A Multi-Nuclear Solid State NMR, Density Functional Theory and X-Ray Diffraction Study of Hydrogen Bonds in Group I Hemibenzoates

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Supplementary Information

S1: Experimental

General IR spectra were recorded on Perkin Elmer Spectrum 100 FT-IR Spectrometer using Attenuated Total Reflection sampling unless otherwise stated, and are reported in cm^{-1}. Mass spectra were recorded at the EPSRC Mass Spectrometry Centre at the University of Swansea. GCMS was carried out at NTU using Agilent Technologies 6890N GC equipped with a 5975 mass detector. Chemical analysis data were obtained from Mr Stephen Boyer, London Metropolitan University. All ^{17}O labelled water was purchased from Cortecnet.

Lithium hydrogen dibenzoate

Lithium hydroxide monohydrate (0.056 g) dissolved in water (0.5 ml) was added to a solution of benzoic acid (0.33 g, 2 equiv.) in warm methanol (1.5 ml). The mixture was heated for 5 min., methanol added dropwise until a solution was formed and the product left to crystallise out at room temperature. Colourless flat needles of the product were collected, washed with water and dried under vacuum. Yield 35%. m.p. 119-121 °C; IR (ATR): $\tilde{\nu}$= 3072, 2829, 2667, 2552, 1678 (C=O), 1601, 1583, 1453, 1420, 1324, 1288, 1179, 1128, 1073, 932, 805,704, 684, 666 cm^{-1}; elemental analysis calcd (%) for. $C_{14}H_{11}O_4Li$: C 67.21, H 4.43; found: C 67.19, H 4.54. ^{17}O-Enriched lithium hydrogen dibenzoate was prepared from 64% ^{17}O-enriched benzoic acid: elemental analysis calcd (%) for. $C_{14}H_{11}O_4Li$: C 66.53, H 4.39; found: C 66.21, H 4.42.

Sodium benzoate.benzoic acid 1:2[1]

Thick needle shaped crystals of this material were obtained by treatment of an ethanolic solution of benzoic acid with 0.5 equivalent of sodium hydroxide in water, and subsequent slow evaporation of the mixture, m.p. > 300 °C; IR (ATR): $\tilde{\nu}$= 1698 and 1673 (C=O), 1600, 1584, 1563, 1451, 1376, 1318, 1287, 1249, 1177, 1118, 1072, 1025, 1004, 934, 903, 800, 787, 704, 684, 663 cm^{-1}.

Potassium hydrogen dibenzoate [2]

Method A. Potassium hydroxide (0.077 g) in water (1 ml) was added to a hot solution of benzoic acid(0.33 g, 2 equiv.) in ethanol (2 ml) and a precipitate started form. The mixture was heated for 5 min., and then water was added dropwise with heating until a solution was just formed, and the product left to crystallise out at room temperature. Colourless flat needles of the product were collected by filtration, washed with ethanol and ether, and dried *in vacuo*. Yield 45%, m.p. > 300 ^{o}C; IR (ATR): $\tilde{\nu}$= 3056, 1690 br (C=O), 1580, 1448, 1070, 802, 702, 683, 660 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{11}O_4K$: C 59.55, H 3.93; found: C 59.44, H 3.83. ^{17}O-Enriched potassium hydrogen dibenzoate was prepared from 64% ^{17}O-enriched benzoic acid: elemental analysis calcd (%) for $C_{14}H_{11}O_4K$: C 58.90, H 3.88; found: C 58.79, H 3.86.

Method B. Potassium hydroxide (0.077 g) in methanol (1.5 ml) was added to a hot solution of benzoic acid (0.33 g, 2 equiv.) in THF (2.5 ml) and the immediately formed precipitate heated for 5 min. Methanol was added dropwise until a solution was just formed, and the product left to crystallise, to give the same polymorphic form of potassium hydrogen dibenzoate as obtained from ethanol/water.

Rubidium hydrogen dibenzoate

Method A above was employed but using a commercial 50% solution of rubidium hydroxide to give the product as colourless flat needles. Yield 60%. m.p. > 300°C; IR (ATR): $\tilde{\nu}$= 3059, 1690 br (C=O), 1581, 1448, 1352, 1317, 1307, 1208, 1071, 804, 702, 683, 661 cm^{-1}; elemental analysis

calcd (%) for $C_{14}H_{11}O_4Rb$: C 51.15, H 3.37; found: C 51.08, H 3.23. ^{17}O-Enriched rubidium hydrogen dibenzoate was prepared from 64% enriched ^{17}O-enriched benzoic acid: elemental analysis calcd (%) for $C_{14}H_{11}O_4Rb$: C 50.76, H 3.35; found: C 50.37, H 3.34.

Cesium hydrogen dibenzoate .

Following Method A above but using cesium hydroxide monohydrate gave colourless plates of cesium hydrogen dibenzoate. Yield 76%. m.p. > 300 °C; IR (ATR): $\tilde{\nu}$= 3055, 1671 sh and 1634 (C=O), 1600, 1577, 1448, 1343, 1314, 1281, 1067, 803, 688, 669 cm^{-1}; elemental analysis calcd (%) for $C_{14}H_{11}O_4Cs$: C 44.70, H 2.95; found: C 44.75, H 2.87. ^{17}O-Enriched cesium hydrogen dibenzoate was prepared from 64% ^{17}O-enriched benzoic acid: elemental analysis calcd (%) for $C_{14}H_{11}O_4Cs$: C 44.40, H 2.93; found: C 44.20, H 3.00. ^{133}Cs SSNMR on the unlabelled material showed this to be mixture of two polymorphs. The crystal structure of the monoclinic polymorph was obtained from this preparation. The material was also prepared from cesium hydroxide monhydrate in methanol and benzoic acid in THF (2.5 ml) (36% yield), and the crystal structure of the orthorhombic polymorph was obtained from this batch.

^{13}C isotopically enriched hydrogen dibenzoates

^{13}C labelled hydrogen dibenzoates were prepared as above but using benzoic acid isotopically labelled with ^{13}C at the carbonyl group.

S2: X-ray Crystallography

The crystallographic structure determination of BZA has been previously completed by numerous workers; we have chosen to use the relatively recent study by Wilson[3] using neutron diffraction at 20 K for DFT calculations. The hydrogen dibenzoates of Li, K, Rb and Cs were prepared by reaction of BZA with half an equivalent of the corresponding metal hydroxide under conditions where the product slowly crystallised from the reaction mixture. The corresponding reaction with sodium hydroxide gave crystals of a 1:2 benzoate/benzoic acid or dihydrogen tribenzoate complex. The Li, Rb and Cs hydrogen dibenzoates (HD) complexes and the Na dihydrogen tribenzoate (DT) complex have not been previously reported. The crystal structures of these materials were determined at low temperature (typically 120 K) and their coordination motifs and crystal packing schemes are given in Figures 2 and 3, respectively, with their structural parameters summarised in Table 1.

The LiHD crystallises in space group *P*–1, with one lithium cation, a benzoate anion and a benzoic acid moiety all crystallographically unique. Two Li atoms and an O (O4) from each of two benzoate anions form a centrosymmetric Li_2O_2 grouping in an approximate square arrangement, and the second oxygen atoms (O3) from the two benzoates act as coordinating ligands to the next Li_2O_2 'squares' in the +*a* and –*a* directions to form a linear coordination polymer, in which the 'squares' are linked by an eight-membered ring involving four O, two C and with the carbonyl oxygen atom (O2) providing the fourth coordination site at the Li position, and the -OH group forming a hydrogen bond with the benzoate O atom (O3) (O···O: 2.6128(17), O-H: 1.03(3), OH---O: 1.59(3) Å, angle at H: 171(3) °), and so bridging across the eight-membered ring (Figure 2(a)). This O···O separation is almost identical to that observed by neutron diffraction in benzoic acid at 125 K (2.616(7) Å), though the hydrogen atom is in dynamic disorder between attachment to either oxygen.[3] This leads to the two C,O bonds of the carboxylic acid being similar in length at 125 K (1.263 Å) in contrast to the benzoic acid molecule in LiHD where these two bonds are quite different (1.231(2) and 1.316(2) Å). There are thus four distinct O atom environments: an OH (O1), a C=O group (O2) which coordinates one Li, and two benzoate O atoms, one of which (O3) coordinates one Li ion and forms a H bond, while the second (O4) coordinates two Li ions as part of the Li_2O_2 square. The coordination polymers lie side by side in the –*b* and +*b* directions to form a layer in the *ab* plane, and the interface between the layers in the –*c* and +*c* directions involves only the benzene rings but with no interdigitation of aromatic residues (Figure 3(a)). Benzene rings of the benzoic acid and benzoate residues lie at 8.8°.

From the Na benzoate/benzoic acid system Flammersheim has identified two 1:2 complexes and one 2:1 complex, but no 1:1 hydrogen dibenzoate has been prepared.[2] We isolated crystals of a 1:2 complex, which crystallised in the monoclinic space group $P2_1/c$ and forms coordination polymers oriented along the *a* axis. The structure is related to that of LiHD except that an extra benzoic acid molecule is incorporated so that the coordination of the metal can be expanded to six. Two Na ions and two O atoms (O2A) from different benzoate anions form a Na_2O_2 unit in an approximately square arrangement (angles 84 and 96°). These are linked together as for LiHD by the second benzoate O atom (O1A), forming an eight membered ring between "squares" and by one benzoic acid coordinating Na by its carbonyl O atom (O2C) while the hydroxyl group forms a H bond to the bridging inequivalent, one coordinating a Na ion at both oxygen atoms and the other just coordinating a single Na via the carbonyl O atom. The two benzoic acid molecules lie roughly perpendicular. The shortest Na-O bonds are those to carbonyl O atoms (2.3322(11) and 2.3436(11) Å) and the longest are to the doubly H bonded benzoate oxygen (2.6693(10) Å) and the OH group (2.6461(11) Å). The bonds in the Na_2O_2 group are 2.3326(10) and 2.3859(10) Å. Adjacent coordination polymers in the *b* direction are related by a unit cell translation, while adjacent chains in the *c* direction are related by the *c* glide plane (Figure 3(b)). We were not able to find a reproducible way of crystallising this phase and thus did not attempt SSNMR studies.

The crystal structures of the K, Rb and Cs hydrogen dibenzoates are quite different from the Li and Na salts, and comprise two-dimensional coordination polymers with tight hydrogen bonds in which the O···O separations lie in the narrow range 2.456 – 2.475 Å, significantly shorter than in the Li and Na salts (2.562-2.664 Å). KHD crystallises in the monoclinic space group *C*2/*c* with four KHD moieties per unit cell. The six-coordinate K ions are organised in layers perpendicular to the *a* axis (Figure 2(c)). There are chains of coplanar K_2O_2 motifs in an approximately square arrangement (angles: 87° and 95°) which share K ions running along the *b* direction. A two-fold axis parallel to *b* cuts the line of K ions, so that the K_2O_2 motif has two-fold symmetry. In contrast the M_2O_2 motifs in the Li and Na salts are centrosymmetric and do not share metal ions. The benzoate O positions which bridge two K positions are not involved in H bonding, and these K-O bonds are 2.6895(14) and 2.8110(14) Å long. The second benzoate O atoms coordinate K ions in adjacent lines (K-O 2.7641(14) Å) and so eight-membered rings are formed.

As in the Na salt, the acidic H atom is located between two O atoms of this ring (Figure 3(c)). These two O atoms are 2.456(3) Å apart, and related by a centre of symmetry. Difference electron density maps showed two positions for this H atom, which were refined as each 50% occupied (O-H: 0.84(3)); H···O: 1.62(3) Å, angle at H: 174(4)°). The benzene rings project to either side of the layer, and are related by a unit cell translation in the *b* direction and by the glide plane in the *c* direction, with the best planes of the glide related benzene rings lying at 49.1°. Adjacent layers are related by the *C*-centring.

RbHD crystallises in the monoclinic space group *C*2/*c* and is isostructural to the KHD and contains six-coordinate Rb ions. However, on one occasion a crystal of a polymorph with eight coordinate Rb ions was obtained and this is isostructural with the monoclinic Cs analogue described below. Powder diffraction data shows that the six coordinate polymorph is predominant in our samples of RbHD. The crystal structure of the six-coordinate polymorph at 100 K (Figure 3(d)) shows Rb-O distances of 2.8206(13) and 2.9688(13) Å to the O atoms in the Rb_2O_2 units and 2.9448(15) Å to the H bonded O atoms. The difference electron density map did not show clear evidence for two positions for the (O)H atom, unlike the K analogue, and so the H atom is positioned on a centre of symmetry between the two O atoms which are 2.475(3) Å apart. However, the H atom refines with a large isotropic displacement parameter (0.083(17) $Å^2$), indicative of some disorder in its position.

The minor polymorph of RbHD crystallises in the monoclinic space group *C*2/*c* (Figure 3(e)). The eight-coordinate Rb ions are organised in layers and coordinated by benzoate anions such that each metal ion is involved in four centrosymmetric Rb_2O_2 rhombus-like motifs, two formed by bonds to non-hydrogen bonded benzoate O atoms (Rb-O: 2.9641(18) and 2.9956(19) Å, angles at Rb and O: 81.1 and 98.9°), and two by longer bonds to the H bonded benzoate O atoms (Rb-O: 3.1561(19) and 3.210(2) Å, angles at Rb and O: 73.8 and 106.2°). The H bonds between these latter rings involve two O atoms 2.456(3) Å apart, and these two O atoms subtend an angle of 44.98(5)° at the Rb position. Difference electron density maps found only one position for the acidic H atom, equidistant from the O atoms and lying on a two-fold axis passing between the O atoms and through the Rb ion and which refined with a high displacement parameter (O···H: 1.249(13) Å, angle at H 159(6)°, 0.07(2) $Å^2$). The benzene rings project to either side of the layer (Figure 3(d)), and the layers are packed along the long *a* axis (29.03 Å) and related by the *C*-centring. Within a layer the benzene rings make edge-to-face contacts with each other, with the planes of benzenes related by the *c* glide lying at 76.8° to each other.

The CsHD analogue has two polymorphs, one monoclinic in space group *C*2/*c* and one orthorhombic in space group *Pbcn*, though their overall crystal packing arrangements are similar (Figures 3(f)-(g)). The monoclinic form is very similar to that of the eight-coordinate RbHD, with the Cs cations linked by two sets of two centrosymmetric Cs_2O_2 rhombus-like motifs into a layer (Figure 2(d)). The Cs-O distances are 3.0631(13), 3.0660(14), 3.2230(14) and 3.2459(15) Å and, as for the Rb salt, the two longer Cs-O distances are to the O atoms involved in the H bonding. The two types of Cs_2O_2 motifs have bond angles at Cs and O of 75.1 and 104.8° and 80.9 and 99.1° similar to RbHD. The two O atoms involved in H bonding are 2.457(2) Å apart. Difference electron density maps found only one position for the acidic H atom located on the two fold axis between the two O atoms (O···H: 1.236(16) Å, angle at H 168(7)°, U_{iso}: 0.076(19) $Å^2$). The benzene rings project from the surface of each layer. The best planes of the two crystallographically distinct benzene rings lie at 83.02° to each other.

For the orthorhombic phase of CsHD at 150 K the unit cell lengths are very similar to those of the monoclinic phase, but the β angle has decreased by 10° (90 vs 99.97°). There is the same mode of linking of Cs ions with bridging O atoms into Cs_2O_2 motifs. The Cs-O bond lengths are a little different (3.063(2), 3.090(2), 3.231(2) and 3.286(2) Å) and in most cases slightly longer than in the monoclinic case. The O···O distance between hydrogen bonded oxygen atoms is identical to the monoclinic case, and only one position for the acidic hydrogen atom was located from difference electron density maps (O···H: 1.233(5) Å, angle at H 170(7)°, U_{iso}: 0.09(2) $Å^2$). The relative orientations of the benzene rings are almost the same (82.63°) and they lie at 76.90° to the Cs ion plane. There is a significant amount of crystallographic evidence for such symmetrical O—H—O hydrogen bonds (*vide supra*), and it is notable that we have both symmetrical and unsymmetrical tight OHO hydrogen bonds among the K, Rb and Cs hydrogen dibenzoates, though we emphasise that for the Rb and Cs salts, there is less certainty in the interpretation of the electron density in the O—H—O region, and the high isotropic displacement parameter for the H atom in these cases may indicate variation in the position of the H atom The nearest comparison is to the neutron diffraction studies on K and Cs hydrogen trifluoroacetates which both show short symmetrical O—H—O hydrogen bonds with O---O separation of 2.436 Å and isotropic displacement parameters of 0.016 $Å^2$ for both salts at 20 K.[4] Future neutron diffraction studies on the hydrogen dibenzoate salts will provide useful further insight.

References

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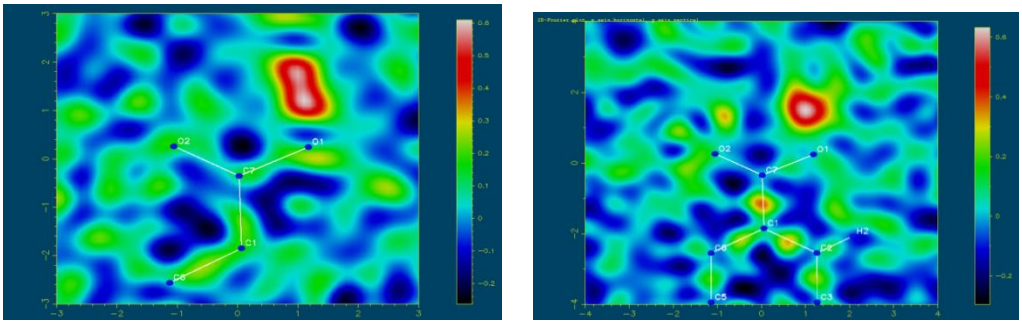
S3: Difference electron density maps for potassium hydrogen dibenzoate (left) and the monoclinic polymorph of cesium hydrogen dibenzoate (right) to locate electron density corresponding to the (O)H atom.[5]



S4: GIPAW DFT (SEDC) and experimentally determined paramters for LiHD. The GIPAW DFT (without the use of the SEDC scheme) calculations are showin in Table 2.

Sample	$\delta_{iso(MAS)}$ $^{1}H^{(a)}$	δ_{iso} ^{1}H CASTEP	$\delta_{iso(MAS)}$ $^{13}C^{(b)}$	$\delta_{iso(CSA)}$ $^{13}C^{(c)}$	δ_{11} ^{13}C	δ_{22} ^{13}C	δ_{33} ^{13}C	$\Omega^{(d)}$	$K^{(d)}$	$\Delta\delta^{(e)}$	$\eta_{\delta}^{(e)}$
Site	=O···^{1}HO	–^{13}COOH	–^{13}COOH	–^{13}COOH	–^{13}COOH	–^{13}COOH	–^{13}COOH				
Error (ppm/±)	±0.25		±0.5	±2	±2	±2	±2	±2	±0.05	±2	±0.05
LiHB	13.00	13.73	173.5	173.5	226.6	189.2	104.6	176.22	237.4	188.2	103.1

S5: The LiHD lattice parameters before and after geometry optimisation.

Parameters	After Lattice Relaxation	Original Lattice Parameters
Cell Length a	5.306663647173393	5.3600(3)
Cell Length b	8.357233498018864	8.5693(7)
Cell Length c	13.391084191542832	13.4999(11)
Cell Angle Alpha	97.471125277253336	98.830(4)
Cell Angle Beta	94.945701269298496	93.800(5)
Cell Angle Gamma	94.187405697170931	95.524(5)

S6: Tables; The atomic positions of LiHD (eith and without SEDC), KHD, RbHD and CsHD before and after geometry optimisations. The absolute difference between the two positions is also given. The change in key bond lengths and angles is presented at the foot of each table.

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Crystallography		Fractional Co-ordiantes				After Geometry Optimisation		Fractional Co-ordinates				Absolute Differences		
		Elmt	x	y	z			Elmt	x	y	z	Δx	Δy	Δz
1	C1	C	0.3403	0.0044	0.3373	1	C1	C	0.3417	0.005	0.3375	0.0014	0.0006	0.0002
2	C1	C	0.6597	0.9956	0.6627	2	C1	C	0.6583	0.995	0.6625	0.0014	0.0006	0.0002
3	C2	C	0.4472	0.9703	0.2467	3	C2	C	0.45	0.9713	0.246	0.0028	0.001	0.0007
4	C2	C	0.5528	0.0297	0.7533	4	C2	C	0.55	0.0287	0.754	0.0028	0.001	0.0007
5	C3	C	0.3373	0.8466	0.1744	5	C3	C	0.3391	0.8486	0.1723	0.0018	0.002	0.0021
6	C3	C	0.6627	0.1534	0.8256	6	C3	C	0.6609	0.1514	0.8277	0.0018	0.002	0.0021
7	C4	C	0.121	0.7565	0.1914	7	C4	C	0.1204	0.7575	0.1896	0.0006	0.001	0.0018
8	C4	C	0.879	0.2435	0.8086	8	C4	C	0.8796	0.2425	0.8104	0.0006	0.001	0.0018
9	C5	C	0.0155	0.79	0.281	9	C5	C	0.0123	0.7904	0.2808	0.0032	0.0004	0.0002
10	C5	C	0.9845	0.21	0.719	10	C5	C	0.9877	0.2096	0.7192	0.0032	0.0004	0.0002
11	C6	C	0.1233	0.9138	0.3542	11	C6	C	0.122	0.914	0.3546	0.0013	0.0002	0.0004
12	C6	C	0.8767	0.0862	0.6458	12	C6	C	0.878	0.086	0.6454	0.0013	0.0002	0.0004
13	C7	C	0.4566	0.1407	0.4128	13	C7	C	0.4588	0.1416	0.4124	0.0022	0.0009	0.0004
14	C7	C	0.5434	0.8593	0.5872	14	C7	C	0.5412	0.8584	0.5876	0.0022	0.0009	0.0004
15	C11	C	0.2738	0.4015	0.2525	15	C11	C	0.276	0.403	0.252	0.0022	0.0015	0.0005
16	C11	C	0.7262	0.5985	0.7475	16	C11	C	0.724	0.597	0.748	0.0022	0.0015	0.0005
17	C12	C	0.4527	0.4233	0.1848	17	C12	C	0.4548	0.4258	0.183	0.0021	0.0025	0.0018
18	C12	C	0.5473	0.5767	0.8152	18	C12	C	0.5452	0.5742	0.817	0.0021	0.0025	0.0018
19	C13	C	0.4171	0.3423	0.0864	19	C13	C	0.4187	0.3435	0.085	0.0016	0.0012	0.0014
20	C13	C	0.5829	0.6577	0.9136	20	C13	C	0.5813	0.6565	0.915	0.0016	0.0012	0.0014
21	C14	C	0.2044	0.2361	0.0567	21	C14	C	0.2052	0.2353	0.0551	0.0008	0.0008	0.0016
22	C14	C	0.7956	0.7639	0.9433	22	C14	C	0.7948	0.7647	0.9449	0.0008	0.0008	0.0016

23	C15	C	0.0266	0.2121	0.1243	23	C15	C	0.0272	0.2113	0.1237		0.0006	0.0008	0.0006
24	C15	C	0.9734	0.7879	0.8757	24	C15	C	0.9728	0.7887	0.8763		0.0006	0.0008	0.0006
25	C16	C	0.0602	0.2948	0.2218	25	C16	C	0.0614	0.2949	0.2216		0.0012	1.00E-04	0.0002
26	C16	C	0.9398	0.7052	0.7782	26	C16	C	0.9386	0.7051	0.7784		0.0012	0.0001	0.0002
27	C17	C	0.315	0.4908	0.3582	27	C17	C	0.3178	0.4928	0.3574		0.0028	0.002	0.0008
28	C17	C	0.685	0.5092	0.6418	28	C17	C	0.6822	0.5072	0.6426		0.0028	0.002	0.0008
29	H1	H	0.411	0.269	0.543	29	H1	H	0.4174	0.2733	0.5401		0.0064	0.0043	0.0029
30	H1	H	0.589	0.731	0.457	30	H1	H	0.5826	0.7267	0.4599		0.0064	0.0043	0.0029
31	H2	H	0.597	0.039	0.2359	31	H2	H	0.6211	0.043	0.2342		0.0241	0.004	0.0017
32	H2	H	0.403	0.961	0.7641	32	H2	H	0.3789	0.957	0.7658		0.0241	0.004	0.0017
33	H3	H	0.41	0.828	0.114	33	H3	H	0.4232	0.8238	0.101		0.0132	0.0042	0.013
34	H3	H	0.59	0.172	0.886	34	H3	H	0.5768	0.1762	0.899		0.0132	0.0042	0.013
35	H4	H	0.044	0.667	0.1363	35	H4	H	0.0358	0.66	0.1319		0.0082	0.007	0.0044
36	H4	H	0.956	0.333	0.8637	36	H4	H	0.9642	0.34	0.8681		0.0082	0.007	0.0044
37	H5	H	0.865	0.727	0.2938	37	H5	H	0.8427	0.7196	0.2952		0.0223	0.0074	0.0014
38	H5	H	0.135	0.273	0.7062	38	H5	H	0.1573	0.2804	0.7048		0.0223	0.0074	0.0014
39	H6	H	0.05	0.938	0.4181	39	H6	H	0.036	0.9394	0.4252		0.014	0.0014	0.0071
40	H6	H	0.95	0.062	0.5819	40	H6	H	0.964	0.0606	0.5748		0.014	0.0014	0.0071
41	H12	H	0.602	0.5	0.2057	41	H12	H	0.6222	0.5088	0.2071		0.0202	0.0088	0.0014
42	H12	H	0.398	0.5	0.7943	42	H12	H	0.3778	0.4912	0.7929		0.0202	0.0088	0.0014
43	H13	H	0.55	0.358	0.0375	43	H13	H	0.5585	0.3637	0.0319		0.0085	0.0057	0.0056
44	H13	H	0.45	0.642	0.9625	44	H13	H	0.4415	0.6363	0.9681		0.0085	0.0057	0.0056
45	H14	H	0.187	0.177	0.9871	45	H14	H	0.1773	0.17	0.9786		0.0097	0.007	0.0085
46	H14	H	0.813	0.823	0.0129	46	H14	H	0.8227	0.83	0.0214		0.0097	0.007	0.0085
47	H15	H	0.939	0.272	0.2719	47	H15	H	0.923	0.2743	0.275		0.016	0.0023	0.0031
48	H15	H	0.061	0.728	0.7281	48	H15	H	0.077	0.7257	0.725		0.016	0.0023	0.0031
49	H61	H	0.879	0.132	0.1036	49	H61	H	0.8604	0.1267	0.1007		0.0186	0.0053	0.0029

50	H61	H	0.121	0.868	0.8964	50	H61	H	0.1396	0.8733	0.8993		0.0186	0.0053	0.0029
51	Li1	Li	0.7918	0.4407	0.4387	51	Li1	Li	0.7952	0.4407	0.4376		0.0034	0	0.0011
52	Li1	Li	0.2082	0.5593	0.5613	52	Li1	Li	0.2048	0.5593	0.5624		0.0034	0	0.0011
53	O1	O	0.3417	0.1645	0.496	53	O1	O	0.3426	0.1682	0.4958		0.0009	0.0037	0.0002
54	O1	O	0.6583	0.8355	0.504	54	O1	O	0.6574	0.8318	0.5042		0.0009	0.0037	0.0002
55	O2	O	0.6437	0.2258	0.3972	55	O2	O	0.6486	0.226	0.3963		0.0049	0.0002	0.0009
56	O2	O	0.3563	0.7742	0.6028	56	O2	O	0.3514	0.774	0.6037		0.0049	0.0002	0.0009
57	O3	O	0.5327	0.5632	0.3867	57	O3	O	0.5374	0.5657	0.3853		0.0047	0.0025	0.0014
58	O3	O	0.4673	0.4368	0.6133	58	O3	O	0.4626	0.4343	0.6147		0.0047	0.0025	0.0014
59	O4	O	0.1375	0.4886	0.4146	59	O4	O	0.1401	0.4918	0.4146		0.0026	0.0032	0
60	O4	O	0.8625	0.5114	0.5854	60	O4	O	0.8599	0.5082	0.5854		0.0026	0.0032	0
												Max Value	**0.0241**	**0.0088**	**0.013**
												In Angstoms	**0.129176**	**0.07540984**	**0.1754987**

Lattice Parameters	a	b	c
	5.36	8.5693	13.4999

OHO	1.032	A
	1.566	
OHO	163.81	degrees
O-O	2.579	A
O-C-O	1.322	A
	1.241	
M-O x2 /Å	1.988	A
	87.215	

		89.579	degrees
	M2O2	1.915	A

Li Hydrogen Dibenzoate SEDC Scheme

Crystallography		Fractional Co-ordiantes			
		Elmt	x	y	z
1	C1	C	0.3403	0.0044	0.3373
2	C1	C	0.6597	0.9956	0.6627
3	C2	C	0.4472	0.9703	0.2467
4	C2	C	0.5528	0.0297	0.7533
5	C3	C	0.3373	0.8466	0.1744
6	C3	C	0.6627	0.1534	0.8256
7	C4	C	0.121	0.7565	0.1914
8	C4	C	0.879	0.2435	0.8086
9	C5	C	0.0155	0.79	0.281
10	C5	C	0.9845	0.21	0.719
11	C6	C	0.1233	0.9138	0.3542
12	C6	C	0.8767	0.0862	0.6458
13	C7	C	0.4566	0.1407	0.4128
14	C7	C	0.5434	0.8593	0.5872
15	C11	C	0.2738	0.4015	0.2525
16	C11	C	0.7262	0.5985	0.7475
17	C12	C	0.4527	0.4233	0.1848
18	C12	C	0.5473	0.5767	0.8152
19	C13	C	0.4171	0.3423	0.0864
20	C13	C	0.5829	0.6577	0.9136
21	C14	C	0.2044	0.2361	0.0567
22	C14	C	0.7956	0.7639	0.9433
23	C15	C	0.0266	0.2121	0.1243
24	C15	C	0.9734	0.7879	0.8757

After Geometry Optimisation		Fractional Co-ordinates			
		Elmt	x	y	z
1	C1	C	0.3414	0.0044	0.3377
2	C1	C	0.6586	0.9956	0.6623
3	C2	C	0.4496	0.9716	0.2463
4	C2	C	0.5504	0.0284	0.7537
5	C3	C	0.3381	0.8488	0.1723
6	C3	C	0.6619	0.1512	0.8277
7	C4	C	0.1185	0.7574	0.1893
8	C4	C	0.8815	0.2426	0.8107
9	C5	C	0.0093	0.7903	0.2802
10	C5	C	0.9907	0.2097	0.7198
11	C6	C	0.1201	0.9136	0.3543
12	C6	C	0.8799	0.0864	0.6457
13	C7	C	0.4608	0.1388	0.4139
14	C7	C	0.5392	0.8612	0.5861
15	C11	C	0.277	0.4034	0.2515
16	C11	C	0.723	0.5966	0.7485
17	C12	C	0.4551	0.4262	0.1822
18	C12	C	0.5449	0.5738	0.8178
19	C13	C	0.419	0.3428	0.0845
20	C13	C	0.581	0.6572	0.9155
21	C14	C	0.205	0.2338	0.055
22	C14	C	0.795	0.7662	0.945
23	C15	C	0.0269	0.2102	0.1237
24	C15	C	0.9731	0.7898	0.8763

25	C16	C	0.0602	0.2948	0.2218
26	C16	C	0.9398	0.7052	0.7782
27	C17	C	0.315	0.4908	0.3582
28	C17	C	0.685	0.5092	0.6418
29	H1	H	0.411	0.269	0.543
30	H1	H	0.589	0.731	0.457
31	H2	H	0.597	0.039	0.2359
32	H2	H	0.403	0.961	0.7641
33	H3	H	0.41	0.828	0.114
34	H3	H	0.59	0.172	0.886
35	H4	H	0.044	0.667	0.1363
36	H4	H	0.956	0.333	0.8637
37	H5	H	0.865	0.727	0.2938
38	H5	H	0.135	0.273	0.7062
39	H6	H	0.05	0.938	0.4181
40	H6	H	0.95	0.062	0.5819
41	H12	H	0.602	0.5	0.2057
42	H12	H	0.398	0.5	0.7943
43	H13	H	0.55	0.358	0.0375
44	H13	H	0.45	0.642	0.9625
45	H14	H	0.187	0.177	0.9871
46	H14	H	0.813	0.823	0.0129
47	H15	H	0.939	0.272	0.2719
48	H15	H	0.061	0.728	0.7281
49	H61	H	0.879	0.132	0.1036
50	H61	H	0.121	0.868	0.8964
51	Li1	Li	0.7918	0.4407	0.4387

25	C16	C	0.0623	0.2945	0.2215
26	C16	C	0.9377	0.7055	0.7785
27	C17	C	0.3201	0.4948	0.3565
28	C17	C	0.6799	0.5052	0.6435
29	H1	H	0.4133	0.2717	0.5409
30	H1	H	0.5867	0.7283	0.4591
31	H2	H	0.6201	0.0442	0.2345
32	H2	H	0.3799	0.9558	0.7655
33	H3	H	0.4224	0.8237	0.1012
34	H3	H	0.5776	0.1763	0.8988
35	H4	H	0.0346	0.6588	0.132
36	H4	H	0.9654	0.3412	0.868
37	H5	H	0.8391	0.7191	0.2943
38	H5	H	0.1609	0.2809	0.7057
39	H6	H	0.0346	0.9385	0.4249
40	H6	H	0.9654	0.0615	0.5751
41	H12	H	0.6214	0.5109	0.2058
42	H12	H	0.3786	0.4891	0.7942
43	H13	H	0.559	0.363	0.0314
44	H13	H	0.441	0.637	0.9686
45	H14	H	0.1761	0.1678	0.9786
46	H14	H	0.8239	0.8322	0.0214
47	H15	H	0.9252	0.2729	0.2754
48	H15	H	0.0748	0.7271	0.7246
49	H61	H	0.8599	0.1252	0.1009
50	H61	H	0.1401	0.8748	0.8991
51	Li1	Li	0.8048	0.4349	0.439

52	Li1	Li	0.2082	0.5593	0.5613
53	O1	O	0.3417	0.1645	0.496
54	O1	O	0.6583	0.8355	0.504
55	O2	O	0.6437	0.2258	0.3972
56	O2	O	0.3563	0.7742	0.6028
57	O3	O	0.5327	0.5632	0.3867
58	O3	O	0.4673	0.4368	0.6133
59	O4	O	0.1375	0.4886	0.4146
60	O4	O	0.8625	0.5114	0.5854

Lattice Parameters	a	b	c
	5.36	8.5693	13.4999
	alpha	beta	gamma
	98.83	93.8	95.524

52	Li1	Li	0.1952	0.5651	0.561
53	O1	O	0.3371	0.1676	0.495
54	O1	O	0.6629	0.8324	0.505
55	O2	O	0.6585	0.2194	0.401
56	O2	O	0.3415	0.7806	0.599
57	O3	O	0.5402	0.5687	0.3838
58	O3	O	0.4598	0.4313	0.6162
59	O4	O	0.1426	0.4937	0.4139
60	O4	O	0.8574	0.5063	0.5861

Lattice Parameters	a	b	c
	5.30666	8.35723	13.39108
	alpha	beta	gamma
	97.471	94.946	94.187

Potassium Hydrogen Dibenzoate

Crystallography		Fractional Co-ordiantes			
		Elmt	x	y	z
1	C1	C	0.6142	0.2898	0.0388
2	C1	C	0.1142	0.7898	0.0388
3	C1	C	0.3858	0.2898	0.4612
4	C1	C	0.8858	0.7898	0.4612
5	C1	C	0.3858	0.7102	0.9612
6	C1	C	0.8858	0.2102	0.9612
7	C1	C	0.6142	0.7102	0.5388
8	C1	C	0.1142	0.2102	0.5388
9	C2	C	0.6454	0.1392	0.9694
10	C2	C	0.1454	0.6392	0.9694
11	C2	C	0.3546	0.1392	0.5306
12	C2	C	0.8546	0.6392	0.5306
13	C2	C	0.3546	0.8608	0.0306
14	C2	C	0.8546	0.3608	0.0306
15	C2	C	0.6454	0.8608	0.4694
16	C2	C	0.1454	0.3608	0.4694
17	C3	C	0.6904	0.0906	0.0183
18	C3	C	0.1904	0.5906	0.0183
19	C3	C	0.3096	0.0906	0.4817
20	C3	C	0.8096	0.5906	0.4817
21	C3	C	0.3096	0.9094	0.9817
22	C3	C	0.8096	0.4094	0.9817
23	C3	C	0.6904	0.9094	0.5183
24	C3	C	0.1904	0.4094	0.5183

After Geometry Optimisation			Fractional Co-ordinates		
		Elmt	x	y	z
1	C1	C	0.6139	0.2894	0.0384
2	C1	C	0.1139	0.7894	0.0384
3	C1	C	0.3861	0.2894	0.4616
4	C1	C	0.8861	0.7894	0.4616
5	C1	C	0.3861	0.7106	0.9616
6	C1	C	0.8861	0.2106	0.9616
7	C1	C	0.6139	0.7106	0.5384
8	C1	C	0.1139	0.2106	0.5384
9	C2	C	0.6452	0.1384	0.9688
10	C2	C	0.1452	0.6384	0.9688
11	C2	C	0.3548	0.1384	0.5312
12	C2	C	0.8548	0.6384	0.5312
13	C2	C	0.3548	0.8616	0.0312
14	C2	C	0.8548	0.3616	0.0312
15	C2	C	0.6452	0.8616	0.4688
16	C2	C	0.1452	0.3616	0.4688
17	C3	C	0.6904	0.0918	0.0178
18	C3	C	0.1904	0.5918	0.0178
19	C3	C	0.3096	0.0918	0.4822
20	C3	C	0.8096	0.5918	0.4822
21	C3	C	0.3096	0.9082	0.9822
22	C3	C	0.8096	0.4082	0.9822
23	C3	C	0.6904	0.9082	0.5178
24	C3	C	0.1904	0.4082	0.5178

Absolute Differences		
Δx	Δy	Δz
0.0003	0.0004	0.0004
0.0003	0.0004	0.0004
0.0003	0.0004	0.0004
0.0003	0.0004	0.0004
0.0003	0.0004	0.0004
0.0003	0.0004	0.0004
0.0003	0.0004	0.0004
0.0003	0.0004	0.0004
0.0002	0.0008	0.0006
0.0002	0.0008	0.0006
0.0002	0.0008	0.0006
0.0002	0.0008	0.0006
0.0002	0.0008	0.0006
0.0002	0.0008	0.0006
0.0002	0.0008	0.0006
0.0002	0.0008	0.0006
0	0.0012	0.0005
0	0.0012	0.0005
0	0.0012	0.0005
0	0.0012	0.0005
0	0.0012	0.0005
0	0.0012	0.0005
0	0.0012	0.0005
0	0.0012	0.0005

25	C4	C	0.7046	0.1941	0.1374		25	C4	C	0.7046	0.1974	0.1367		0	0.0033	0.0007
26	C4	C	0.2046	0.6941	0.1374		26	C4	C	0.2046	0.6974	0.1367		0	0.0033	0.0007
27	C4	C	0.2954	0.1941	0.3626		27	C4	C	0.2954	0.1974	0.3633		0	0.0033	0.0007
28	C4	C	0.7954	0.6941	0.3626		28	C4	C	0.7954	0.6974	0.3633		0	0.0033	0.0007
29	C4	C	0.2954	0.8059	0.8626		29	C4	C	0.2954	0.8026	0.8633		0	0.0033	0.0007
30	C4	C	0.7954	0.3059	0.8626		30	C4	C	0.7954	0.3026	0.8633		0	0.0033	0.0007
31	C4	C	0.7046	0.8059	0.6374		31	C4	C	0.7046	0.8026	0.6367		0	0.0033	0.0007
32	C4	C	0.2046	0.3059	0.6374		32	C4	C	0.2046	0.3026	0.6367		0	0.0033	0.0007
33	C5	C	0.6737	0.3425	0.2068		33	C5	C	0.6735	0.3474	0.2064		0.0002	0.0049	0.0004
34	C5	C	0.1737	0.8425	0.2068		34	C5	C	0.1735	0.8474	0.2064		0.0002	0.0049	0.0004
35	C5	C	0.3263	0.3425	0.2932		35	C5	C	0.3265	0.3474	0.2936		0.0002	0.0049	0.0004
36	C5	C	0.8263	0.8425	0.2932		36	C5	C	0.8265	0.8474	0.2936		0.0002	0.0049	0.0004
37	C5	C	0.3263	0.6575	0.7932		37	C5	C	0.3265	0.6526	0.7936		0.0002	0.0049	0.0004
38	C5	C	0.8263	0.1575	0.7932		38	C5	C	0.8265	0.1526	0.7936		0.0002	0.0049	0.0004
39	C5	C	0.6737	0.6575	0.7068		39	C5	C	0.6735	0.6526	0.7064		0.0002	0.0049	0.0004
40	C5	C	0.1737	0.1575	0.7068		40	C5	C	0.1735	0.1526	0.7064		0.0002	0.0049	0.0004
41	C6	C	0.6285	0.3893	0.1587		41	C6	C	0.6282	0.3924	0.158		0.0003	0.0031	0.0007
42	C6	C	0.1285	0.8893	0.1587		42	C6	C	0.1282	0.8924	0.158		0.0003	0.0031	0.0007
43	C6	C	0.3715	0.3893	0.3413		43	C6	C	0.3718	0.3924	0.342		0.0003	0.0031	0.0007
44	C6	C	0.8715	0.8893	0.3413		44	C6	C	0.8718	0.8924	0.342		0.0003	0.0031	0.0007
45	C6	C	0.3715	0.6107	0.8413		45	C6	C	0.3718	0.6076	0.842		0.0003	0.0031	0.0007
46	C6	C	0.8715	0.1107	0.8413		46	C6	C	0.8718	0.1076	0.842		0.0003	0.0031	0.0007
47	C6	C	0.6285	0.6107	0.6587		47	C6	C	0.6282	0.6076	0.658		0.0003	0.0031	0.0007
48	C6	C	0.1285	0.1107	0.6587		48	C6	C	0.1282	0.1076	0.658		0.0003	0.0031	0.0007
49	C7	C	0.5662	0.3463	0.983		49	C7	C	0.566	0.3463	0.9821		0.0002	0	0.0009
50	C7	C	0.0662	0.8463	0.983		50	C7	C	0.066	0.8463	0.9821		0.0002	0	0.0009
51	C7	C	0.4338	0.3463	0.517		51	C7	C	0.434	0.3463	0.5179		0.0002	0	0.0009

52	C7	C	0.9338	0.8463	0.517	52	C7	C	0.934	0.8463	0.5179	0.0002	0	0.0009
53	C7	C	0.4338	0.6537	0.017	53	C7	C	0.434	0.6537	0.0179	0.0002	0	0.0009
54	C7	C	0.9338	0.1537	0.017	54	C7	C	0.934	0.1537	0.0179	0.0002	0	0.0009
55	C7	C	0.5662	0.6537	0.483	55	C7	C	0.566	0.6537	0.4821	0.0002	0	0.0009
56	C7	C	0.0662	0.1537	0.483	56	C7	C	0.066	0.1537	0.4821	0.0002	0	0.0009
57	H1	H	0.5	0.5	0	57	H1	H	0.5	0.5	0	0	0	0
58	H1	H	0	0	0	58	H1	H	0	0	0	0	0	0
59	H1	H	0.5	0.5	0.5	59	H1	H	0.5	0.5	0.5	0	0	0
60	H1	H	0	0	0.5	60	H1	H	0	0	0.5	0	0	0
61	H1	H	1	0	0	61	H1	H	1	0	0	0	0	0
62	H1	H	1	0	0.5	62	H1	H	1	0	0.5	0	0	0
63	H1	H	0	1	0	63	H1	H	0	1	0	0	0	0
64	H1	H	0	1	0.5	64	H1	H	0	1	0.5	0	0	0
65	H1	H	1	1	0	65	H1	H	1	1	0	0	0	0
66	H1	H	1	1	0.5	66	H1	H	1	1	0.5	0	0	0
67	H1	H	0.5	0.5	1	67	H1	H	0.5	0.5	1	0	0	0
68	H1	H	0	0	1	68	H1	H	0	0	1	0	0	0
69	H1	H	1	0	1	69	H1	H	1	0	1	0	0	0
70	H1	H	0	1	1	70	H1	H	0	1	1	0	0	0
71	H1	H	1	1	1	71	H1	H	1	1	1	0	0	0
72	H2	H	0.6346	0.07	0.887	72	H2	H	0.6334	0.0593	0.876	0.0012	0.0107	0.011
73	H2	H	0.1346	0.57	0.887	73	H2	H	0.1334	0.5593	0.876	0.0012	0.0107	0.011
74	H2	H	0.3654	0.07	0.613	74	H2	H	0.3666	0.0593	0.624	0.0012	0.0107	0.011
75	H2	H	0.8654	0.57	0.613	75	H2	H	0.8666	0.5593	0.624	0.0012	0.0107	0.011
76	H2	H	0.3654	0.93	0.113	76	H2	H	0.3666	0.9407	0.124	0.0012	0.0107	0.011
77	H2	H	0.8654	0.43	0.113	77	H2	H	0.8666	0.4407	0.124	0.0012	0.0107	0.011
78	H2	H	0.6346	0.93	0.387	78	H2	H	0.6334	0.9407	0.376	0.0012	0.0107	0.011

79	H2	H	0.1346	0.43	0.387	79	H2	H	0.1334	0.4407	0.376	0.0012	0.0107	0.011
80	H3	H	0.712	0.989	0.971	80	H3	H	0.7146	0.9727	0.9636	0.0026	0.0163	0.0074
81	H3	H	0.212	0.489	0.971	81	H3	H	0.2146	0.4727	0.9636	0.0026	0.0163	0.0074
82	H3	H	0.288	0.989	0.529	82	H3	H	0.2854	0.9727	0.5364	0.0026	0.0163	0.0074
83	H3	H	0.788	0.489	0.529	83	H3	H	0.7854	0.4727	0.5364	0.0026	0.0163	0.0074
84	H3	H	0.288	0.011	0.029	84	H3	H	0.2854	0.0273	0.0364	0.0026	0.0163	0.0074
85	H3	H	0.788	0.511	0.029	85	H3	H	0.7854	0.5273	0.0364	0.0026	0.0163	0.0074
86	H3	H	0.712	0.011	0.471	86	H3	H	0.7146	0.0273	0.4636	0.0026	0.0163	0.0074
87	H3	H	0.212	0.511	0.471	87	H3	H	0.2146	0.5273	0.4636	0.0026	0.0163	0.0074
88	H4	H	0.7375	0.164	0.1694	88	H4	H	0.74	0.163	0.1753	0.0025	0.001	0.0059
89	H4	H	0.2375	0.664	0.1694	89	H4	H	0.24	0.663	0.1753	0.0025	0.001	0.0059
90	H4	H	0.2625	0.164	0.3306	90	H4	H	0.26	0.163	0.3247	0.0025	0.001	0.0059
91	H4	H	0.7625	0.664	0.3306	91	H4	H	0.76	0.663	0.3247	0.0025	0.001	0.0059
92	H4	H	0.2625	0.836	0.8306	92	H4	H	0.26	0.837	0.8247	0.0025	0.001	0.0059
93	H4	H	0.7625	0.336	0.8306	93	H4	H	0.76	0.337	0.8247	0.0025	0.001	0.0059
94	H4	H	0.7375	0.836	0.6694	94	H4	H	0.74	0.837	0.6753	0.0025	0.001	0.0059
95	H4	H	0.2375	0.336	0.6694	95	H4	H	0.24	0.337	0.6753	0.0025	0.001	0.0059
96	H5	H	0.6828	0.43	0.289	96	H5	H	0.6846	0.4325	0.2991	0.0018	0.0025	0.0101
97	H5	H	0.1828	0.93	0.289	97	H5	H	0.1846	0.9325	0.2991	0.0018	0.0025	0.0101
98	H5	H	0.3172	0.43	0.211	98	H5	H	0.3154	0.4325	0.2009	0.0018	0.0025	0.0101
99	H5	H	0.8172	0.93	0.211	99	H5	H	0.8154	0.9325	0.2009	0.0018	0.0025	0.0101
100	H5	H	0.3172	0.57	0.711	100	H5	H	0.3154	0.5675	0.7009	0.0018	0.0025	0.0101
101	H5	H	0.8172	0.07	0.711	101	H5	H	0.8154	0.0675	0.7009	0.0018	0.0025	0.0101
102	H5	H	0.6828	0.57	0.789	102	H5	H	0.6846	0.5675	0.7991	0.0018	0.0025	0.0101
103	H5	H	0.1828	0.07	0.789	103	H5	H	0.1846	0.0675	0.7991	0.0018	0.0025	0.0101
104	H6	H	0.607	0.501	0.204	104	H6	H	0.6039	0.5125	0.2119	0.0031	0.0115	0.0079
105	H6	H	0.107	0.001	0.204	105	H6	H	0.1039	0.0125	0.2119	0.0031	0.0115	0.0079

106	H6	H	0.393	0.501	0.296		106	H6	H	0.3961	0.5125	0.2881		0.0031	0.0115	0.0079
107	H6	H	0.893	0.001	0.296		107	H6	H	0.8961	0.0125	0.2881		0.0031	0.0115	0.0079
108	H6	H	0.393	0.499	0.796		108	H6	H	0.3961	0.4875	0.7881		0.0031	0.0115	0.0079
109	H6	H	0.893	0.999	0.796		109	H6	H	0.8961	0.9875	0.7881		0.0031	0.0115	0.0079
110	H6	H	0.607	0.499	0.704		110	H6	H	0.6039	0.4875	0.7119		0.0031	0.0115	0.0079
111	H6	H	0.107	0.999	0.704		111	H6	H	0.1039	0.9875	0.7119		0.0031	0.0115	0.0079
112	K1	K	0.5	0.1789	0.25		112	K1	K	0.5	0.1776	0.25		0	0.0013	0
113	K1	K	0	0.6789	0.25		113	K1	K	0	0.6776	0.25		0	0.0013	0
114	K1	K	0.5	0.8211	0.75		114	K1	K	0.5	0.8224	0.75		0	0.0013	0
115	K1	K	0	0.3211	0.75		115	K1	K	0	0.3224	0.75		0	0.0013	0
116	K1	K	1	0.6789	0.25		116	K1	K	1	0.6776	0.25		0	0.0013	0
117	K1	K	1	0.3211	0.75		117	K1	K	1	0.3224	0.75		0	0.0013	0
118	O1	O	0.538	0.4533	0.0553		118	O1	O	0.5376	0.4527	0.055		0.0004	0.0006	0.0003
119	O1	O	0.038	0.9533	0.0553		119	O1	O	0.0376	0.9527	0.055		0.0004	0.0006	0.0003
120	O1	O	0.462	0.4533	0.4447		120	O1	O	0.4624	0.4527	0.445		0.0004	0.0006	0.0003
121	O1	O	0.962	0.9533	0.4447		121	O1	O	0.9624	0.9527	0.445		0.0004	0.0006	0.0003
122	O1	O	0.462	0.5467	0.9447		122	O1	O	0.4624	0.5473	0.945		0.0004	0.0006	0.0003
123	O1	O	0.962	0.0467	0.9447		123	O1	O	0.9624	0.0473	0.945		0.0004	0.0006	0.0003
124	O1	O	0.538	0.5467	0.5553		124	O1	O	0.5376	0.5473	0.555		0.0004	0.0006	0.0003
125	O1	O	0.038	0.0467	0.5553		125	O1	O	0.0376	0.0473	0.555		0.0004	0.0006	0.0003
126	O2	O	0.555	0.2978	0.8727		126	O2	O	0.555	0.2971	0.871		0	0.0007	0.0017
127	O2	O	0.055	0.7978	0.8727		127	O2	O	0.055	0.7971	0.871		0	0.0007	0.0017
128	O2	O	0.445	0.2978	0.6273		128	O2	O	0.445	0.2971	0.629		0	0.0007	0.0017
129	O2	O	0.945	0.7978	0.6273		129	O2	O	0.945	0.7971	0.629		0	0.0007	0.0017
130	O2	O	0.445	0.7022	0.1273		130	O2	O	0.445	0.7029	0.129		0	0.0007	0.0017
131	O2	O	0.945	0.2022	0.1273		131	O2	O	0.945	0.2029	0.129		0	0.0007	0.0017
132	O2	O	0.555	0.7022	0.3727		132	O2	O	0.555	0.7029	0.371		0	0.0007	0.0017

133	O2	O	0.055	0.2022	0.3727

133	O2	O	0.055	0.2029	0.371

	0	0.0007	0.0017
Max Value	**0.0031**	**0.0163**	**0.011**
In Angstoms	**0.0917166**	**0.06188132**	**0.1223354**

Lattice Parameters	a	b	c
	29.586	3.7964	11.1214

OHO	1.214	A
	1.214	
OHO	180	degrees
O-O	2.428	A
O-C-O	1.252	A
	1.304	A
M-O x2 /Å	2.761	A
	87.524	degrees
	89.579	degrees
	97.952	degrees
M2O2	2.81	A

Rubidium Hydrogen Dibenzoate

Crystallography		Fractional Co-ordiantes			
		Elmt	x	y	z
1	C1	C	0.1173	0.2401	0.2682
2	C1	C	0.8827	0.2401	0.2318
3	C1	C	0.8827	0.7599	0.7318
4	C1	C	0.1173	0.7599	0.7682
5	C1	C	0.6173	0.7401	0.2682
6	C1	C	0.3827	0.7401	0.2318
7	C1	C	0.3827	0.2599	0.7318
8	C1	C	0.6173	0.2599	0.7682
9	C2	C	0.1294	0.352	0.1098
10	C2	C	0.8706	0.352	0.3902
11	C2	C	0.8706	0.648	0.8902
12	C2	C	0.1294	0.648	0.6098
13	C2	C	0.6294	0.852	0.1098
14	C2	C	0.3706	0.852	0.3902
15	C2	C	0.3706	0.148	0.8902
16	C2	C	0.6294	0.148	0.6098
17	C3	C	0.1758	0.3589	0.0775
18	C3	C	0.8242	0.3589	0.4225
19	C3	C	0.8242	0.6411	0.9225
20	C3	C	0.1758	0.6411	0.5775
21	C3	C	0.6758	0.8589	0.0775
22	C3	C	0.3242	0.8589	0.4225
23	C3	C	0.3242	0.1411	0.9225
24	C3	C	0.6758	0.1411	0.5775

After Geometry Optimisation		Fractional Co-ordinates			
		Elmt	x	y	z
1	C1	C	0.1171	0.2387	0.2689
2	C1	C	0.8829	0.2387	0.2311
3	C1	C	0.8829	0.7613	0.7311
4	C1	C	0.1171	0.7613	0.7689
5	C1	C	0.6171	0.7387	0.2689
6	C1	C	0.3829	0.7387	0.2311
7	C1	C	0.3829	0.2613	0.7311
8	C1	C	0.6171	0.2613	0.7689
9	C2	C	0.1292	0.3494	0.1086
10	C2	C	0.8708	0.3494	0.3914
11	C2	C	0.8708	0.6506	0.8914
12	C2	C	0.1292	0.6506	0.6086
13	C2	C	0.6292	0.8494	0.1086
14	C2	C	0.3708	0.8494	0.3914
15	C2	C	0.3708	0.1506	0.8914
16	C2	C	0.6292	0.1506	0.6086
17	C3	C	0.1754	0.3578	0.0762
18	C3	C	0.8246	0.3578	0.4238
19	C3	C	0.8246	0.6422	0.9238
20	C3	C	0.1754	0.6422	0.5762
21	C3	C	0.6754	0.8578	0.0762
22	C3	C	0.3246	0.8578	0.4238
23	C3	C	0.3246	0.1422	0.9238
24	C3	C	0.6754	0.1422	0.5762

Absolute Differences		
Δx	Δy	Δz
0.0002	0.0014	0.0007
0.0002	0.0014	0.0007
0.0002	0.0014	0.0007
0.0002	0.0014	0.0007
0.0002	0.0014	0.0007
0.0002	0.0014	0.0007
0.0002	0.0014	0.0007
0.0002	0.0014	0.0007
0.0002	0.0026	0.0012
0.0002	0.0026	0.0012
0.0002	0.0026	0.0012
0.0002	0.0026	0.0012
0.0002	0.0026	0.0012
0.0002	0.0026	0.0012
0.0002	0.0026	0.0012
0.0002	0.0026	0.0012
0.0004	0.0011	0.0013
0.0004	0.0011	0.0013
0.0004	0.0011	0.0013
0.0004	0.0011	0.0013
0.0004	0.0011	0.0013
0.0004	0.0011	0.0013
0.0004	0.0011	0.0013
0.0004	0.0011	0.0013

25	C4	C	0.2098	0.2569	0.2047	25	C4	C	0.21	0.2569	0.2055		0.0002	0	0.0008
26	C4	C	0.7902	0.2569	0.2953	26	C4	C	0.79	0.2569	0.2945		0.0002	0	0.0008
27	C4	C	0.7902	0.7431	0.7953	27	C4	C	0.79	0.7431	0.7945		0.0002	0	0.0008
28	C4	C	0.2098	0.7431	0.7047	28	C4	C	0.21	0.7431	0.7055		0.0002	0	0.0008
29	C4	C	0.7098	0.7569	0.2047	29	C4	C	0.71	0.7569	0.2055		0.0002	0	0.0008
30	C4	C	0.2902	0.7569	0.2953	30	C4	C	0.29	0.7569	0.2945		0.0002	0	0.0008
31	C4	C	0.2902	0.2431	0.7953	31	C4	C	0.29	0.2431	0.7945		0.0002	0	0.0008
32	C4	C	0.7098	0.2431	0.7047	32	C4	C	0.71	0.2431	0.7055		0.0002	0	0.0008
33	C5	C	0.1977	0.1454	0.363	33	C5	C	0.198	0.1456	0.3647		0.0003	0.0002	0.0017
34	C5	C	0.8023	0.1454	0.137	34	C5	C	0.802	0.1456	0.1353		0.0003	0.0002	0.0017
35	C5	C	0.8023	0.8546	0.637	35	C5	C	0.802	0.8544	0.6353		0.0003	0.0002	0.0017
44	C5	C	0.1977	0.8546	0.863	36	C5	C	0.198	0.8544	0.8647		0.0003	0.0002	0.0017
37	C5	C	0.6977	0.6454	0.363	37	C5	C	0.698	0.6456	0.3647		0.0003	0.0002	0.0017
36	C5	C	0.3023	0.6454	0.137	38	C5	C	0.302	0.6456	0.1353		0.0003	0.0002	0.0017
39	C5	C	0.3023	0.3546	0.637	39	C5	C	0.302	0.3544	0.6353		0.0003	0.0002	0.0017
40	C5	C	0.6977	0.3546	0.863	40	C5	C	0.698	0.3544	0.8647		0.0003	0.0002	0.0017
41	C6	C	0.1515	0.1364	0.3948	41	C6	C	0.1517	0.1354	0.396		0.0002	0.001	0.0012
42	C6	C	0.8485	0.1364	0.1052	42	C6	C	0.8483	0.1354	0.104		0.0002	0.001	0.0012
43	C6	C	0.8485	0.8636	0.6052	43	C6	C	0.8483	0.8646	0.604		0.0002	0.001	0.0012
47	C6	C	0.1515	0.8636	0.8948	44	C6	C	0.1517	0.8646	0.896		0.0002	0.001	0.0012
45	C6	C	0.6515	0.6364	0.3948	45	C6	C	0.6517	0.6354	0.396		0.0002	0.001	0.0012
38	C6	C	0.3485	0.6364	0.1052	46	C6	C	0.3483	0.6354	0.104		0.0002	0.001	0.0012
46	C6	C	0.3485	0.3636	0.6052	47	C6	C	0.3483	0.3646	0.604		0.0002	0.001	0.0012
48	C6	C	0.6515	0.3636	0.8948	48	C6	C	0.6517	0.3646	0.896		0.0002	0.001	0.0012
49	C7	C	0.0676	0.2312	0.3065	49	C7	C	0.0677	0.2297	0.3083		0.0001	0.0015	0.0018
50	C7	C	0.9324	0.2312	0.1935	50	C7	C	0.9323	0.2297	0.1917		1.00E-04	0.0015	0.0018
51	C7	C	0.9324	0.7688	0.6935	51	C7	C	0.9323	0.7703	0.6917		1.00E-04	0.0015	0.0018

52	C7	C	0.0676	0.7688	0.8065		52	C7	C	0.0677	0.7703	0.8083		0.0001	0.0015	0.0018
53	C7	C	0.5676	0.7312	0.3065		53	C7	C	0.5677	0.7297	0.3082		1.00E-04	0.0015	0.0017
54	C7	C	0.4324	0.7312	0.1935		54	C7	C	0.4323	0.7297	0.1918		1.00E-04	0.0015	0.0017
55	C7	C	0.4324	0.2688	0.6935		55	C7	C	0.4323	0.2703	0.6918		1.00E-04	0.0015	0.0017
56	C7	C	0.5676	0.2688	0.8065		56	C7	C	0.5677	0.2703	0.8082		1.00E-04	0.0015	0.0017
57	H1	H	0	0.319	0.25		57	H1	H	0	0.3392	0.25		**0**	**0.0202**	**0**
58	H1	H	0	0.681	0.75		58	H1	H	0	0.6608	0.75		**0**	**0.0202**	**0**
59	H1	H	1	0.319	0.25		59	H1	H	1	0.3392	0.25		**0**	**0.0202**	**0**
60	H1	H	1	0.681	0.75		60	H1	H	1	0.6608	0.75		**0**	**0.0202**	**0**
61	H1	H	0.5	0.819	0.25		61	H1	H	0.5	0.8392	0.25		**0**	**0.0202**	**0**
62	H1	H	0.5	0.181	0.75		62	H1	H	0.5	0.1608	0.75		**0**	**0.0202**	**0**
63	H2	H	0.1062	0.4235	0.0239		63	H2	H	0.1022	0.4289	0.0093		0.004	0.0054	0.0146
64	H2	H	0.8938	0.4235	0.4761		64	H2	H	0.8978	0.4289	0.4907		0.004	0.0054	0.0146
65	H2	H	0.8938	0.5765	0.9761		65	H2	H	0.8978	0.5711	0.9907		0.004	0.0054	0.0146
66	H2	H	0.1062	0.5765	0.5239		66	H2	H	0.1022	0.5711	0.5093		0.004	0.0054	0.0146
67	H2	H	0.6062	0.9235	0.0239		67	H2	H	0.6022	0.9289	0.0093		0.004	0.0054	0.0146
68	H2	H	0.3938	0.9235	0.4761		68	H2	H	0.3978	0.9289	0.4907		0.004	0.0054	0.0146
69	H2	H	0.3938	0.0765	0.9761		69	H2	H	0.3978	0.0711	0.9907		0.004	0.0054	0.0146
70	H2	H	0.6062	0.0765	0.5239		70	H2	H	0.6022	0.0711	0.5093		0.004	0.0054	0.0146
71	H3	H	0.184	0.4335	0.9685		71	H3	H	0.1843	0.4439	0.9503		0.0003	0.0104	0.0182
72	H3	H	0.816	0.4335	0.5315		72	H3	H	0.8157	0.4439	0.5497		0.0003	0.0104	0.0182
73	H3	H	0.816	0.5665	0.0315		73	H3	H	0.8157	0.5561	0.0497		0.0003	0.0104	0.0182
74	H3	H	0.184	0.5665	0.4685		74	H3	H	0.1843	0.5561	0.4503		0.0003	0.0104	0.0182
75	H3	H	0.684	0.9335	0.9685		75	H3	H	0.6843	0.9439	0.9503		0.0003	0.0104	0.0182
76	H3	H	0.316	0.9335	0.5315		76	H3	H	0.3157	0.9439	0.5497		0.0003	0.0104	0.0182
77	H3	H	0.316	0.0665	0.0315		77	H3	H	0.3157	0.0561	0.0497		0.0003	0.0104	0.0182
78	H3	H	0.684	0.0665	0.4685		78	H3	H	0.6843	0.0561	0.4503		0.0003	0.0104	0.0182

79	H4	H	0.2414	0.2628	0.184	79	H4	H	0.2463	0.2647	0.1831		0.0049	0.0019	0.0009
80	H4	H	0.7586	0.2628	0.316	80	H4	H	0.7537	0.2647	0.3169		0.0049	0.0019	0.0009
81	H4	H	0.7586	0.7372	0.816	81	H4	H	0.7537	0.7353	0.8169		0.0049	0.0019	0.0009
82	H4	H	0.2414	0.7372	0.684	82	H4	H	0.2463	0.7353	0.6831		0.0049	0.0019	0.0009
83	H4	H	0.7414	0.7628	0.184	83	H4	H	0.7463	0.7647	0.1831		0.0049	0.0019	0.0009
84	H4	H	0.2586	0.7628	0.316	84	H4	H	0.2537	0.7647	0.3169		0.0049	0.0019	0.0009
85	H4	H	0.2586	0.2372	0.816	85	H4	H	0.2537	0.2353	0.8169		0.0049	0.0019	0.0009
86	H4	H	0.7414	0.2372	0.684	86	H4	H	0.7463	0.2353	0.6831		0.0049	0.0019	0.0009
87	H5	H	0.2211	0.0753	0.4496	87	H4	H	0.2249	0.0671	0.4655		0.0038	0.0082	0.0159
88	H5	H	0.7789	0.0753	0.0504	88	H5	H	0.7751	0.0671	0.0345		0.0038	0.0082	0.0159
89	H5	H	0.7789	0.9247	0.5504	89	H5	H	0.7751	0.9329	0.5345		0.0038	0.0082	0.0159
90	H5	H	0.2211	0.9247	0.9496	90	H5	H	0.2249	0.9329	0.9655		0.0038	0.0082	0.0159
91	H5	H	0.7211	0.5753	0.4496	91	H5	H	0.7249	0.5671	0.4655		0.0038	0.0082	0.0159
92	H5	H	0.2789	0.5753	0.0504	92	H5	H	0.2751	0.5671	0.0345		0.0038	0.0082	0.0159
93	H5	H	0.2789	0.4247	0.5504	93	H5	H	0.2751	0.4329	0.5345		0.0038	0.0082	0.0159
94	H5	H	0.7211	0.4247	0.9496	94	H5	H	0.7249	0.4329	0.9655		0.0038	0.0082	0.0159
95	H6	H	0.1433	0.0597	0.5024	95	H6	H	0.1418	0.0487	0.519		0.0015	0.011	0.0166
96	H6	H	0.8567	0.0597	0.9976	96	H6	H	0.8582	0.0487	0.981		0.0015	0.011	0.0166
97	H6	H	0.8567	0.9403	0.4976	97	H6	H	0.8582	0.9513	0.481		0.0015	0.011	0.0166
98	H6	H	0.1433	0.9403	0.0024	98	H6	H	0.1418	0.9513	0.019		0.0015	0.011	0.0166
99	H6	H	0.6433	0.5597	0.5024	99	H6	H	0.6418	0.5487	0.519		0.0015	0.011	0.0166
100	H6	H	0.3567	0.5597	0.9976	100	H6	H	0.3582	0.5487	0.981		0.0015	0.011	0.0166
101	H6	H	0.3567	0.4403	0.4976	101	H6	H	0.3582	0.4513	0.481		0.0015	0.011	0.0166
102	H6	H	0.6433	0.4403	0.0024	102	H6	H	0.6418	0.4513	0.019		0.0015	0.011	0.0166
103	O1	O	0.0391	0.3521	0.2022	103	O1	O	0.0388	0.3511	0.2032		0.0003	0.001	0.001
105	O1	O	0.9609	0.3521	0.2978	104	O1	O	0.9612	0.3511	0.2968		0.0003	0.001	0.001
104	O1	O	0.9609	0.6479	0.7978	105	O1	O	0.9612	0.6489	0.7968		0.0003	0.001	0.001

106	O1	O	0.0391	0.6479	0.7022	106	O1	O	0.0388	0.6489	0.7032		0.0003	0.001	0.001
110	O1	O	0.5391	0.8521	0.2022	107	O1	O	0.5388	0.8511	0.2032		0.0003	0.001	0.001
109	O1	O	0.4609	0.8521	0.2978	108	O1	O	0.4612	0.8511	0.2968		0.0003	0.001	0.001
108	O1	O	0.4609	0.1479	0.7978	109	O1	O	0.4612	0.1489	0.7968		0.0003	0.001	0.001
107	O1	O	0.5391	0.1479	0.7022	110	O1	O	0.5388	0.1489	0.7032		0.0003	0.001	0.001
111	O2	O	0.0561	0.1155	0.4304	111	O2	O	0.0562	0.1139	0.4351		0.0001	0.0016	0.0047
113	O2	O	0.9439	0.1155	0.0696	112	O2	O	0.9438	0.1139	0.0649		1.00E-04	0.0016	0.0047
112	O2	O	0.9439	0.8845	0.5696	113	O9	O	0.9438	0.8861	0.5649		1.00E-04	0.0016	0.0047
114	O2	O	0.0561	0.8845	0.9304	114	O2	O	0.0562	0.8861	0.9351		0.0001	0.0016	0.0047
115	O2	O	0.5561	0.6155	0.4304	115	O2	O	0.5562	0.6139	0.4351		1.00E-04	0.0016	0.0047
116	O2	O	0.4439	0.6155	0.0696	116	O2	O	0.4438	0.6139	0.0649		0.0001	0.0016	0.0047
117	O2	O	0.4439	0.3845	0.5696	117	O2	O	0.4438	0.3861	0.5649		0.0001	0.0016	0.0047
118	O2	O	0.5561	0.3845	0.9304	118	O2	O	0.5562	0.3861	0.9351		1.00E-04	0.0016	0.0047
119	Rb1	Rb	0	0.7779	0.25	119	Rb1	Rb	0	0.7861	0.25		0	0.0082	0
120	Rb1	Rb	0	0.2221	0.75	120	Rb1	Rb	0	0.2139	0.75		0	0.0082	0
121	Rb1	Rb	1	0.7779	0.25	121	Rb1	Rb	1	0.7861	0.25		0	0.0082	0
122	Rb1	Rb	1	0.2221	0.75	122	Rb1	Rb	1	0.2139	0.75		0	0.0082	0
123	Rb1	Rb	0.5	0.278	0.25	123	Rb1	Rb	0.5	0.2861	0.25		0	0.0081	0
124	Rb1	Rb	0.5	0.7221	0.75	124	Rb1	Rb	0.5	0.7139	0.75		0	0.0082	0
												Max Value	**0.0049**	**0.0202**	**0.0182**
												In Angstoms	**0.14225435**	**0.1406526**	**0.12040392**

Lattice Parameters	a	b	c
	29.0315	6.963	6.6156

OHO 1.218 A

	1.218	A
OHO	172.199	degrees
O-O	2.431	A
O-C-O	1.248	A
	1.31	A
M-O x2 /Å	2.954	A
	98.327	degrees
	81.673	degrees
M2O2	2.93	A

Caesium Hydrogen Dibenzoate

CRYSTALLOGRAPHY		Fractional Co-ordiantes			
		Elmt	x	y	z
1	C1	C	0.1185	0.2395	0.2715
2	C1	C	0.6185	0.7395	0.2715
3	C1	C	0.8815	0.2395	0.2285
4	C1	C	0.3815	0.7395	0.2285
5	C1	C	0.8815	0.7605	0.7285
6	C1	C	0.3815	0.2605	0.7285
7	C1	C	0.1185	0.7605	0.7715
8	C1	C	0.6185	0.2605	0.7715
9	C2	C	0.1306	0.3571	0.1228
10	C2	C	0.6306	0.8571	0.1228
11	C2	C	0.8694	0.3571	0.3772
12	C2	C	0.3694	0.8571	0.3772
13	C2	C	0.8694	0.6429	0.8772
14	C2	C	0.3694	0.1429	0.8772
15	C2	C	0.1306	0.6429	0.6228
16	C2	C	0.6306	0.1429	0.6228
17	C3	C	0.1769	0.3651	0.0912
18	C3	C	0.6769	0.8651	0.0912
19	C3	C	0.8231	0.3651	0.4088
20	C3	C	0.3231	0.8651	0.4088
21	C3	C	0.8231	0.6349	0.9088
22	C3	C	0.3231	0.1349	0.9088
23	C3	C	0.1769	0.6349	0.5912

After Geometry Optimisation		Fractional Co-ordinates			
		Elmt	x	y	z
1	C1	C	0.1155	0.2404	0.2737
2	C1	C	0.6155	0.7404	0.2736
3	C1	C	0.8845	0.2404	0.2264
4	C1	C	0.3845	0.7404	0.2263
5	C1	C	0.8845	0.7596	0.7263
6	C1	C	0.3845	0.2596	0.7264
7	C1	C	0.1155	0.7596	0.7736
8	C1	C	0.6155	0.2596	0.7737
9	C2	C	0.1272	0.3585	0.1242
10	C2	C	0.6272	0.8585	0.1242
11	C2	C	0.8728	0.3585	0.3758
12	C2	C	0.3728	0.8585	0.3759
13	C2	C	0.8728	0.6415	0.8759
14	C2	C	0.3728	0.1415	0.8758
15	C2	C	0.1272	0.6415	0.6242
16	C2	C	0.6272	0.1415	0.6241
17	C3	C	0.172	0.3674	0.0924
18	C3	C	0.672	0.8674	0.0924
19	C3	C	0.828	0.3674	0.4076
20	C3	C	0.328	0.8674	0.4076
21	C3	C	0.828	0.6326	0.9076
22	C3	C	0.328	0.1326	0.9076
23	C3	C	0.172	0.6326	0.5924

Absolute Differences		
Δx	Δy	Δz
0.003	0.0009	0.0022
0.003	0.0009	0.0021
0.003	0.0009	0.0021
0.003	0.0009	0.0022
0.003	0.0009	0.0022
0.003	0.0009	0.0021
0.003	0.0009	0.0021
0.003	0.0009	0.0022
0.0034	0.0014	0.0014
0.0034	0.0014	0.0014
0.0034	0.0014	0.0014
0.0034	0.0014	0.0013
0.0034	0.0014	0.0013
0.0034	0.0014	0.0014
0.0034	0.0014	0.0014
0.0034	0.0014	0.0013
0.0049	0.0023	0.0012
0.0049	0.0023	0.0012
0.0049	0.0023	0.0012
0.0049	0.0023	0.0012
0.0049	0.0023	0.0012
0.0049	0.0023	0.0012
0.0049	0.0023	0.0012

24	C3	C	0.6769	0.1349	0.5912		24	C3	C	0.672	0.1326	0.5924		0.0049	0.0023	0.0012
25	C4	C	0.2113	0.2565	0.2097		25	C4	C	0.2055	0.2596	0.211		0.0058	0.0031	0.0013
26	C4	C	0.7113	0.7565	0.2097		26	C4	C	0.7055	0.7596	0.211		0.0058	0.0031	0.0013
27	C4	C	0.7887	0.2565	0.2903		27	C4	C	0.7944	0.2596	0.289		0.0057	0.0031	0.0013
28	C4	C	0.2887	0.7565	0.2903		28	C4	C	0.2945	0.7596	0.289		0.0058	0.0031	0.0013
29	C4	C	0.7887	0.7435	0.7903		29	C4	C	0.7945	0.7404	0.789		0.0058	0.0031	0.0013
30	C4	C	0.2887	0.2435	0.7903		30	C4	C	0.2945	0.2404	0.789		0.0058	0.0031	0.0013
31	C4	C	0.2113	0.7435	0.7097		31	C4	C	0.2056	0.7404	0.711		0.0057	0.0031	0.0013
32	C4	C	0.7113	0.2435	0.7097		32	C4	C	0.7055	0.2404	0.711		0.0058	0.0031	0.0013
33	C5	C	0.1992	0.139	0.3587		33	C5	C	0.1942	0.1423	0.3609		0.005	0.0033	0.0022
34	C5	C	0.6992	0.639	0.3587		34	C5	C	0.6941	0.6423	0.3608		0.0051	0.0033	0.0021
35	C5	C	0.8008	0.139	0.1413		35	C5	C	0.8059	0.1423	0.1392		0.0051	0.0033	0.0021
36	C5	C	0.3008	0.639	0.1413		36	C5	C	0.3058	0.6423	0.1391		0.005	0.0033	0.0022
37	C5	C	0.8008	0.861	0.6413		37	C5	C	0.8058	0.8577	0.6391		0.005	0.0033	0.0022
38	C5	C	0.3008	0.361	0.6413		38	C5	C	0.3059	0.3577	0.6392		0.0051	0.0033	0.0021
39	C5	C	0.1992	0.861	0.8587		39	C5	C	0.1941	0.8577	0.8608		0.0051	0.0033	0.0021
40	C5	C	0.6992	0.361	0.8587		40	C5	C	0.6942	0.3577	0.8609		0.005	0.0033	0.0022
41	C6	C	0.153	0.1301	0.3887		41	C6	C	0.1494	0.1322	0.3917		0.0036	0.0021	0.003
42	C6	C	0.6529	0.6301	0.3887		42	C6	C	0.6494	0.6322	0.3918		0.0035	0.0021	0.0031
43	C6	C	0.8471	0.1301	0.1113		43	C6	C	0.8506	0.1322	0.1082		0.0035	0.0021	0.0031
44	C6	C	0.3471	0.6301	0.1113		44	C6	C	0.3506	0.6322	0.1083		0.0035	0.0021	0.003
45	C6	C	0.8471	0.8699	0.6113		45	C6	C	0.8506	0.8678	0.6083		0.0035	0.0021	0.003
46	C6	C	0.3471	0.3699	0.6113		46	C6	C	0.3506	0.3678	0.6082		0.0035	0.0021	0.0031
47	C6	C	0.153	0.8699	0.8887		47	C6	C	0.1494	0.8678	0.8918		0.0036	0.0021	0.0031
48	C6	C	0.6529	0.3699	0.8887		48	C6	C	0.6494	0.3678	0.8917		0.0035	0.0021	0.003
49	C7	C	0.0689	0.2283	0.3097		49	C7	C	0.0677	0.225	0.3118		0.0012	0.0033	0.0021

50	C7	C	0.5689	0.7283	0.3097	50	C7	C	0.5677	0.725	0.3119	0.0012	0.0033	0.0022
51	C7	C	0.9311	0.2283	0.1903	51	C7	C	0.9323	0.225	0.1881	0.0012	0.0033	0.0022
52	C7	C	0.4311	0.7283	0.1903	52	C7	C	0.4323	0.725	0.1882	0.0012	0.0033	0.0021
53	C7	C	0.9311	0.7717	0.6903	53	C7	C	0.9323	0.775	0.6882	0.0012	0.0033	0.0021
54	C7	C	0.4311	0.2717	0.6903	54	C7	C	0.4323	0.275	0.6881	0.0012	0.0033	0.0022
55	C7	C	0.0689	0.7717	0.8097	55	C7	C	0.0677	0.775	0.8119	0.0012	0.0033	0.0022
56	C7	C	0.5689	0.2717	0.8097	56	C7	C	0.5677	0.275	0.8118	0.0012	0.0033	0.0021
57	Cs1	Cs	0	0.7728	0.25	57	Cs1	Cs	0	0.7725	0.25	0	0.0003	0
58	Cs1	Cs	0.5	0.2728	0.25	58	Cs1	Cs	0.5	0.2725	0.25	0	0.0003	0
59	Cs1	Cs	0	0.2272	0.75	59	Cs1	Cs	0	0.2275	0.75	0	0.0003	0
60	Cs1	Cs	0.5	0.7272	0.75	60	Cs1	Cs	0.5	0.7275	0.75	0	0.0003	0
61	Cs1	Cs	1	0.7728	0.25	61	Cs1	Cs	1	0.7725	0.25	0	0.0003	0
62	Cs1	Cs	1	0.2272	0.75	62	Cs1	Cs	1	0.2275	0.75	0	0.0003	0
63	H1	H	0	0.336	0.25	63	H1	H	0	0.3233	0.25	0	0.0127	0
64	H1	H	0.5	0.836	0.25	64	H1	H	0.5	0.8233	0.25	0	0.0127	0
65	H1	H	0	0.664	0.75	65	H1	H	0	0.6767	0.75	0	0.0127	0
66	H1	H	0.5	0.164	0.75	66	H1	H	0.5	0.1767	0.75	0	0.0127	0
67	H1	H	1	0.336	0.25	67	H1	H	1	0.3233	0.25	0	0.0127	0
68	H1	H	1	0.664	0.75	68	H1	H	1	0.6767	0.75	0	0.0127	0
69	H2	H	0.1061	0.429	0.047	69	H2	H	0.101	0.4436	0.0332	0.0051	0.0146	0.0138
70	H2	H	0.6061	0.929	0.047	70	H2	H	0.601	0.9436	0.0332	0.0051	0.0146	0.0138
71	H2	H	0.8939	0.429	0.453	71	H2	H	0.899	0.4436	0.4668	0.0051	0.0146	0.0138
72	H2	H	0.3939	0.929	0.453	72	H2	H	0.399	0.9436	0.4668	0.0051	0.0146	0.0138
73	H2	H	0.8939	0.571	0.953	73	H2	H	0.899	0.5564	0.9668	0.0051	0.0146	0.0138
74	H2	H	0.3939	0.071	0.953	74	H2	H	0.399	0.0564	0.9668	0.0051	0.0146	0.0138
75	H2	H	0.1061	0.571	0.547	75	H2	H	0.101	0.5564	0.5332	0.0051	0.0146	0.0138

76	H2	H	0.6061	0.071	0.547		76	H2	H	0.601	0.0564	0.5332		0.0051	0.0146	0.0138
77	H3	H	0.1855	0.442	0.989		77	H3	H	0.1806	0.4591	0.9751		0.0049	0.0171	0.0139
78	H3	H	0.6855	0.942	0.989		78	H3	H	0.6806	0.9591	0.9751		0.0049	0.0171	0.0139
79	H3	H	0.8145	0.442	0.511		79	H3	H	0.8194	0.4591	0.5249		0.0049	0.0171	0.0139
80	H3	H	0.3145	0.942	0.511		80	H3	H	0.3194	0.9591	0.5249		0.0049	0.0171	0.0139
81	H3	H	0.8145	0.558	0.011		81	H3	H	0.8194	0.5409	0.0249		0.0049	0.0171	0.0139
82	H3	H	0.3145	0.058	0.011		82	H3	H	0.3194	0.0409	0.0249		0.0049	0.0171	0.0139
83	H3	H	0.1855	0.558	0.489		83	H3	H	0.1806	0.5409	0.4751		0.0049	0.0171	0.0139
84	H3	H	0.6855	0.058	0.489		84	H3	H	0.6806	0.0409	0.4751		0.0049	0.0171	0.0139
85	H4	H	0.2417	0.263	0.196		85	H4	H	0.2407	0.2673	0.1876		0.001	0.0043	0.0084
86	H4	H	0.7417	0.763	0.196		86	H4	H	0.7407	0.7673	0.1875		0.001	0.0043	0.0085
87	H4	H	0.7583	0.263	0.304		87	H4	H	0.7593	0.2673	0.3125		0.001	0.0043	0.0085
88	H4	H	0.2583	0.763	0.304		88	H4	H	0.2593	0.7673	0.3124		0.001	0.0043	0.0084
89	H4	H	0.7583	0.737	0.804		89	H4	H	0.7593	0.7327	0.8124		0.001	0.0043	0.0084
90	H4	H	0.2583	0.237	0.804		90	H4	H	0.2593	0.2327	0.8125		0.001	0.0043	0.0085
91	H4	H	0.2417	0.737	0.696		91	H4	H	0.2407	0.7327	0.6875		0.001	0.0043	0.0085
92	H4	H	0.7417	0.237	0.696		92	H4	H	0.7407	0.2327	0.6875		0.001	0.0043	0.0085
93	H5	H	0.2225	0.062	0.439		93	H5	H	0.2203	0.0585	0.4543		0.0022	0.0035	0.0153
94	H5	H	0.7225	0.562	0.439		94	H5	H	0.7203	0.5585	0.4543		0.0022	0.0035	0.0153
95	H5	H	0.7775	0.062	0.061		95	H5	H	0.7797	0.0585	0.0457		0.0022	0.0035	0.0153
96	H5	H	0.2775	0.562	0.061		96	H5	H	0.2797	0.5585	0.0457		0.0022	0.0035	0.0153
97	H5	H	0.7775	0.938	0.561		97	H5	H	0.7797	0.9415	0.5457		0.0022	0.0035	0.0153
98	H5	H	0.2775	0.438	0.561		98	H5	H	0.2797	0.4415	0.5457		0.0022	0.0035	0.0153
99	H5	H	0.2225	0.938	0.939		99	H5	H	0.2203	0.9415	0.9543		0.0022	0.0035	0.0153
100	H5	H	0.7225	0.438	0.939		100	H5	H	0.7203	0.4415	0.9543		0.0022	0.0035	0.0153
101	H6	H	0.1455	0.053	0.486		101	H6	H	0.1399	0.0411	0.5075		0.0056	0.0119	0.0215

102	H6	H	0.6455	0.553	0.486	102	H6	H	0.6399	0.5411	0.5076		0.0056	0.0119	0.0216
103	H6	H	0.8545	0.053	0.014	103	H6	H	0.8601	0.0411	0.0076		0.0056	0.0119	0.0064
104	H6	H	0.3545	0.553	0.014	104	H6	H	0.3601	0.5411	0.0075		0.0056	0.0119	0.0065
105	H6	H	0.8545	0.947	0.514	105	H6	H	0.8601	0.9589	0.4924		0.0056	0.0119	0.0216
106	H6	H	0.3545	0.447	0.514	106	H6	H	0.3601	0.4589	0.4924		0.0056	0.0119	0.0216
107	H6	H	0.1455	0.947	0.986	107	H6	H	0.1399	0.9589	0.9924		0.0056	0.0119	0.0064
108	H6	H	0.6455	0.447	0.986	108	H6	H	0.6399	0.4589	0.9924		0.0056	0.0119	0.0064
109	O1	O	0.0396	0.3468	0.207	109	O1	O	0.0379	0.3378	0.2062		0.0017	0.009	0.0008
110	O1	O	0.5396	0.8468	0.207	110	O1	O	0.5379	0.8378	0.2062		0.0017	0.009	0.0008
111	O1	O	0.9604	0.3468	0.293	111	O1	O	0.9621	0.3378	0.2938		0.0017	0.009	0.0008
112	O1	O	0.4604	0.8468	0.293	112	O1	O	0.4621	0.8378	0.2938		0.0017	0.009	0.0008
113	O1	O	0.9604	0.6532	0.793	113	O1	O	0.9621	0.6622	0.7938		0.0017	0.009	0.0008
114	O1	O	0.4604	0.1532	0.793	114	O1	O	0.4621	0.1622	0.7937		0.0017	0.009	0.0007
115	O1	O	0.0396	0.6532	0.707	115	O1	O	0.0379	0.6622	0.7062		0.0017	0.009	0.0008
116	O1	O	0.5396	0.1532	0.707	116	O1	O	0.5379	0.1622	0.7062		0.0017	0.009	0.0008
117	O2	O	0.058	0.1142	0.431	117	O2	O	0.0581	0.1109	0.4384		1E-04	0.0033	0.0074
118	O2	O	0.558	0.6142	0.431	118	O2	O	0.5581	0.6109	0.4384		1E-04	0.0033	0.0074
119	O2	O	0.942	0.1142	0.069	119	O2	O	0.9419	0.1109	0.0616		1E-04	0.0033	0.0074
120	O2	O	0.4419	0.6142	0.069	120	O2	O	0.4419	0.6109	0.0616		0	0.0033	0.0074
121	O2	O	0.942	0.8858	0.569	121	O2	O	0.9419	0.8891	0.5616		1E-04	0.0033	0.0074
122	O2	O	0.4419	0.3858	0.569	122	O2	O	0.4419	0.3891	0.5616		0	0.0033	0.0074
123	O2	O	0.058	0.8858	0.931	123	O2	O	0.0581	0.8891	0.9384		1E-04	0.0033	0.0074
124	O2	O	0.558	0.3858	0.931	124	O2	O	0.5581	0.3891	0.9384		1E-04	0.0033	0.0074
												Max Value	**0.0058**	**0.0171**	**0.0216**
												In Angstoms	**0.1734751**	**0.12057039**	**0.14640264**

Lattice Parameters	a	b	c
	29.9095	7.0509	6.7779

OHO	1.262	A
	1.262	
OHO	171.331	degrees
O-O	2.516	A
O-C-O	1.245	A
	1.318	
M-O x2 /Å	3.11	A
M2O2	3.095	A
	82.803	degrees
	97.19	