0.0008 (3)	0.0002 (3)	0.0001 (3)
C5	0.0254 (5)	0.0179 (4)	0.0159 (4)	-0.0095 (3)	0.0001 (3)	0.0012 (3)
C6	0.0377 (6)	0.0347 (6)	0.0207 (5)	-0.0232 (5)	-0.0017 (4)	0.0076 (4)
C7	0.0483 (7)	0.0235 (5)	0.0181 (4)	-0.0183 (5)	-0.0036 (4)	-0.0012 (4)
C8	0.0450 (7)	0.0245 (5)	0.0158 (4)	-0.0085 (4)	0.0000(4)	-0.0021 (3)
C9	0.1150 (17)	0.0468 (8)	0.0168 (5)	-0.0332 (10)	-0.0024(7)	-0.0059 (5)
C10	0.0254 (5)	0.0222 (4)	0.0163 (4)	-0.0016 (3)	0.0023 (3)	0.0043 (3)
C11	0.0153 (4)	0.0153 (4)	0.0185 (4)	-0.0014 (3)	-0.0002 (3)	0.0045 (3)
C12	0.0252 (5)	0.0237 (4)	0.0292 (5)	-0.0120 (4)	-0.0081 (4)	0.0124 (4)

Geometric parameters (Å, º)

O1—C1	1.2062 (11)	C5—C6	1.5030 (14)
O2—C3	1.2115 (11)	C5—C7	1.3975 (13)
N1—N1A	1.3855 (13)	C6—H6A	0.966
N1—C1	1.4178 (11)	C6—H6B	0.959
N1—N3	1.4349 (10)	C6—H6C	0.996
N2—C1	1.3694 (11)	C7—C8	1.3896 (15)
N2—C2	1.4567 (12)	C7—H7	0.942
N2—C3	1.4003 (11)	C8—C9	1.5035 (17)
C2—H2A	0.968	C8—C10	1.3945 (14)
C2—H2B	0.991	C9—H9A	0.926
C2—H2C	0.964	C9—H9B	0.923
C2—H2D	0.975	C9—H9C	0.958
C2—H2E	0.966	C10—C11	1.3891 (13)
C2—H2F	0.988	C10—H10	0.957
N3—C3	1.3714 (11)	C11—C12	1.5080 (13)
N3—C4	1.4331 (11)	C12—H12A	0.965
C4—C5	1.3953 (12)	C12—H12B	0.979
C4—C11	1.4030 (12)	C12—H12C	0.949

N1A—N1—N3	113.27 (8)	C6—C5—C7	119.96 (9)
N1A—N1—C1	118.68 (5)	C5—C6—H6A	113.6
N3—N1—C1	106.82 (6)	C5—C6—H6B	113.9
C1—N2—C2	124.36 (8)	C5—C6—H6C	112.1
C1—N2—C3	111.66 (7)	H6A—C6—H6B	107.6
C2—N2—C3	123.92 (8)	H6A—C6—H6C	103.6
N1—N3—C3	107.79 (7)	H6B—C6—H6C	105.3
N1—N3—C4	118.40 (7)	C5—C7—C8	121.89 (9)
C3—N3—C4	125.83 (7)	C5—C7—H7	117.6
O1—C1—N1	125.18 (8)	C8—C7—H7	120.5
O1—C1—N2	129.74 (8)	C7—C8—C9	120.93 (11)
N1—C1—N2	105.05 (7)	C7—C8—C10	118.95 (9)
N2—C2—H2A	109.9	C9—C8—C10	120.10 (10)
N2—C2—H2B	107.8	C8—C9—H9A	113.5
N2—C2—H2C	110.6	C8—C9—H9B	112.3
N2—C2—H2D	109.8	C8—C9—H9C	110.2
N2—C2—H2E	110.5	H9A—C9—H9B	110.6
N2—C2—H2F	108.9	H9A—C9—H9C	103.6

H2A—C2—H2B	106.8	H9B—C9—H9C	106.0
H2A—C2—H2C	111.9	C8—C10—C11	121.33 (9)
H2B—C2—H2C	109.7	C8—C10—H10	119.6
H2D—C2—H2E	110.7	C11—C10—H10	119.1
H2D—C2—H2F	108.7	C4—C11—C10	118.07 (8)
H2E—C2—H2F	108.3	C4—C11—C12	120.93 (8)
N2—C3—N3	106.27 (7)	C10—C11—C12	121.00 (8)
O2—C3—N2	126.08 (8)	C11—C12—H12A	110.7
O2—C3—N3	127.65 (8)	C11—C12—H12B	109.6
N3—C4—C5	117.84 (8)	C11—C12—H12C	111.6
N3—C4—C11	119.81 (8)	H12A—C12—H12B	106.5
C5—C4—C11	122.33 (8)	H12A—C12—H12C	109.6
C4—C5—C6	122.60 (9)	H12B—C12—H12C	108.8
C4—C5—C7	117.42 (9)		

N3A—N1A—N1—N3	-140.6	C4—N3—C3—N2	156.86 (8)
N3A—N1A—N1—C1	93.0	N1—N3—C4—C5	-104.43 (10)
C1A—N1A—N1—C1	-33.5	N1—N3—C4—C11	73.77 (10)
N1A—N1—N3—C3	-147.65 (6)	C3—N3—C4—C5	110.61 (10)
N1A—N1—N3—C4	61.61 (8)	C3—N3—C4—C11	-71.19 (12)
C1—N1—N3—C3	-15.15 (9)	N3—C4—C5—C6	-0.96 (15)
C1—N1—N3—C4	-165.89 (7)	N3—C4—C5—C7	177.43 (9)
N1A—N1—C1—O1	-37.29 (14)	C11—C4—C5—C6	-179.11 (10)
N1A—N1—C1—N2	144.56 (9)	C11—C4—C5—C7	-0.72 (15)
N3—N1—C1—O1	-166.76 (8)	N3—C4—C11—C10	-176.98 (8)
N3—N1—C1—N2	15.09 (9)	N3—C4—C11—C12	3.13 (13)
C2—N2—C1—O1	-5.46 (16)	C5—C4—C11—C10	1.14 (14)
C2—N2—C1—N1	172.58 (9)	C5—C4—C11—C12	-178.75 (9)
C3—N2—C1—O1	171.90 (9)	C4—C5—C7—C8	-0.46 (18)
C3—N2—C1—N1	-10.06 (10)	C6—C5—C7—C8	177.98 (13)
C1—N2—C3—O2	-178.74 (9)	C5—C7—C8—C9	-177.41 (15)
C1—N2—C3—N3	0.76 (10)	C5—C7—C8—C10	1.2 (2)
C2—N2—C3—O2	-1.37 (15)	C7—C8—C10—C11	-0.72 (18)
C2—N2—C3—N3	178.13 (9)	C9—C8—C10—C11	177.87 (14)
N1—N3—C3—O2	-171.62 (9)	C8—C10—C11—C4	-0.40 (15)
N1—N3—C3—N2	8.89 (9)	C8—C10—C11—C12	179.50 (10)
C4—N3—C3—O2	-23.65 (15)		

Figure S1 ^{1}H NMR Spectrum of Urazole Radical Dimer **2c**-**2c** at 25°C

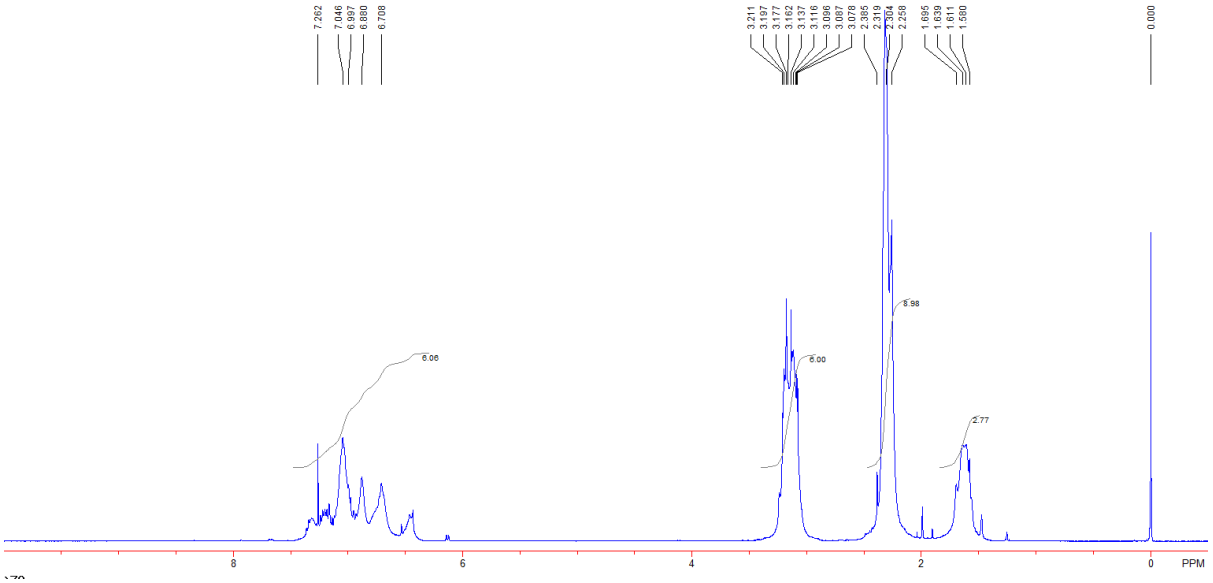


Figure S2 ^{1}H NMR Spectrum of Urazole Radical Dimer **2c**-**2c** at –30°C

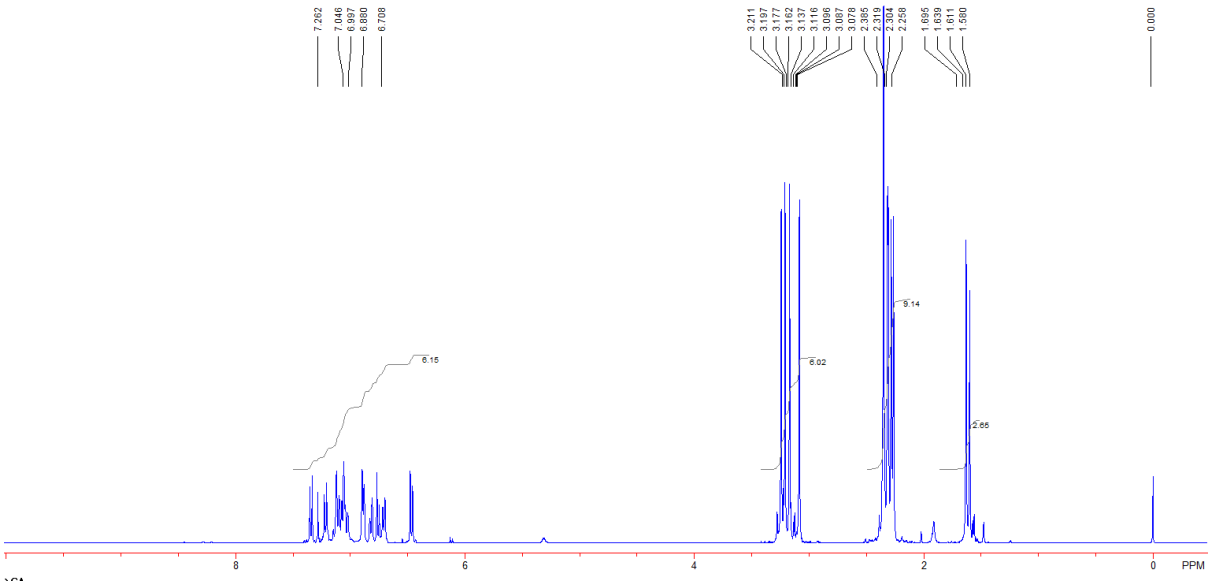
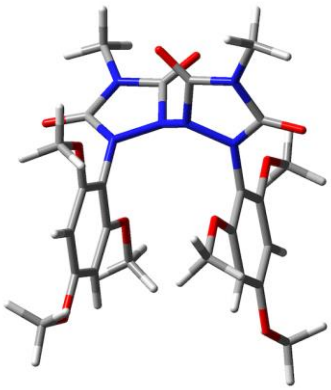


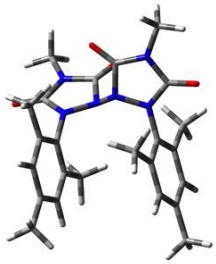
Figure S3 Computationally Optimized Geometry for Urazole Radical Dimer **2b**-**2b**



S3. Computational Details for Urazole Dimers *syn*-2a-2a, *anti*-2a-2a and 2b-2b

All calculations were performed using Gaussian 09 Revision E.01 software (Frisch *et al*., 2009). Density functional theory was used to optimize geometries at the ground state. Geometry optimizations for the urazole radical dimers below employed the B3LYP hybrid functional and 6-311G(d,p) basis set.

Urazole Radical Dimer *syn* **2a-2a**
E = –1561.24955720 Hartrees
Imaginary Frequencies = 0

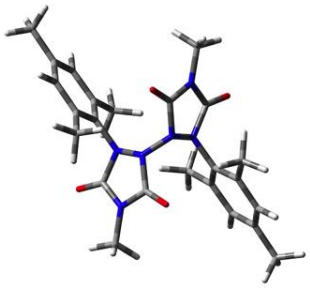


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.459605	0.091746	-2.487462
2	6	0	-1.277612	-0.584047	-2.356517
3	7	0	-0.689354	-0.110486	-1.140220
4	7	0	-1.466880	1.023488	-0.730976
5	6	0	-2.600769	1.096332	-1.512897
6	6	0	-3.386223	-0.093644	-3.593456
7	1	0	-3.624749	-1.151865	-3.699697
8	1	0	-2.948851	0.271533	-4.524739
9	1	0	-4.285267	0.474157	-3.360930
10	8	0	-0.790376	-1.417611	-3.079448
11	8	0	-3.540344	1.843465	-1.387347
12	6	0	-1.357670	1.570931	0.588215
13	6	0	-1.139602	2.699336	3.131204
14	6	0	-1.751012	0.815602	1.705295
15	6	0	-0.893100	2.888613	0.710788
16	6	0	-0.790376	3.428541	1.994922
17	6	0	-1.619186	1.397619	2.965106
18	1	0	-0.429635	4.446338	2.105603
19	1	0	-1.912280	0.822601	3.837995
20	6	0	-0.562290	3.722595	-0.500785
21	1	0	-0.013889	3.155951	-1.254604
22	1	0	0.025473	4.597667	-0.217868
23	1	0	-1.483146	4.074729	-0.976905
24	6	0	-1.043677	3.314012	4.506643
25	1	0	-0.734472	2.577775	5.252514
26	1	0	-2.013936	3.711436	4.823668
27	1	0	-0.328944	4.139308	4.525817
28	6	0	-2.321170	-0.571664	1.557544
29	1	0	-1.575969	-1.274667	1.179378
30	1	0	-3.163901	-0.576682	0.859799
31	1	0	-2.680869	-0.941532	2.518548

32	7	0	0.689354	0.110486	-1.140220
33	7	0	1.466880	-1.023488	-0.730976
34	6	0	2.600769	-1.096332	-1.512897
35	7	0	2.459605	-0.091746	-2.487462
36	6	0	1.277612	0.584047	-2.356517
37	8	0	0.790376	1.417611	-3.079448
38	8	0	3.540344	-1.843465	-1.387347
39	6	0	3.386223	0.093644	-3.593456
40	1	0	4.285267	-0.474157	-3.360930
41	1	0	3.624749	1.151865	-3.699697
42	1	0	2.948851	-0.271533	-4.524739
43	6	0	1.357670	-1.570931	0.588215
44	6	0	1.139602	-2.699336	3.131204
45	6	0	0.893100	-2.888613	0.710788
46	6	0	1.751012	-0.815602	1.705295
47	6	0	1.619186	-1.397619	2.965106
48	6	0	0.790376	-3.428541	1.994922
49	1	0	1.912280	-0.822601	3.837995
50	1	0	0.429635	-4.446338	2.105603
51	6	0	0.562290	-3.722595	-0.500785
52	1	0	-0.025473	-4.597667	-0.217868
53	1	0	1.483146	-4.074729	-0.976905
54	1	0	0.013889	-3.155951	-1.254604
55	6	0	1.043677	-3.314012	4.506643
56	1	0	2.013936	-3.711436	4.823668
57	1	0	0.328944	-4.139308	4.525817
58	1	0	0.734472	-2.577775	5.252514
59	6	0	2.321170	0.571664	1.557544
60	1	0	2.680869	0.941532	2.518548
61	1	0	1.575969	1.274667	1.179378
62	1	0	3.163901	0.576682	0.859799

Urazole Radical Dimer *anti* **2a-2a**
E = –1561.24955720 Hartrees
Imaginary Frequencies = 0



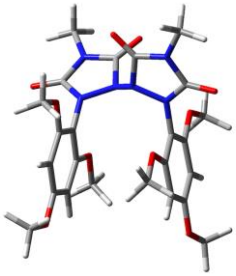
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.932880	2.588987	0.477235
2	6	0	0.159007	1.799263	1.299799
3	7	0	0.509808	0.457941	0.973692
4	7	0	1.409697	0.497453	-0.157971
5	6	0	1.726435	1.836609	-0.393773

6	6	0	0.915199	4.043448	0.505947
7	1	0	1.023389	4.390646	1.533431
8	1	0	-0.023228	4.423336	0.097564
9	1	0	1.749709	4.391111	-0.100208
10	8	0	-0.637774	2.150278	2.128706
11	8	0	2.537508	2.264224	-1.176800
12	6	0	2.434732	-0.521863	-0.262545
13	6	0	4.399769	-2.493303	-0.543203
14	6	0	3.323777	-0.760658	0.801429
15	6	0	2.537508	-1.221101	-1.473417
16	6	0	3.526275	-2.200926	-1.588714
17	6	0	4.284674	-1.756929	0.636903
18	1	0	3.615550	-2.741642	-2.525500
19	1	0	4.970822	-1.953106	1.454849
20	6	0	1.645023	-0.909980	-2.646933
21	1	0	0.589661	-0.987966	-2.381777
22	1	0	1.843582	-1.595762	-3.472082
23	1	0	1.817060	0.109595	-3.002464
24	6	0	5.438153	-3.580453	-0.674690
25	1	0	5.111805	-4.495391	-0.168584
26	1	0	6.386865	-3.280663	-0.222421
27	1	0	5.624330	-3.830013	-1.721167
28	6	0	3.266978	0.008505	2.096439
29	1	0	2.410966	-0.310524	2.694601
30	1	0	3.178676	1.085488	1.929431
31	1	0	4.176171	-0.162018	2.674941
32	7	0	-0.509808	-0.457941	0.973692
33	7	0	-1.409697	-0.497453	-0.157971
34	6	0	-1.726435	-1.836609	-0.393773
35	7	0	-0.932880	-2.588987	0.477235
36	6	0	-0.159007	-1.799263	1.299799
37	8	0	0.637774	-2.150278	2.128706
38	8	0	-2.537508	-2.264224	-1.176800
39	6	0	-0.915199	-4.043448	0.505947
40	1	0	-1.749709	-4.391111	-0.100208
41	1	0	-1.023389	-4.390646	1.533431
42	1	0	0.023228	-4.423336	0.097564
43	6	0	-2.434732	0.521863	-0.262545
44	6	0	-4.399769	2.493303	-0.543203
45	6	0	-2.537508	1.221101	-1.473417
46	6	0	-3.323777	0.760658	0.801429
47	6	0	-4.284674	1.756929	0.636903
48	6	0	-3.526275	2.200926	-1.588714
49	1	0	-4.970822	1.953106	1.454849
50	1	0	-3.615550	2.741642	-2.525500
51	6	0	-1.645023	0.909980	-2.646933
52	1	0	-1.843582	1.595762	-3.472082
53	1	0	-1.817060	-0.109595	-3.002464
54	1	0	-0.589661	0.987966	-2.381777
55	6	0	-5.438153	3.580453	-0.674690
56	1	0	-6.386865	3.280663	-0.222421
57	1	0	-5.624330	3.830013	-1.721167
58	1	0	-5.111805	4.495391	-0.168584
59	6	0	-3.266978	-0.008505	2.096439
60	1	0	-4.176171	0.162018	2.674941

61	1	0	-2.410966	0.310524	2.694601
62	1	0	-3.178676	-1.085488	1.929431

Urazole Radical Dimer **2b-2b**
E = –2012,59824939 Hartrees
Imaginary Frequencies = 0



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.931885	1.674773	-2.807181
2	6	0	-1.385072	0.413033	-2.808514
3	7	0	-0.585140	0.354498	-1.635667
4	7	0	-0.490328	1.697734	-1.123590
5	6	0	-1.407619	2.484509	-1.785374
6	6	0	-2.849373	2.159453	-3.822893
7	1	0	-3.712087	1.495877	-3.895227
8	1	0	-2.355627	2.207860	-4.795640
9	1	0	-3.167116	3.155522	-3.519587
10	8	0	-1.539768	-0.477505	-3.605156
11	8	0	-1.717312	3.627630	-1.548125
12	6	0	0.004741	1.947831	0.173015
13	6	0	0.993627	2.540586	2.709606
14	6	0	-0.805544	1.769594	1.310460
15	6	0	1.312712	2.430157	0.325872
16	6	0	1.817226	2.729930	1.598659
17	6	0	-0.313692	2.062611	2.578465
18	1	0	2.820358	3.107747	1.710225
19	1	0	-0.902836	1.936924	3.474129
20	7	0	0.585140	-0.354498	-1.635667
21	7	0	0.490328	-1.697734	-1.123590
22	6	0	1.407619	-2.484509	-1.785374
23	7	0	1.931885	-1.674773	-2.807181
24	6	0	1.385072	-0.413033	-2.808514
25	8	0	1.539768	0.477505	-3.605156
26	8	0	1.717312	-3.627630	-1.548125
27	6	0	2.849373	-2.159453	-3.822893
28	1	0	3.167116	-3.155522	-3.519587
29	1	0	3.712087	-1.495877	-3.895227
30	1	0	2.355627	-2.207860	-4.795640
31	6	0	-0.004741	-1.947831	0.173015
32	6	0	-0.993627	-2.540586	2.709606
33	6	0	-1.312712	-2.430157	0.325872

34	6	0	0.805544	-1.769594	1.310460
35	6	0	0.313692	-2.062611	2.578465
36	6	0	-1.817226	-2.729930	1.598659
37	1	0	0.902836	-1.936924	3.474129
38	1	0	-2.820358	-3.107747	1.710225
39	8	0	1.385072	2.790968	3.990302
40	8	0	2.016742	2.584076	-0.814810
41	8	0	-2.055071	1.311189	1.066289
42	8	0	2.055071	-1.311189	1.066289
43	8	0	-2.016742	-2.584076	-0.814810
44	8	0	-1.385072	-2.790968	3.990302
45	6	0	-3.344679	-3.084256	-0.757321
46	1	0	-3.997007	-2.424928	-0.174202
47	1	0	-3.687822	-3.108635	-1.789551
48	1	0	-3.374158	-4.096101	-0.338987
49	6	0	-2.670293	-3.352749	4.218888
50	1	0	-2.745725	-3.489104	5.296339
51	1	0	-3.469225	-2.681576	3.884473
52	1	0	-2.777549	-4.323055	3.722445
53	6	0	2.954380	-1.175754	2.160873
54	1	0	3.891301	-0.828992	1.728982
55	1	0	2.590558	-0.438806	2.883584
56	1	0	3.117056	-2.136367	2.659661
57	6	0	2.670293	3.352749	4.218888
58	1	0	2.745725	3.489104	5.296339
59	1	0	3.469225	2.681576	3.884473
60	1	0	2.777549	4.323055	3.722445
61	6	0	3.344679	3.084256	-0.757321
62	1	0	3.997007	2.424928	-0.174202
63	1	0	3.687822	3.108635	-1.789551
64	1	0	3.374158	4.096101	-0.338987
65	6	0	-2.954380	1.175754	2.160873
66	1	0	-3.891301	0.828992	1.728982
67	1	0	-2.590558	0.438806	2.883584
68	1	0	-3.117056	2.136367	2.659661