Title
THE DISORDERED STRUCTURE OF DIBENZOURANOCENE, [C8H6(C4H4)]2U

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and A. Streitwieser, Jr.

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Abstract. M_r = 546.46, monoclinic, $P2_1/c$, a = 9.524(4) A, b = 8.558(4) A, c = 11.758(6) A, β = 113.52(4)°, V = 878.7 A^3, Z = 2, D_x = 2.065 g/cm^3, T = 296 K, MoKα, λ = 0.71073, μ = 88 cm^{-1}, F(000) = 512, R = 0.052 for 944 observed data. The benzo-[8]annulene ligand is planar and consists of a benzene ring fused to an octagonal [8]annulene ring. The uranium atom is sandwiched by two of these ligands and is centered between the two 8-membered rings. The [8]annulene rings in the sandwich are about 6° from an eclipsed configuration. The molecules pack in a disordered manner with the uranium atom sometimes on one side of the center of symmetry and sometimes on the other.

Introduction. The structure of a number of derivatives of uranocene, di-[8]annulene uranium(IV), have now been established (Zalkin & Raymond, 1969; Avdeef, Raymond, Hodgson & Zalkin, 1972; Hodgson, Dempf & Raymond, 1971; Hodgson & Raymond, 1973; Templeton, Templeton & Walker, 1976; Zalkin, Templeton, Berryhill & Luke, 1979; Zalkin, Templeton, Luke & Streitwieser, 1982). Some of the examples are not centrosymmetric, some

contain strained rings, but all show the uranium atom accurately centered between planar 8-membered rings. Bis-(benzo[8]annulene)uranium(IV), 1, (Streitwieser, Kluttz, Smith & Luke, 1983), provides the further feature of extensive delocalization to the benzene ring. In benzocyclooctatetraene radical anion, for example, a substantial fraction of the odd electron spin density is on the benzene ring (Dodd, 1973). In the corresponding dianion, a substantial amount of charge is delocalized to the benzene ring (Paquette, Ewing, Traynor & Gardik, 1977). Using HMO π-electron populations as a model the electrostatic minimum is located 0.4 Å away from the center of the [8]annulene ring towards the benzene ring. Accordingly, for a wholly ionic structure we would expect the uranium atom in 1 not to be located between the centers of the 8-membered rings. For this compound, a structure determination thus provides a unique contribution to the nature of the ring-metal bonding in these organoactinide compounds.

Experimental. The preparation of 1 has been described (Streitwieser, Kluttz, Smith & Luke, 1983). The low solubility makes the compound difficult to crystallize under normal conditions. An inverted U-tube equipped with a single joint and with 100 mg of solid crude 1 in one arm was filled with 1:2 benzene:hexane. This arm was maintained at 40°C and the other at 25°C for a period of 2 mo without stirring. About 10 mg of crystalline product was obtained from the cooler arm. The solid is an intense olive green but the liquid phase was only faintly tinted. Attempted crystallization at a faster rate gave poorly formed disordered crystals.

A dark opaque crystal, because of its reactivity in the atmosphere, was sealed in a quartz capillary. Crystal size 0.2 x 0.2 x 0.05 mm; Picker automatic diffractometer, graphite monochromator; cell dimensions from 12

manually centered reflections, 43° < 2θ < 49°; θ-2θ scan, 2°/min, 4° < 2θ < 45°, h -11 to 10, k 0 to 9, ℓ -14 to 13, 2θ scan width (1.8 + 0.693 tanθ); analytical absorption correction (Templeton & Templeton, 1973), range 1.47-3.84; 3 reference reflections, every 250 scans, 3% decrease; 4668 scans, 1727 unique, 944 with $F^2 > 3\sigma(F^2)$, $R_{int} = 0.052$; structure solved by Patterson and Fourier methods; refined on F; local unpublished programs.

The uranium atom position was deduced from a three-dimensional Patterson function, and was found to be in the general position of the space group. The short U-U vector of length 2.5 Å observed in the Patterson function indicated disorder problems. The electron density map, using phases derived from the uranium positions, showed a collection of peaks in a plane about 2 Å from uranium. The pattern of peaks in the electron density map suggested a disorder of the type found in the structure of azulene (Robertson, Shearer, Sim & Watson, 1962), a planar molecule consisting of a 5- and 7- membered ring fused to each other, in which successive azulene molecules are subject to random reversals. A scaled paper model of the $C_8H_6(C_4H_4)$ ligand was moved about the electron density map to obtain trial positions for the carbon atoms. Figure 1 shows the electron density map through the plane of the ligand, with the final structure superimposed on it. As the peaks are not well resolved, restraints were imposed in the least-squares refinement (Waser, 1963) as follows: C-C distance of bonded carbons 1.40 ± 0.01 Å, 2nd neighbors in the benzene ring, 2.43 ± 0.06 Å; 2nd neighbors in the [8]annulene ring, 2.60 ± 0.03 Å; 3rd neighbors in the benzene ring, 2.80 ± 0.05 Å; 3rd neighbors in the [8]annulene ring, 3.38 ± 0.05 Å; 4th neighbors in the [8]annulene ring, 3.66 ± 0.05 Å. The planarity of the rings is restrained by imposing restraining distances to 2nd, 3rd and 4th neighbors within the ring. Only the uranium atom was

assigned anisotropic thermal parameters in the full-matrix least-squares refinement. Atomic scattering factors of Doyle and Turner (1968) were used and anomalous dispersion corrections were applied (Cromer & Liberman, 1970). With 106 parameters, 84 distance restraints, and 944 data [$F^2 > 3\sigma(F^2)$], $R = 0.052$, $R_w = 0.062$, and $S = 2.37$. For all 1811 data, $R = 0.107$, $(\Delta/\sigma)_{max} = 0.06$. Atomic coordinates are given in Table 1 with the numbering scheme indicated in Fig. 2.*

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*Lists of structure factors, anisotropic thermal parameters, and interatomic distances have been deposited with the British Library Lending Division as Supplementary Publication No. (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. The disorder precludes a quantitatively precise description of the structure, however, the results are adequate to describe the overall geometry. The uranium atom is sandwiched in the center of two [8]annulene rings at an average distance of 1.91 Å from their least-squares planes, and is within 0.01 Å of comparable distances found in uranocene (Zalkin & Raymond, 1969; Avdeef, Raymond, Hodgson & Zalkin, 1972), octamethyluranocene (Hodgson, Dempf & Raymond, 1971), octaphenyluranocene (Templeton, Templeton & Walker, 1976), dicyclobutenouranocene (Zalkin, Templeton, Berryhill & Luke, 1979), and dicyclopentenouranocene (Zalkin, Templeton, Luke & Streitwieser, 1982). The 8-membered rings of the ligands in the sandwich are about 6° from an eclipsed conformation, Fig. 3.

The carbon atoms in each 8-membered ring are within 0.03 Å of a common plane and the uranium atom is centered between these rings. Thus, the present determination provides structural evidence (Baker, Halstead & Raymond, 1976) for ring-metal covalency in uranocenes.

In some of the substituted uranocenes mentioned above the substituents were found to be bent in towards the metal by several degrees. Because of the disorder problem, the present structure determination is not sufficiently precise to establish this point with respect to the benzene rings. The benzene rings are clearly not bent in severely; we can only state that they are within several degrees (~5°) of coplanarity with the [8]annulene rings.

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Table 1. Positional and Thermal Parameters in $[C_8H_6(C_4H_4)]_2U$.

Atom	x	y	z	B(A^2)
U	.14113(13)	.00689(17)	.02844(8)	2.34 *
C(1)	.1206(24)	.032(3)	.2440(24)	3.4(6)
C(2)	.2788(28)	.040(3)	.2696(26)	2.1(6)
C(3)	.3682(29)	.128(4)	.2202(29)	2.7(6)
C(4)	.325(3)	.239(4)	.122(3)	3.2(7)
C(5)	.1864(28)	.310(4)	.047(3)	2.9(7)
C(6)	.0328(29)	.298(4)	.023(3)	3.8(8)
C(7)	-.0612(27)	.215(3)	.0686(26)	3.9(7)
C(8)	-.223(3)	.242(5)	-.006(4)	5.1(10)
C(9)	-.332(4)	.162(4)	.026(3)	4.6(9)
C(10)	-.303(3)	.051(4)	.127(3)	4.3(8)
C(11)	-.1461(29)	.037(4)	.185(3)	2.8(8)
C(12)	-.0207(24)	.101(3)	.1624(23)	2.7(5)
C(13)	.024(3)	-.029(6)	-.205(4)	10.4(16)
C(14)	.183(3)	-.016(5)	-.179(3)	4.2(9)
C(15)	.3051(29)	-.097(3)	-.0943(25)	2.4(6)
C(16)	.3270(26)	-.209(3)	.0012(23)	1.7(5)
C(17)	.2232(28)	-.285(4)	.042(3)	2.7(7)
C(18)	.0639(27)	-.292(3)	.0102(24)	2.3(6)
C(19)	-.0718(24)	-.222(3)	-.0824(23)	2.7(5)
C(20)	-.214(3)	-.269(5)	-.082(4)	4.3(9)
C(21)	-.357(4)	-.209(5)	-.163(4)	4.7(9)
C(22)	-.368(4)	-.092(6)	-.249(4)	6.3(12)
C(23)	-.235(3)	-.044(5)	-.260(3)	4.2(10)
C(24)	-.0888(26)	-.1081(29)	-.1773(22)	2.5(5)

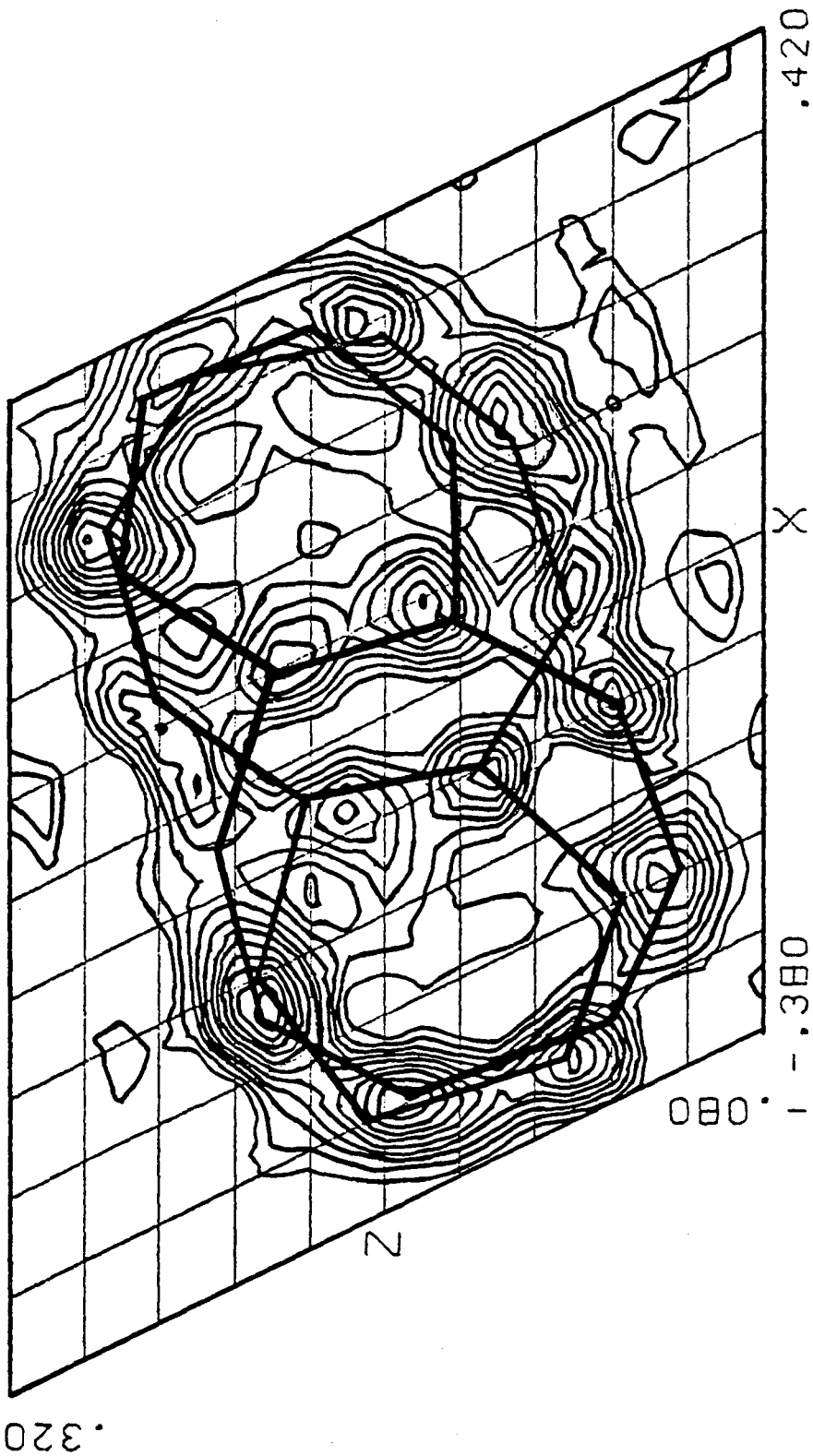
* $B_{eq} = \Sigma_i \Sigma_j a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

Figure Captions

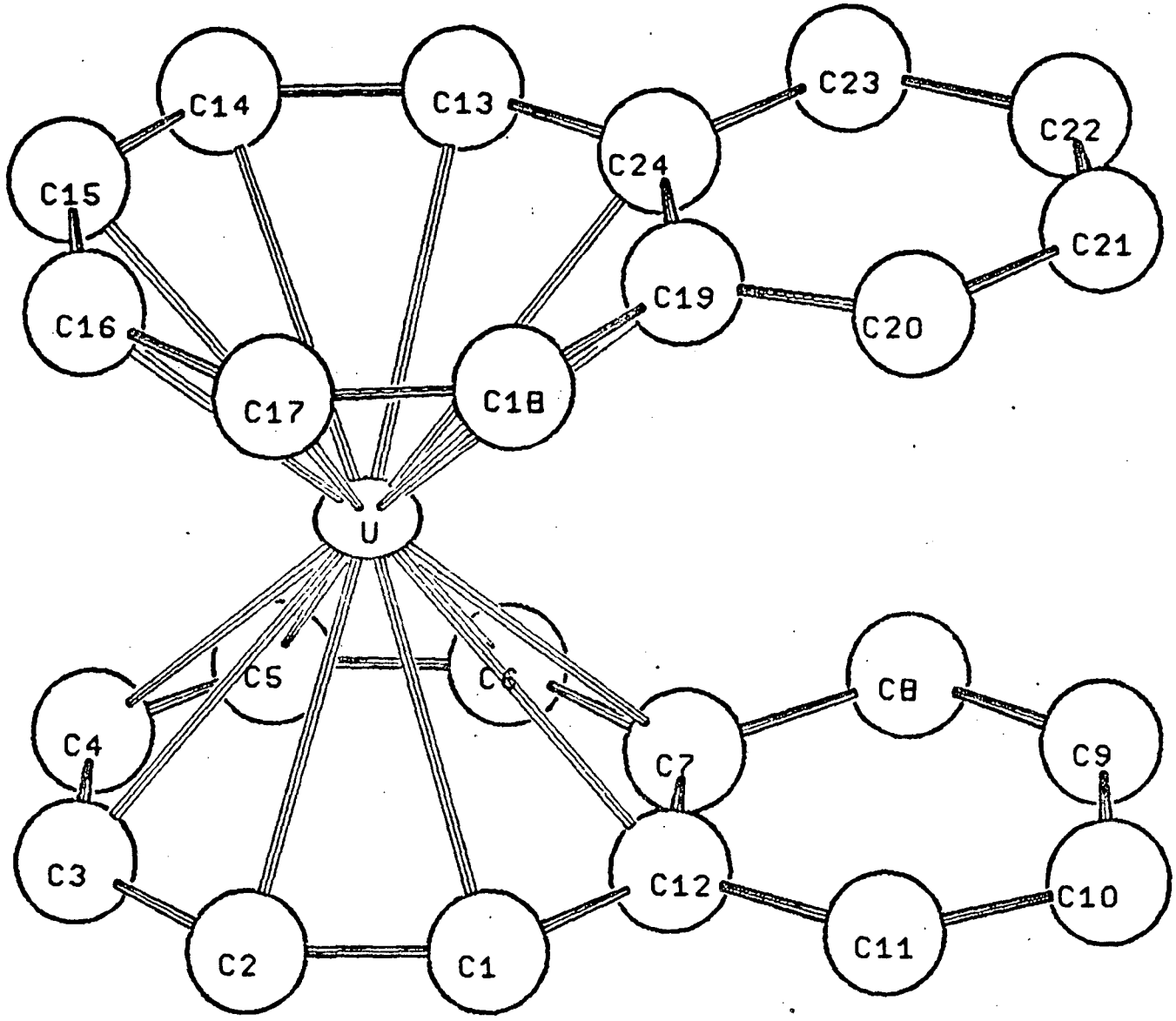
Fig. 1. Electron density map through the plane of the ligand with the backbone of the disordered ligands superimposed.

Fig. 2. ORTEP (Johnson, 1965) view of molecule showing the numbering scheme.

Fig. 3. ORTEP view perpendicular to the planes of the ligands.

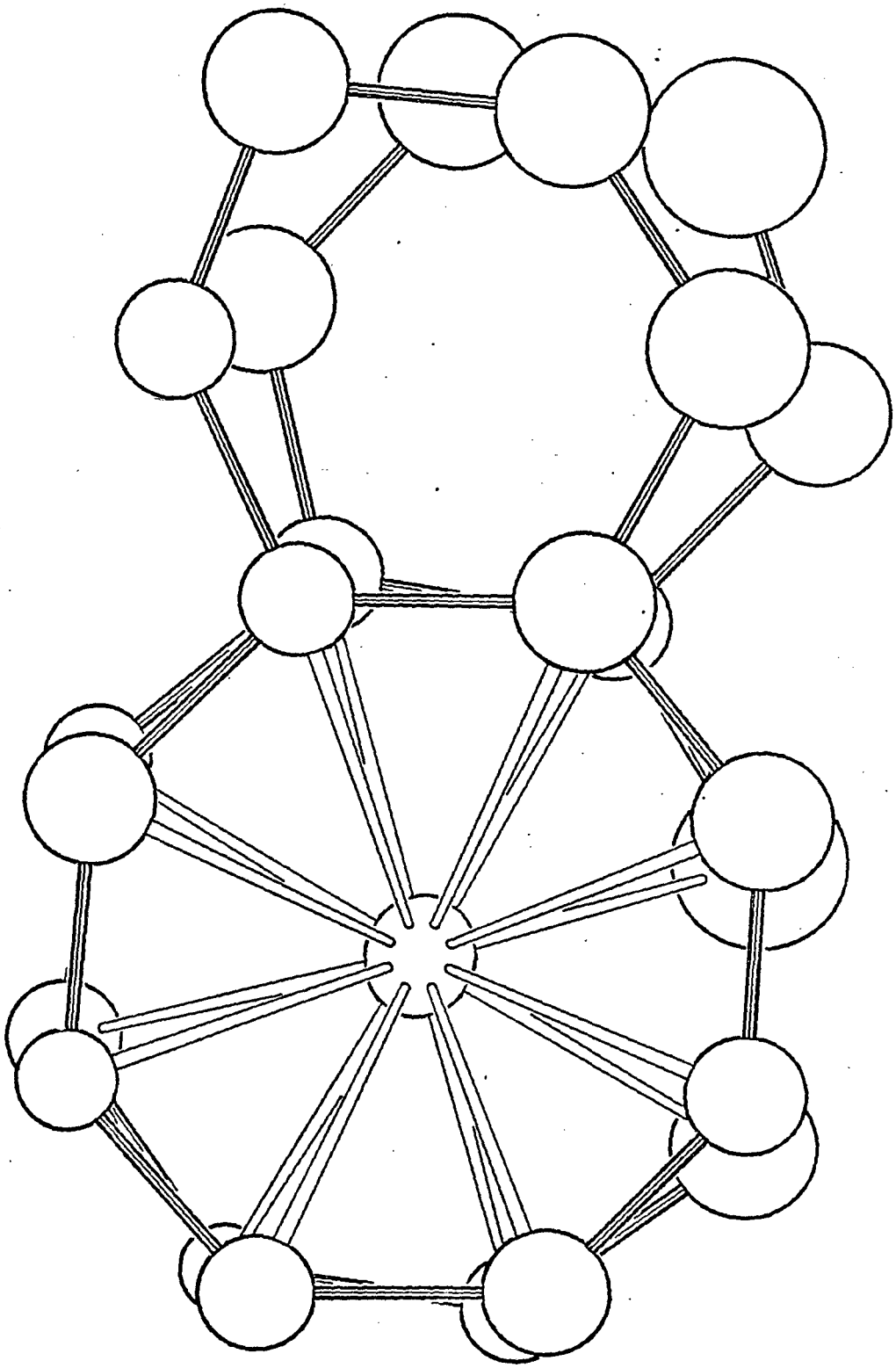


XBL 817-10794



XBL 816-10255

Fig. 2



XBL 816-10259

Fig. 3

Supplementary Material

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Selected Interatomic Distances (Å)*

U-C(1)	2.63(3)	U-C(13)	2.53(5)
U-C(2)	2.62(2)	U-C(14)	2.63(4)
U-C(3)	2.64(3)	U-C(15)	2.67(3)
U-C(4)	2.58(3)	U-C(16)	2.67(3)
U-C(5)	2.62(3)	U-C(17)	2.60(3)
U-C(6)	2.69(4)	U-C(18)	2.65(3)
U-C(7)	2.80(3)	U-C(19)	2.75(3)
U-C(12)	2.73(3)	U-C(24)	2.72(3)
C(1)-C(2)	1.42(2)	C(13)-C(14)	1.43(2)
C(2)-C(3)	1.43(2)	C(14)-C(15)	1.38(2)
C(3)-C(4)	1.42(2)	C(15)-C(16)	1.43(2)
C(4)-C(5)	1.40(2)	C(16)-C(17)	1.42(2)
C(5)-C(6)	1.38(2)	C(17)-C(18)	1.41(2)
C(6)-C(7)	1.40(2)	C(18)-C(19)	1.45(2)
C(7)-C(12)	1.41(2)	C(19)-C(24)	1.44(2)
C(7)-C(8)	1.46(2)	C(19)-C(20)	1.41(2)
C(8)-C(9)	1.41(2)	C(20)-C(21)	1.41(2)
C(9)-C(10)	1.46(2)	C(21)-C(22)	1.39(2)
C(10)-C(11)	1.38(2)	C(22)-C(23)	1.39(2)
C(11)-C(12)	1.43(2)	C(23)-C(24)	1.45(2)

* C-C interatomic distances were restrained to values given in the text, and the resulting standard deviations are not significant.

Selected Angles (°)

C(12)-C(1) -C(2)	140(3)	C(24)-C(13)-C(14)	146(4)
C(1) -C(2) -C(3)	134(3)	C(13)-C(14)-C(15)	129(3)
C(2)- C(3) -C(4)	131(3)	C(14)-C(15)-C(16)	136(3)
C(3)- C(4) -C(5)	135(3)	C(15)-C(16)-C(17)	132(2)
C(4)- C(5) -C(6)	138(3)	C(16)-C(17)-C(18)	139(2)
C(5) -C(6) -C(7)	138(3)	C(17)-C(18)-C(19)	136(3)
C(6) -C(7) -C(12)	129(3)	C(18)-C(19)-C(24)	131(2)
C(7) -C(12)-C(1)	134(2)	C(19)-C(24)-C(13)	130(3)
C(12)-C(7) -C(8)	118(3)	C(24)-C(19)-C(20)	112(3)
C(7) -C(8) -C(9)	119(3)	C(19)-C(20)-C(21)	125(3)
C(8) -C(9) -C(10)	128(3)	C(20)-C(21)-C(22)	121(4)
C(9) -C(10)-C(11)	106(3)	C(21)-C(22)-C(23)	118(3)
C(10)-C(11)-C(12)	134(3)	C(22)-C(23)-C(24)	120(3)
C(11)-C(12)-C(7)	115(2)	C(23)-C(24)-C(19)	124(2)

Anisotropic Thermal Parameters* for U ($Å^2$)

B_{11} = 3.07(4)	B_{12} = -0.15(3)
B_{22} = 1.98(3)	B_{13} = 1.08(3)
B_{33} = 2.03(3)	B_{23} = -0.41(8)

* The anisotropic temperature factor has the form $\exp[-0.25(B_{11}h^2a^{*2} + 2B_{12}hka^*b^* + \ldots)]$.

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
BENZYL URANOCENE F(0,0,0) = 2707

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	0,	0		2	699	11	14	6	139	8	21	9	352	10	-14	7	232	9	15
2	873	13	18	3	27	33	-20*	7	75	15	8*	10	78	15	31*	8	118	24	-6*
4	829	13	60	4	494	8	24	8	55	65	45*	11	236	8	-5	9	270	7	-23
6	323	6	7	5	82	11	5	H,K=	0,	9		12	0	50	-5*	10	31	53	13*
8	144	13	50	6	248	7	21	1	285	7	-9	H,K=	1,	2		11	244	7	-5
10	86	13	12	7	43	68	2*	2	38	46	8*	-13	62	21	28*	12	49	57	12*
12	118	9	11	8	112	50	42*	3	195	6	-3	-12	90	14	8	H,K=	1,	4	
H,K=	0,	1		9	61	63	-12*	4	45	49	5*	-11	0	56	-5*	-12	89	15	4
11	077	20	-44	10	70	33	5*	5	140	15	-7	-10	230	7	14	-11	62	22	39*
2	419	9	8	11	81	26	36*	6	52	28	-16*	-9	39	53	34*	-10	222	9	5
3	452	9	-1	12	140	12	18	7	61	31	16*	-8	418	7	-0	-9	33	51	-12*
4	35	42	-22*	H,K=	0,	5		H,K=	0,	10		-7	33	49	-9*	-8	373	8	8
5	486	8	10	1	519	9	-9	0	272	8	15	-6	599	9	-21	-7	48	77	13*
6	38	25	7*	2	126	6	21	1	53	46	-0*	-5	110	6	14	-6	410	7	-6
7	173	5	-7	3	441	7	-4	2	234	8	-8	-4	677	10	-21	-5	81	14	21
8	45	29	40*	4	65	14	9*	3	77	19	43*	-3	86	11	62	-4	788	13	19
9	87	14	50	5	306	6	25	4	167	9	14	-2	178	6	-35	-3	199	6	-6
10	70	15	56*	6	74	26	54*	H,K=	1,	0		-1	113	5	-2	-2	607	10	-17
11	96	13	14	7	140	14	13	-10	278	7	31	0	579	9	59	-1	50	17	28*
12	0	56	-12*	8	0	79	-64*	-8	413	8	1	1	58	23	29*	0	526	8	11
13	174	10	10	9	0	78	-13*	-6	726	11	14	2	326	5	31	1	142	4	1
H,K=	0,	2		10	50	86	15*	-4	987	15	56	3	52	14	27*	2	183	6	2
0	689	11	-17	11	120	15	36	-2	879	13	-6	4	105	9	65	3	155	5	-11
1	425	7	12	H,K=	0,	6		0	917	22	-21	5	0	45	-20*	4	115	7	55
2	164	13	-65	0	435	7	-4	2	312	5	8	6	156	9	27	5	65	19	-14*
3	20	46	-18*	1	79	10	-4	4	150	4	62	7	78	15	6*	6	216	7	16
4	532	8	9	2	441	7	-5	6	219	5	16	8	270	9	-16	7	101	23	-25*
5	50	17	1*	3	46	24	12*	8	374	7	-12	9	0	63	-6*	8	247	8	-14
6	236	5	5	4	366	6	-7	10	313	8	3	10	264	8	-16	9	45	57	-13*
7	48	38	15*	5	96	11	9	12	212	7	-4	11	54	59	47*	10	258	10	2
8	98	11	38	6	202	9	11	H,K=	1,	1		12	227	10	-5	11	45	54	3*
9	48	32	12*	7	71	18	11*	-13	74	18	42*	H,K=	1,	3		H,K=	1,	5	
10	118	14	19	8	42	64	16*	-11	145	14	-8	-13	43	55	14*	-12	48	59	21*
11	23	48	4*	9	59	35	-28*	-10	21	44	17*	-12	37	47	10*	-11	109	16	5
12	145	8	1	10	45	58	-26*	-9	349	6	14	-11	153	9	15	-10	15	66	-27*
13	37	55	-7*	H,K=	0,	7		-8	45	29	15*	-10	29	48	-3*	-9	266	8	15
H,K=	0,	3		1	410	7	-1	-7	450	7	7	-9	375	9	6	-8	0	57	-30*
1	811	12	40	2	51	53	43*	-6	154	8	25	-8	59	21	42*	-7	253	9	-10
2	53	9	-0	3	358	6	-2	-5	865	13	1	-7	470	8	-6	-6	111	9	19
3	644	10	28	4	60	32	-10*	-4	134	7	-18	-6	38	47	13*	-5	368	6	-26
4	94	8	29	5	266	7	13	-3	342	7	-26	-5	871	14	12	-4	58	14	1*
5	415	7	28	6	97	14	7	-2	299	8	-21	-4	447	7	55	-3	478	8	-10
6	83	18	12*	7	96	29	24*	-1	745	11	-23	-3	749	12	22	-2	38	23	24*
7	170	9	10	8	93	19	-16*	0	61	5	-1	-2	27	28	12*	-1	366	6	1
8	57	30	-28*	9	67	24	45*	1	371	7	10	-1	687	10	31	0	99	7	-5
9	65	31	20*	H,K=	0,	8		2	162	18	51	0	95	5	8	1	266	6	25
10	47	49	3*	0	327	7	-13	3	234	6	47	1	490	10	27	2	93	8	4
11	104	14	-12	1	30	42	9*	4	47	13	35*	2	68	10	-2	3	91	9	36
12	46	53	-16*	2	283	6	-6	5	178	5	5	3	151	5	51	4	105	8	-10
H,K=	0,	4		3	45	50	31*	6	21	44	-3*	4	175	5	12	5	120	9	0
0	874	14	8	4	203	7	-8	7	241	6	21	5	149	9	-3	6	81	27	14*
1	164	4	-10	5	77	35	-6*	8	9	60	5*	6	55	37	-20*	7	230	11	21

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
8	80	21	0*	-2	289	6	-9	-7	408	7	-2	-3	282	5	-2	2	74	11	1
9	215	11	-8	-1	83	17	9*	-6	30	32	-24*	-2	136	4	9	3	279	6	13
10	25	54	-7*	0	219	6	9	-5	513	8	14	-1	146	8	137	4	94	11	0
11	203	16	-13	1	99	11	5	-4	78	13	28	0	113	8	2	5	443	15	-1
H,K=		1,	6	2	90	18	13*	-3	347	7	51	1	323	6	36	6	39	77	-14*
-11	0	84	-39*	3	99	11	-15	-2	208	12	16	2	99	6	-11	7	340	8	-8
-10	163	10	5	4	73	17	54*	-1	191	6	47	3	395	6	27	8	44	77	10*
-9	0	53	-32*	5	84	21	-0*	0	47	34	32*	4	96	10	32	9	251	7	-11
-8	294	6	12	6	102	12	8	1	265	8	8	5	452	8	8	10	0	60	-14*
-7	0	53	-30*	7	70	18	-11*	2	156	5	18	6	39	51	-8*	H,K=		2,	6
-6	360	7	-3	8	155	10	12	3	570	9	13	7	371	7	8	-11	51	61	43*
-5	57	38	-11*	H,K=		1,	9	4	30	55	5*	8	28	69	-4*	-10	318	7	8
-4	468	9	5	-7	174	9	-24	5	469	8	-5	9	282	7	-5	-9	124	15	-1
-3	72	13	-16	-6	34	48	19*	6	46	31	5*	10	38	52	37*	-8	358	7	-1
-2	385	6	-4	-5	216	6	1	7	429	7	-10	11	199	10	13	-7	73	14	-19*
-1	57	23	16*	-4	35	44	-19*	8	19	59	6*	H,K=		2,	4	-6	275	6	-12
0	332	6	27	-3	234	6	-6	9	325	7	-24	-13	46	60	42*	-5	68	24	-30*
1	110	11	9	-2	24	66	-48*	10	33	63	28*	-12	205	7	-13	-4	250	8	14
2	158	19	3	-1	215	6	-1	11	222	8	-1	-11	45	49	23*	-3	124	10	2
3	127	9	1	0	95	16	-14	12	0	57	-4*	-10	375	7	-7	-2	114	8	32
4	100	13	79	1	144	16	9	H,K=		2,	2	-9	42	46	28*	-1	134	10	-33
5	91	65	-12*	2	88	11	-3	-13	66	17	62*	-8	373	7	2	8	120	9	33
6	160	9	11	3	64	17	49*	-11	60	21	3*	-7	12	48	-6*	1	96	10	24
7	99	14	16	4	91	12	-16	-10	405	7	-7	-6	373	7	-1	2	224	6	20
8	183	9	3	5	56	27	7*	-9	55	21	-2*	-5	66	12	-8	3	166	13	-8
9	53	56	15*	6	89	17	19*	-8	440	7	-2	-4	338	6	10	4	322	6	-3
10	187	11	-17	H,K=		1,	10	-7	42	21	11*	-3	97	8	33	5	91	12	3
H,K=		1,	7	-4	204	13	0	-6	434	7	-6	-2	110	5	32	6	324	9	-6
-10	50	55	-16*	-3	29	50	-11*	-5	16	32	-67*	-1	152	5	-16	7	31	51	-5*
-9	204	9	7	-2	208	7	0	-4	374	6	58	0	216	5	-0	8	256	7	3
-8	20	45	5*	-1	55	36	-12*	-3	107	18	-9	1	38	34	-10*	9	0	59	-30*
-7	330	7	5	0	176	6	11	-2	258	5	36	2	257	6	17	H,K=		2,	7
-6	42	56	4*	1	90	21	-13*	-1	144	8	-0	3	0	48	-39*	-10	55	27	46*
-5	426	7	14	2	84	26	16*	0	207	7	40	4	430	15	-2	-9	319	6	8
-4	60	37	-12*	3	85	24	-19*	1	99	8	12	5	67	19	48*	-8	131	14	-4
-3	425	7	5	H,K=		2,	8	2	344	13	58	6	460	10	17	-7	333	6	-4
-2	69	21	-9*	-14	216	8	19	3	96	9	-7	7	30	66	-23*	-6	66	17	-8*
-1	340	7	5	-10	405	8	-31	4	458	8	-7	8	305	7	-6	-5	267	6	3
0	89	20	-6*	-8	450	7	-11	5	0	55	-12*	9	30	75	18*	-4	136	9	8
1	230	7	15	-6	560	9	-28	6	377	7	0	10	235	8	-0	-3	153	14	-5
2	117	10	9	-4	571	9	25	7	75	19	2*	11	64	43	46*	-2	123	20	-20
3	59	33	15*	-2	148	4	46	8	353	14	-15	H,K=		2,	5	-1	90	15	88
4	133	8	-18	0	444	8	14	9	17	52	11*	-12	34	68	5*	0	148	12	15
5	73	17	-1*	2	451	7	23	10	259	7	-17	-11	225	9	-13	1	158	11	6
6	88	20	9*	4	683	11	-4	11	51	43	46*	-10	18	60	4*	2	101	15	-7
7	150	10	19	6	465	8	2	H,K=		2,	3	-9	363	8	15	3	246	6	3
8	95	27	18*	8	424	7	-11	-13	220	8	5	-8	56	23	-27*	4	115	9	-3
9	147	13	-28	10	263	11	-17	-12	0	46	-17*	-7	234	6	-5	5	260	7	-10
H,K=		1,	8	12	161	11	12	-11	302	6	-14	-6	68	33	44*	6	66	35	28*
-9	70	23	49*	H,K=		2,	1	-10	40	57	27*	-5	272	5	6	7	228	7	-8
-8	178	7	2	-14	17	52	4*	-9	511	8	-4	-4	100	11	-2	8	42	54	18*
-7	41	43	30*	-13	260	6	6	-8	76	13	17	-3	130	6	2	H,K=		2,	8
-6	271	8	-7	-11	312	6	-10	-7	446	7	-1	-2	105	7	-13	-9	0	52	-38*
-5	37	45	32*	-10	23	43	-8*	-6	40	69	-47*	-1	90	11	44	-8	225	9	-7
-4	296	7	11	-9	448	7	-15	-5	539	9	23	0	79	9	-11	-7	72	15	-1*
-3	105	10	-1	-8	43	24	20*	-4	80	9	-21	1	173	7	0	-6	211	7	1

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-5	90	12	9	-6	68	9	4	-2	51	11	15*	5	329	7	-7	1	25	46	15*
-4	154	7	-3	-5	225	4	23	-1	711	11	15	6	32	50	-7*	2	299	6	0
-3	130	8	29	-4	0	41	-61*	0	57	14	-4*	7	212	10	13	3	43	47	33*
-2	48	29	21*	-3	358	6	14	1	628	10	1	8	61	32	40*	4	250	7	5
-1	131	13	-5	-2	146	10	38	2	44	30	26*	9	114	21	17*	5	46	55	37*
0	88	12	26	-1	491	8	7	3	536	9	-1	H,K=	3,	6		6	188	9	-1
1	89	11	25	0	96	10	1	4	47	52	34*	-11	57	71	-14*	H,K=	3,	9	
2	173	7	-2	1	638	14	12	5	426	7	-1	-10	201	8	4	-7	64	25	26*
3	98	13	-4	2	110	7	8	6	31	70	1*	-9	99	16	-12	-6	75	30	-31*
4	212	7	-7	3	616	10	-16	7	258	7	19	-8	134	8	8	-5	78	18	48*
5	62	23	12*	4	35	43	29*	8	37	53	1*	-7	114	11	-11	-4	94	17	9*
6	227	6	1	5	458	8	-16	9	127	12	18	-6	82	13	70	-3	138	9	-8
7	30	56	-5*	6	35	49	34*	10	66	27	47*	-5	94	16	-16	-2	98	11	2
H,K=	2,	9		7	290	7	19	H,K=	3,	4		-4	130	12	16	-1	167	7	6
-7	178	8	-10	8	15	56	10*	-13	38	52	5*	-3	64	16	-1*	0	46	33	-5*
-6	71	22	4*	9	101	15	-10	-12	209	6	-11	-2	298	6	24	1	236	7	-7
-5	145	10	2	10	69	24	63*	-11	0	47	-20*	-1	80	12	-21	2	60	24	35*
-4	104	12	5	11	63	35	39*	-10	253	7	9	0	426	7	-2	3	229	8	1
-3	96	10	16	H,K=	3,	2		-9	67	18	-0*	1	43	50	6*	4	0	53	-17*
-2	109	12	-7	-14	234	8	9	-8	182	8	4	2	370	7	0	H,K=	3,	10	
-1	44	48	39*	-13	48	50	14*	-7	106	11	12	3	41	44	-10*	-4	73	24	9*
0	68	19	-20*	-11	40	55	-4*	-6	95	12	82	4	308	7	-3	-3	85	16	14*
1	110	11	20	-10	252	6	1	-5	84	13	-11	5	26	58	9*	-2	135	10	8
2	95	10	9	-9	65	35	6*	-4	241	5	0	6	238	8	4	-1	46	58	-20*
3	181	7	2	-8	156	6	24	-3	99	7	26	7	51	52	20*	0	170	9	5
4	81	14	2	-7	40	41	-3*	-2	390	6	2	8	129	14	-3	1	34	63	-9*
5	200	8	-1	-6	106	7	41	-1	57	20	-22*	H,K=	3,	7		H,K=	4,	0	
H,K=	2,	10		-5	23	36	-31*	0	558	9	-17	-10	51	55	-15*	-14	141	10	12
-4	113	13	-4	-4	236	6	3	1	34	42	6*	-9	170	7	12	-18	127	20	22
-3	97	15	-7	-3	65	26	20*	2	468	8	9	-8	92	18	1*	-8	274	7	34
-2	37	50	4*	-2	472	7	43	3	45	29	39*	-7	91	12	36	-6	553	9	43
-1	94	15	-16	-1	15	40	-19*	4	445	8	1	-6	101	11	-15	-4	762	12	-18
0	57	22	34*	0	724	11	11	5	44	52	26*	-5	62	18	16*	-2	624	10	8
1	79	22	-13*	1	180	4	3	6	267	7	-14	-4	74	15	18*	0	604	11	-15
2	115	13	-22	2	653	10	-9	7	56	37	-6*	-3	218	6	11	2	341	6	19
H,K=	3,	0		3	0	41	-5*	8	155	10	13	-2	117	9	-22	4	123	14	-11
-14	280	7	-17	4	534	9	-15	9	61	41	39*	-1	336	7	5	6	58	49	22*
-10	318	8	-7	5	63	21	38*	10	0	68	-57*	0	40	58	19*	8	55	45	-18*
-8	230	5	-3	6	420	8	1	H,K=	3,	5		1	366	7	-10	10	119	16	-3
-6	128	5	107	7	52	40	18*	-12	48	51	-5*	2	0	50	-11*	H,K=	4,	1	
-4	427	7	43	8	205	8	14	-11	174	10	-21	3	295	7	8	-14	43	53	34*
-2	458	7	9	9	56	36	49*	-10	50	55	-13*	4	0	46	-2*	-13	120	10	30
0	440	7	5	10	79	20	-12*	-9	181	7	10	5	241	8	2	-11	59	61	54*
2	703	11	18	11	19	67	6*	-8	103	15	18	6	21	59	-5*	-10	35	47	16*
4	498	10	10	H,K=	3,	3		-7	96	15	16	7	163	10	-1	-9	204	6	-3
6	377	8	17	-13	233	9	-7	-6	147	7	-15	H,K=	3,	8	-8	54	55	41*	
8	141	9	23	-12	36	49	-9*	-5	106	9	3	-9	50	67	-18*	-7	299	6	20
10	85	14	22	-11	249	9	-13	-4	36	40	-17*	-8	93	17	12*	-6	47	23	-11*
H,K=	3,	1		-10	43	44	-24*	-3	194	5	2	-7	94	13	10	-5	626	11	-4
-14	24	59	12*	-9	259	6	15	-2	114	7	-4	-6	68	18	61*	-4	90	8	9
-13	280	9	5	-8	73	30	-7*	-1	409	7	0	-5	79	17	-10*	-3	744	12	21
-11	254	6	-13	-7	119	9	12	0	14	39	-26*	-4	134	8	12	-2	63	13	-1*
-10	38	70	33*	-6	32	54	-31*	1	426	7	-1	-3	127	11	29	-1	650	11	-5
-9	262	8	25	-5	220	5	26	2	94	10	13	-2	221	6	1	0	45	23	-5*
-8	44	23	38*	-4	48	36	31*	3	414	7	5	-1	80	14	-14	1	586	10	20
-7	109	7	9	-3	334	6	41	4	40	46	27*	0	270	7	-5	2	126	7	6

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	248	9	4	9	116	20	17	-3	53	21	30*	2	57	46	7*	1	50	22	10*
4	49	49	21*	H,K=		4,	4	-2	407	7	-6	3	123	12	2	2	78	12	64
5	151	10	-6	-13	56	24	19*	-1	34	42	15*	H,K=		5,	0	3	53	23	9*
6	60	73	19*	-12	82	11	26	0	381	6	2	-14	34	53	-58*	4	185	7	6
7	48	53	18*	-11	81	11	17	1	8	41	-21*	-12	170	11	3	5	53	30	14*
8	16	53	-6*	-10	79	14	24	2	272	6	2	-10	404	7	-3	6	248	6	-10
9	122	13	19	-9	60	34	32*	3	105	11	17	-8	491	8	5	7	34	47	27*
10	97	18	69*	-8	231	7	31	4	134	10	8	-6	456	7	-21	8	192	10	-19
H,K=		4,	2	-7	94	14	32	5	61	22	5*	-4	391	6	10	9	50	59	38*
-14	130	11	15	-6	429	8	7	6	63	20	46*	-2	359	7	-1	H,K=		5,	3
-13	29	57	5*	-5	80	11	-9	7	83	16	9*	0	192	5	19	-13	149	11	20
-11	39	45	-5*	-4	431	8	-7	8	66	30	1*	2	95	19	54*	-12	39	46	14*
-10	120	16	3	-3	38	41	10*	H,K=		4,	7	4	168	8	10	-11	259	5	20
-9	39	46	33*	-2	487	8	-11	-10	27	46	-40*	6	239	6	11	-10	26	50	15*
-8	193	7	-15	-1	52	17	-5*	-9	107	12	17	8	188	13	14	-9	382	7	-2
-7	51	17	30*	0	429	8	-0	-8	69	16	24*	H,K=		5,	1	-8	45	38	23*
-6	376	9	2	1	56	16	22*	-7	182	6	-3	-14	29	56	26*	-7	449	8	-7
-5	62	20	-8*	2	350	7	-5	-6	8	52	-29*	-13	131	9	11	-6	28	50	15*
-4	610	10	-9	3	57	24	37*	-5	288	6	-12	-12	80	27	45*	-5	435	8	-11
-3	77	10	9	4	145	16	18	-4	43	24	38*	-11	279	6	1	-4	46	38	13*
-2	710	11	-9	5	0	56	-23*	-3	328	6	-13	-10	38	61	11*	-3	366	7	-8
-1	40	20	39*	6	42	52	17*	-2	23	48	5*	-9	427	7	-8	-2	44	20	16*
0	577	9	-3	7	72	21	23*	-1	309	7	-2	-8	24	39	8*	-1	106	9	1
1	72	12	-23	8	96	19	28*	0	41	46	-5*	-7	501	8	1	0	66	12	42
2	442	7	23	9	33	57	-11*	1	240	5	-8	-6	51	14	2*	1	81	15	41*
3	37	47	12*	H,K=		4,	5	2	94	9	10	-5	466	8	-15	2	47	39	-12*
4	249	6	23	-12	54	29	6*	3	159	7	17	-4	29	42	18*	3	149	9	15
5	50	53	23*	-11	58	17	48*	4	70	16	10*	-3	517	8	56	4	90	13	26
6	126	23	52	-10	78	19	18*	5	79	18	29*	-2	57	13	27*	5	187	7	-8
7	68	30	28*	-9	134	11	13	6	58	62	-23*	-1	283	5	-9	6	50	29	30*
8	89	22	16*	-8	44	40	-9*	H,K=		4,	8	0	72	12	2	7	183	9	-7
9	0	58	-33*	-7	296	6	7	-9	44	47	-12*	1	132	7	28	8	64	58	37*
10	153	12	11	-6	55	18	-4*	-8	114	13	-3	2	60	23	30*	H,K=		5,	4
H,K=		4,	3	-5	392	7	-10	-7	55	35	-14*	3	104	10	8	-13	32	51	26*
-13	92	14	-12	-4	20	38	1*	-6	191	6	-1	4	50	35	23*	-12	151	8	-8
-12	38	57	-17*	-3	418	7	-12	-5	45	30	11*	5	232	6	-3	-11	16	44	-14*
-11	57	23	49*	-2	0	41	-5*	-4	261	7	-21	6	28	46	24*	-10	281	6	-0
-10	0	50	-59*	-1	460	8	-7	-3	16	42	-2*	7	207	7	-11	-9	12	47	-18*
-9	145	8	-1	0	21	44	15*	-2	249	6	-4	8	62	33	59*	-8	407	8	-14
-8	51	25	20*	1	426	7	-8	-1	13	42	-6*	9	203	12	-6	-7	96	20	39*
-7	312	6	21	2	38	41	-19*	0	254	6	-12	H,K=		5,	2	-6	380	7	-4
-6	107	12	10	3	252	7	-8	1	25	44	-13*	-14	114	12	19	-5	75	13	-10
-5	471	10	-3	4	69	23	28*	2	179	9	-2	-13	18	45	7*	-4	409	7	1
-4	51	19	-21*	5	88	12	4	3	54	54	-4*	-12	194	10	16	-3	118	8	-15
-3	575	9	-12	6	41	53	-24*	4	96	12	2	-11	48	24	2*	-2	251	5	13
-2	45	17	13*	7	47	51	20*	5	62	33	3*	-10	340	6	-4	-1	59	15	-23*
-1	500	8	-22	8	36	56	-21*	H,K=		4,	9	-9	14	53	-4*	0	120	8	4
0	36	37	-4*	H,K=		4,	6	-7	135	13	7	-8	434	7	-5	1	74	13	-27
1	425	7	13	-11	75	19	1*	-6	45	47	-15*	-7	26	40	17*	2	92	11	42
2	0	51	-35*	-10	85	15	29	-5	198	6	-6	-6	503	8	-8	3	72	15	-14*
3	262	6	28	-9	48	49	3*	-4	53	19	39*	-5	52	21	47*	4	129	13	-8
4	0	49	-32*	-8	174	9	3	-3	226	7	-6	-4	551	9	9	5	54	26	-7*
5	112	12	14	-7	64	15	2*	-2	34	41	20*	-3	55	16	-32*	6	181	7	-4
6	56	38	9*	-6	307	6	6	-1	232	5	3	-2	336	6	11	7	53	54	25*
7	71	22	46*	-5	15	61	-7*	0	30	41	19*	-1	17	37	7*	8	166	11	-0
8	61	73	35*	-4	386	7	-1	1	194	7	-7	0	179	6	3	H,K=		5,	5

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-12	29	46	3*	H,K=	5,	8		4	45	45	29*	-9	60	26	36*	-10	0	58	-46*
-11	182	8	-8	-9	52	57	49*	5	312	7	-6	-8	224	7	-11	-9	187	8	-16
-10	56	61	25*	-8	201	8	-8	6	16	49	4*	-7	106	23	0*	-8	62	22	-20*
-9	304	10	-6	-7	32	45	16*	7	202	18	-25	-6	131	11	4	-7	170	7	1
-8	34	49	7*	-6	234	6	-5	8	42	68	29*	-5	98	12	-7	-6	49	57	-18*
-7	362	7	-23	-5	46	35	-2*	H,K=	6,	2		-4	79	14	17	-5	47	34	-22*
-6	36	62	-33*	-4	215	6	6	-14	230	7	6	-3	92	11	-24	-4	51	31	-40*
-5	392	7	9	-3	99	13	-28	-13	38	52	34*	-2	108	9	21	-3	42	57	21*
-4	76	11	39	-2	167	9	6	-12	284	8	0	-1	74	28	18*	-2	38	48	-35*
-3	380	7	0	-1	93	18	8	-11	39	41	14*	0	219	6	15	-1	98	15	-5
-2	112	7	14	0	67	17	8*	-10	311	6	6	1	34	68	2*	0	81	17	6*
-1	206	6	5	1	83	21	-6*	-9	0	65	-12*	2	230	7	-13	1	146	15	-13
0	71	15	2*	2	22	52	1*	-8	390	7	0	3	44	48	35*	2	76	26	47*
1	109	9	35	3	70	35	-7*	-7	69	19	24*	4	247	6	-0	3	181	9	4
2	108	10	-20	4	121	13	29	-6	251	7	-2	5	73	27	46*	4	74	25	23*
3	91	15	11	H,K=	5,	9		-5	27	56	14*	6	229	10	-6	H,K=	6,	8	
4	57	37	-14*	-6	54	37	21*	-4	124	8	18	7	0	57	-6*	-8	145	11	-21
5	152	8	-8	-5	207	8	7	-3	45	51	-15*	H,K=	6,	5	-7	102	12	-0	
6	62	46	9*	-4	89	12	37	-2	142	8	32	-12	60	42	38*	-6	106	11	-10
7	173	10	-11	-3	164	8	1	-1	66	20	34*	-11	238	7	-4	-5	86	13	1
H,K=	5,	6		-2	68	18	-10*	0	269	7	8	-10	75	51	32*	-4	46	41	15*
-11	23	71	-11*	-1	114	10	-10	1	51	58	35*	-9	243	8	-11	-3	93	12	-20
-10	214	9	3	0	60	34	-9*	2	336	6	-1	-8	74	25	-2*	-2	31	47	-4*
-9	46	38	26*	1	63	28	51*	3	20	52	-6*	-7	170	7	9	-1	84	15	3
-8	295	6	-4	H,K=	6,	0		4	300	7	-6	-6	41	58	-20*	0	130	10	10
-7	26	45	-10*	-14	209	10	-3	5	32	50	5*	-5	123	13	7	1	43	54	-21*
-6	345	7	0	-12	298	14	-8	6	253	7	-18	-4	86	28	-4*	2	162	11	6
-5	2	41	-8*	-10	280	5	-14	7	0	63	-19*	-3	60	65	50*	H,K=	6,	9	
-4	338	6	-6	-8	329	6	12	8	151	14	-11	-2	70	14	-16*	-4	51	54	-21*
-3	51	26	1*	-6	132	8	32	H,K=	6,	3		-1	152	8	18	-3	12	62	1*
-2	208	6	0	-4	88	13	54	-13	241	6	-8	0	85	11	1	-2	88	18	8*
-1	52	24	15*	-2	192	6	-6	-12	24	44	3*	1	255	6	-7	H,K=	7,	0	
0	64	21	-12*	0	310	7	3	-11	287	7	1	2	62	18	34*	-14	219	8	8
1	100	12	11	2	282	6	-2	-10	25	45	15*	3	254	6	-9	-12	179	7	-12
2	57	18	34*	4	283	6	10	-9	312	7	-8	4	38	58	-44*	-10	74	12	12
3	83	14	17	6	253	7	-11	-8	29	53	9*	5	273	9	-20	-8	77	13	37
4	106	14	1	8	199	10	7	-7	254	7	2	6	33	67	23*	-6	150	7	-12
5	91	17	29*	H,K=	6,	1		-6	53	32	-17*	H,K=	6,	6	-4	303	6	2	
6	156	11	3	-14	34	59	33*	-5	117	11	-15	-11	44	66	9*	-2	279	7	13
H,K=	5,	7	-13	250	9	-7	-4	80	13	28	-10	225	9	2	0	313	6	10	
-10	76	19	63*	-12	0	58	-12*	-3	85	12	38	-9	71	23	25*	2	295	6	7
-9	208	7	-4	-11	286	6	-18	-2	48	25	-6*	-8	205	7	-7	4	160	8	-8
-8	38	48	34*	-10	25	48	-28*	-1	154	10	5	-7	60	40	1*	6	133	13	22
-7	267	7	1	-9	339	8	6	0	59	21	30*	-6	114	9	-11	H,K=	7,	1	
-6	24	43	-12*	-8	60	16	-11*	1	290	6	4	-5	61	17	41*	-14	27	60	9*
-5	283	6	-6	-7	313	7	13	2	42	59	31*	-4	69	15	42*	-13	213	9	-2
-4	31	47	-19*	-6	64	15	-10*	3	221	6	-5	-3	95	11	12	-12	58	42	-15*
-3	192	6	-10	-5	120	10	-1	4	42	45	24*	-2	83	13	-1	-11	130	9	17
-2	123	8	10	-4	18	55	-21*	5	268	7	10	-1	78	13	12	-10	64	15	-3*
-1	106	9	15	-3	98	15	77	6	0	65	-14*	0	193	7	9	-9	68	15	7*
0	38	42	-13*	-2	73	21	0*	7	144	13	-9	1	76	13	15	-8	11	63	-49*
1	25	43	16*	-1	236	6	1	H,K=	6,	4		2	221	6	-9	-7	134	11	25
2	88	12	3	0	38	44	27*	-13	43	53	20*	3	83	27	23*	-6	35	52	13*
3	72	23	15*	1	342	6	6	-12	249	6	-4	4	225	10	-11	-5	216	6	10
4	56	38	-2*	2	31	48	28*	-11	63	31	22*	5	55	59	10*	-4	36	45	8*
5	129	13	11	3	309	7	11	-10	272	11	-9	H,K=	6,	7	-3	361	7	4	

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	37	47	-9*	-9	35	53	-18*	-6	62	37	2*	-6	293	6	7	-5	256	7	-4
-1	312	7	-4	-8	81	16	59*	-5	115	11	-10	-5	57	50	23*	-4	49	53	16*
0	56	22	26*	-7	24	53	-44*	-4	0	67	-52*	-4	413	7	-2	-3	260	8	2
1	417	8	-11	-6	125	11	-9	-3	185	8	-9	-3	103	10	10	-2	39	47	-2*
2	42	68	32*	-5	42	52	12*	-2	18	46	-15*	-2	296	6	-20	-1	198	8	-9
3	235	9	-13	-4	262	9	-5	-1	210	9	4	-1	30	53	3*	0	42	49	19*
4	24	47	14*	-3	25	62	18*	0	79	14	62	0	248	6	-7	1	84	24	-19*
5	177	11	20	-2	269	6	1	1	178	10	-12	1	70	17	57*	2	48	65	27*
6	18	61	11*	-1	40	51	4*	2	36	56	21*	2	111	11	-1	3	41	58	0*
7	91	23	12*	0	292	6	2	H,K=		7,	8	3	48	57	31*	H,K=		8,	6
H,K=		7,	2	1	42	56	-7*	-7	63	65	-10*	4	0	55	-10*	-10	140	16	23
-13	0	59	-22*	2	198	7	9	-6	79	21	16*	5	26	56	10*	-9	57	40	24*
-12	155	12	-2	3	72	25	15*	-5	0	59	-64*	H,K=		8,	3	-8	185	9	-6
-11	24	46	-11*	4	200	9	8	-4	147	10	3	-12	30	52	11*	-7	44	52	36*
-10	84	12	-4	5	85	30	47*	-3	21	48	-11*	-11	88	20	-20*	-6	199	10	-4
-9	38	51	23*	6	84	32	-13*	-2	174	10	-12	-10	66	22	46*	-5	15	51	4*
-8	83	25	78*	H,K=		7,	5	-1	32	55	3*	-9	183	9	-16	-4	222	8	2
-7	59	64	41*	-12	64	51	-11*	0	173	11	2	-8	63	28	55*	-3	44	51	16*
-6	182	7	14	-11	126	14	3	H,K=		8,	0	-7	239	9	-28	-2	220	7	-1
-5	69	21	41*	-10	54	63	-9*	-12	66	18	10*	-6	41	46	-27*	-1	56	26	36*
-4	334	9	20	-9	63	26	18*	-10	157	7	8	-5	292	6	-2	0	143	9	1
-3	45	39	16*	-8	43	52	-48*	-8	290	6	5	-4	26	57	-4*	1	64	80	35*
-2	353	7	-2	-7	56	29	2*	-6	312	6	-1	-3	305	6	-1	2	0	60	-48*
-1	83	15	22*	-6	85	15	27	-4	408	8	-18	-2	35	46	29*	H,K=		8,	7
0	459	9	-16	-5	185	7	8	-2	147	10	12	-1	221	7	-16	-8	8	56	-12*
1	39	50	-23*	-4	36	58	-7*	0	194	7	31	0	47	39	29*	-7	131	14	-29
2	341	7	-13	-3	253	6	-16	2	83	18	-1*	1	116	14	-15	-6	7	56	4*
3	36	55	21*	-2	55	26	38*	4	50	53	42*	2	19	52	-9*	-5	172	10	-7
4	198	7	-11	-1	282	8	-8	H,K=		8,	1	3	42	56	-15*	-4	42	57	40*
5	52	55	37*	0	38	45	12*	-13	47	53	43*	4	0	62	-16*	-3	185	8	-6
6	102	17	1	1	243	7	-8	-12	55	30	29*	5	14	59	-17*	-2	32	49	16*
H,K=		7,	3	2	33	47	16*	-11	90	17	-12	H,K=		8,	4	-1	143	15	-15
-13	175	11	9	3	206	10	2	-10	45	56	28*	-12	78	23	31*	0	97	17	43
-12	44	51	15*	4	79	22	71*	-9	243	6	19	-11	56	34	20*	H,K=		9,	0
-11	120	10	15	5	147	14	-8	-8	50	66	39*	-10	150	12	34	-12	195	7	0
-10	40	47	20*	H,K=		7,	6	-7	290	6	7	-9	76	20	35*	-10	271	6	-2
-9	93	11	55	-11	64	64	-1*	-6	56	66	34*	-8	227	13	1	-8	272	7	-5
-8	79	15	48*	-10	93	36	14*	-5	405	7	1	-7	45	48	42*	-6	232	7	-12
-7	119	14	10	-9	51	65	-7*	-4	116	15	-10	-6	265	7	-1	-4	175	7	4
-6	63	65	55*	-8	0	52	-13*	-3	326	6	-12	-5	37	54	0*	-2	92	17	21
-5	236	8	-4	-7	54	61	-9*	-2	90	23	-7*	-4	270	7	-3	0	54	26	36*
-4	65	30	26*	-6	115	11	10	-1	207	6	-2	-3	0	48	-52*	2	82	23	10*
-3	306	6	-6	-5	60	25	-3*	0	41	45	39*	-2	222	7	-11	4	142	21	18
-2	52	27	17*	-4	205	7	-4	1	177	11	5	-1	37	51	30*	H,K=		9,	1
-1	336	7	-1	-3	33	45	2*	2	67	18	46*	0	163	8	16	-12	23	51	17*
0	79	20	-4*	-2	241	6	-9	3	60	31	6*	1	57	27	25*	-11	219	8	-0
1	326	6	-4	-1	12	54	-52*	4	0	59	-16*	2	96	20	14*	-10	37	49	33*
2	74	19	15*	0	260	9	4	5	19	59	-9*	3	71	39	40*	-9	278	7	-11
3	185	7	-11	1	68	23	62*	H,K=		8,	2	4	30	66	13*	-8	65	42	30*
4	23	56	-10*	2	192	11	-6	-13	75	59	67*	H,K=		8,	5	-7	225	7	1
5	134	17	-6	3	18	57	-29*	-12	52	40	-16*	-11	54	63	-19*	-6	32	59	-5*
6	46	59	41*	4	102	21	-39*	-11	38	46	31*	-10	28	56	1*	-5	241	6	2
H,K=		7,	4	H,K=		7,	7	-10	155	11	6	-9	189	8	30	-4	41	53	-17*
-12	156	9	0	-9	44	56	10*	-9	19	51	4*	-8	43	50	10*	-3	133	8	13
-11	62	26	-0*	-8	59	38	-38*	-8	280	6	5	-7	250	7	10	-2	39	46	27*
-10	91	16	13	-7	84	16	38*	-7	0	67	-6*	-6	35	48	22*	-1	69	27	39*

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
0	46	60	30*	-9	237	8	-4	H,K=	10,	3		H,K=	11,	3					
1	83	15	15	-8	77	19	27*	-10	0	80	-30*	-8	12	61	-4*				
2	46	59	35*	-7	237	8	-12	-9	116	14	6	-7	77	35	-15*				
3	92	28	-15*	-6	0	51	-42*	-8	40	62	13*	-6	0	62	-8*				
4	24	56	13*	-5	156	9	-1	-7	14	58	-36*	-5	170	10	25				
H,K=	9,	2		-4	49	52	-2*	-6	55	33	17*	-4	22	60	0*				
-12	178	10	-16	-3	103	24	3*	-5	52	34	23*	-3	125	15	-12				
-11	39	53	26*	-2	69	22	25*	-4	56	27	16*								
-10	222	8	-11	-1	63	26	42*	-3	97	14	5								
-9	46	50	30*	0	56	58	16*	-2	40	50	13*								
-8	224	10	-6	1	28	66	-23*	-1	119	11	2								
-7	18	58	-4*	H,K=	9,	6		0	0	80	-4*								
-6	204	9	16	-8	194	16	6	1	152	12	-1								
-5	31	46	27*	-7	40	64	-6*	H,K=	10,	4									
-4	187	7	10	-6	133	14	-16	-9	33	59	-27*								
-3	15	48	-10*	-5	19	52	-14*	-8	33	54	-56*								
-2	36	55	-27*	-4	103	14	7	-7	34	53	-13*								
-1	36	50	10*	-3	37	61	-5*	-6	44	53	29*								
0	42	48	-9*	-2	60	63	15*	-5	42	54	-9*								
1	0	69	-22*	-1	43	63	-7*	-4	66	30	7*								
2	117	15	15	H,K=	10,	0		-3	40	51	10*								
3	70	25	43*	-10	166	10	4	-2	112	14	24								
H,K=	9,	3		-8	85	19	1*	-1	74	26	51*								
-12	39	56	36*	-6	81	17	76*	H,K=	10,	5									
-11	154	12	-24	-4	93	13	14	-8	42	58	-2*								
-10	30	52	17*	-2	134	15	-5	-7	81	23	25*								
-9	241	9	-3	0	158	9	3	-6	0	63	-42*								
-8	0	50	-26*	2	130	13	-16	-5	72	28	51*								
-7	189	7	0	H,K=	10,	1		-4	0	57	-28*								
-6	55	28	-8*	-11	170	12	6	-3	46	58	-27*								
-5	150	10	3	-10	61	35	49*	-2	69	33	44*								
-4	0	49	-12*	-9	121	16	-18	H,K=	11,	0									
-3	36	50	-51*	-8	85	16	63*	-10	27	61	-6*								
-2	30	63	3*	-7	73	20	16*	-9	103	24	-2*								
-1	13	49	7*	-6	54	32	50*	-6	128	14	10								
0	71	20	35*	-5	65	45	28*	-4	165	8	2								
1	61	65	-13*	-4	57	58	41*	-2	198	11	-14								
2	41	55	12*	-3	126	9	21	H,K=	11,	1									
3	110	16	-1	-2	42	42	37*	-9	86	24	28*								
H,K=	9,	4		-1	144	9	-11	-8	26	56	23*								
-11	108	31	92*	0	50	32	25*	-7	87	23	-21*								
-10	184	13	-14	1	136	16	1	-6	43	57	37*								
-9	66	26	17*	H,K=	10,	2		-5	148	10	9								
-8	280	7	1	-11	0	58	-9*	-4	40	50	1*								
-7	55	62	14*	-10	163	9	21	-3	171	9	-18								
-6	180	7	-6	-9	0	65	-15*	-2	0	62	-15*								
-5	42	58	29*	-8	120	12	30	-1	140	12	-12								
-4	116	14	-4	-7	55	30	42*	H,K=	11,	2									
-3	36	50	-12*	-6	70	27	41*	-9	35	64	15*								
-2	40	52	-14*	-5	59	34	47*	-8	91	21	23*								
-1	52	36	11*	-4	91	14	16	-7	32	52	27*								
0	41	55	19*	-3	35	49	19*	-6	134	11	11								
1	34	60	3*	-2	133	11	10	-5	12	54	-11*								
2	71	31	-0*	-1	41	50	31*	-4	154	9	4								
H,K=	9,	5		0	131	15	-6	-3	60	70	28*								
-10	56	62	39*	1	57	40	51*	-2	134	13	-8								

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