

PLATON(V-311206)-Run for: k1a0005 in P2(1)/c

TIME: Mar 21 17:55:47 2011

(C) 1980-2007 A.L.Spek

Crystal Data

Input Cell (Lattice Type: P)		Temp = 200K	Reduced Cell (Acta Cryst.(1976), A32, 297-298)	
a = 20.712(2) Angstrom	alpha = 90 Degree		a = 14.769	alpha = 103.77 V = 6713.1
b = 14.7695(15)	beta = 103.771(2)		b = 20.712	beta = 90.00
c = 22.595(2)	gamma = 90		c = 22.595	gamma = 90.00
V = 6713.1(11) Cubic-Angstrom	d(100) = 20.1163 Angstrom		Niggli Values	
	d(010) = 14.7695		218.138	428.975 510.525
Lambda(MoKa) = 0.71073 Angstrom	d(001) = 21.9453		-111.398	0.000 0.000

Orthogonalization Matrices

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(X0) (20.71200 0 -5.37856) (X) , (X) (0.04828 0 0.01183) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 14.76950 0)*(Y) , (Y) = (0 0.06771 0)*(Y0) are defined as:
 (Z0) (0 0 21.94550) (Z) , (Z) (0 0 0.04557) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P21/c No: 14, Laue: 2/m [Hall: -P 2ybc]

Lattice Type mP, Centric, Monoclinic, Order 4(2) [Schoenflies: C2h^5]

Nr ***** Symmetry Operation(s) *****

1	X ,	Y ,	Z
2	- X ,	1/2 + Y ,	1/2 - Z
3	- X ,	- Y ,	- Z
4	X ,	1/2 - Y ,	1/2 + Z

(Not-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

 Site = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
 ***** Move = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
 SYMBOLS: Type = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
 ***** El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
 ARU = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
 RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
 FLAGS : d = determined, c = calculated, R = riding G = group

Atom Types : C H B Cr N O
 Cov.Rad(Ang): 0.68 0.35 0.83 1.35 0.68 0.68
 Atom Volume : 13.87 5.08 13.24 28.10 11.80 11.39
 Atom Number : 6 1 5 24 7 8
 Atom Weight : 12.010 1.008 10.81 52.00 14.01 16.00
 Scat.Fact.f0: 5.999 1.000 4.999 23.994 6.995 7.999
 Scat.Fact.f': 0.003 0.000 0.001 0.321 0.006 0.011
 Scat.Fact.f": 0.002 0.000 0.001 0.624 0.003 0.006
 Mu/Rho(MoKa): 0.58 0.37 0.37 29.88 0.84 1.22
 Elem. Type : -- -- -- TR -- --

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
 - Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
 - Atomic Wt. : SHELXL97
 - Scat. Fact.: SHELXL97 (International Tables)
 - mu/rho : International Tables C, table 4.2.4.2, p193-199

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
-	Cr(1)	0.29029	0.99045	0.38685	3.9318	14.6285	8.4896	1	1	1	-	Met
-	Cr(2)	0.20926	0.85839	0.41432	2.1057	12.6780	9.0925	1	1	1	-	Met
-	O(1)	0.21528	0.93465	0.34874	2.5832	13.8043	7.6533	1	1	1	-	D/A
-	O(2)	0.27415	0.92650	0.45584	3.2264	13.6839	10.0036	1	1	1	-	D/A
-	N(1)	0.30540	1.06901	0.30972	4.6596	15.7887	6.7970	1	1	1	-	D/A
-	N(2)	0.36933	1.10442	0.32050	5.9257	16.3117	7.0335	1	1	1	-	D/A
-	N(3)	0.32492	1.11309	0.43857	4.3709	16.4398	9.6246	1	1	1	-	D/A
-	N(4)	0.38352	1.14773	0.42926	5.6347	16.9514	9.4203	1	1	1	-	D/A
-	N(5)	0.38564	0.93770	0.38962	5.8918	13.8494	8.5504	1	1	1	-	D/A
-	N(6)	0.43475	1.00324	0.40255	6.8394	14.8174	8.8342	1	1	1	-	D/A
-	N(7)	0.21824	0.74927	0.47929	1.9423	11.0663	10.5183	1	1	1	-	D/A
-	N(8)	0.20321	0.66912	0.44666	1.8065	9.8826	9.8022	1	1	1	-	D/A
-	N(9)	0.10656	0.81969	0.38245	0.1500	12.1064	8.3931	1	1	1	-	D/A
-	N(10)	0.10737	0.72969	0.36787	0.2452	10.7772	8.0731	1	1	1	-	D/A
-	N(11)	0.22799	0.54631	0.35006	2.8393	8.0687	7.6822	1	1	1	-	D/A
-	N(12)	0.18558	0.61840	0.33340	2.0505	9.1335	7.3166	1	1	1	-	D/A
-	C(1)	0.27524	1.09137	0.25137	4.3488	16.1190	5.5164	1	1	1	-	-
-	C(2)	0.32024	1.13972	0.22603	5.4171	16.8331	4.9603	1	1	1	-	-
-	C(3)	0.37807	1.14718	0.26981	6.3794	16.9433	5.9211	1	1	1	-	-

-	C(4)	0.20405	1.06889	0.22066	3.0395	15.7870	4.8425	1	1	1	-	-
-	C(5)	0.18455	1.11722	0.15823	2.9714	16.5008	3.4724	1	1	1	-	-
-	C(6)	0.15784	1.10186	0.25972	1.8723	16.2739	5.6997	1	1	1	-	-
-	C(7)	0.19572	0.96610	0.20966	2.9261	14.2688	4.6011	1	1	1	-	-
-	C(8)	0.44111	1.19411	0.26634	7.7037	17.6364	5.8450	1	1	1	-	-
-	C(9)	0.30393	1.17228	0.47561	3.7369	17.3140	10.4375	1	1	1	-	-
-	C(10)	0.35034	1.24291	0.49005	4.6205	18.3572	10.7544	1	1	1	-	-
-	C(11)	0.39861	1.22607	0.45952	5.7845	18.1084	10.0844	1	1	1	-	-
-	C(12)	0.24037	1.16242	0.49644	2.3084	17.1684	10.8946	1	1	1	-	-
-	C(13)	0.24864	1.09242	0.54704	2.2075	16.1345	12.0051	1	1	1	-	-
-	C(14)	0.22182	1.25443	0.52069	1.7938	18.5273	11.4268	1	1	1	-	-
-	C(15)	0.18323	1.13650	0.44247	1.4152	16.7855	9.7102	1	1	1	-	-
-	C(16)	0.45793	1.28100	0.45714	7.0259	18.9197	10.0322	1	1	1	-	-
-	C(17)	0.41746	0.85733	0.39315	6.5319	12.6623	8.6279	1	1	1	-	-
-	C(18)	0.48615	0.87228	0.41148	7.8560	12.8831	9.0301	1	1	1	-	-
-	C(19)	0.49509	0.96409	0.41669	8.0131	14.2391	9.1445	1	1	1	-	-
-	C(20)	0.38375	0.76661	0.37608	5.9255	11.3224	8.2533	1	1	1	-	-
-	C(21)	0.32650	0.77538	0.31868	5.0484	11.4520	6.9936	1	1	1	-	-
-	C(22)	0.35903	0.72833	0.43023	5.1222	10.7571	9.4416	1	1	1	-	-
-	C(23)	0.43485	0.69882	0.36169	7.0612	10.3212	7.9375	1	1	1	-	-
-	C(24)	0.55887	1.01706	0.43401	9.2410	15.0215	9.5246	1	1	1	-	-
-	C(25)	0.23025	0.72695	0.53851	1.8725	10.7367	11.8179	1	1	1	-	-
-	C(26)	0.22091	0.63392	0.54348	1.6523	9.3627	11.9269	1	1	1	-	-
-	C(27)	0.20338	0.59911	0.48518	1.6028	8.8486	10.6475	1	1	1	-	-
-	C(28)	0.24933	0.79564	0.58907	1.9958	11.7512	12.9274	1	1	1	-	-
-	C(29)	0.19796	0.87130	0.57906	0.9856	12.8687	12.7078	1	1	1	-	-
-	C(30)	0.31813	0.83456	0.59043	3.4134	12.3260	12.9573	1	1	1	-	-
-	C(31)	0.25128	0.74946	0.65039	1.7064	11.0691	14.2731	1	1	1	-	-
-	C(32)	0.18561	0.50415	0.46630	1.3363	7.4460	10.2332	1	1	1	-	-
-	C(33)	0.04255	0.84248	0.37641	-1.1432	12.4430	8.2605	1	1	1	-	-
-	C(34)	0.00273	0.76710	0.35803	-1.8691	11.3297	7.8571	1	1	1	-	-
-	C(35)	0.04512	0.69599	0.35371	-0.9679	10.2794	7.7623	1	1	1	-	-
-	C(36)	0.02239	0.93779	0.38840	-1.6253	13.8507	8.5236	1	1	1	-	-
-	C(37)	0.04066	1.00162	0.34180	-0.9962	14.7934	7.5010	1	1	1	-	-
-	C(38)	0.05916	0.96706	0.45209	-1.2063	14.2830	9.9213	1	1	1	-	-
-	C(39)	-0.05264	0.94120	0.38355	-3.1532	13.9011	8.4172	1	1	1	-	-
-	C(40)	0.03067	0.59829	0.33842	-1.1850	8.8364	7.4268	1	1	1	-	-
-	C(41)	0.23112	0.50534	0.29830	3.1825	7.4636	6.5463	1	1	1	-	-
-	C(42)	0.19199	0.55094	0.24821	2.6415	8.1371	5.4471	1	1	1	-	-
-	C(43)	0.16453	0.62323	0.27125	1.9488	9.2048	5.9527	1	1	1	-	-
-	C(44)	0.27248	0.42102	0.29835	4.0389	6.2183	6.5474	1	1	1	-	-
-	C(45)	0.25046	0.34884	0.33527	3.3843	5.1522	7.3577	1	1	1	-	-
-	C(46)	0.25424	0.38053	0.23804	3.9855	5.6202	5.2239	1	1	1	-	-
-	C(47)	0.33938	0.44150	0.32307	5.2916	6.5207	7.0899	1	1	1	-	-
-	C(48)	0.12277	0.69748	0.23827	1.2613	10.3014	5.2290	1	1	1	-	-
-	B(1)	0.41725	1.10196	0.38410	6.5762	16.2754	8.4293	1	1	1	-	-
-	B(2)	0.17767	0.68958	0.37802	1.6467	10.1848	8.2958	1	1	1	-	-

-	H(1)	0.45956	1.13991	0.38409	7.4526	16.8359	8.4290	1	1	1	-	A-H
-	H(2)	0.20822	0.75675	0.36795	2.3336	11.1768	8.0748	1	1	1	-	-
-	H(2A)	0.31202	1.16305	0.18574	5.4635	17.1777	4.0762	1	1	1	-	-
-	H(5A)	0.19104	1.18263	0.16414	3.0740	17.4669	3.6021	1	1	1	-	-
-	H(5B)	0.13776	1.10484	0.13905	2.1054	16.3179	3.0515	1	1	1	-	-
-	H(5C)	0.21249	1.09484	0.13195	3.6914	16.1702	2.8957	1	1	1	-	-
-	H(6A)	0.16007	1.16803	0.26279	1.9019	17.2512	5.7671	1	1	1	-	-
-	H(6B)	0.17169	1.07537	0.30055	1.9395	15.8827	6.5957	1	1	1	-	-
-	H(6C)	0.11213	1.08334	0.24089	1.0268	16.0004	5.2865	1	1	1	-	-
-	H(7A)	0.20272	0.93471	0.24889	2.8601	13.8052	5.4620	1	1	1	-	-
-	H(7B)	0.22837	0.94480	0.18777	3.7201	13.9542	4.1207	1	1	1	-	-
-	H(7C)	0.15076	0.95344	0.18533	2.1257	14.0818	4.0672	1	1	1	-	-
-	H(8A)	0.47901	1.15421	0.28251	8.4018	17.0471	6.1998	1	1	1	-	-
-	H(8B)	0.44584	1.24991	0.29046	7.6720	18.4605	6.3743	1	1	1	-	-
-	H(8C)	0.43977	1.20895	0.22379	7.9048	17.8556	4.9112	1	1	1	-	-
-	H(10A)	0.34854	1.29287	0.51608	4.4432	19.0950	11.3256	1	1	1	-	-
-	H(13A)	0.25823	1.03323	0.53150	2.4898	15.2603	11.6640	1	1	1	-	-
-	H(13B)	0.20756	1.08871	0.56126	1.2802	16.0797	12.3171	1	1	1	-	-
-	H(13C)	0.28547	1.11022	0.58097	2.7879	16.3974	12.7497	1	1	1	-	-
-	H(14A)	0.25869	1.27560	0.55348	2.3811	18.8400	12.1464	1	1	1	-	-
-	H(14B)	0.18193	1.24711	0.53643	0.8829	18.4192	11.7722	1	1	1	-	-
-	H(14C)	0.21308	1.29886	0.48752	1.7912	19.1835	10.6989	1	1	1	-	-
-	H(15A)	0.19049	1.07512	0.42890	1.6386	15.8790	9.4124	1	1	1	-	-
-	H(15B)	0.18154	1.17921	0.40894	1.5605	17.4163	8.9744	1	1	1	-	-
-	H(15C)	0.14113	1.13860	0.45505	0.4756	16.8166	9.9863	1	1	1	-	-
-	H(16A)	0.49803	1.24388	0.47014	7.7865	18.3715	10.3175	1	1	1	-	-
-	H(16B)	0.46071	1.33325	0.48437	6.9370	19.6914	10.6297	1	1	1	-	-
-	H(16C)	0.45422	1.30214	0.41535	7.1738	19.2320	9.1151	1	1	1	-	-
-	H(18A)	0.51998	0.82740	0.41888	8.5169	12.2203	9.1925	1	1	1	-	-
-	H(21A)	0.34395	0.79803	0.28480	5.5921	11.7865	6.2501	1	1	1	-	-
-	H(21B)	0.29316	0.81774	0.32669	4.3148	12.0776	7.1694	1	1	1	-	-
-	H(21C)	0.30596	0.71595	0.30805	4.6802	10.5742	6.7603	1	1	1	-	-
-	H(22A)	0.39719	0.71577	0.46424	5.7297	10.5716	10.1880	1	1	1	-	-
-	H(22B)	0.33428	0.67219	0.41783	4.6763	9.9279	9.1695	1	1	1	-	-
-	H(22C)	0.32989	0.77270	0.44305	4.4497	11.4124	9.7230	1	1	1	-	-
-	H(23A)	0.45384	0.72345	0.32928	7.6289	10.6850	7.2262	1	1	1	-	-
-	H(23B)	0.41267	0.64121	0.34828	6.6740	9.4704	7.6432	1	1	1	-	-
-	H(23C)	0.47039	0.68884	0.39837	7.6001	10.1738	8.7424	1	1	1	-	-
-	H(24A)	0.55526	1.06299	0.46436	9.0030	15.6998	10.1906	1	1	1	-	-
-	H(24B)	0.56718	1.04674	0.39774	9.6082	15.4598	8.7286	1	1	1	-	-
-	H(24C)	0.59570	0.97595	0.45119	9.9114	14.4143	9.9016	1	1	1	-	-
-	H(26A)	0.22574	0.60067	0.58027	1.5545	8.8716	12.7343	1	1	1	-	-
-	H(29A)	0.15453	0.84632	0.58052	0.0783	12.4997	12.7398	1	1	1	-	-
-	H(29B)	0.19504	0.89922	0.53916	1.1398	13.2810	11.8321	1	1	1	-	-
-	H(29C)	0.21123	0.91707	0.61105	1.0884	13.5447	13.4098	1	1	1	-	-
-	H(30A)	0.31718	0.86488	0.55165	3.6024	12.7738	12.1062	1	1	1	-	-
-	H(30B)	0.35084	0.78541	0.59668	4.0573	11.6001	13.0944	1	1	1	-	-
-	H(30C)	0.33043	0.87831	0.62383	3.4886	12.9722	13.6903	1	1	1	-	-

-	H(31A)	0.20800	0.72175	0.64921	0.8163	10.6599	14.2472	1	1	1	-	-
-	H(31B)	0.26133	0.79459	0.68309	1.7386	11.7357	14.9908	1	1	1	-	-
-	H(31C)	0.28576	0.70259	0.65799	2.3796	10.3769	14.4399	1	1	1	-	-
-	H(32A)	0.14690	0.50388	0.43152	0.7216	7.4421	9.4699	1	1	1	-	-
-	H(32B)	0.17497	0.47096	0.50033	0.9329	6.9558	10.9800	1	1	1	-	-
-	H(32C)	0.22323	0.47500	0.45462	2.1783	7.0155	9.9769	1	1	1	-	-
-	H(34A)	-0.04440	0.76471	0.34997	-2.8019	11.2944	7.6803	1	1	1	-	-
-	H(37A)	0.01705	0.98322	0.30067	-1.2640	14.5217	6.5984	1	1	1	-	-
-	H(37B)	0.08871	0.99896	0.34530	-0.0199	14.7541	7.5778	1	1	1	-	-
-	H(37C)	0.02797	1.06363	0.34952	-1.3006	15.7093	7.6704	1	1	1	-	-
-	H(38A)	0.05253	0.92176	0.48178	-1.5033	13.6139	10.5729	1	1	1	-	-
-	H(38B)	0.04191	1.02564	0.46169	-1.6152	15.1482	10.1320	1	1	1	-	-
-	H(38C)	0.10672	0.97261	0.45381	-0.2305	14.3650	9.9591	1	1	1	-	-
-	H(39A)	-0.07647	0.92037	0.34305	-3.4290	13.5934	7.5284	1	1	1	-	-
-	H(39B)	-0.06584	1.00353	0.38978	-3.4601	14.8216	8.5539	1	1	1	-	-
-	H(39C)	-0.06359	0.90187	0.41470	-3.5476	13.3202	9.1008	1	1	1	-	-
-	H(40A)	0.07231	0.56638	0.33904	-0.3259	8.3651	7.4404	1	1	1	-	-
-	H(40B)	0.00090	0.59344	0.29774	-1.5828	8.7648	6.5341	1	1	1	-	-
-	H(40C)	0.00934	0.57110	0.36848	-1.7884	8.4349	8.0865	1	1	1	-	-
-	H(42A)	0.18571	0.53496	0.20650	2.7358	7.9011	4.5317	1	1	1	-	-
-	H(45A)	0.22926	0.29978	0.30837	3.0898	4.4276	6.7673	1	1	1	-	-
-	H(45B)	0.21859	0.37424	0.35661	2.6094	5.5273	7.8260	1	1	1	-	-
-	H(45C)	0.28905	0.32505	0.36511	4.0230	4.8008	8.0125	1	1	1	-	-
-	H(46A)	0.28110	0.40737	0.21225	4.6805	6.0167	4.6579	1	1	1	-	-
-	H(46B)	0.20705	0.39180	0.21989	3.1057	5.7867	4.8256	1	1	1	-	-
-	H(46C)	0.26227	0.31513	0.24131	4.1342	4.6543	5.2957	1	1	1	-	-
-	H(47A)	0.35476	0.48498	0.29667	5.7521	7.1629	6.5106	1	1	1	-	-
-	H(47B)	0.36592	0.38601	0.32617	5.8246	5.7012	7.1580	1	1	1	-	-
-	H(47C)	0.34435	0.46786	0.36372	5.1759	6.9101	7.9820	1	1	1	-	-
-	H(48A)	0.11852	0.69064	0.19437	1.4094	10.2004	4.2655	1	1	1	-	-
-	H(48B)	0.14359	0.75587	0.25180	1.6197	11.1638	5.5259	1	1	1	-	-
-	H(48C)	0.07860	0.69501	0.24686	0.3002	10.2649	5.4175	1	1	1	-	-

Ordered Structure							Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)						
Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	B	Cr	N	O
1	1	0.253	0.876	0.389	982.86	1	4	48	80	2	2	12	2
Unit Cell Weight =					3931.44			192	320	8	8	48	8
Calculated Analysis (Percent) =								58.7	8.2	2.2	10.6	17.1	3.3
Moiety_Formula = C48 H80 B2 Cr2 N12 O2													
Sum_Formula = C48 H80 B2 Cr2 N12 O2													
Formula_Weight =					982.86 [Note: Based on SHELXL97 Atomic Weights]								
Formula_Z =					4								
SpaceGroup_Z =					4 ==> Z' = 4 / 4 = 1.000								
Calculated Density =					0.9725(2) g cm-3 [= Mg m-3]				** WARNING **				
F(000) =					2104.0 [2107.10]				Please Check the Derived Crystal Data. They may be Incorrect for Disordered, Incomplete or Polymeric Structures.				
mu(MoKa) =					3.62 cm-1 = 0.362 mm-1								
Resonant Scattering =					2.03 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)								
Predicted Volume =					5276.9[5227.8] Ang**3, 298[200]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)								

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f, f' & f''

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6

van der Waals (or ion) Radii used in the Analysis

C	H	B	Cr	N	O
1.70	1.20	1.63	2.15	1.55	1.52

:: Grid: Y-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.21
 :: Grid: X-Axis Step = 0.0093 = Points 108, Angstrom Step = 0.19
 :: Grid: Z-Axis Step = 0.0093 = Points 108, Angstrom Step = 0.21

:: Total Potential Solvent Area Vol 1922.1 Ang^3
 per Unit Cell Vol 6713.1 Ang^3 [28.6%]

Note: Expected volumes for solvent molecules are:
 A hydrogen bonded H2O-molecule 40 Ang^3
 Small molecules (e.g. Toluene) 100-300 Ang^3

Values below for gridpoints and volumes in []
 refer to areas where atom centers may reside.

Area	#GridPoint	VolPerc.	Vol(A^3)	X(av)	Y(av)	Z(av)	Eigenvector(frac)	Sig(Ang)
1	54256[14331]	6	434[114.6]	0.000	0.000	0.000	1 -0.150-1.000 0.738	3.90
							2 -0.221 1.000 0.472	1.94
							3 -1.000-0.133-0.446	1.50
2	131940[29546]	16	1055[236.2]	0.500	-0.118	0.113	1 -0.079-0.910 1.000	7.29
							2 0.209 1.000 0.441	3.85
							3 -1.000 0.328-0.154	2.05
3	54263[14331]	6	434[114.6]	1.000	0.500	0.500	1 -0.150 1.000 0.738	3.90
							2 0.220 1.000-0.473	1.94
							3 -1.000 0.131-0.445	1.50

x	y	z	Shortest Contacts within 4.5 Angstrom (Excl. H)
1	0.000	0.000	0.000
2	0.500	-0.118	0.113
3	1.000	0.500	0.500

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

=====
 (An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]
 =====

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Cr1	0.03066	0.03014	0.03065	0.00099	0.00370	-0.00199	0.03109	0.0275	0.0294	0.0363	1.32
		[0.2909	0.9896	0.3862]	[0.2897	0.9913	0.3875]					
2	Cr2	0.03094	0.03004	0.02933	0.00094	0.00503	-0.00129	0.03046	0.0282	0.0292	0.0339	1.20
		[0.2097	0.8577	0.4140]	[0.2088	0.8590	0.4146]					
3	O1	0.03477	0.03953	0.03259	0.00682	0.00064	-0.00723	0.03687	0.0276	0.0300	0.0530	1.92
		[0.2141	0.9382	0.3498]	[0.2164	0.9311	0.3477]					
4	O2	0.04284	0.03388	0.03038	0.00022	0.00424	-0.00567	0.03645	0.0294	0.0319	0.0481	1.64
		[0.2760	0.9248	0.4555]	[0.2723	0.9282	0.4562]					
5	N1	0.03487	0.03506	0.03846	0.00184	0.00620	-0.00368	0.03656	0.0313	0.0357	0.0428	1.37
		[0.3058	1.0676	0.3089]	[0.3050	1.0704	0.3105]					
6	N2	0.03820	0.03980	0.04606	0.00730	0.00847	-0.00618	0.04162	0.0304	0.0403	0.0541	1.78
		[0.3690	1.1074	0.3221]	[0.3696	1.1014	0.3189]					
7	N3	0.04561	0.03340	0.03756	0.00039	0.00380	-0.00608	0.03988	0.0307	0.0362	0.0527	1.72
		[0.3269	1.1115	0.4378]	[0.3229	1.1147	0.4393]					
8	N4	0.04348	0.03663	0.04563	0.00288	-0.00151	-0.00988	0.04395	0.0291	0.0384	0.0643	2.21
		[0.3855	1.1448	0.4271]	[0.3815	1.1507	0.4314]					
9	N5	0.03059	0.03922	0.04324	0.00410	0.00401	-0.00341	0.03849	0.0292	0.0367	0.0496	1.70
		[0.3855	0.9400	0.3913]	[0.3858	0.9354	0.3880]					
10	N6	0.03267	0.04442	0.04929	0.00475	0.00164	-0.00673	0.04349	0.0292	0.0416	0.0597	2.05
		[0.4342	1.0066	0.4048]	[0.4353	0.9999	0.4003]					
11	N7	0.03496	0.03272	0.03013	-0.00057	0.00624	-0.00299	0.03286	0.0294	0.0316	0.0376	1.28
		[0.2190	0.7483	0.4792]	[0.2174	0.7502	0.4794]					
12	N8	0.03956	0.02926	0.03303	0.00019	0.00720	-0.00315	0.03419	0.0284	0.0330	0.0413	1.46
		[0.2047	0.6683	0.4465]	[0.2017	0.6700	0.4468]					
13	N9	0.03301	0.03364	0.03830	0.00112	0.00838	0.00115	0.03500	0.0321	0.0343	0.0386	1.20
		[0.1069	0.8200	0.3832]	[0.1062	0.8194	0.3817]					
14	N10	0.03151	0.03734	0.03766	-0.00423	0.00745	-0.00238	0.03564	0.0304	0.0348	0.0417	1.37
		[0.1078	0.7280	0.3686]	[0.1070	0.7313	0.3671]					
15	N11	0.05037	0.03557	0.03939	-0.00264	0.00530	0.00663	0.04268	0.0326	0.0382	0.0572	1.75
		[0.2302	0.5482	0.3494]	[0.2258	0.5444	0.3507]					
16	N12	0.03701	0.03648	0.03389	-0.00251	0.00400	0.00218	0.03654	0.0314	0.0347	0.0435	1.39
		[0.1864	0.6198	0.3328]	[0.1848	0.6170	0.3340]					
17	C1	0.04897	0.03075	0.03346	0.00163	0.01184	0.00279	0.03739	0.0300	0.0328	0.0494	1.65
		[0.2776	1.0920	0.2519]	[0.2728	1.0907	0.2509]					
18	C2	0.05898	0.04579	0.03822	0.00750	0.01692	0.00404	0.04676	0.0322	0.0471	0.0611	1.90
		[0.3233	1.1416	0.2271]	[0.3172	1.1378	0.2250]					
19	C3	0.04977	0.04080	0.05432	0.00848	0.02334	-0.00100	0.04646	0.0313	0.0454	0.0626	2.00
		[0.3808	1.1489	0.2722]	[0.3753	1.1455	0.2674]					
20	C4	0.05225	0.04476	0.03190	0.00426	0.00051	-0.00051	0.04457	0.0291	0.0452	0.0595	2.05
		[0.2071	1.0676	0.2197]	[0.2010	1.0702	0.2216]					
21	C5	0.07543	0.07775	0.04193	0.02060	-0.00291	-0.00765	0.06788	0.0316	0.0689	0.1032	3.27

=====											
		[	0.1877	1.1095	0.1562]	[	0.1814	1.1249	0.1602]		
22	C6		0.04324	0.06419	0.05345		0.01087	0.00719	0.00839	0.05435	0.0380 0.0540 0.0711 1.87
		[	0.1587	1.1063	0.2609]	[	0.1570	1.0974	0.2585]		
23	C7		0.08927	0.05504	0.03749		-0.00463	0.00262	-0.01782	0.06270	0.0342 0.0517 0.1022 2.99
		[	0.2014	0.9620	0.2093]	[	0.1900	0.9702	0.2101]		
24	C8		0.06259	0.07196	0.07628		0.01859	0.03051	-0.01340	0.06793	0.0332 0.0774 0.0931 2.80
		[	0.4422	1.2010	0.2694]	[	0.4400	1.1872	0.2632]		
25	C9		0.05877	0.03166	0.03877		0.00007	0.00109	-0.00046	0.04484	0.0317 0.0362 0.0666 2.10
		[	0.3074	1.1722	0.4745]	[	0.3005	1.1724	0.4767]		
26	C10		0.07236	0.03646	0.04734		-0.00648	-0.00008	-0.00824	0.05446	0.0307 0.0488 0.0838 2.73
		[	0.3552	1.2418	0.4885]	[	0.3455	1.2441	0.4916]		
27	C11		0.05672	0.03908	0.05106		0.00101	-0.00843	-0.01197	0.05253	0.0304 0.0426 0.0847 2.79
		[	0.4021	1.2232	0.4566]	[	0.3951	1.2290	0.4624]		
28	C12		0.06932	0.03980	0.05427		-0.00919	0.02212	0.00021	0.05322	0.0340 0.0545 0.0712 2.10
		[	0.2443	1.1618	0.4981]	[	0.2364	1.1630	0.4948]		
29	C13		0.11219	0.05803	0.07369		0.00223	0.04686	0.00407	0.07714	0.0538 0.0577 0.1199 2.23
		[	0.2541	1.0931	0.5495]	[	0.2432	1.0917	0.5446]		
30	C14		0.10227	0.04973	0.09324		-0.01997	0.03722	0.00324	0.07940	0.0387 0.0885 0.1109 2.87
		[	0.2278	1.2526	0.5246]	[	0.2159	1.2562	0.5168]		
31	C15		0.05947	0.06195	0.08660		-0.02435	0.01826	-0.00474	0.06919	0.0470 0.0589 0.1017 2.17
		[	0.1848	1.1319	0.4459]	[	0.1817	1.1411	0.4391]		
32	C16		0.07566	0.05863	0.08213		-0.00652	-0.00024	-0.03323	0.07534	0.0310 0.0815 0.1135 3.67
		[	0.4625	1.2745	0.4542]	[	0.4533	1.2875	0.4601]		
33	C17		0.03553	0.04254	0.03924		0.00502	0.00852	0.00057	0.03917	0.0353 0.0359 0.0463 1.31
		[	0.4177	0.8590	0.3937]	[	0.4173	0.8557	0.3926]		
34	C18		0.03183	0.05571	0.06060		0.01289	0.00690	0.00453	0.05007	0.0307 0.0476 0.0720 2.34
		[	0.4871	0.8770	0.4143]	[	0.4852	0.8675	0.4087]		
35	C19		0.03248	0.05957	0.05412		0.01188	0.00059	-0.00397	0.05036	0.0306 0.0465 0.0740 2.42
		[	0.4949	0.9696	0.4190]	[	0.4953	0.9586	0.4144]		
36	C20		0.03601	0.04276	0.05590		-0.00074	0.01389	0.00376	0.04439	0.0328 0.0444 0.0559 1.70
		[	0.3851	0.7663	0.3785]	[	0.3824	0.7669	0.3737]		
37	C21		0.04673	0.05578	0.04568		-0.00863	0.01162	-0.00054	0.04929	0.0404 0.0467 0.0608 1.51
		[	0.3262	0.7783	0.3179]	[	0.3268	0.7725	0.3194]		
38	C22		0.04096	0.04826	0.06048		0.01378	0.00703	-0.00063	0.05075	0.0390 0.0412 0.0720 1.85
		[	0.3593	0.7316	0.4326]	[	0.3587	0.7250	0.4279]		
39	C23		0.04832	0.05549	0.10145		-0.01313	0.02778	0.00999	0.06675	0.0330 0.0623 0.1049 3.18
		[	0.4380	0.6954	0.3676]	[	0.4317	0.7023	0.3558]		
40	C24		0.03646	0.07330	0.08962		0.01243	-0.00147	-0.01240	0.06923	0.0322 0.0667 0.1088 3.38
		[	0.5587	1.0235	0.4391]	[	0.5591	1.0106	0.4289]		
41	C25		0.04277	0.03659	0.03394		0.00423	0.00950	-0.00292	0.03771	0.0298 0.0387 0.0447 1.50
		[	0.2317	0.7253	0.5384]	[	0.2288	0.7286	0.5386]		
42	C26		0.07328	0.04132	0.03783		0.00954	0.01185	-0.00584	0.05104	0.0286 0.0486 0.0760 2.66
		[	0.2258	0.6317	0.5436]	[	0.2160	0.6362	0.5434]		
43	C27		0.06249	0.03671	0.03649		0.00378	0.01187	-0.00441	0.04522	0.0316 0.0403 0.0638 2.02
		[	0.2069	0.5978	0.4855]	[	0.1998	0.6004	0.4849]		
44	C28		0.06098	0.04495	0.02764		0.00351	0.00872	-0.00751	0.04483	0.0265 0.0425 0.0655 2.47
		[	0.2532	0.7925	0.5891]	[	0.2454	0.7988	0.5890]		
45	C29		0.08002	0.04773	0.03625		-0.00337	0.01363	0.00253	0.05470	0.0346 0.0485 0.0810 2.34

72	H5C	0.10182	0.10182
73	H6A	0.08153	0.08153
74	H6B	0.08153	0.08153
75	H6C	0.08153	0.08153
76	H7A	0.09405	0.09405
77	H7B	0.09405	0.09405
78	H7C	0.09405	0.09405
79	H8A	0.10189	0.10189
80	H8B	0.10189	0.10189
81	H8C	0.10189	0.10189
82	H10A	0.06536	0.06536
83	H13A	0.11572	0.11572
84	H13B	0.11572	0.11572
85	H13C	0.11572	0.11572
86	H14A	0.11910	0.11910
87	H14B	0.11910	0.11910
88	H14C	0.11910	0.11910
89	H15A	0.10379	0.10379
90	H15B	0.10379	0.10379
91	H15C	0.10379	0.10379
92	H16A	0.11301	0.11301
93	H16B	0.11301	0.11301
94	H16C	0.11301	0.11301
95	H18A	0.06008	0.06008
96	H21A	0.07394	0.07394
97	H21B	0.07394	0.07394
98	H21C	0.07394	0.07394
99	H22A	0.07612	0.07612
100	H22B	0.07612	0.07612
101	H22C	0.07612	0.07612
102	H23A	0.10012	0.10012
103	H23B	0.10012	0.10012
104	H23C	0.10012	0.10012
105	H24A	0.10385	0.10385
106	H24B	0.10385	0.10385
107	H24C	0.10385	0.10385
108	H26A	0.06125	0.06125
109	H29A	0.08205	0.08205
110	H29B	0.08205	0.08205
111	H29C	0.08205	0.08205
112	H30A	0.08893	0.08893
113	H30B	0.08893	0.08893
114	H30C	0.08893	0.08893
115	H31A	0.09172	0.09172
116	H31B	0.09172	0.09172
117	H31C	0.09172	0.09172
118	H32A	0.10013	0.10013
119	H32B	0.10013	0.10013

=====

120	H32C	0.10013
121	H34A	0.06065

0.10013
0.06065

=====										
-3	-2	3	0.11	78.87	50.62	31.97	82.48	2.58	6219.83	225.98
-3	2	3	0.11	80.32	51.85	31.89	83.66	2.63	6451.75	208.38
3	-2	-3	0.11	77.69	51.85	31.89	83.66	4.39	6035.23	219.54
3	-2	-3	0.11	78.34	51.85	31.89	83.66	3.81	6136.82	226.23
-2	-2	3	0.10	13.50	8.10	23.71	16.13	5.41	182.37	14.37
-2	-2	3	0.10	13.96	8.10	23.71	16.13	3.10	194.76	21.06
-2	2	3	0.10	15.56	10.30	24.11	13.82	2.27	242.08	22.55
2	2	-3	0.10	14.35	8.10	23.71	16.13	3.65	205.91	14.87
2	2	-3	0.10	14.41	8.10	23.71	16.13	2.58	207.64	20.32
1	2	-3	0.10	29.73	69.03	47.07	22.94	8.16	884.09	43.86
-1	-2	3	0.10	27.10	69.03	47.07	22.94	5.16	734.67	40.39
1	-2	-3	0.10	28.69	69.24	47.16	22.41	8.30	823.13	38.65
1	-2	-3	0.10	27.81	69.24	47.16	22.41	6.51	773.33	41.63
-1	2	3	0.10	29.76	69.24	47.16	22.41	7.85	885.57	48.81
-1	-2	3	0.10	27.79	69.03	47.07	22.94	5.70	772.09	43.11
0	2	-3	0.10	219.19	186.46	17.36	203.80	4.04	48043.24	1611.08
0	-2	-3	0.10	226.37	183.59	18.58	202.02	6.48	51245.32	1610.58
0	-2	3	0.10	221.52	186.46	17.36	203.80	4.43	49070.05	1702.02
0	2	3	0.10	220.71	183.59	18.58	202.02	4.75	48712.50	1662.12
0	-2	-3	0.10	223.06	183.59	18.58	202.02	5.83	49754.67	1534.52
0	2	-3	0.10	227.13	186.46	17.36	203.80	6.51	51587.52	1544.67
0	2	3	0.10	221.61	183.59	18.58	202.02	4.85	49112.42	1711.18
0	-2	3	0.10	220.34	186.46	17.36	203.80	4.23	48550.70	1659.89
-1	2	-3	0.10	228.62	150.39	49.84	200.18	7.34	52265.45	1660.39
1	2	3	0.10	223.43	149.43	49.42	198.85	5.92	49920.44	1752.07
-1	-2	-3	0.10	220.92	149.43	49.42	198.85	5.59	48805.66	1657.17
1	-2	3	0.10	224.76	150.39	49.84	200.18	5.96	50516.85	1753.06
1	-2	3	0.10	226.43	150.39	49.84	200.18	6.55	51269.61	1709.95
1	2	3	0.10	223.13	149.43	49.42	198.85	5.98	49785.15	1711.93
-1	2	-3	0.10	229.41	150.39	49.84	200.18	7.94	52629.44	1580.85
-1	-2	-3	0.10	229.81	149.43	49.42	198.85	8.39	52814.29	1581.10
-2	-2	-3	0.12	56.30	8.13	51.56	59.38	3.22	3169.63	110.76
2	2	3	0.12	56.53	8.13	51.56	59.38	2.67	3195.40	124.14
2	2	3	0.12	55.88	8.13	51.56	59.38	3.21	3123.05	125.63
2	-2	3	0.12	55.32	10.32	50.17	60.29	5.14	3060.61	111.75
-2	2	-3	0.12	56.15	10.32	50.17	60.29	4.50	3152.29	107.29
-2	-2	-3	0.12	55.53	8.13	51.56	59.38	4.04	3083.15	109.77
-2	2	-3	0.12	54.47	10.32	50.17	60.29	5.67	2966.70	117.70
2	-2	3	0.12	55.25	10.32	50.17	60.29	4.69	3052.18	124.14
3	-2	3	0.13	153.23	184.82	46.87	137.98	5.19	23479.60	855.59
3	2	3	0.13	160.91	182.97	46.20	136.99	8.51	25892.99	837.26
-3	2	-3	0.13	154.95	184.82	46.87	137.98	6.47	24010.59	768.62
-3	2	-3	0.13	161.99	184.82	46.87	137.98	8.88	26240.63	811.24
3	-2	3	0.13	157.84	184.82	46.87	137.98	7.08	24914.01	829.33
-3	-2	-3	0.13	152.51	182.97	46.20	136.99	5.84	23259.07	770.11
-3	-2	-3	0.13	156.72	182.97	46.20	136.99	7.21	24561.17	804.05
3	2	3	0.13	156.43	182.97	46.20	136.99	6.68	24469.73	853.61
4	-2	3	0.15	109.81	54.84	47.12	101.97	4.15	12057.58	400.17

4	-2	3	0.15	109.32	54.84	47.12	101.97	3.92	11951.78	396.70
-4	2	-3	0.15	108.97	54.84	47.12	101.97	3.92	11874.96	377.12
-4	-2	-3	0.15	109.23	53.46	48.01	101.38	4.02	11931.21	411.07
-4	-2	-3	0.15	107.17	53.46	48.01	101.38	3.19	11484.46	378.36
4	2	3	0.15	108.37	53.46	48.01	101.38	3.49	11743.39	419.74
4	-2	3	0.15	106.15	54.84	47.12	101.97	2.07	11267.40	420.73
-4	-2	-3	0.15	108.34	53.46	48.01	101.38	3.77	11738.19	387.28
-4	3	3	0.15	140.48	157.32	25.72	131.77	3.62	19734.12	655.38
-4	3	3	0.15	138.44	157.32	25.72	131.77	2.95	19164.96	609.79
4	-3	-3	0.15	136.86	157.32	25.72	131.77	2.04	18729.86	670.75
4	-3	-3	0.15	140.49	157.32	25.72	131.77	3.70	19737.84	642.00
4	3	-3	0.15	142.88	157.32	25.70	132.26	4.31	20413.29	677.68
-4	-3	3	0.15	139.65	157.32	25.70	132.26	3.32	19500.96	604.09
-3	3	3	0.13	55.40	18.03	34.74	52.71	2.57	3069.03	113.24
-2	-3	3	0.13	231.70	182.59	30.51	212.98	4.68	53686.48	1780.07
2	-3	-3	0.13	222.07	182.59	30.15	212.70	2.42	49315.60	1684.18
-2	-3	3	0.13	222.69	182.59	30.51	212.98	2.44	49589.15	1736.21
-2	-3	3	0.13	228.89	182.59	30.51	212.98	4.38	52391.07	1606.12
2	3	-3	0.13	229.91	182.59	30.51	212.98	4.45	52858.39	1683.93
2	-3	-3	0.13	231.47	182.59	30.15	212.70	5.19	53580.67	1605.38
2	-3	-3	0.13	230.82	182.59	30.15	212.70	4.52	53279.87	1780.07
-2	3	3	0.13	221.88	182.59	30.15	212.70	2.30	49228.63	1735.71
1	-3	-3	0.12	74.59	39.70	31.43	70.95	2.69	5564.20	197.23
1	-3	-3	0.12	74.89	39.70	31.43	70.95	3.09	5608.06	186.08
-1	-3	3	0.12	74.14	39.70	31.78	71.39	2.25	5496.80	177.66
-1	-3	3	0.12	76.39	39.70	31.78	71.39	3.57	5835.02	206.65
1	3	-3	0.12	74.66	39.70	31.78	71.39	2.44	5573.86	195.50
1	-3	-3	0.12	75.40	39.70	31.43	70.95	3.33	5684.62	195.75
0	-3	-3	0.12	90.74	76.87	10.30	85.94	3.15	8233.80	268.84
0	-3	3	0.12	89.21	76.87	9.20	85.46	2.27	7958.02	287.43
0	-3	-3	0.12	89.72	76.87	10.30	85.94	2.37	8049.21	280.24
0	3	-3	0.12	90.23	76.87	9.20	85.46	2.95	8142.12	283.71
0	-3	3	0.12	90.73	76.87	9.20	85.46	3.11	8231.57	298.33
0	3	-3	0.12	93.27	76.87	9.20	85.46	5.31	8698.39	262.65
0	3	3	0.12	93.30	76.87	10.30	85.94	4.45	8704.59	296.10
0	3	3	0.12	90.02	76.87	10.30	85.94	2.46	8103.47	291.39
2	3	3	0.14	111.30	75.82	26.28	102.09	4.55	12387.38	432.13
2	3	3	0.14	111.29	75.82	26.28	102.09	4.57	12384.65	429.16
2	-3	3	0.14	109.40	75.82	26.48	102.24	3.62	11969.12	418.01
-2	-3	-3	0.14	110.38	75.82	26.28	102.09	4.33	12183.20	406.12
-2	-3	-3	0.14	109.67	75.82	26.28	102.09	4.09	12028.09	392.73
2	-3	3	0.14	110.27	75.82	26.48	102.24	3.91	12160.41	436.34
-2	3	-3	0.14	113.15	75.82	26.48	102.24	5.65	12802.66	416.03
-2	3	-3	0.14	111.25	75.82	26.48	102.24	4.94	12377.22	389.02
-5	0	4	0.14	42.15	62.66	17.08	45.59	4.48	1776.60	67.40
5	0	-4	0.14	40.31	62.66	17.08	45.59	5.58	1624.96	81.27
-5	0	4	0.14	42.11	62.66	17.08	45.59	4.08	1773.38	74.83
5	0	-4	0.14	41.33	62.66	17.08	45.59	4.70	1707.96	78.79

=====										
4	0	-4	0.12	114.55	51.05	54.77	105.82	4.21	13121.56	457.65
-4	0	4	0.12	113.05	51.05	54.77	105.82	3.85	12781.35	411.81
-4	0	4	0.12	116.03	51.05	54.77	105.82	5.05	13463.25	448.73
4	0	-4	0.12	113.74	51.05	54.77	105.82	4.00	12937.70	435.35
-3	0	4	0.10	171.22	170.54	12.47	158.08	4.93	29315.12	878.14
3	0	-4	0.10	167.06	170.54	12.47	158.08	3.00	27908.45	973.04
-3	0	4	0.10	164.98	170.54	12.47	158.08	2.34	27218.13	951.73
3	0	-4	0.10	168.72	170.54	12.47	158.08	3.77	28466.46	923.48
2	0	-4	0.09	207.82	201.30	20.34	181.01	7.07	43189.43	1474.80
2	0	-4	0.09	215.71	201.30	20.34	181.01	9.79	46530.28	1406.16
-2	0	4	0.09	212.59	201.30	20.34	181.01	8.17	45195.97	1521.88
-2	0	4	0.09	215.48	201.30	20.34	181.01	8.76	46431.66	1559.54
-1	0	4	0.09	88.80	90.70	10.16	81.50	4.53	7885.42	274.05
-1	0	4	0.09	88.34	90.70	10.16	81.50	4.19	7803.41	276.77
1	0	-4	0.09	90.27	90.70	10.16	81.50	5.66	8149.31	266.12
1	0	-4	0.09	88.19	90.70	10.16	81.50	4.55	7777.14	249.52
0	0	4	0.09	208.32	194.36	5.51	188.86	5.29	43398.56	1461.42
0	0	4	0.09	210.37	194.36	5.51	188.86	5.74	44257.38	1497.10
0	0	-4	0.09	206.57	194.36	5.51	188.86	4.94	42670.33	1416.32
0	0	-4	0.09	209.29	194.36	5.51	188.86	6.03	43802.94	1349.42
-1	0	-4	0.10	11.23	26.41	34.24	9.50	2.16	126.12	16.60
-2	0	-4	0.11	166.58	144.33	2.62	146.70	6.79	27749.38	917.04
2	0	4	0.11	167.22	144.33	2.62	146.70	6.63	27961.23	970.56
2	0	4	0.11	166.58	144.33	2.62	146.70	6.58	27748.88	946.28
-2	0	-4	0.11	169.60	144.33	2.62	146.70	8.28	28762.56	874.67
3	0	4	0.13	150.51	99.72	44.02	143.73	2.44	22651.76	817.43
3	0	4	0.13	152.12	99.72	44.02	143.73	3.12	23139.39	795.63
-3	0	-4	0.13	152.86	99.72	44.02	143.73	3.52	23367.35	770.35
-3	0	-4	0.13	157.72	99.72	44.02	143.73	5.72	24876.84	737.40
-5	1	4	0.14	56.51	57.30	8.47	48.85	6.80	3193.42	118.69
-5	-1	4	0.14	57.88	58.30	8.91	49.40	7.39	3350.26	123.15
5	-1	-4	0.14	54.79	57.30	8.47	48.85	4.90	3002.38	125.87
5	1	-4	0.14	57.34	58.30	8.91	49.40	6.67	3288.07	127.11
-5	-1	4	0.14	56.10	58.30	8.91	49.40	6.52	3147.08	108.53
-5	1	4	0.14	53.99	57.30	8.47	48.85	4.82	2914.66	109.77
5	1	-4	0.14	55.15	58.30	8.91	49.40	5.13	3042.02	117.45
5	-1	-4	0.14	55.32	57.30	8.47	48.85	5.56	3060.61	121.41
4	1	-4	0.12	43.88	43.62	2.55	46.08	2.38	1925.27	83.25
-3	-1	4	0.11	97.92	89.26	0.20	89.45	5.10	9587.93	311.21
-3	-1	4	0.11	95.01	89.26	0.20	89.45	3.65	9026.21	281.23
-3	1	4	0.11	93.82	88.89	0.94	89.81	2.59	8802.46	284.45
-3	1	4	0.11	96.40	88.89	0.94	89.81	3.96	9292.82	309.73
3	1	-4	0.11	93.56	89.26	0.20	89.45	2.51	8752.66	300.06
-3	-1	4	0.11	93.57	89.26	0.20	89.45	2.40	8755.88	315.18
2	1	-4	0.10	42.40	34.64	5.28	39.88	2.73	1797.66	75.82
2	-1	-4	0.10	43.75	36.46	5.65	41.89	2.05	1914.12	77.56
-2	1	4	0.10	44.59	36.46	5.65	41.89	2.98	1987.96	78.30
-2	-1	4	0.10	46.26	34.64	5.28	39.88	6.91	2140.09	79.54

=====										
-2	-1	4	0.10	43.24	34.64	5.28	39.88	4.35	1869.76	64.18
-2	-1	4	0.10	43.85	34.64	5.28	39.88	4.30	1923.04	77.31
-1	-1	4	0.09	291.51	239.20	14.47	253.63	7.61	84979.39	2712.72
1	-1	-4	0.09	283.89	238.16	15.27	253.42	5.80	80592.16	2820.75
-1	1	4	0.09	286.56	238.16	15.27	253.42	6.33	82115.52	2828.43
1	1	-4	0.09	277.31	239.20	14.47	253.63	4.78	76899.46	2628.72
-1	-1	4	0.09	280.52	239.20	14.47	253.63	5.17	78693.16	2777.64
1	-1	-4	0.09	279.61	238.16	15.27	253.42	5.58	78183.96	2503.84
1	1	-4	0.09	285.34	239.20	14.47	253.63	6.74	81420.25	2535.56
1	-1	-4	0.09	290.23	238.16	15.27	253.42	7.61	84232.58	2630.21
-1	1	4	0.09	286.36	238.16	15.27	253.42	6.56	82001.55	2712.22
0	-1	-4	0.10	26.49	25.20	3.43	28.51	3.11	701.72	35.68
0	1	4	0.10	24.98	25.20	3.43	28.51	5.44	623.92	34.69
0	1	-4	0.10	24.07	23.62	3.44	27.05	5.21	579.31	29.24
0	-1	-4	0.10	26.07	25.20	3.43	28.51	3.38	679.42	39.40
1	1	4	0.11	241.64	231.13	27.20	203.94	8.86	58390.13	1896.28
1	1	4	0.11	237.68	231.13	27.20	203.94	7.67	56491.37	1941.62
1	-1	4	0.11	236.40	229.33	26.91	202.42	7.87	55882.82	1894.05
-1	1	-4	0.11	240.33	229.33	26.91	202.42	9.13	57758.53	1838.05
-1	-1	-4	0.11	234.87	231.13	27.20	203.94	7.76	55165.25	1749.59
1	-1	4	0.11	236.18	229.33	26.91	202.42	7.63	55780.73	1940.88
-1	-1	-4	0.11	239.87	231.13	27.20	203.94	8.68	57539.25	1836.81
-1	1	-4	0.11	234.95	229.33	26.91	202.42	8.13	55202.41	1749.34
2	-1	4	0.12	155.27	113.59	20.23	133.79	7.83	24107.97	793.40
2	-1	4	0.12	153.46	113.59	20.23	133.79	6.92	23548.48	815.95
-2	1	-4	0.12	153.80	113.59	20.23	133.79	7.46	23653.04	771.59
-2	-1	-4	0.12	152.81	112.52	20.40	132.87	7.75	23351.74	734.92
2	1	4	0.12	155.76	112.52	20.40	132.87	8.28	24259.86	797.86
-2	-1	-4	0.12	150.10	112.52	20.40	132.87	6.35	22530.59	768.12
-2	1	-4	0.12	151.14	113.59	20.23	133.79	6.75	22844.78	733.19
2	1	4	0.12	153.73	112.52	20.40	132.87	7.34	23632.97	815.20
3	1	4	0.14	39.66	11.13	32.24	43.32	3.78	1572.92	80.28
3	1	4	0.14	38.66	11.13	32.24	43.32	4.35	1494.87	87.71
-3	1	-4	0.14	39.22	9.35	32.64	41.79	3.17	1537.98	65.91
-3	-1	-4	0.14	39.13	11.13	32.24	43.32	5.09	1531.05	67.89
-3	-1	-4	0.14	39.98	11.13	32.24	43.32	4.24	1598.44	65.66
3	-1	4	0.14	39.26	9.35	32.64	41.79	3.02	1541.45	67.89
4	2	-4	0.14	79.47	79.37	5.59	73.79	3.74	6315.23	232.67
4	-2	-4	0.14	77.49	79.37	5.40	73.98	2.32	6004.01	228.70
4	2	-4	0.14	79.20	79.37	5.59	73.79	3.80	6272.61	218.05
-4	-2	4	0.14	80.38	79.37	5.59	73.79	5.00	6460.18	202.93
-4	2	4	0.14	79.73	79.37	5.40	73.98	4.23	6357.60	209.13
-4	-2	4	0.14	79.31	79.37	5.59	73.79	3.72	6289.70	227.22
4	-2	-4	0.14	78.48	79.37	5.40	73.98	3.10	6158.88	221.77
-4	2	4	0.14	82.02	79.37	5.40	73.98	5.58	6727.54	224.99
3	-2	-4	0.12	46.57	45.56	4.70	49.68	3.23	2168.59	92.92
-2	2	4	0.11	36.33	21.19	10.46	31.43	5.11	1319.69	64.92
2	2	-4	0.11	35.02	21.19	10.47	31.64	3.70	1226.52	60.95

=====										
2	-2	-4	0.11	33.89	21.19	10.46	31.43	2.91	1148.72	55.26
2	-2	-4	0.11	34.83	21.19	10.46	31.43	3.50	1213.39	64.42
-2	-2	4	0.11	34.36	21.19	10.47	31.64	2.96	1180.93	60.71
-2	-2	4	0.11	33.55	21.19	10.47	31.64	2.10	1125.43	59.22
-1	-2	4	0.11	140.15	117.66	10.66	128.29	4.89	19641.45	651.67
-1	2	4	0.11	137.81	117.66	10.82	128.45	3.82	18991.02	653.15
1	2	-4	0.11	134.72	117.66	10.66	128.29	2.68	18148.56	632.09
1	-2	-4	0.11	142.13	117.66	10.82	128.45	6.15	20202.18	602.61
1	-2	-4	0.11	139.55	117.66	10.82	128.45	4.71	19473.95	632.09
-1	-2	4	0.11	135.70	117.66	10.66	128.29	2.93	18414.18	667.03
0	-2	4	0.11	72.31	79.86	12.22	67.83	3.39	5229.20	185.59
0	-2	-4	0.11	71.01	79.86	12.85	67.52	2.68	5043.11	180.39
0	2	-4	0.11	72.24	79.86	12.22	67.83	3.36	5218.05	184.10
0	2	4	0.11	75.31	79.86	12.85	67.52	5.74	5671.73	194.01
0	-2	4	0.11	70.73	79.86	12.22	67.83	2.09	5002.23	192.03
0	2	-4	0.11	71.60	79.86	12.22	67.83	3.16	5125.87	166.26
0	2	4	0.11	72.30	79.86	12.85	67.52	3.57	5226.72	186.83
0	-2	-4	0.11	70.69	79.86	12.85	67.52	2.54	4997.52	172.70
1	2	4	0.12	83.26	77.23	1.51	75.75	4.83	6931.71	247.04
1	-2	4	0.12	81.60	77.23	1.95	75.67	3.90	6659.15	239.11
-1	2	-4	0.12	84.51	77.23	1.95	75.67	5.93	7141.83	238.61
-1	-2	-4	0.12	80.65	77.23	1.51	75.75	3.29	6504.04	232.42
-1	2	-4	0.12	84.49	77.23	1.95	75.67	6.41	7138.85	220.28
1	-2	4	0.12	84.79	77.23	1.95	75.67	5.82	7189.15	251.50
1	2	4	0.12	82.24	77.23	1.51	75.75	4.14	6763.96	247.78
-1	-2	-4	0.12	81.32	77.23	1.51	75.75	3.89	6612.32	224.74
2	-2	4	0.13	94.18	54.30	32.52	86.81	4.38	8869.36	304.03
-2	2	-4	0.13	92.92	54.30	32.52	86.81	3.64	8633.48	301.55
2	2	4	0.13	94.52	54.30	32.64	86.93	4.38	8933.29	313.94
-2	2	-4	0.13	94.93	54.30	32.52	86.81	5.22	9012.09	282.72
-2	-2	-4	0.13	94.74	54.30	32.64	86.93	4.80	8976.41	295.36
2	-2	4	0.13	91.50	54.30	32.52	86.81	2.63	8372.07	317.90
2	2	4	0.13	95.24	54.30	32.64	86.93	4.77	9071.55	317.66
-2	-2	-4	0.13	93.19	54.30	32.64	86.93	3.93	8683.53	286.19
3	2	4	0.15	96.87	89.90	2.49	87.48	5.38	9384.01	321.87
3	-2	4	0.15	95.07	89.90	2.46	87.54	4.44	9038.60	310.22
-3	2	-4	0.15	97.77	89.90	2.46	87.54	6.11	9558.94	310.47
-3	2	-4	0.15	93.31	89.90	2.46	87.54	3.59	8706.08	290.40
3	2	4	0.15	96.74	89.90	2.49	87.48	5.21	9358.49	327.32
3	-2	4	0.15	93.85	89.90	2.46	87.54	3.50	8807.17	327.07
-3	-2	-4	0.15	93.20	89.90	2.49	87.48	3.44	8686.01	300.31
-3	-2	-4	0.15	92.69	89.90	2.49	87.48	3.20	8591.35	293.37
3	3	-4	0.14	188.72	173.36	1.67	171.96	4.96	35613.49	1218.84
3	-3	-4	0.14	196.27	172.84	0.78	172.17	7.62	38520.22	1164.33
-3	3	4	0.14	189.94	172.84	0.78	172.17	5.12	36077.59	1257.25
3	-3	-4	0.14	192.80	172.84	0.78	172.17	5.85	37172.54	1286.49
-3	-3	4	0.14	196.28	173.36	1.67	171.96	6.94	38527.66	1290.70
-3	-3	4	0.14	190.49	173.36	1.67	171.96	5.79	36287.46	1160.86

=====										
3	-3	-4	0.14	195.17	172.84	0.78	172.17	6.91	38089.58	1222.56
-3	-3	4	0.14	196.44	173.36	1.67	171.96	7.15	38587.62	1260.47
2	-3	-4	0.14	15.42	2.09	18.93	17.15	3.61	237.62	15.61
2	-3	-4	0.14	14.68	2.09	18.93	17.15	2.62	215.57	29.98
2	-3	-4	0.14	15.49	2.09	18.93	17.15	2.10	239.85	25.77
1	-3	-4	0.13	89.26	72.09	8.41	80.48	5.92	7967.69	251.99
-1	-3	4	0.13	85.81	71.15	8.66	79.76	3.71	7362.60	269.83
-1	3	4	0.13	85.97	72.09	8.41	80.48	3.39	7390.10	269.34
-1	3	4	0.13	89.10	72.09	8.41	80.48	5.29	7939.19	276.28
1	-3	-4	0.13	87.83	72.09	8.41	80.48	4.69	7714.95	264.14
1	3	-4	0.13	86.63	71.15	8.66	79.76	4.71	7505.32	242.58
1	3	-4	0.13	90.10	71.15	8.66	79.76	6.61	8118.83	265.87
-1	-3	4	0.13	86.97	71.15	8.66	79.76	4.31	7563.80	278.76
0	3	-4	0.14	108.78	79.53	23.10	102.56	3.68	11832.34	356.81
0	-3	4	0.14	111.00	79.53	23.10	102.56	4.44	12320.72	405.37
0	3	4	0.14	105.90	78.39	23.13	101.49	2.32	11215.37	395.21
0	3	4	0.14	107.08	78.39	23.13	101.49	2.94	11467.11	397.19
1	3	4	0.14	56.59	47.14	2.52	49.66	5.67	3202.59	129.84
-1	3	-4	0.14	55.04	48.25	2.60	50.49	3.94	3029.14	121.66
-1	-3	-4	0.14	55.34	47.14	2.52	49.66	5.28	3062.84	112.99
1	-3	4	0.14	55.17	48.25	2.60	50.49	4.22	3043.51	116.95
-1	3	-4	0.14	55.80	48.25	2.60	50.49	5.34	3113.63	105.56
1	3	4	0.14	55.02	47.14	2.52	49.66	4.71	3027.16	118.94
1	-3	4	0.14	57.91	48.25	2.60	50.49	6.29	3353.48	127.86
-1	-3	-4	0.14	56.07	47.14	2.52	49.66	5.86	3143.61	115.47
-4	1	5	0.14	185.64	152.40	21.13	173.51	4.01	34460.81	1086.28
4	1	-5	0.14	185.40	152.40	21.24	173.61	3.51	34372.84	1204.47
4	-1	-5	0.14	184.30	152.40	21.13	173.51	3.21	33965.00	1201.99
4	-1	-5	0.14	186.87	152.40	21.13	173.51	4.21	34918.96	1142.77
-4	-1	5	0.14	190.93	152.40	21.24	173.61	5.35	36453.23	1179.20
-4	-1	5	0.14	189.65	152.40	21.24	173.61	5.37	35966.33	1084.30
-4	1	5	0.14	187.82	152.40	21.13	173.51	4.39	35277.50	1177.46
4	1	-5	0.14	184.39	152.40	21.24	173.61	3.38	33998.94	1141.28
-3	-1	5	0.13	37.48	47.50	14.88	32.63	5.36	1404.43	63.43
3	-1	-5	0.13	37.33	47.50	15.58	32.04	6.24	1393.53	58.72
-3	1	5	0.13	36.79	47.50	15.58	32.04	5.10	1353.14	63.93
-3	-1	5	0.13	35.92	47.50	14.88	32.63	4.52	1289.95	49.80
-3	-1	5	0.13	37.59	47.50	14.88	32.63	5.31	1413.10	65.66
3	-1	-5	0.13	36.69	47.50	15.58	32.04	4.63	1345.95	68.88
3	1	-5	0.13	38.17	47.50	14.88	32.63	5.61	1456.71	69.87
3	-1	-5	0.13	36.46	47.50	15.58	32.04	5.24	1329.10	57.73
2	-1	-5	0.12	89.20	93.78	14.24	79.55	6.25	7955.79	260.67
-2	1	5	0.12	92.98	93.78	14.24	79.55	8.07	8644.63	287.18
2	-1	-5	0.12	89.64	93.78	14.24	79.55	6.15	8035.08	277.76
-2	-1	5	0.12	91.34	93.78	14.35	79.45	7.01	8343.57	289.66
2	1	-5	0.12	90.79	93.78	14.35	79.45	6.94	8242.97	278.26
-2	1	5	0.12	90.83	93.78	14.24	79.55	6.75	8250.40	284.95
2	1	-5	0.12	88.22	93.78	14.35	79.45	5.73	7782.10	256.45

=====											
-2	-1	5	0.12	88.71	93.78	14.35	79.45	5.46	7868.82	284.95	
1	1	-5	0.12	6.16	19.92	17.24	3.04	2.57	37.91	11.15	
-1	-1	5	0.12	8.09	19.92	17.24	3.04	3.06	65.41	18.34	
-1	1	5	0.12	6.81	19.92	17.30	2.75	3.07	46.34	12.64	
-1	1	5	0.12	7.92	19.92	17.30	2.75	2.71	62.69	20.32	
1	1	-5	0.12	8.01	19.92	17.24	3.04	2.55	64.18	21.56	
0	-1	-5	0.12	412.33	350.97	18.26	369.23	6.31	170013.05	5335.49	
0	1	-5	0.12	425.42	350.97	18.39	369.35	7.95	180985.09	5602.85	
0	-1	5	0.12	416.90	350.97	18.39	369.35	6.47	173808.08	5776.55	
0	-1	-5	0.12	417.06	350.97	18.26	369.23	6.71	173936.67	5601.61	
0	-1	5	0.12	410.74	350.97	18.39	369.35	5.45	168706.48	5923.98	
0	1	5	0.12	416.08	350.97	18.26	369.23	6.20	173119.25	5931.66	
0	1	-5	0.12	414.87	350.97	18.39	369.35	6.68	172121.17	5346.65	
0	1	5	0.12	414.15	350.97	18.26	369.23	6.08	171521.80	5785.96	
1	1	5	0.13	43.50	31.97	8.14	40.09	3.33	1892.31	85.48	
-1	1	-5	0.13	43.71	31.97	7.97	39.89	4.64	1910.65	68.88	
-1	1	-5	0.13	44.74	31.97	7.97	39.89	5.11	2001.58	80.28	
-4	2	5	0.15	236.03	195.06	16.60	211.66	5.90	55708.38	1850.44	
4	2	-5	0.15	233.81	192.77	16.49	209.22	6.07	54668.69	1793.70	
-4	-2	5	0.15	233.10	192.77	16.49	209.22	5.70	54337.16	1851.68	
-4	-2	5	0.15	237.82	192.77	16.49	209.22	6.74	56557.04	1896.03	
-4	2	5	0.15	231.55	195.06	16.60	211.66	5.16	53617.10	1709.45	
-4	-2	5	0.15	241.44	192.77	16.49	209.22	8.49	58293.75	1710.19	
4	-2	-5	0.15	235.73	195.06	16.60	211.66	5.68	55566.40	1895.78	
4	-2	-5	0.15	228.60	195.06	16.60	211.66	4.15	52256.78	1794.93	
-2	-2	5	0.13	9.25	2.27	15.02	13.54	4.94	85.48	19.82	
2	2	-5	0.13	6.57	2.27	15.02	13.54	6.16	43.11	22.80	
2	-2	-5	0.13	8.68	3.61	15.19	12.05	2.61	75.33	26.76	
-2	2	5	0.13	9.92	3.61	15.19	12.05	2.12	98.37	22.05	
-2	-2	5	0.13	7.90	2.27	15.02	13.54	5.96	62.44	20.32	
1	-2	-5	0.13	168.52	144.49	7.56	152.04	6.17	28398.82	856.34	
-1	-2	5	0.13	160.53	142.28	8.48	150.69	3.31	25768.86	925.71	
1	2	-5	0.13	163.14	142.28	8.48	150.69	4.34	26614.79	899.70	
-1	2	5	0.13	172.90	144.49	7.56	152.04	7.28	29893.19	930.67	
1	-2	-5	0.13	165.38	144.49	7.56	152.04	4.71	27350.20	898.71	
-1	-2	5	0.13	162.74	142.28	8.48	150.69	3.98	26483.21	948.76	
0	-2	-5	0.13	64.63	65.56	4.61	61.08	2.93	4177.36	152.63	
0	-2	-5	0.13	64.33	65.56	4.61	61.08	2.80	4137.72	145.45	
0	2	-5	0.13	65.93	66.33	5.01	61.34	4.24	4347.34	138.01	
0	-2	5	0.13	65.14	66.33	5.01	61.34	2.98	4243.02	161.55	
0	2	-5	0.13	65.24	66.33	5.01	61.34	3.18	4256.16	155.61	
0	2	5	0.13	67.97	65.56	4.61	61.08	5.40	4619.90	164.53	
0	-2	5	0.13	64.06	66.33	5.01	61.34	2.20	4103.77	155.11	
0	2	5	0.13	64.13	65.56	4.61	61.08	2.46	4112.69	155.36	
-1	2	-5	0.14	188.30	173.99	6.58	167.44	6.89	35456.40	1077.11	
-1	-2	-5	0.14	180.64	171.18	5.26	165.94	4.72	32629.45	1079.83	
1	2	5	0.14	187.86	171.18	5.26	165.94	6.61	35293.11	1173.00	
1	-2	5	0.14	186.48	173.99	6.58	167.44	5.77	34774.75	1167.30	

-1	-2	-5	0.14	185.80	171.18	5.26	165.94	6.17	34522.26	1131.62
1	2	5	0.14	186.71	171.18	5.26	165.94	6.13	34860.23	1195.80
-1	2	-5	0.14	187.09	173.99	6.58	167.44	6.13	35001.47	1135.83
1	-2	5	0.14	186.51	173.99	6.58	167.44	5.63	34784.16	1199.27
-3	0	6	0.14	176.41	126.57	34.85	161.41	4.74	31121.45	1069.68
3	0	-6	0.14	176.78	126.57	34.85	161.41	5.39	31250.29	965.36
-3	0	6	0.14	180.55	126.57	34.85	161.41	6.23	32597.49	1051.09
3	0	-6	0.14	170.63	126.57	34.85	161.41	3.01	29113.17	1017.15
2	0	-6	0.13	54.88	54.36	3.45	51.54	3.07	3012.29	115.96
-2	0	6	0.13	55.17	54.36	3.45	51.54	3.33	3044.00	116.46
-2	0	6	0.13	53.83	54.36	3.45	51.54	2.18	2897.81	110.51
1	0	-6	0.13	232.53	165.44	39.42	204.85	7.17	54070.79	1689.13
1	0	-6	0.13	234.57	165.44	39.42	204.85	7.35	55020.79	1776.85
-1	0	6	0.13	231.07	165.44	39.42	204.85	6.10	53393.11	1873.23
-1	0	6	0.13	236.24	165.44	39.42	204.85	7.55	55807.99	1833.09
0	0	6	0.14	175.09	167.01	8.95	158.13	5.19	30655.87	1089.99
0	0	6	0.14	179.88	167.01	8.95	158.13	6.88	32357.63	1068.68
0	0	-6	0.14	177.00	167.01	8.95	158.13	6.44	31327.60	982.70
0	0	-6	0.14	179.19	167.01	8.95	158.13	6.86	32110.10	1035.48
1	0	6	0.14	105.40	75.96	17.37	93.33	6.08	11110.06	394.47
-1	0	-6	0.14	105.81	75.96	17.37	93.33	6.62	11196.29	375.64
1	0	6	0.14	106.00	75.96	17.37	93.33	6.50	11235.44	388.27
-1	0	-6	0.14	105.08	75.96	17.37	93.33	6.56	11041.67	355.32
3	1	-6	0.14	52.16	60.15	10.69	49.47	2.59	2720.90	105.80
-3	1	6	0.14	50.66	58.78	10.97	47.80	2.70	2566.53	104.32
3	-1	-6	0.14	52.01	58.78	10.97	47.80	4.47	2705.04	93.91
3	-1	-6	0.14	50.48	58.78	10.97	47.80	2.53	2548.69	104.32
2	1	-6	0.14	165.11	135.05	16.70	151.71	5.02	27262.73	845.68
2	-1	-6	0.14	163.65	134.25	17.15	151.35	4.57	26780.55	847.91
-2	1	6	0.14	167.02	134.25	17.15	151.35	5.31	27896.56	938.85
2	-1	-6	0.14	162.37	134.25	17.15	151.35	3.87	26363.04	893.25
-2	-1	6	0.14	167.83	135.05	16.70	151.71	5.47	28167.63	941.08
-2	1	6	0.14	164.61	134.25	17.15	151.35	4.54	27096.97	922.25
2	1	-6	0.14	162.12	135.05	16.70	151.71	3.66	26283.99	893.50
-2	-1	6	0.14	166.64	135.05	16.70	151.71	5.15	27769.45	922.49
1	1	-6	0.14	102.79	83.60	11.99	95.52	4.34	10566.42	332.52
-1	-1	6	0.14	103.49	83.60	11.99	95.52	4.31	10709.89	368.20
-1	-1	6	0.14	102.60	83.60	11.99	95.52	3.75	10526.53	373.90
1	1	-6	0.14	102.22	83.60	11.99	95.52	3.71	10449.47	357.80
-1	1	6	0.14	101.28	81.71	12.16	93.78	3.97	10257.19	368.45
1	-1	-6	0.14	103.70	81.71	12.16	93.78	5.48	10754.49	357.55
1	-1	-6	0.14	103.54	81.71	12.16	93.78	5.70	10719.55	337.48
-1	1	6	0.14	101.39	81.71	12.16	93.78	4.03	10280.73	368.95
0	1	6	0.14	223.30	189.28	13.99	203.15	4.91	49863.20	1750.83
0	-1	6	0.14	229.15	188.69	14.12	202.78	6.51	52509.51	1750.33
0	1	-6	0.14	232.95	188.69	14.12	202.78	7.74	54266.79	1698.79
0	1	-6	0.14	227.00	188.69	14.12	202.78	6.45	51527.55	1613.31
0	-1	6	0.14	225.88	188.69	14.12	202.78	5.53	51022.82	1791.47

0	1	6	0.14	229.21	189.28	13.99	203.15	6.29	52535.04	1789.73
0	-1	-6	0.14	229.66	189.28	13.99	203.15	6.76	52741.93	1696.81
0	-1	-6	0.14	228.90	189.28	13.99	203.15	6.89	52396.28	1615.29
-1	1	-6	0.15	66.75	69.41	6.14	63.62	2.56	4455.12	159.57
1	1	6	0.15	67.38	67.54	5.97	61.72	4.38	4539.87	166.76
-1	-1	-6	0.15	65.97	67.54	5.97	61.72	3.47	4352.54	156.60
1	1	6	0.15	66.05	67.54	5.97	61.72	3.40	4362.45	162.55
1	-2	-6	0.15	115.38	104.89	5.78	110.63	2.26	13311.85	473.51
-1	-2	6	0.15	120.03	104.89	6.28	110.98	4.17	14408.04	501.26
1	2	-6	0.15	120.50	104.89	6.28	110.98	4.62	14521.28	476.98
1	2	-6	0.15	119.38	104.89	6.28	110.98	4.35	14251.44	445.02
-1	2	6	0.15	120.73	104.89	5.78	110.63	4.74	14576.78	492.59
-1	-2	6	0.15	116.45	104.89	6.28	110.98	2.55	13560.87	488.63
1	-2	-6	0.15	121.40	104.89	5.78	110.63	5.52	14737.59	452.20

=====

SQUEEZE Statistics on the Difference Map Phasing

=====

FcMod = Average contribution to Fc from discrete model
 FcSolv = Average contribution to Fc from solvent region
 FcTot = Average Fc total (= model + solvent contrib.)
 DelMS = Average Phase difference between model and solvent contrib.
 DelMT = Average Phase difference between model and combined contrib.
 N = Number of reflections in Sin(Theta)/Lambda range
 R(Mod) = SIGMA(ABS(ABS(FcMod) - Fo)) / SIGMA(Fo)
 R(Tot) = SIGMA(ABS(ABS(FcTot) - Fo)) / SIGMA(Fo)

SinT/L	<FcMod>	<FcSolv>	<FcTot>	<Fo>	<DelMS>	<DelMT>	N	R(Mod)	R(Tot)
0.05	142.41	72.71	117.31	127.21	118.59	32.23	129.	0.468	0.090
0.10	91.35	35.39	98.54	107.92	84.05	25.32	614.	0.336	0.099
0.15	67.23	17.70	71.78	76.69	86.32	14.76	1382.	0.244	0.085
0.20	51.18	8.69	51.40	53.53	96.66	10.92	2550.	0.160	0.072
0.25	44.21	4.58	44.34	45.74	91.93	5.56	3877.	0.118	0.069
0.30	37.52	2.60	37.62	38.01	90.72	5.39	5677.	0.088	0.060
0.35	28.53	1.71	28.37	28.14	96.36	4.69	7442.	0.087	0.065
0.40	26.23	1.29	26.18	25.92	93.05	3.46	9162.	0.087	0.073
0.45	19.70	1.06	19.64	19.27	94.45	4.24	10322.	0.115	0.103
0.50	16.20	0.92	16.25	15.93	89.03	5.12	11639.	0.142	0.136
0.55	12.61	0.91	12.68	12.51	90.40	7.18	12614.	0.198	0.192
0.60	10.18	0.99	10.33	10.39	88.36	8.98	13633.	0.276	0.267
0.65	8.15	0.86	8.31	8.60	87.15	8.67	11818.	0.389	0.375

Comments on and Analysis of the SQUEEZE run

=====

Note on how to Proceed after SQUEEZE:

=====

- The file .hkp now contains solvent free reflection data.
 - Rename this file .hkp to .hkl
 - Use this new .hkl file to continue SHELXL refinement with a solvent-free .ins.
 - After L.S.-convergence, run PLATON with the new .hkl and .res files with the instruction 'CALC FCF' to produce a final FoFc-CIF on .hkp
 - Rename this .hkp file to .fcf.
 - Append the .sqf file produced by PLATON (detailing the SQUEEZE results) to the .cif produced by SHELXL
- =====

=====

=====

***** N O T I C E *****

=====

- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13
- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow
- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)
- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.
- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.
- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl
- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl
- More INFO can be found on <http://www.cryst.chem.uu.nl/platon/>

=====
Page - Index
=====

Page 1 --- GENERAL
Page 2 --- GEOMETRY
Page 7 --- VOIDS
Page 9 --- ADP-Anal
Page 54 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
=====

N: No S.U.'s (esd) on observed/calculated parameters.

W: Low density (check!) of 0.972 gcm⁻³
N: Number of Ignored Lines on INPUT 8
 of which blank in column 1 8
W: Number of unusual anisotropic displacement parameters 2
N: Total Potential Solvent Accessible Void Vol 1922.1 Ang³
N: Electron Count / Cell = 299 - To be included in D(calc), F000 & Mol.Wght.

=====
:: Input Xtal Data from File kla0005s.ins - Data Type RES

:: NORMAL END of PLATON : 55 Pages on:
:: kla0005s.lis (ASCII, 132 Characters Wide)
:: kla0005s.lps (PostScript Version of .lis)
:: kla0005s.pdf (PDF Version of .lis)

:: SQUEEZE xyz on :kla0005s.sqz
:: SQUEEZE CIF on :kla0005s.sqf