

Electronic supplementary information

Experimental charge density of a potential DHO synthetase inhibitor: dimethyl-*trans*-2-oxohexahydro-pyrimidine-4,6-dicarboxylate

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Fractional coordinates (multipole refinement) plus U_{iso}

O(1)	0.76110(8)	-0.00444(6)	0.47034(5)	1.0000	0.018
O(2)	0.10963(9)	0.50919(6)	0.80628(7)	1.0000	0.023
O(3)	0.13660(9)	0.39928(7)	0.60015(7)	1.0000	0.023
O(4)	0.71801(6)	0.25932(9)	0.98394(9)	1.0000	0.029
O(5)	0.74011(6)	0.00740(11)	0.92443(10)	1.0000	0.030
N(1)	0.48967(7)	0.17752(7)	0.60673(6)	1.0000	0.016
N(2)	0.80996(7)	0.16084(7)	0.60379(7)	1.0000	0.017
C(1)	0.68954(7)	0.10519(6)	0.55888(5)	1.0000	0.013
C(2)	0.39341(7)	0.28363(6)	0.72829(6)	1.0000	0.013
C(3)	0.53255(7)	0.38898(6)	0.72106(6)	1.0000	0.015
C(4)	0.73858(7)	0.26981(6)	0.72038(6)	1.0000	0.015
C(5)	0.19969(6)	0.40251(6)	0.70219(6)	1.0000	0.014
C(6)	-0.07928(8)	0.62749(7)	0.79500(8)	1.0000	0.024
C(7)	0.73254(6)	0.16076(7)	0.88604(6)	1.0000	0.016
C(8)	0.7100(1)	0.1703(1)	1.1450(1)	1.0000	0.029
H(01)	0.40749	0.13047	0.57077	1.0000	0.021
H(02)	0.95627	0.09973	0.57315	1.0000	0.022
H(2)	0.35702	0.20224	0.84728	1.0000	0.018
H(3A)	0.46752	0.45387	0.82314	1.0000	0.020
H(3B)	0.54924	0.48850	0.61270	1.0000	0.020
H(4)	0.84956	0.34564	0.68788	1.0000	0.019
H(6A)	-0.10464	0.73436	0.84930	1.0000	0.035
H(6B)	-0.19503	0.55934	0.86036	1.0000	0.035
H(6C)	-0.06755	0.67624	0.67178	1.0000	0.035
H(8A)	0.56834	0.13723	1.20477	1.0000	0.039
H(8B)	0.72166	0.26032	1.20242	1.0000	0.039
H(8C)	0.83118	0.05664	1.14382	1.0000	0.039

Non-hydrogen temperature factors (U_{iso})

in order U_11 U_22 U_33 U_12 U_13 U_23

O(1)	0.0112(2)	0.0201(2)	0.0184(2)	-0.0003(1)	-0.0047(1)	-0.0109(2)
O(2)	0.0159(2)	0.0205(2)	0.0261(2)	0.0032(2)	-0.0061(2)	-0.0136(2)
O(3)	0.0144(2)	0.0251(2)	0.0262(2)	0.0015(2)	-0.0109(2)	-0.0112(2)
O(4)	0.0470(4)	0.0162(2)	0.0188(2)	-0.0108(2)	-0.0174(2)	-0.0017(2)
O(5)	0.0474(4)	0.0128(3)	0.0206(3)	-0.0069(2)	-0.0100(2)	-0.0038(2)
N(1)	0.0087(1)	0.0166(2)	0.0190(2)	-0.0011(1)	-0.0041(1)	-0.0095(2)
N(2)	0.0088(1)	0.0207(2)	0.0179(2)	-0.0022(1)	-0.0036(1)	-0.0099(2)
C(1)	0.0093(2)	0.0143(2)	0.0134(2)	-0.0014(1)	-0.0035(1)	-0.0060(1)
C(2)	0.0100(2)	0.0122(2)	0.0137(2)	-0.0021(1)	-0.0032(1)	-0.0041(1)
C(3)	0.0126(2)	0.0128(2)	0.0152(2)	-0.0029(1)	-0.0050(1)	-0.0039(1)
C(4)	0.0114(2)	0.0143(2)	0.0150(2)	-0.0034(1)	-0.0048(1)	-0.0046(1)
C(5)	0.0095(1)	0.0126(2)	0.0166(2)	-0.0016(1)	-0.0032(1)	-0.0047(1)
C(6)	0.0148(2)	0.0169(2)	0.0331(3)	0.0025(1)	-0.0048(2)	-0.0097(2)
C(7)	0.0153(2)	0.0125(2)	0.0158(2)	-0.0025(1)	-0.0061(1)	-0.0044(1)
C(8)	0.0432(4)	0.0209(3)	0.0179(2)	-0.0084(2)	-0.0158(2)	-0.0012(2)

Definitions of local coordinate systems:

O(1)	C(1)	X	O(1)	N(2)	Y
O(2)	C(5)	X	O(2)	C(6)	Y
O(3)	C(5)	X	O(3)	O(2)	Y
O(4)	C(7)	X	O(4)	C(8)	Y
O(5)	C(7)	X	O(5)	O(4)	Y
N(1)	C(2)	X	N(1)	C(1)	Y
N(2)	C(4)	X	N(2)	C(1)	Y
C(1)	N(1)	X	C(1)	N(2)	Y
C(2)	C(3)	X	C(2)	N(1)	Y
C(3)	C(4)	X	C(3)	C(2)	Y
C(4)	C(3)	X	C(4)	N(2)	Y
C(5)	O(3)	X	C(5)	O(2)	Y
C(6)	O(2)	Z	C(6)	H(6C)	Y
C(7)	O(5)	X	C(7)	O(4)	Y
C(8)	O(4)	Z	C(8)	H(8C)	Y
H(01)	N(1)	Z	H(01)	C(1)	Y
H(02)	N(2)	Z	H(02)	C(1)	Y
H(2)	C(2)	Z	H(2)	C(5)	Y
H(3A)	C(3)	Z	H(3A)	H(3B)	Y
H(3B)	C(3)	Z	H(3B)	H(3A)	Y
H(4)	C(4)	Z	H(4)	N(2)	Y
H(6A)	C(6)	Z	H(6A)	H(6B)	Y
H(6B)	C(6)	Z	H(6B)	H(6A)	Y
H(6C)	C(6)	Z	H(6C)	H(6B)	Y
H(8A)	C(8)	Z	H(8A)	H(8B)	Y
H(8B)	C(8)	Z	H(8B)	H(8A)	Y

H(8C) C(8) Z H(8C) H(8A) Y

Multipole populations and kappa parameters: (Hansen-Coppens model):

Variables after cycle 10

ATOM # 1 <<< O(1) >>>
Occupation= 1.0000, Core # 1, Kappa Set # 1, Tmax= 2, Lmax= 4, Symm
1
Local System: R(XY) O(1)-C(1) O(1)-N(2), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.761099	0.000000	0.761099	0.000081	1	-7
Y	-0.004438	0.000000	-0.004438	0.000058	16	-7
Z	0.470344	0.000000	0.470344	0.000050	31	-7
U11	0.011216	0.000000	0.011216	0.000174	46	-6
U22	0.020072	0.000000	0.020072	0.000175	61	-6
U33	0.018382	0.000000	0.018382	0.000177	76	-6
U12	-0.000286	0.000000	-0.000286	0.000114	91	-6
U13	-0.004721	0.000000	-0.004721	0.000111	106	-6
U23	-0.010905	0.000000	-0.010905	0.000178	121	-7
M1	6.298165	0.000000	6.298165	0.029178	136	-6
D1+	-0.101707	0.000000	-0.101707	0.014000	155	-8
D1-	0.017034	0.000000	0.017034	0.011714	170	-6
Q0	-0.052608	0.000000	-0.052608	0.012711	197	-6
Q2+	-0.111835	0.000000	-0.111835	0.011470	228	-6
Q2-	0.008085	0.000000	0.008085	0.011113	243	-7
O1+	-0.034193	0.000000	-0.034193	0.009927	266	-6
O1-	0.012193	0.000000	0.012193	0.009185	281	-7
O3+	0.043441	0.000000	0.043441	0.008674	312	-6
O3-	-0.004731	0.000000	-0.004731	0.008653	327	-7

ATOM # 2 <<< O(2) >>>
Occupation= 1.0000, Core # 1, Kappa Set # 5, Tmax= 2, Lmax= 4, Symm
1
Local System: R(XY) O(2)-C(5) O(2)-C(6), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.109634	0.000000	0.109634	0.000086	2	-6
Y	0.509194	0.000000	0.509194	0.000065	17	-6
Z	0.806279	0.000000	0.806279	0.000072	32	-6
U11	0.015939	0.000000	0.015939	0.000153	47	-6
U22	0.020517	0.000000	0.020517	0.000209	62	-7
U33	0.026114	0.000000	0.026114	0.000201	77	-7
U12	0.003158	0.000000	0.003158	0.000152	92	-6
U13	-0.006143	0.000000	-0.006143	0.000172	107	-6
U23	-0.013574	0.000000	-0.013574	0.000200	122	-7

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M1	6.279459	0.000001	6.279459	0.034344	137	-5
D1+	-0.016090	0.000000	-0.016090	0.014109	156	-6
D1-	-0.060596	0.000000	-0.060596	0.014758	171	-6
Q0	0.022427	0.000000	0.022427	0.015135	198	-6
Q2+	-0.008645	0.000000	-0.008645	0.012471	229	-6
Q2-	0.013920	0.000000	0.013920	0.013038	244	-6
O1+	0.003591	0.000000	0.003591	0.010278	267	-6
O1-	-0.025474	0.000000	-0.025474	0.010666	282	-6
O3+	0.112664	0.000000	0.112664	0.009886	313	-6
O3-	-0.000539	0.000000	-0.000539	0.010787	328	-6

ATOM # 3 <<< O(3) >>>
 Occupation= 1.0000, Core # 1, Kappa Set # 1, Tmax= 2, Lmax= 4, Symm # 1
 Local System: R(XY) O(3)-C(5) O(3)-O(2), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.136599	0.000000	0.136599	0.000089	3	-7
Y	0.399280	0.000000	0.399280	0.000073	18	-8
Z	0.600148	0.000000	0.600148	0.000074	33	-6
U11	0.014375	0.000000	0.014375	0.000176	48	-6
U22	0.025121	0.000000	0.025121	0.000212	63	-6
U33	0.026234	0.000000	0.026234	0.000207	78	-6
U12	0.001474	0.000000	0.001474	0.000189	93	-6
U13	-0.010915	0.000000	-0.010915	0.000181	108	-6
U23	-0.011190	0.000000	-0.011190	0.000207	123	-7
M1	6.192161	0.000000	6.192161	0.033925	138	-6
D1+	-0.007201	0.000000	-0.007201	0.017521	157	-6
D1-	-0.017776	0.000000	-0.017776	0.013899	172	-7
Q0	-0.131824	0.000000	-0.131824	0.015909	199	-7
Q2+	-0.023145	0.000000	-0.023145	0.012494	230	-6
Q2-	-0.038129	0.000000	-0.038129	0.014322	245	-6
O1+	-0.005429	0.000000	-0.005429	0.011003	268	-7
O1-	0.013732	0.000000	0.013732	0.009802	283	-6
O3+	0.032854	0.000000	0.032854	0.009579	314	-6
O3-	-0.021862	0.000000	-0.021862	0.009573	329	-7

ATOM # 4 <<< O(4) >>>
 Occupation= 1.0000, Core # 1, Kappa Set # 5, Tmax= 2, Lmax= 4, Symm # 1
 Local System: R(XY) O(4)-C(7) O(4)-C(8), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.718005	0.000000	0.718005	0.000059	4	-6
Y	0.259316	0.000000	0.259316	0.000094	19	-6
Z	0.983936	0.000000	0.983936	0.000087	34	-7
U11	0.047006	0.000000	0.047006	0.000413	49	-6
U22	0.016186	0.000000	0.016186	0.000247	64	-6

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U33	0.018839	0.000000	0.018839	0.000182	79	-6
U12	-0.010760	0.000000	-0.010760	0.000154	94	-6
U13	-0.017414	0.000000	-0.017414	0.000179	109	-6
U23	-0.001723	0.000000	-0.001723	0.000166	124	-6
M1	6.297569	0.000000	6.297570	0.034467	139	-5
D1+	0.012688	0.000000	0.012688	0.016173	158	-6
D1-	-0.037550	0.000000	-0.037550	0.014972	173	-6
Q0	-0.014857	0.000000	-0.014857	0.016704	200	-6
Q2+	-0.026851	0.000000	-0.026851	0.013812	231	-6
Q2-	0.028687	0.000000	0.028687	0.013534	246	-6
O1+	0.051192	0.000000	0.051192	0.011338	269	-6
O1-	-0.012864	0.000000	-0.012864	0.011231	284	-6
O3+	0.118434	0.000000	0.118434	0.010272	315	-6
O3-	0.053218	0.000000	0.053218	0.011280	330	-6

 ATOM # 5 <<< O(5) >>>
 Occupation= 1.0000, Core # 1, Kappa Set # 1, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(XY) O(5)-C(7) O(5)-O(4), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.740114	0.000000	0.740114	0.000059	5	-7
Y	0.007404	0.000000	0.007404	0.000106	20	-8
Z	0.924425	0.000000	0.924425	0.000101	35	-7
U11	0.047442	0.000000	0.047442	0.000441	50	-6
U22	0.012806	0.000000	0.012806	0.000262	65	-6
U33	0.020565	0.000000	0.020565	0.000277	80	-6
U12	-0.006854	0.000000	-0.006854	0.000150	95	-6
U13	-0.010030	0.000000	-0.010030	0.000175	110	-6
U23	-0.003835	0.000000	-0.003835	0.000202	125	-8
M1	6.287558	0.000000	6.287558	0.036615	140	-6
D1+	-0.005674	0.000000	-0.005674	0.019900	159	-7
D1-	0.022833	0.000000	0.022833	0.016508	174	-7
Q0	-0.207368	0.000000	-0.207368	0.019633	201	-7
Q2+	-0.061261	0.000000	-0.061261	0.015681	232	-6
Q2-	-0.037237	0.000000	-0.037237	0.015057	247	-7
O1+	0.045998	0.000000	0.045998	0.012629	270	-6
O1-	0.040996	0.000000	0.040996	0.011041	285	-7
O3+	0.043058	0.000000	0.043058	0.010426	316	-6
O3-	0.035500	0.000000	0.035500	0.010188	331	-6

 ATOM # 6 <<< N(1) >>>
 Occupation= 1.0000, Core # 2, Kappa Set # 2, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(XY) N(1)-C(2) N(1)-C(1), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.489675	0.000000	0.489675	0.000067	6	-8

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Y	0.177522	0.000000	0.177522	0.000067	21	-7
Z	0.606734	0.000000	0.606734	0.000064	36	-7
U11	0.008687	0.000000	0.008687	0.000146	51	-6
U22	0.016588	0.000000	0.016588	0.000195	66	-6
U33	0.019000	0.000000	0.019000	0.000205	81	-6
U12	-0.001090	0.000000	-0.001090	0.000131	96	-7
U13	-0.004136	0.000000	-0.004136	0.000140	111	-7
U23	-0.009547	0.000000	-0.009547	0.000151	126	-6
M1	5.542878	0.000001	5.542879	0.049016	141	-5
D1+	-0.061333	0.000000	-0.061333	0.017377	160	-7
D1-	-0.075905	0.000000	-0.075905	0.017192	175	-7
D0	-0.022876	0.000000	-0.022876	0.014540	185	-6
Q0	-0.001780	0.000000	-0.001780	0.013503	202	-5
Q1+	0.008606	0.000000	0.008606	0.013257	212	-6
Q1-	0.023136	0.000000	0.023136	0.012431	220	-6
Q2+	-0.057885	0.000000	-0.057885	0.015138	233	-6
Q2-	0.062589	0.000000	0.062589	0.013938	248	-8
O0	0.078542	0.000000	0.078542	0.013177	258	-6
O1+	-0.003171	0.000000	-0.003171	0.012145	271	-7
O1-	0.007715	0.000000	0.007715	0.012094	286	-7
O2+	0.081821	0.000000	0.081821	0.012983	296	-7
O2-	-0.039510	0.000000	-0.039510	0.012746	304	-6
O3+	0.307393	0.000000	0.307393	0.013889	317	-5
O3-	0.042308	0.000000	0.042308	0.014084	332	-6

 ATOM # 7 <<< N(2) >>>
 Occupation= 1.0000, Core # 2, Kappa Set # 2, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(XY) N(2)-C(4) N(2)-C(1), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.809963	0.000000	0.809963	0.000069	7	-7
Y	0.160843	0.000000	0.160843	0.000073	22	-7
Z	0.603792	0.000000	0.603792	0.000065	37	-6
U11	0.008847	0.000000	0.008847	0.000149	52	-6
U22	0.020684	0.000000	0.020684	0.000218	67	-6
U33	0.017912	0.000000	0.017912	0.000203	82	-6
U12	-0.002202	0.000000	-0.002202	0.000138	97	-7
U13	-0.003595	0.000000	-0.003595	0.000139	112	-6
U23	-0.009939	0.000000	-0.009939	0.000161	127	-6
M1	5.529831	0.000001	5.529832	0.049383	142	-5
D1+	-0.055035	0.000000	-0.055035	0.018502	161	-7
D1-	-0.059984	0.000000	-0.059984	0.016914	176	-7
D0	0.049910	0.000000	0.049910	0.015329	186	-6
Q0	-0.025402	0.000000	-0.025402	0.014021	203	-5
Q1+	-0.021151	0.000000	-0.021151	0.013904	213	-6
Q1-	-0.038221	0.000000	-0.038221	0.012965	221	-6
Q2+	-0.038366	0.000000	-0.038366	0.016368	234	-6
Q2-	0.018088	0.000000	0.018088	0.013843	249	-6
O0	-0.082020	0.000000	-0.082020	0.013503	259	-6
O1+	-0.006169	0.000000	-0.006169	0.012850	272	-7
O1-	0.026406	0.000000	0.026406	0.012122	287	-6

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O2+	-0.062591	0.000000	-0.062591	0.013472	297	-6
O2-	0.037015	0.000000	0.037015	0.013027	305	-6
O3+	0.330531	0.000000	0.330531	0.014188	318	-5
O3-	0.051478	0.000000	0.051478	0.014249	333	-6

 ATOM # 8 <<< C(1) >>>
 Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(XY) C(1)-N(1) C(1)-N(2), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.689543	0.000000	0.689543	0.000066	8	-7
Y	0.105185	0.000000	0.105185	0.000061	23	-6
Z	0.558882	0.000000	0.558882	0.000055	38	-6
U11	0.009350	0.000000	0.009350	0.000151	53	-6
U22	0.014348	0.000000	0.014348	0.000183	68	-6
U33	0.013404	0.000000	0.013404	0.000173	83	-6
U12	-0.001403	0.000000	-0.001403	0.000125	98	-6
U13	-0.003492	0.000000	-0.003492	0.000129	113	-6
U23	-0.005980	0.000000	-0.005980	0.000131	128	-6
M1	3.826630	-0.000001	3.826629	0.040146	143	-5
D1+	-0.115140	0.000000	-0.115140	0.022228	162	-6
D1-	-0.166903	0.000000	-0.166903	0.023953	177	-6
D0	-0.016310	0.000000	-0.016310	0.015215	187	-7
Q0	-0.430942	0.000000	-0.430942	0.016703	204	-5
Q1+	0.003572	0.000000	0.003572	0.015337	214	-7
Q1-	-0.004745	0.000000	-0.004745	0.014096	222	-6
Q2+	-0.119179	0.000000	-0.119179	0.021199	235	-6
Q2-	0.177798	0.000000	0.177798	0.022023	250	-6
O0	-0.050282	0.000000	-0.050282	0.017391	260	-6
O1+	0.015787	0.000000	0.015787	0.017236	273	-7
O1-	0.013698	0.000000	0.013698	0.017260	288	-7
O2+	-0.001144	0.000000	-0.001144	0.017903	298	-7
O2-	-0.020014	0.000000	-0.020014	0.017156	306	-7
O3+	0.620772	0.000000	0.620771	0.022306	319	-5
O3-	-0.057228	0.000000	-0.057228	0.027639	334	-7

 ATOM # 9 <<< C(2) >>>
 Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(XY) C(2)-C(3) C(2)-N(1), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.393409	0.000000	0.393409	0.000066	9	-6
Y	0.283634	0.000000	0.283634	0.000061	24	-6
Z	0.728293	0.000000	0.728293	0.000056	39	-6
U11	0.010014	0.000000	0.010014	0.000152	54	-6
U22	0.012223	0.000000	0.012223	0.000174	69	-6

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U33	0.013719	0.000000	0.013719	0.000178	84	-6
U12	-0.002139	0.000000	-0.002139	0.000125	99	-6
U13	-0.003171	0.000000	-0.003171	0.000130	114	-6
U23	-0.004142	0.000000	-0.004142	0.000130	129	-7
M1	3.998687	0.000000	3.998687	0.031018	144	-6
D1+	0.053566	0.000000	0.053566	0.019762	163	-6
D1-	-0.135794	0.000000	-0.135794	0.020168	178	-5
D0	-0.217582	0.000000	-0.217582	0.019329	188	-6
Q0	0.018684	0.000000	0.018685	0.016191	205	-6
Q1+	0.041565	0.000000	0.041565	0.017118	215	-6
Q1-	0.131529	0.000000	0.131529	0.017241	223	-8
Q2+	0.089578	0.000000	0.089578	0.018683	236	-5
Q2-	0.031455	0.000000	0.031455	0.017637	251	-6
O0	0.004463	0.000000	0.004463	0.016964	261	-7
O1+	-0.240772	0.000000	-0.240772	0.017817	274	-6
O1-	-0.334637	0.000000	-0.334637	0.016554	289	-6
O2+	0.006409	0.000000	0.006409	0.018928	299	-6
O2-	-0.127238	0.000000	-0.127238	0.017650	307	-6
O3+	0.337313	0.000000	0.337313	0.017417	320	-6
O3-	-0.081769	0.000000	-0.081769	0.019829	335	-6

 ATOM # 10 <<< C(3) >>>
 Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(XY) C(3)-C(4) C(3)-C(2), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.532553	0.000000	0.532553	0.000070	10	-7
Y	0.388983	0.000000	0.388983	0.000062	25	-7
Z	0.721064	0.000000	0.721064	0.000057	40	-7
U11	0.012577	0.000000	0.012577	0.000169	55	-6
U22	0.012774	0.000000	0.012774	0.000182	70	-6
U33	0.015200	0.000000	0.015200	0.000188	85	-6
U12	-0.002885	0.000000	-0.002885	0.000134	100	-6
U13	-0.004998	0.000000	-0.004998	0.000142	115	-6
U23	-0.003916	0.000000	-0.003916	0.000131	130	-6
M1	4.297674	0.000000	4.297674	0.033488	145	-6
D1+	-0.112071	0.000000	-0.112071	0.020678	164	-7
D1-	-0.241423	0.000000	-0.241423	0.020675	179	-6
D0	0.040466	0.000000	0.040466	0.015260	189	-6
Q0	0.125397	0.000000	0.125397	0.016590	206	-6
Q1+	-0.047110	0.000000	-0.047110	0.014587	216	-7
Q1-	0.019627	0.000000	0.019627	0.014334	224	-6
Q2+	-0.016001	0.000000	-0.016001	0.018119	237	-7
Q2-	0.055722	0.000000	0.055722	0.018011	252	-7
O0	0.002942	0.000000	0.002942	0.015369	262	-7
O1+	-0.244443	0.000000	-0.244443	0.016320	275	-6
O1-	-0.343515	0.000000	-0.343515	0.017062	290	-6
O2+	-0.023509	0.000000	-0.023509	0.016963	300	-7
O2-	-0.000769	0.000000	-0.000769	0.015476	308	-6
O3+	0.295050	0.000000	0.295050	0.016952	321	-7
O3-	-0.057712	0.000000	-0.057712	0.018487	336	-7

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ATOM # 11 <<< C(4) >>>
Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
1
Local System: R(XY) C(4)-C(3) C(4)-N(2), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.738582	0.000000	0.738582	0.000068	11	-6
Y	0.269810	0.000000	0.269810	0.000064	26	-6
Z	0.720383	0.000000	0.720383	0.000060	41	-6
U11	0.011436	0.000000	0.011436	0.000166	56	-6
U22	0.014291	0.000000	0.014291	0.000191	71	-6
U33	0.015032	0.000000	0.015032	0.000190	86	-6
U12	-0.003433	0.000000	-0.003433	0.000135	101	-6
U13	-0.004751	0.000000	-0.004751	0.000137	116	-6
U23	-0.004609	0.000000	-0.004609	0.000140	131	-8
M1	4.055180	0.000000	4.055179	0.032880	146	-5
D1+	0.058473	0.000000	0.058473	0.020442	165	-6
D1-	-0.214071	0.000000	-0.214071	0.021662	180	-5
D0	-0.147451	0.000000	-0.147451	0.019755	190	-6
Q0	0.047884	0.000000	0.047884	0.018078	207	-6
Q1+	0.005514	0.000000	0.005515	0.017023	217	-6
Q1-	0.083334	0.000000	0.083334	0.017159	225	-6
Q2+	0.064307	0.000000	0.064308	0.020249	238	-6
Q2-	0.069399	0.000000	0.069400	0.017399	253	-6
O0	-0.032667	0.000000	-0.032667	0.018122	263	-7
O1+	-0.201902	0.000000	-0.201902	0.018359	276	-6
O1-	-0.364021	0.000000	-0.364021	0.016541	291	-6
O2+	-0.011791	0.000000	-0.011791	0.019064	301	-6
O2-	0.011537	0.000000	0.011537	0.017915	309	-6
O3+	0.321459	0.000000	0.321458	0.017501	322	-6
O3-	-0.027047	0.000000	-0.027047	0.019913	337	-6

ATOM # 12 <<< C(5) >>>
Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
1
Local System: R(XY) C(5)-O(3) C(5)-O(2), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.199685	0.000000	0.199685	0.000064	12	-6
Y	0.402505	0.000000	0.402505	0.000056	27	-6
Z	0.702187	0.000000	0.702187	0.000057	42	-6
U11	0.009508	0.000000	0.009508	0.000145	57	-6
U22	0.012574	0.000000	0.012574	0.000167	72	-6
U33	0.016640	0.000000	0.016640	0.000176	87	-6
U12	-0.001597	0.000000	-0.001597	0.000123	102	-6
U13	-0.003175	0.000000	-0.003175	0.000130	117	-6
U23	-0.004749	0.000000	-0.004749	0.000131	132	-6

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M1	4.102254	0.000000	4.102253	0.035054	147	-6
D1+	0.172868	0.000000	0.172868	0.026667	166	-6
D1-	-0.065084	0.000000	-0.065084	0.021063	181	-5
Q0	-0.422129	0.000000	-0.422128	0.016586	208	-5
Q2+	0.155060	0.000000	0.155060	0.021977	239	-8
Q2-	0.095757	0.000000	0.095757	0.020705	254	-6
O1+	0.047519	0.000000	0.047519	0.018366	277	-6
O1-	-0.045281	0.000000	-0.045281	0.015764	292	-6
O3+	0.720580	0.000000	0.720580	0.021903	323	-5
O3-	0.032094	0.000000	0.032094	0.026533	338	-6

 ATOM # 13 <<< C(6) >>>
 Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(ZY) C(6)-O(2) C(6)-H(6C), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	-0.079282	0.000000	-0.079282	0.000080	13	-6
Y	0.627487	0.000000	0.627487	0.000075	28	-7
Z	0.795002	0.000000	0.795002	0.000078	43	-6
U11	0.014792	0.000000	0.014792	0.000185	58	-6
U22	0.016864	0.000000	0.016864	0.000235	73	-6
U33	0.033128	0.000000	0.033128	0.000287	88	-6
U12	0.002450	0.000000	0.002450	0.000143	103	-7
U13	-0.004754	0.000000	-0.004754	0.000185	118	-6
U23	-0.009704	0.000000	-0.009704	0.000202	133	-6
M1	4.337735	0.000000	4.337735	0.034238	148	-6
D1+	-0.031607	0.000000	-0.031607	0.013091	167	-8
D1-	0.090739	0.000000	0.090739	0.013492	182	-6
D0	-0.235884	0.000000	-0.235884	0.017622	191	-6
Q0	-0.171468	0.000000	-0.171468	0.015700	209	-6
Q1+	-0.054085	0.000000	-0.054085	0.012266	218	-6
Q1-	-0.033474	0.000000	-0.033474	0.012867	226	-6
Q2+	0.052666	0.000000	0.052666	0.012325	240	-7
Q2-	-0.046062	0.000000	-0.046061	0.012896	255	-6
O0	0.540368	0.000000	0.540368	0.019160	264	-5
O1+	0.069061	0.000000	0.069061	0.014045	278	-6
O1-	0.093603	0.000000	0.093603	0.015000	293	-6
O2+	0.008352	0.000000	0.008352	0.013773	302	-7
O2-	0.061096	0.000000	0.061096	0.014157	310	-6
O3+	-0.037437	0.000000	-0.037437	0.013162	324	-7
O3-	-0.170716	0.000000	-0.170716	0.015625	339	-6

 ATOM # 14 <<< C(7) >>>
 Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(XY) C(7)-O(5) C(7)-O(4), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
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X	0.732544	0.000000	0.732544	0.000057	14	-6
Y	0.160759	0.000000	0.160759	0.000069	29	-7
Z	0.886041	0.000000	0.886041	0.000061	44	-6
U11	0.015270	0.000000	0.015270	0.000180	59	-6
U22	0.012490	0.000000	0.012490	0.000189	74	-6
U33	0.015758	0.000000	0.015758	0.000189	89	-6
U12	-0.002524	0.000000	-0.002524	0.000119	104	-6
U13	-0.006115	0.000000	-0.006115	0.000128	119	-6
U23	-0.004402	0.000000	-0.004402	0.000139	134	-7
M1	4.111821	0.000000	4.111821	0.035710	149	-6
D1+	0.109140	0.000000	0.109140	0.028947	168	-7
D1-	-0.097625	0.000000	-0.097625	0.022093	183	-6
Q0	-0.433381	0.000000	-0.433381	0.015877	210	-6
Q2+	0.193158	0.000000	0.193158	0.024231	241	-6
Q2-	-0.003945	0.000000	-0.003945	0.021261	256	-6
O1+	0.044444	0.000000	0.044444	0.018898	279	-6
O1-	-0.064242	0.000000	-0.064242	0.016156	294	-6
O3+	0.611046	0.000000	0.611045	0.023040	325	-6
O3-	0.064347	0.000000	0.064347	0.027991	340	-6

 ATOM # 15 <<< C(8) >>>
 Occupation= 1.0000, Core # 3, Kappa Set # 3, Tmax= 2, Lmax= 4, Symm
 # 1
 Local System: R(ZY) C(8)-O(4) C(8)-H(8C), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.710014	0.000000	0.710014	0.000112	15	-6
Y	0.170266	0.000000	0.170266	0.000080	30	-7
Z	1.145023	0.000000	1.145023	0.000072	45	-6
U11	0.043201	0.000000	0.043201	0.000363	60	-6
U22	0.020854	0.000000	0.020854	0.000260	75	-6
U33	0.017870	0.000000	0.017870	0.000199	90	-6
U12	-0.008393	0.000000	-0.008393	0.000235	105	-6
U13	-0.015781	0.000000	-0.015781	0.000238	120	-6
U23	-0.001245	0.000000	-0.001245	0.000168	135	-7
M1	4.317573	0.000000	4.317573	0.035555	150	-7
D1+	-0.111780	0.000000	-0.111779	0.014029	169	-6
D1-	-0.020226	0.000000	-0.020226	0.014074	184	-6
D0	-0.244000	0.000000	-0.244000	0.017473	192	-6
Q0	-0.128589	0.000000	-0.128589	0.016253	211	-6
Q1+	0.021123	0.000000	0.021122	0.013588	219	-6
Q1-	-0.008608	0.000000	-0.008608	0.012566	227	-8
Q2+	0.023936	0.000000	0.023936	0.013357	242	-6
Q2-	0.008189	0.000000	0.008189	0.013887	257	-6
O0	0.507586	0.000000	0.507585	0.019344	265	-6
O1+	-0.033532	0.000000	-0.033532	0.015692	280	-6
O1-	0.115953	0.000000	0.115953	0.014822	295	-6
O2+	0.034995	0.000000	0.034995	0.014061	303	-7
O2-	-0.070349	0.000000	-0.070349	0.014362	311	-6
O3+	-0.010611	0.000000	-0.010611	0.013916	326	-7

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03- -0.263318 0.000000 -0.263318 0.015744 341 -6

ATOM # 16 <<< H(01) >>>
Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1
Local System: R(ZY) H(01)-N(1) H(01)-C(1), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.407490		0.407490			
Y	0.130473		0.130473			
Z	0.570765		0.570765			
U11	0.020990		0.020990			
M1	0.582451	0.000000	0.582450	0.015789	151	-5
D0	0.091037	0.000000	0.091037	0.009848	193	-5

ATOM # 17 <<< H(02) >>>
Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1
Local System: R(ZY) H(02)-N(2) H(02)-C(1), Constrain: H(01)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.956268		0.956268			
Y	0.099735		0.099735			
Z	0.573153		0.573153			
U11	0.022431		0.022431			
M1	0.582451	0.000000	0.582450	0.015789	151	-5
D0	0.091037	0.000000	0.091037	0.009848	193	-5

ATOM # 18 <<< H(2) >>>
Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1
Local System: R(ZY) H(2)-C(2) H(2)-C(5), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.357018		0.357018			
Y	0.202242		0.202242			
Z	0.847276		0.847276			
U11	0.017955		0.017955			
M1	0.715622	0.000000	0.715622	0.014877	152	-6
D0	0.104948	0.000000	0.104948	0.008582	194	-6

ATOM # 19 <<< H(3A) >>>

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Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1

Local System: R(ZY) H(3A)-C(3) H(3A)-H(3B), Constrain: No

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.467521		0.467521			
Y	0.453869		0.453869			
Z	0.823145		0.823145			
U11	0.019712		0.019712			
M1	0.776993	0.000000	0.776993	0.014300	153	-6
D0	0.073373	0.000000	0.073373	0.008025	195	-7

ATOM # 20 <<< H(3B) >>>

Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1

Local System: R(ZY) H(3B)-C(3) H(3B)-H(3A), Constrain: H(3A)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.549238		0.549238			
Y	0.488503		0.488503			
Z	0.612702		0.612702			
U11	0.019712		0.019712			
M1	0.776993	0.000000	0.776993	0.014300	153	-6
D0	0.073373	0.000000	0.073373	0.008025	195	-7

ATOM # 21 <<< H(4) >>>

Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1

Local System: R(ZY) H(4)-C(4) H(4)-N(2), Constrain: H(2)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.849560		0.849560			
Y	0.345640		0.345640			
Z	0.687877		0.687877			
U11	0.019465		0.019465			
M1	0.715622	0.000000	0.715622	0.014877	152	-6
D0	0.104948	0.000000	0.104948	0.008582	194	-6

ATOM # 22 <<< H(6A) >>>

Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1

Local System: R(ZY) H(6A)-C(6) H(6A)-H(6B), Constrain: No

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PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	-0.104637		-0.104637			
Y	0.734365		0.734365			
Z	0.849300		0.849300			
U11	0.034533		0.034533			
M1	0.729299	0.000000	0.729299	0.009546	154	-6
D0	0.114890	0.000000	0.114890	0.005500	196	-6

ATOM # 23 <<< H(6B) >>>
Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1
Local System: R(ZY) H(6B)-C(6) H(6B)-H(6A), Constrain: H(6A)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	-0.195033		-0.195033			
Y	0.559344		0.559344			
Z	0.860360		0.860360			
U11	0.034533		0.034533			
M1	0.729299	0.000000	0.729299	0.009546	154	-6
D0	0.114890	0.000000	0.114890	0.005500	196	-6

ATOM # 24 <<< H(6C) >>>
Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1
Local System: R(ZY) H(6C)-C(6) H(6C)-H(6B), Constrain: H(6A)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	-0.067549		-0.067549			
Y	0.676239		0.676239			
Z	0.671781		0.671781			
U11	0.034533		0.034533			
M1	0.729299	0.000000	0.729299	0.009546	154	-6
D0	0.114890	0.000000	0.114890	0.005500	196	-6

ATOM # 25 <<< H(8A) >>>
Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
1
Local System: R(ZY) H(8A)-C(8) H(8A)-H(8B), Constrain: H(6A)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.568336		0.568336			
Y	0.137234		0.137234			

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Z	1.204774		1.204774			
U11	0.038695		0.038695			
M1	0.729299	0.000000	0.729299	0.009546	154	-6
D0	0.114890	0.000000	0.114890	0.005500	196	-6

 ATOM # 26 <<< H(8B) >>>
 Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
 # 1
 Local System: R(ZY) H(8B)-C(8) H(8B)-H(8A), Constrain: H(6A)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.721662		0.721662			
Y	0.260316		0.260316			
Z	1.202424		1.202424			
U11	0.038695		0.038695			
M1	0.729299	0.000000	0.729299	0.009546	154	-6
D0	0.114890	0.000000	0.114890	0.005500	196	-6

 ATOM # 27 <<< H(8C) >>>
 Occupation= 1.0000, Core # 4, Kappa Set # 4, Tmax= 1, Lmax= 2, Symm
 # 1
 Local System: R(ZY) H(8C)-C(8) H(8C)-H(8A), Constrain: H(6A)

PARAMETER	OLD	SHIFT	NEW	ESD	VAR	S/E
X	0.831185		0.831185			
Y	0.056645		0.056645			
Z	1.143819		1.143819			
U11	0.038695		0.038695			
M1	0.729299	0.000000	0.729299	0.009546	154	-6
D0	0.114890	0.000000	0.114890	0.005500	196	-6

KAPPA TBL	OLD	SHIFT	NEW	ESD	VAR	S/E
KS 1	0.995444	0.000000	0.995444	0.001381	342	-5
K0 1	0.934478		0.934478			
K1 1	0.934478		0.934478			
K2 1	0.934478		0.934478			
K3 1	0.934478		0.934478			
K4 1	0.934478		0.934478			

KS 2	0.975800	0.000000	0.975800	0.002080	343	-5
K0 2	0.800737		0.800737			
K1 2	0.800737		0.800737			
K2 2	0.800737		0.800737			
K3 2	0.800737		0.800737			

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K4	2	0.800737		0.800737			

KS	3	1.014854	0.000000	1.014854	0.002012	344	-5
K0	3	0.780222		0.780222			
K1	3	0.780222		0.780222			
K2	3	0.780222		0.780222			
K3	3	0.780222		0.780222			
K4	3	0.780222		0.780222			

KS	4	1.200000		1.200000			
K0	4	1.200000		1.200000			
K1	4	1.200000		1.200000			
K2	4	1.200000		1.200000			
K3	4	1.200000		1.200000			
K4	4	1.200000		1.200000			

KS	1	0.999580	0.000000	0.999580	0.001681	345	-4
K0	1	0.926442		0.926442			
K1	1	0.926442		0.926442			
K2	1	0.926442		0.926442			
K3	1	0.926442		0.926442			
K4	1	0.926442		0.926442			