ADDSYM - CHECK (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)

- ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
- Number of Input Atoms Included in Search 124 (Unitcell 248)
- Density based on Input Atom Set = 1.426 g.cm-3 - Vol / Non-H atom = 24.3 Ang+3
- The Structure Implies the Following Symmetry Elements Subject to the Criteria:

Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm. Elem	Input Cell_Row	Reduced Cell_Row	(Ang) d	Typ	Dot	(Deg) Angle	(%) Fit	(Ang) MaxDev.		Input Cell x	y	z
-1	==========	==========	100		0	at				0	0	0

T.R.A.N.S.F.O.R.M.A.T.I.O.N M.A.T.R.I.X for CELL and HKL DATA

Reduced->Convent			Input->Reduced			T = Input->Convent:			a' = T a
(1	0	0)	(1	0	0)	(1	0	0)	Det(T)
(0	1	0) X	(0	1	0) =	(0	1	0)	=
(0	0	1)	(0	0	1)	(0	0	1)	1.000

Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	aP	15.740	19.162	22.348	67.31	82.50	76.07	6030	Triclinic	-1
Reduced	P	15.740	19.162	22.348	67.30	82.50	76.07	6030		
Convent	aP	15.740	19.162	22.348	67.31	82.50	76.07	6030	Triclinic	-1

:: *** No Obvious Extra Crystallographic Symmetry was Detected ***

:: Note: Rerun in EQUAL Atom Type Mode for more Checks

(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	Cr	N	Te
Cov.Rad(Ang):	0.68	0.35	1.35	0.68	1.49
Atom Volume :	13.87	5.08	28.10	11.80	46.70
Atom Number :	6	1	24	7	52
Atom Weight :	12.010	1.008	52.00	14.01	127.60
Scat.Fact.f0:	5.999	1.000	23.994	6.995	51.999
Scat.Fact.f':	0.003	0.000	0.321	0.006	-0.531
Scat.Fact.f":	0.002	0.000	0.624	0.003	1.675
Mu/Rho(MoKa):	0.58	0.37	29.88	0.84	33.79
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

Residue = 1

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN	*SSOF = S.O.F	Move	Type
-	Te(1)	0.15889	0.13723	0.15156	3.5763	3.7890	3.1220	1	1	1	-	-
-	Te(2)	0.15579	0.00094	0.24873	3.1825	2.0471	5.1237	1	1	1	-	-
-	Te(3)	-0.06629	0.21229	0.20830	0.5438	5.6480	4.2908	1	1	1	-	-
-	Te(4)	-0.04428	0.09138	0.32056	0.6602	4.3152	6.6033	1	1	1	-	-
-	Cr(1)	0.09998	0.14341	0.26629	3.0125	4.8401	5.4854	1	1	1	-	Met
-	Cr(2)	0.00379	0.07790	0.19637	0.9922	3.0512	4.0451	1	1	1	-	Met
-	N(1)	0.09893	0.24429	0.27517	3.4872	6.7887	5.6683	1	1	1	-	D/A
-	N(2)	0.20128	0.11142	0.32315	4.6253	4.7091	6.6567	1	1	1	-	D/A
-	N(3)	-0.08505	0.01332	0.21497	-0.6498	2.0018	4.4282	1	1	1	-	D/A
-	N(4)	0.00625	0.06623	0.11140	0.7290	2.1408	2.2948	1	1	1	-	D/A
-	C(1)	0.16267	0.24062	0.31005	4.5753	7.0051	6.3868	1	1	1	-	-
-	C(2)	0.21835	0.16860	0.33644	5.1966	5.8810	6.9304	1	1	1	-	-
-	C(3)	0.06442	0.37339	0.18976	3.2902	8.4929	3.9089	1	1	1	-	-
-	C(4)	0.01274	0.44925	0.16868	2.7651	9.7318	3.4747	1	1	1	-	-

-	C(5)	-0.05635	0.46959	0.20527	1.8783	10.4086	4.2284	1	1	1	- -
-	C(6)	-0.07709	0.41714	0.26505	1.4844	9.9209	5.4598	1	1	1	- -
-	C(7)	-0.02758	0.34031	0.28993	1.9819	8.6950	5.9724	1	1	1	- -
-	C(8)	0.04340	0.32010	0.25051	2.8909	7.9975	5.1603	1	1	1	- -
-	C(9)	0.14027	0.35118	0.14578	4.2532	7.7210	3.0030	1	1	1	- -
-	C(10)	0.10450	0.35377	0.08262	3.5178	7.2538	1.7019	1	1	1	- -
-	C(11)	0.20659	0.40105	0.13035	5.4821	8.5226	2.6851	1	1	1	- -
-	C(12)	-0.04910	0.28435	0.35554	1.5766	8.1896	7.3239	1	1	1	- -
-	C(13)	-0.01927	0.30692	0.40846	2.3047	9.0412	8.4140	1	1	1	- -
-	C(14)	-0.14764	0.28487	0.36525	0.0563	8.2785	7.5239	1	1	1	- -
-	C(15)	0.34095	0.02221	0.32178	6.4083	3.0387	6.6284	1	1	1	- -
-	C(16)	0.40143	-0.04955	0.35347	7.1217	1.9627	7.2812	1	1	1	- -
-	C(17)	0.37889	-0.09981	0.41278	6.7082	1.5119	8.5030	1	1	1	- -
-	C(18)	0.29894	-0.08296	0.44247	5.6142	2.0675	9.1146	1	1	1	- -
-	C(19)	0.23680	-0.01327	0.41272	4.8707	3.1209	8.5017	1	1	1	- -
-	C(20)	0.25947	0.03844	0.35272	5.2909	3.5930	7.2658	1	1	1	- -
-	C(21)	0.36922	0.07788	0.25509	6.9153	3.5299	5.2547	1	1	1	- -
-	C(22)	0.43671	0.12143	0.26459	8.2063	4.4174	5.4504	1	1	1	- -
-	C(23)	0.40724	0.03413	0.20885	7.1770	2.3389	4.3022	1	1	1	- -
-	C(24)	0.15113	0.00480	0.44812	3.7090	3.7458	9.2310	1	1	1	- -
-	C(25)	0.11349	-0.07016	0.48782	2.8866	2.6756	10.0488	1	1	1	- -
-	C(26)	0.16040	0.04437	0.49265	4.1674	4.8451	10.1483	1	1	1	- -
-	C(27)	-0.09244	-0.01040	0.16647	-1.0171	1.1649	3.4292	1	1	1	- -
-	C(28)	-0.04234	0.01729	0.11076	-0.2634	1.2253	2.2816	1	1	1	- -
-	C(29)	-0.12607	-0.07512	0.32286	-1.3884	1.2373	6.6507	1	1	1	- -
-	C(30)	-0.18853	-0.09581	0.37325	-2.3199	1.2637	7.6887	1	1	1	- -
-	C(31)	-0.27320	-0.04867	0.36785	-3.4509	2.0964	7.5775	1	1	1	- -
-	C(32)	-0.29319	0.01884	0.31352	-3.6128	2.9086	6.4583	1	1	1	- -
-	C(33)	-0.23288	0.03939	0.26360	-2.7144	2.8835	5.4300	1	1	1	- -
-	C(34)	-0.14843	-0.00796	0.26855	-1.5891	2.0432	5.5319	1	1	1	- -
-	C(35)	-0.03527	-0.13006	0.32673	-0.2014	0.2471	6.7304	1	1	1	- -
-	C(36)	-0.04359	-0.20808	0.32488	-0.6976	-1.2191	6.6923	1	1	1	- -
-	C(37)	0.00885	-0.14336	0.38856	0.6122	0.5043	8.0041	1	1	1	- -
-	C(38)	-0.25792	0.11021	0.20091	-2.9649	3.6891	4.1386	1	1	1	- -
-	C(39)	-0.30882	0.08977	0.15773	-3.9863	2.9566	3.2491	1	1	1	- -
-	C(40)	-0.31396	0.18002	0.21800	-3.4750	5.1269	4.4907	1	1	1	- -
-	C(41)	0.12219	0.04082	0.03184	2.2045	1.0190	0.6559	1	1	1	- -
-	C(42)	0.16061	0.06389	-0.03119	2.7317	0.9338	-0.6425	1	1	1	- -
-	C(43)	0.13243	0.13979	-0.07653	2.5059	1.9754	-1.5765	1	1	1	- -
-	C(44)	0.06747	0.19117	-0.05774	1.7752	3.0843	-1.1894	1	1	1	- -
-	C(45)	0.02964	0.17063	0.00573	1.2703	3.2202	0.1180	1	1	1	- -
-	C(46)	0.05402	0.09402	0.04959	1.4287	2.1533	1.0215	1	1	1	- -
-	C(47)	0.15683	-0.04110	0.07923	2.5102	-0.1179	1.6321	1	1	1	- -
-	C(48)	0.25610	-0.05367	0.09101	4.0491	-0.2556	1.8747	1	1	1	- -
-	C(49)	0.13844	-0.10160	0.05563	1.8728	-1.4357	1.1459	1	1	1	- -
-	C(50)	-0.03767	0.23119	0.02576	0.5487	4.5100	0.5306	1	1	1	- -
-	C(51)	-0.13373	0.22252	0.02532	-1.0046	4.3452	0.5216	1	1	1	- -
-	C(52)	-0.02686	0.31347	-0.01691	0.9738	5.6921	-0.3483	1	1	1	- -

Residue = 2

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	Te(5)	0.47629	0.55338	0.15772	10.5097	11.5790	3.2489	1	1	1	-	-
-	Te(6)	0.43051	0.69768	0.15664	10.4516	14.2540	3.2267	1	1	1	-	-
-	Te(7)	0.64938	0.50849	0.27431	13.3674	11.6955	5.6506	1	1	1	-	-
-	Te(8)	0.56804	0.63483	0.29979	12.7443	14.2531	6.1755	1	1	1	-	-
-	Cr(3)	0.59895	0.63221	0.17208	12.8459	13.1623	3.5447	1	1	1	-	Met
-	Cr(4)	0.46392	0.56291	0.27298	10.6954	12.6967	5.6232	1	1	1	-	Met
-	N(5)	0.66147	0.61856	0.09342	13.5374	12.2666	1.9244	1	1	1	-	D/A
-	N(6)	0.68315	0.70207	0.15464	14.4426	14.3193	3.1855	1	1	1	-	D/A
-	N(7)	0.34307	0.59103	0.30526	9.0172	13.4831	6.2881	1	1	1	-	D/A
-	N(8)	0.45323	0.46492	0.34518	10.2859	11.4634	7.1105	1	1	1	-	D/A
-	C(53)	0.73110	0.65538	0.07053	14.7364	12.7646	1.4529	1	1	1	-	-
-	C(54)	0.74050	0.69867	0.10600	15.1876	13.8592	2.1835	1	1	1	-	-
-	C(55)	0.59042	0.62369	0.00081	12.1724	11.6063	0.0167	1	1	1	-	-
-	C(56)	0.57407	0.58285	-0.03677	11.6170	10.5401	-0.7574	1	1	1	-	-
-	C(57)	0.61165	0.50577	-0.02302	11.8931	9.2187	-0.4742	1	1	1	-	-
-	C(58)	0.66941	0.46486	0.02929	12.7663	8.8847	0.6034	1	1	1	-	-
-	C(59)	0.68688	0.50287	0.06735	13.3277	9.9022	1.3874	1	1	1	-	-
-	C(60)	0.64710	0.58010	0.05374	13.0180	11.2275	1.1070	1	1	1	-	-
-	C(61)	0.54550	0.70110	-0.01570	11.7743	12.9113	-0.3234	1	1	1	-	-
-	C(62)	0.61630	0.75610	-0.06700	12.9926	13.5157	-1.3802	1	1	1	-	-
-	C(63)	0.45936	0.72308	-0.03283	10.4698	13.1803	-0.6763	1	1	1	-	-
-	C(64)	0.75080	0.45760	0.12180	14.2839	9.5045	2.5090	1	1	1	-	-
-	C(65)	0.84060	0.43056	0.09268	15.4876	8.7640	1.9091	1	1	1	-	-
-	C(66)	0.71774	0.38948	0.17365	13.6006	8.6607	3.5771	1	1	1	-	-
-	C(67)	0.63631	0.83180	0.15658	14.3094	16.7479	3.2254	1	1	1	-	-
-	C(68)	0.64254	0.88613	0.18351	14.7367	17.9781	3.7802	1	1	1	-	-
-	C(69)	0.69926	0.86270	0.23539	15.6728	17.9657	4.8489	1	1	1	-	-
-	C(70)	0.74788	0.78976	0.25942	16.1718	16.8052	5.3439	1	1	1	-	-
-	C(71)	0.74444	0.73634	0.23287	15.7937	15.5950	4.7970	1	1	1	-	-
-	C(72)	0.68825	0.75693	0.18259	14.8575	15.5677	3.7612	1	1	1	-	-
-	C(73)	0.57927	0.85573	0.09935	13.3549	16.7260	2.0465	1	1	1	-	-
-	C(74)	0.48576	0.90208	0.10857	12.1238	17.6633	2.2365	1	1	1	-	-
-	C(75)	0.62269	0.90313	0.03542	14.0704	17.0859	0.7296	1	1	1	-	-
-	C(76)	0.80342	0.65640	0.25769	16.4258	14.3108	5.3082	1	1	1	-	-
-	C(77)	0.89650	0.66092	0.22682	17.8216	14.1429	4.6723	1	1	1	-	-
-	C(78)	0.80812	0.62262	0.33284	16.5633	14.2957	6.8563	1	1	1	-	-
-	C(79)	0.31720	0.53719	0.35949	8.5199	12.9243	7.4052	1	1	1	-	-
-	C(80)	0.37598	0.46752	0.38194	9.1893	11.8117	7.8677	1	1	1	-	-
-	C(81)	0.21460	0.64655	0.23727	7.0527	13.9609	4.8876	1	1	1	-	-
-	C(82)	0.14528	0.70916	0.20913	6.1683	14.8958	4.3079	1	1	1	-	-

-	C(83)	0.13402	0.77845	0.21915	6.3399	16.2662	4.5143	1	1	1	- -
-	C(84)	0.19188	0.78576	0.25766	7.3967	16.7164	5.3076	1	1	1	- -
-	C(85)	0.26075	0.72487	0.28653	8.2841	15.8195	5.9023	1	1	1	- -
-	C(86)	0.27147	0.65582	0.27705	8.1067	14.4579	5.7070	1	1	1	- -
-	C(87)	0.22502	0.57250	0.22543	6.8406	12.4871	4.6437	1	1	1	- -
-	C(88)	0.22152	0.59140	0.15039	6.6536	12.2263	3.0979	1	1	1	- -
-	C(89)	0.15623	0.52600	0.26531	5.6597	11.9477	5.4652	1	1	1	- -
-	C(90)	0.32178	0.73480	0.33002	9.4175	16.3591	6.7982	1	1	1	- -
-	C(91)	0.37634	0.79529	0.29046	10.4398	17.1613	5.9833	1	1	1	- -
-	C(92)	0.27039	0.75701	0.38588	8.8741	17.2280	7.9489	1	1	1	- -
-	C(93)	0.50571	0.34157	0.33184	10.5040	9.0604	6.8357	1	1	1	- -
-	C(94)	0.56448	0.26948	0.34745	11.1421	7.8470	7.1572	1	1	1	- -
-	C(95)	0.62454	0.24756	0.39325	12.1200	7.8131	8.1007	1	1	1	- -
-	C(96)	0.62888	0.29639	0.42718	12.5126	8.9981	8.7996	1	1	1	- -
-	C(97)	0.56942	0.36930	0.41191	11.8685	10.2295	8.4851	1	1	1	- -
-	C(98)	0.51181	0.39036	0.36412	10.9193	10.2312	7.5006	1	1	1	- -
-	C(99)	0.43475	0.36262	0.28490	9.3472	9.0689	5.8687	1	1	1	- -
-	C(100)	0.46898	0.34032	0.22198	9.5995	8.1407	4.5726	1	1	1	- -
-	C(101)	0.35778	0.32437	0.31784	8.0554	8.6263	6.5473	1	1	1	- -
-	C(102)	0.57368	0.41872	0.44954	12.2733	11.4557	9.2602	1	1	1	- -
-	C(103)	0.52072	0.38710	0.51745	11.4921	11.4217	10.6591	1	1	1	- -
-	C(104)	0.66597	0.42336	0.46012	13.7782	11.6283	9.4782	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	Cr	N	Te
1	1	0.052	0.111	0.231	1294.96	1	2	52	-	2	4	4
2	1	0.530	0.597	0.220	1294.96	1	2	52	-	2	4	4
				Unit Cell Weight =	5179.84			208	0	8	16	16

Calculated Analysis (Percent) = 48.2 0.0 8.0 4.3 39.4

Moiety_Formula = C52 Cr2 N4 Te4

Sum_Formula = C52 Cr2 N4 Te4

Formula_Weight = 1294.96 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

SpaceGroup_Z = 2 ===> Z' = 4 / 2 = 2.000

Calculated Density = 1.4264(7) g cm-3 [= Mg m-3]

F(000) = 2384.0 [2378.76]

mu(MoKa) = 22.87 cm-1 = 2.287 mm-1

** WARNING **
Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Resonant Scattering = 4.16 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 4045.8[4008.1] 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"

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

Residue = 1

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Te1	0.02970	0.03960	0.04220	-0.02170	0.00200	-0.01150	0.03467	0.0260	0.0314	0.0467	1.80
		[0.1604	0.1344	0.1533]	[0.1574	0.1401	0.1498]					
2	Te2	0.03390	0.02910	0.05400	-0.01970	-0.01400	-0.00010	0.03764	0.0253	0.0281	0.0596	2.36
		[0.1533	-0.0021	0.2520]	[0.1583	0.0039	0.2455]					
3	Te3	0.03050	0.03310	0.05090	-0.02200	-0.00710	-0.00090	0.03667	0.0261	0.0306	0.0533	2.04
		[-0.0673	0.2092	0.2110]	[-0.0653	0.2153	0.2056]					
4	Te4	0.04030	0.04990	0.03780	-0.02040	0.00420	-0.02090	0.03981	0.0292	0.0342	0.0561	1.92
		[-0.0475	0.0944	0.3196]	[-0.0410	0.0883	0.3215]					
5	Cr1	0.02580	0.02800	0.03590	-0.01630	-0.00340	-0.00500	0.02840	0.0221	0.0258	0.0373	1.68
		[0.0997	0.1413	0.2680]	[0.1003	0.1455	0.2646]					
6	Cr2	0.02360	0.02770	0.03270	-0.01370	-0.00270	-0.00650	0.02684	0.0208	0.0264	0.0333	1.60
		[0.0037	0.0761	0.1979]	[0.0039	0.0797	0.1948]					
7	N1	0.03260	0.02890	0.04880	-0.02260	-0.00330	-0.00500	0.03430	0.0206	0.0324	0.0500	2.43
		[0.0987	0.2406	0.2784]	[0.0992	0.2480	0.2719]					
8	N2	0.01590	0.03280	0.05400	-0.02270	-0.00420	-0.00120	0.03260	0.0156	0.0277	0.0546	3.51
		[0.2011	0.1065	0.3277]	[0.2014	0.1163	0.3186]					
9	N3	0.01990	0.02780	0.03650	-0.01570	-0.00170	-0.00420	0.02696	0.0198	0.0241	0.0370	1.87
		[-0.0849	0.0109	0.2171]	[-0.0852	0.0158	0.2129]					
10	N4	0.02870	0.03350	0.02880	-0.01430	-0.00450	-0.00710	0.02902	0.0216	0.0312	0.0343	1.59
		[0.0059	0.0684	0.1104]	[0.0066	0.0641	0.1124]					
11	C1	0.02770	0.05290	0.05830	-0.03310	-0.00550	-0.00620	0.04244	0.0255	0.0358	0.0660	2.59
		[0.1631	0.2354	0.3133]	[0.1622	0.2458	0.3068]					
12	C2	0.03130	0.05020	0.05650	-0.03140	-0.01000	-0.00710	0.04182	0.0227	0.0384	0.0644	2.84
		[0.2180	0.1633	0.3400]	[0.2187	0.1739	0.3328]					
13	C3	0.04040	0.03140	0.05070	-0.01820	-0.00420	-0.01000	0.03919	0.0261	0.0404	0.0511	1.96
		[0.0634	0.3710	0.1926]	[0.0654	0.3758	0.1869]					
14	C4	0.05870	0.02890	0.08700	-0.03090	-0.01450	0.00110	0.05600	0.0207	0.0564	0.0909	4.39
		[0.0089	0.4435	0.1750]	[0.0166	0.4550	0.1623]					
15	C5	0.05780	0.03910	0.08540	-0.02830	-0.02170	0.00320	0.05972	0.0333	0.0514	0.0945	2.84
		[-0.0604	0.4654	0.2099]	[-0.0523	0.4737	0.2006]					
16	C6	0.04520	0.04570	0.08000	-0.04190	-0.00930	0.00740	0.05361	0.0235	0.0500	0.0874	3.72
		[-0.0789	0.4104	0.2702]	[-0.0752	0.4239	0.2599]					
17	C7	0.03110	0.05180	0.06240	-0.03740	0.00320	-0.00610	0.04434	0.0275	0.0356	0.0699	2.54
		[-0.0262	0.3351	0.2933]	[-0.0290	0.3455	0.2865]					
18	C8	0.02950	0.03210	0.05420	-0.03050	-0.00690	-0.00510	0.03382	0.0135	0.0292	0.0588	4.36
		[0.0427	0.3140	0.2554]	[0.0441	0.3262	0.2457]					

19	C9	0.04830	0.03700	0.05390	-0.01820	0.00720	-0.01880	0.04504	0.0284	0.0454	0.0613	2.16
		[0.1439	0.3483	0.1482]	[0.1367	0.3540	0.1433]					
20	C10	0.09100	0.08020	0.05240	-0.02530	0.01460	-0.03100	0.07356	0.0463	0.0742	0.1002	2.17
		[0.1107	0.3507	0.0838]	[0.0983	0.3568	0.0815]					
21	C11	0.06720	0.08850	0.13320	-0.05850	0.03170	-0.05570	0.08709	0.0261	0.0822	0.1530	5.87
		[0.2148	0.3909	0.1382]	[0.1984	0.4112	0.1225]					
22	C12	0.04500	0.06790	0.06370	-0.04150	0.00090	-0.00410	0.05524	0.0356	0.0504	0.0797	2.24
		[-0.0485	0.2791	0.3583]	[-0.0497	0.2896	0.3528]					
23	C13	0.10370	0.14220	0.07380	-0.06080	-0.01780	-0.00820	0.10188	0.0503	0.1007	0.1546	3.07
		[-0.0181	0.3162	0.4052]	[-0.0204	0.2976	0.4117]					
24	C14	0.04620	0.07430	0.10190	-0.03320	0.02740	-0.01460	0.07649	0.0339	0.0739	0.1217	3.59
		[-0.1425	0.2806	0.3721]	[-0.1528	0.2891	0.3584]					
25	C15	0.03800	0.03530	0.05160	-0.01550	-0.01060	-0.00730	0.04100	0.0316	0.0355	0.0559	1.77
		[0.3388	0.0208	0.3241]	[0.3431	0.0236	0.3195]					
26	C16	0.04420	0.04600	0.07370	-0.02350	-0.02530	0.00060	0.05379	0.0308	0.0453	0.0853	2.77
		[0.3974	-0.0532	0.3578]	[0.4055	-0.0459	0.3491]					
27	C17	0.06580	0.03820	0.05710	-0.00230	-0.02160	-0.00210	0.05816	0.0299	0.0628	0.0817	2.73
		[0.3851	-0.0992	0.4096]	[0.3727	-0.1004	0.4160]					
28	C18	0.07730	0.05010	0.04540	-0.01120	-0.01760	-0.01120	0.05849	0.0386	0.0542	0.0827	2.15
		[0.3047	-0.0828	0.4412]	[0.2932	-0.0831	0.4438]					
29	C19	0.04210	0.04100	0.04730	-0.01490	-0.00930	-0.01150	0.04264	0.0327	0.0416	0.0536	1.64
		[0.2342	-0.0136	0.4143]	[0.2394	-0.0130	0.4111]					
30	C20	0.03090	0.03320	0.04210	-0.01440	-0.01240	-0.00280	0.03489	0.0236	0.0327	0.0483	2.05
		[0.2570	0.0365	0.3551]	[0.2619	0.0404	0.3503]					
31	C21	0.02680	0.04530	0.05120	-0.01750	0.00010	-0.01230	0.04047	0.0242	0.0455	0.0517	2.14
		[0.3692	0.0756	0.2585]	[0.3693	0.0802	0.2517]					
32	C22	0.06350	0.07860	0.07910	-0.02930	0.00140	-0.04310	0.06889	0.0320	0.0790	0.0956	2.98
		[0.4296	0.1268	0.2639]	[0.4438	0.1160	0.2653]					
33	C23	0.05470	0.06380	0.05500	-0.02370	0.00460	-0.00440	0.05940	0.0445	0.0596	0.0740	1.66
		[0.4092	0.0364	0.2091]	[0.4053	0.0319	0.2086]					
34	C24	0.04700	0.07560	0.04350	-0.02220	0.00230	-0.01480	0.05532	0.0406	0.0485	0.0769	1.89
		[0.1492	0.0090	0.4475]	[0.1531	0.0006	0.4487]					
35	C25	0.06860	0.10360	0.07220	-0.02050	-0.00130	-0.03860	0.08151	0.0535	0.0729	0.1181	2.21
		[0.1082	-0.0653	0.4884]	[0.1187	-0.0750	0.4873]					
36	C26	0.09510	0.11720	0.07960	-0.05740	0.02030	-0.04020	0.08977	0.0563	0.0815	0.1315	2.33
		[0.1546	0.0503	0.4902]	[0.1662	0.0384	0.4951]					
37	C27	0.03050	0.02810	0.04560	-0.01470	-0.00620	-0.00050	0.03496	0.0244	0.0337	0.0467	1.91
		[-0.0936	-0.0125	0.1690]	[-0.0913	-0.0083	0.1639]					
38	C28	0.03060	0.03280	0.03330	-0.00980	0.00210	-0.01140	0.03242	0.0249	0.0356	0.0368	1.48
		[-0.0433	0.0179	0.1120]	[-0.0414	0.0166	0.1096]					
39	C29	0.03380	0.03990	0.03780	-0.01210	-0.00260	-0.01550	0.03631	0.0256	0.0373	0.0460	1.80
		[-0.1291	-0.0733	0.3234]	[-0.1231	-0.0770	0.3224]					
40	C30	0.05250	0.06800	0.04210	-0.01750	0.00100	-0.02640	0.05281	0.0402	0.0430	0.0752	1.87
		[-0.1922	-0.0925	0.3730]	[-0.1848	-0.0991	0.3735]					
41	C31	0.04200	0.10380	0.05760	-0.04400	0.01530	-0.03050	0.06227	0.0312	0.0494	0.1062	3.41
		[-0.2784	-0.0406	0.3653]	[-0.2680	-0.0568	0.3704]					
42	C32	0.03500	0.05730	0.06370	-0.03100	0.00560	-0.01690	0.04871	0.0308	0.0462	0.0691	2.24
		[-0.2909	0.0144	0.3164]	[-0.2955	0.0233	0.3106]					

43	C33	0.03020	0.04040	0.06140	-0.02980	-0.00120	-0.00580	0.04094	0.0291	0.0305	0.0633	2.18
		[-0.2323	0.0355	0.2668]	[-0.2334	0.0433	0.2604]					
44	C34	0.02620	0.03560	0.03850	-0.01930	0.00310	-0.01250	0.03101	0.0210	0.0291	0.0430	2.05
		[-0.1464	-0.0111	0.2705]	[-0.1505	-0.0048	0.2666]					
45	C35	0.03530	0.04440	0.05210	-0.00880	-0.01430	-0.00300	0.04646	0.0276	0.0480	0.0639	2.32
		[-0.0386	-0.1296	0.3300]	[-0.0319	-0.1305	0.3235]					
46	C36	0.06170	0.04250	0.10300	-0.03410	0.00940	-0.01090	0.06805	0.0360	0.0596	0.1086	3.01
		[-0.0402	-0.2132	0.3309]	[-0.0469	-0.2030	0.3189]					
47	C37	0.06350	0.07950	0.06950	-0.02290	-0.02680	-0.01130	0.07055	0.0397	0.0813	0.0907	2.29
		[0.0033	-0.1436	0.3915]	[0.0144	-0.1431	0.3856]					
48	C38	0.03430	0.03180	0.07650	-0.01870	-0.01750	-0.00210	0.04732	0.0283	0.0319	0.0817	2.89
		[-0.2609	0.1068	0.2060]	[-0.2549	0.1136	0.1958]					
49	C39	0.07140	0.05020	0.07680	-0.01750	-0.03050	0.00300	0.06816	0.0401	0.0638	0.1006	2.51
		[-0.3144	0.0872	0.1612]	[-0.3032	0.0923	0.1542]					
50	C40	0.04380	0.05030	0.13860	-0.04410	-0.00350	-0.00440	0.07571	0.0392	0.0485	0.1394	3.56
		[-0.3137	0.1734	0.2260]	[-0.3142	0.1867	0.2100]					
51	C41	0.02510	0.03500	0.04070	-0.01690	-0.00610	-0.00560	0.03234	0.0223	0.0323	0.0424	1.90
		[0.1215	0.0383	0.0341]	[0.1228	0.0434	0.0296]					
52	C42	0.04000	0.05300	0.03550	-0.02060	0.00300	-0.01750	0.04051	0.0317	0.0343	0.0555	1.75
		[0.1581	0.0667	-0.0320]	[0.1632	0.0610	-0.0304]					
53	C43	0.04090	0.05640	0.04380	-0.02170	0.00340	-0.02180	0.04439	0.0313	0.0410	0.0609	1.94
		[0.1292	0.1432	-0.0775]	[0.1357	0.1364	-0.0756]					
54	C44	0.04770	0.04340	0.04310	-0.01520	0.00150	-0.01580	0.04413	0.0371	0.0440	0.0513	1.38
		[0.0695	0.1900	-0.0574]	[0.0654	0.1923	-0.0581]					
55	C45	0.03730	0.03730	0.03220	-0.01310	-0.00390	-0.01080	0.03471	0.0286	0.0349	0.0406	1.42
		[0.0277	0.1716	0.0059]	[0.0316	0.1697	0.0056]					
56	C46	0.03060	0.03410	0.02990	-0.01290	-0.00810	-0.00780	0.03033	0.0199	0.0341	0.0369	1.85
		[0.0511	0.0937	0.0509]	[0.0569	0.0943	0.0483]					
57	C47	0.04020	0.03160	0.04320	-0.01160	-0.00440	-0.00460	0.03927	0.0312	0.0414	0.0452	1.45
		[0.1558	-0.0419	0.0808]	[0.1579	-0.0403	0.0776]					
58	C48	0.03680	0.06150	0.06690	-0.02850	-0.00660	-0.00260	0.05453	0.0357	0.0575	0.0705	1.98
		[0.2558	-0.0577	0.0936]	[0.2564	-0.0497	0.0884]					
59	C49	0.07080	0.03350	0.05720	-0.02350	-0.01120	-0.01170	0.05075	0.0242	0.0534	0.0746	3.09
		[0.1455	-0.1007	0.0536]	[0.1313	-0.1025	0.0576]					
60	C50	0.04820	0.03240	0.04920	-0.01840	-0.00680	-0.00470	0.04244	0.0295	0.0440	0.0539	1.83
		[-0.0405	0.2296	0.0275]	[-0.0349	0.2328	0.0240]					
61	C51	0.03870	0.05590	0.08380	-0.03020	-0.00790	0.00110	0.05957	0.0352	0.0592	0.0843	2.39
		[-0.1345	0.2183	0.0298]	[-0.1330	0.2267	0.0209]					
62	C52	0.09230	0.03490	0.06800	-0.01690	0.00070	-0.01330	0.06609	0.0337	0.0695	0.0950	2.82
		[-0.0189	0.3123	-0.0160]	[-0.0348	0.3146	-0.0178]					
U(i,j)-Average		0.0451	0.0499	0.0584	-0.0239	-0.0036	-0.0108	0.0496	0.0423	0.0474	0.0591	1.40

Residue = 2

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Te5	0.03810	0.04010	0.03670	-0.01690	-0.00170	-0.01480	0.03621	0.0269	0.0371	0.0447	1.66
		[0.4737	0.5554	0.1573]	[0.4789	0.5514	0.1582]					
2	Te6	0.02910	0.03240	0.04280	-0.00650	-0.00470	-0.00420	0.03713	0.0272	0.0332	0.0511	1.88
		[0.4293	0.6979	0.1593]	[0.4317	0.6974	0.1540]					
3	Te7	0.02750	0.03300	0.03520	-0.00600	-0.00190	-0.00310	0.03446	0.0261	0.0309	0.0463	1.77
		[0.6492	0.5098	0.2761]	[0.6496	0.5072	0.2726]					
4	Te8	0.03340	0.04360	0.03730	-0.02060	0.00240	-0.01420	0.03558	0.0276	0.0318	0.0473	1.71
		[0.5660	0.6375	0.2987]	[0.5701	0.6322	0.3009]					
5	Cr3	0.02530	0.02580	0.02930	-0.01020	-0.00040	-0.00670	0.02660	0.0237	0.0265	0.0296	1.25
		[0.5991	0.6316	0.1729]	[0.5988	0.6329	0.1713]					
6	Cr4	0.02360	0.02360	0.03180	-0.00880	-0.00240	-0.00360	0.02689	0.0225	0.0252	0.0330	1.47
		[0.4635	0.5622	0.2745]	[0.4643	0.5636	0.2715]					
7	N5	0.03620	0.02460	0.03380	-0.00970	-0.00150	-0.00710	0.03171	0.0242	0.0347	0.0362	1.50
		[0.6637	0.6182	0.0935]	[0.6592	0.6189	0.0933]					
8	N6	0.02880	0.02450	0.03240	-0.00770	-0.00120	-0.00870	0.02886	0.0220	0.0296	0.0350	1.59
		[0.6821	0.7017	0.1564]	[0.6842	0.7024	0.1529]					
9	N7	0.02490	0.01990	0.04060	-0.01060	-0.00220	-0.00110	0.02921	0.0183	0.0276	0.0417	2.28
		[0.3430	0.5889	0.3086]	[0.3431	0.5931	0.3020]					
10	N8	0.02650	0.02140	0.04110	-0.01050	0.00130	-0.00200	0.03079	0.0200	0.0282	0.0442	2.21
		[0.4545	0.4631	0.3483]	[0.4519	0.4667	0.3420]					
11	C53	0.04800	0.04110	0.03970	-0.01420	0.00360	-0.01390	0.04282	0.0359	0.0416	0.0510	1.42
		[0.7333	0.6544	0.0711]	[0.7289	0.6564	0.0700]					
12	C54	0.04010	0.04540	0.04370	-0.01800	0.01120	-0.02190	0.04145	0.0248	0.0420	0.0575	2.32
		[0.7364	0.7021	0.1042]	[0.7446	0.6952	0.1078]					
13	C55	0.05050	0.09300	0.03680	-0.02950	0.00370	-0.02490	0.05708	0.0316	0.0457	0.0940	2.97
		[0.5859	0.6306	-0.0006]	[0.5949	0.6167	0.0022]					
14	C56	0.04770	0.11210	0.05370	-0.04560	0.00160	-0.02220	0.06585	0.0391	0.0461	0.1124	2.88
		[0.5705	0.5906	-0.0390]	[0.5777	0.5751	-0.0346]					
15	C57	0.05770	0.10400	0.06870	-0.05010	0.01270	-0.03760	0.06883	0.0438	0.0503	0.1123	2.56
		[0.6067	0.5123	-0.0254]	[0.6166	0.4992	-0.0206]					
16	C58	0.05670	0.07020	0.07160	-0.04540	0.01060	-0.02120	0.06003	0.0403	0.0511	0.0887	2.20
		[0.6728	0.4600	0.0321]	[0.6660	0.4697	0.0265]					
17	C59	0.03470	0.05200	0.05390	-0.03470	0.00880	-0.01570	0.04198	0.0289	0.0306	0.0664	2.30
		[0.6896	0.4984	0.0700]	[0.6841	0.5074	0.0647]					
18	C60	0.03770	0.04590	0.03100	-0.01560	0.00190	-0.01430	0.03705	0.0295	0.0339	0.0478	1.62
		[0.6449	0.5824	0.0533]	[0.6493	0.5778	0.0542]					
19	C61	0.05000						0.05000				
20	C62	0.05000						0.05000				

21	C63	0.17400	0.13040	0.10450	-0.05830	-0.07760	0.07500	0.14422	0.0506	0.0905	0.2916	5.76
		[0.4727	0.7342	-0.0379]	[0.4460	0.7119	-0.0278]					
22	C64	0.04020	0.05110	0.06370	-0.02540	0.00090	-0.00240	0.05195	0.0361	0.0555	0.0642	1.78
		[0.7516	0.4549	0.1245]	[0.7500	0.4603	0.1191]					
23	C65	0.04060	0.10790	0.12440	-0.07620	0.00950	0.00420	0.08550	0.0298	0.0846	0.1421	4.77
		[0.8426	0.4196	0.0995]	[0.8386	0.4415	0.0859]					
24	C66	0.06300	0.04480	0.09560	-0.01380	0.00000	-0.01550	0.07107	0.0425	0.0632	0.1074	2.53
		[0.7178	0.3871	0.1795]	[0.7177	0.3918	0.1678]					
25	C67	0.03140	0.02880	0.05140	-0.01850	0.00690	-0.00970	0.03626	0.0248	0.0288	0.0552	2.23
		[0.6385	0.8289	0.1597]	[0.6341	0.8347	0.1534]					
26	C68	0.05020	0.04720	0.07340	-0.02750	0.01060	-0.01900	0.05496	0.0370	0.0479	0.0800	2.16
		[0.6456	0.8826	0.1869]	[0.6395	0.8897	0.1801]					
27	C69	0.06710	0.07380	0.09330	-0.05780	0.02100	-0.03320	0.06868	0.0362	0.0535	0.1164	3.22
		[0.7051	0.8557	0.2399]	[0.6934	0.8697	0.2309]					
28	C70	0.05200	0.05260	0.07410	-0.03770	0.00160	-0.02550	0.05286	0.0231	0.0562	0.0793	3.44
		[0.7515	0.7834	0.2639]	[0.7443	0.7962	0.2550]					
29	C71	0.03640	0.04150	0.04300	-0.01370	0.00040	-0.01610	0.03961	0.0284	0.0437	0.0467	1.65
		[0.7419	0.7380	0.2333]	[0.7470	0.7347	0.2324]					
30	C72	0.02480	0.02890	0.04320	-0.01640	0.00550	-0.01330	0.03059	0.0167	0.0293	0.0459	2.75
		[0.6906	0.7533	0.1859]	[0.6859	0.7606	0.1793]					
31	C73	0.02420	0.03020	0.06560	-0.00770	-0.00460	-0.00030	0.04379	0.0218	0.0345	0.0751	3.45

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