Electronic Supporting Information

for

# Electronic Structure of Cesium Butyratouranylate(VI) as Derived from DFT-assisted Powder X-Ray Diffraction Data

*Anna V. Vologzhanina,*[*,†] *Anton V. Savchenkov,*[‡] *Artem O. Dmitrienko,*[†] *Alexander A. Korlyukov,*[†,§] *Ivan S. Bushmarinov,*[†] *Denis V. Pushkin,*[‡] *Larisa B. Serezhkina*[‡]

[†] Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, 119991 Moscow, Russia. [‡] Samara State University, 443011 Samara, Russia. [§] Pirogov Russian National Research Medical University, 117997 Moscow, Russia.

**Table S1.** Topological parameters of ρ(r) function for weak interactions in **1-calc**.[a]

| Bond | $\rho(\mathbf{r})$, e Å$^{-3}$ | $\nabla^2\rho(\mathbf{r})$, e Å$^{-5}$ | $G_e(\mathbf{r})$, a.u. | $V_e(\mathbf{r})$, a.u. | $h_e(\mathbf{r})$, a.u. | E, kcal/mol |
|---|---|---|---|---|---|---|
| C4...C4 | 0.002 | 0.008 | 0.001 | -0.001 | 0.0005 | -0.26 |
| C12...H4A | 0.006 | 0.019 | 0.004 | -0.003 | 0.001 | -0.86 |
| C16...H3B | 0.004 | 0.013 | 0.002 | -0.002 | 0.0007 | -0.55 |
| H2A...O10 | 0.009 | 0.040 | 0.008 | -0.005 | 0.002 | -1.82 |
| H2B...O9 | 0.006 | 0.025 | 0.005 | -0.003 | 0.002 | -1.02 |
| H6A...O2 | 0.010 | 0.041 | 0.008 | -0.006 | 0.002 | -1.87 |
| H6B...O1 | 0.009 | 0.040 | 0.008 | -0.006 | 0.002 | -1.80 |
| H8C...O5 | 0.004 | 0.017 | 0.003 | -0.002 | 0.001 | -0.62 |
| H8C...O4 | 0.004 | 0.015 | 0.003 | -0.002 | 0.001 | -0.55 |
| H10A...O13 | 0.005 | 0.020 | 0.004 | -0.003 | 0.001 | -0.81 |
| H10A...O10 | 0.003 | 0.013 | 0.002 | -0.002 | 0.001 | -0.51 |
| H10A...O9 | 0.005 | 0.020 | 0.004 | -0.002 | 0.001 | -0.77 |
| H10B...O3 | 0.008 | 0.032 | 0.006 | -0.004 | 0.002 | -1.39 |
| H10B...O1 | 0.006 | 0.027 | 0.005 | -0.004 | 0.002 | -1.10 |
| H11C...O1 | 0.006 | 0.028 | 0.005 | -0.003 | 0.002 | -1.09 |
| H11C...O2 | 0.004 | 0.013 | 0.002 | -0.002 | 0.001 | -0.50 |
| H11D...O3 | 0.006 | 0.014 | 0.003 | -0.002 | 0.0006 | -0.67 |
| H11D...O9 | 0.005 | 0.022 | 0.004 | -0.003 | 0.001 | -0.85 |
| H12B...O4 | 0.004 | 0.012 | 0.002 | -0.002 | 0.0007 | -0.47 |
| H16B...O14 | 0.005 | 0.014 | 0.003 | -0.002 | 0.0008 | -0.58 |
| H16B...O13 | 0.009 | 0.040 | 0.008 | -0.006 | 0.002 | -1.76 |
| H16C...O5 | 0.004 | 0.017 | 0.003 | -0.002 | 0.001 | -0.66 |
| H2B...H11D | 0.006 | 0.020 | 0.004 | -0.003 | 0.001 | -0.83 |
| H2B...H12C | 0.005 | 0.018 | 0.003 | -0.002 | 0.001 | -0.75 |
| H3A...H12B | 0.003 | 0.011 | 0.002 | -0.001 | 0.0008 | -0.39 |
| H3A...H16A | 0.003 | 0.010 | 0.002 | -0.001 | 0.0007 | -0.36 |
| H3A...H3A | 0.008 | 0.025 | 0.005 | -0.004 | 0.001 | -1.25 |
| H3B...H8A | 0.003 | 0.009 | 0.002 | -0.001 | 0.0005 | -0.32 |
| H4B...H14A | 0.005 | 0.016 | 0.003 | -0.002 | 0.001 | -0.70 |
| H4B...H15A | 0.007 | 0.021 | 0.004 | -0.003 | 0.001 | -1.06 |
| H4C...H12D | 0.005 | 0.014 | 0.003 | -0.002 | 0.0007 | -0.59 |
| H4C...H15B | 0.005 | 0.017 | 0.003 | -0.002 | 0.001 | -0.68 |
| H7A...H12D | 0.005 | 0.015 | 0.003 | -0.002 | 0.0008 | -0.68 |
| H7A...H15B | 0.005 | 0.014 | 0.003 | -0.002 | 0.0008 | -0.59 |
| H7B...H8B | 0.009 | 0.026 | 0.006 | -0.004 | 0.001 | -1.37 |
| H7B...H16C | 0.005 | 0.015 | 0.003 | -0.002 | 0.0009 | -0.62 |
| H7B...H14B | 0.003 | 0.010 | 0.002 | -0.001 | 0.0007 | -0.37 |
| H8A...H14A | 0.003 | 0.010 | 0.002 | -0.001 | 0.0007 | -0.37 |
| H8B...H16C | 0.006 | 0.016 | 0.003 | -0.002 | 0.0008 | -0.73 |
| H8B...H14B | 0.005 | 0.015 | 0.003 | -0.002 | 0.0008 | -0.63 |
| H8C...H12B | 0.004 | 0.014 | 0.003 | -0.002 | 0.0008 | -0.55 |
| H8C...H16A | 0.003 | 0.015 | 0.003 | -0.002 | 0.001 | -0.55 |
| H14B...H16B | 0.006 | 0.019 | 0.004 | -0.03 | 0.001 | -0.81 |

[a] For all $\rho(\mathbf{r})$ is the ED at the bcp; $\nabla^2\rho(\mathbf{r})$ is the corresponding Laplacian; $G_e(\mathbf{r})$ - kinetic energy density; $V_e(\mathbf{r})$ - potential energy density; $h_e(\mathbf{r})$ – local energy density, E - bond energy estimated from the correlation proposed by Espinosa, Molins and Lecomte as $1/2V_e(\mathbf{r})$.

**Table S2.** Calculation of coordination numbers of Cs1, U1 and U2 atoms in the structure of **1-calc** using "intersecting spheres" algorithm.[a]

| VDP of the metal atom | | | | Intersection volume (Å$^3$) of two spheres with radii | | | | Type of intersection |
|---|---|---|---|---|---|---|---|---|
| Atom A | Atom B | rA-B), Å | Ω(A-B), % | $r_S \cdot r_S$ | $r_S \cdot R_{SD}$ | $R_{SD} \cdot r_S$ | $R_{SD} \cdot R_{SD}$ | |
| Cs1 | **O3** | **2.998** | **11.03** | 0.06 | 3.04 | 0 | 0.25 | **$I_3$** |
| CN = 5 | **O8** | **3.027** | **10.62** | 0.04 | 3.76 | 0 | 0.38 | **$I_3$** |
| | **O9** | **3.039** | **12.19** | 0.04 | 3.80 | 0 | 0.38 | **$I_3$** |
| | **O2** | **3.207** | **9.79** | 0 | 3.06 | 0 | 0.16 | **$I_2$** |
| | H11C | 3.228 | 6.44 | 0 | 1.71 | 0 | 0.01 | $I_2^{agostic}$ |
| | O11 | 3.229 | 6.27 | 0 | 1.00 | 0 | 0 | $I_1$ |
| | H6B | 2.323 | 4.92 | 0 | 1.32 | 0 | 0 | $I_1^{agostic}$ |
| | H11A | 3.345 | 3.29 | 0 | 0.89 | 0 | 0 | $I_1$ |
| | **O10** | **3.343** | **7.77** | 0 | 2.10 | 0 | 0.01 | **$I_2$** |
| | H6A | 3.365 | 4.07 | 0 | 1.20 | 0 | 0 | $I_1$ |
| | O1 | 3.445 | 5.18 | 0 | 1.55 | 0 | 0 | $I_1$ |
| | O7 | 3.465 | 6.45 | 0 | 0.81 | 0 | 0 | $I_1$ |
| | H11B | 3.669 | 3.91 | 0 | 0.28 | 0 | 0 | $I_1$ |
| | O12 | 3.667 | 2.63 | 0 | 0.26 | 0 | 0 | $I_1$ |
| | #H11B | 3.669 | 0.27 | 0 | 0.21 | 0 | 0 | $I_0$ |
| | H10B | 3.819 | 2.04 | 0 | 0.16 | 0 | 0 | $I_1$ |
| | #C9 | 3.888 | 0.77 | 0 | 0 | 0 | 0 | $I_0$ |
| | #O11 | 3.905 | 0.25 | 0 | 0 | 0 | 0 | $I_0$ |
| | #H2A | 3.937 | 0.36 | 0 | 0.04 | 0 | 0 | $I_0$ |
| | H11D' | 4.007 | 1.77 | 0 | 0.01 | 0 | 0 | $I_1$ |
| | #O8 | 4.760 | 0.00 | 0 | 0 | 0 | 0 | $I_0$ |
| U1 | **O1** | 1.815 | 21.41 | 0.32 | 5.07 | 0.02 | 2.35 | **$I_4$** |
| CN = 8 | **O2** | 1.819 | 21.39 | 0.32 | 5.59 | 0.01 | 2.64 | **$I_4$** |
| | **O3** | 2.420 | 10.16 | 0 | 1.48 | 0 | 0.30 | **$I_2$** |
| | **O4** | 2.451 | 10.13 | 0 | 1.35 | 0 | 0.24 | **$I_2$** |
| | **O5** | 2.500 | 9.65 | 0 | 1.32 | 0 | 0.23 | **$I_2$** |
| | **O6** | 2.537 | 8.80 | 0 | 0.52 | 0 | 0.01 | **$I_2$** |
| | **O7** | 2.491 | 9.33 | 0 | 1.03 | 0 | 0.13 | **$I_2$** |
| | **O8** | 2.494 | 9.14 | 0 | 1.76 | 0 | 0.40 | **$I_2$** |
| U2 | **O9** | 1.823 | 21.12 | 0.32 | 5.30 | 0.01 | 2.39 | **$I_4$** |
| CN = 6 | **O10** | 1.819 | 20.92 | 0.32 | 5.22 | 0.01 | 2.43 | **$I_4$** |
| | O11 | 2.596 | 8.70 | 0 | 0.39 | 0 | 0 | $I_1$ |
| | **O12** | 2.364 | 11.87 | 0 | 1.28 | 0 | 0.22 | **$I_2$** |
| | **O12'** | 2.302 | 12.83 | 0.01 | 1.49 | 0 | 0.31 | **$I_3$** |
| | **O13** | 2.459 | 11.13 | 0 | 1.22 | 0 | 0.19 | **$I_2$** |
| | **O14** | 2.317 | 12.90 | 0.01 | 1.97 | 0 | 0.51 | **$I_3$** |
| | #H12A | 2.811 | 0.15 | 0 | 0 | 0 | 0 | $I_0$ |
| | #H12A' | 2.853 | 0.32 | 0 | 0 | 0 | 0 | $I_0$ |
| | #O14 | 3.465 | 0.06 | 0 | 0 | 0 | 0 | $I_0$ |

[a] $r_s$ is the Slater radius and $R_{SD}$ is the radius of the sphere whose volume is equal to the *A* or B VD polyhedron volume; the first radius in each term is that of the central atom *A* and the second that of the B atom. The # sign marks the atoms for which the mid-point of the *A*-*B* segment does not lie on the VD polyhedron surface of the central atom. The agostic contacts are marked by superscripts.

**Table S3.** Calculation of coordination numbers of Cs1, U1 and U2 atoms in the structure of **1-calc** using sectors algorithm[a]

| VDP of the metal atom | | | | Intersection volume (Å$^3$) of two spheres with radii | | | | Type of intersection |
|---|---|---|---|---|---|---|---|---|
| Atom A | Atom B | rA-B), Å | Ω(A-B), % | $r_S \cdot r_S$ | $r_S \cdot R_{SD}$ | $R_{SD} \cdot r_S$ | $R_{SD} \cdot R_{SD}$ | |
| Cs1 | **O3** | **2.998** | **11.03** | 0.06 | 5.03 | 0 | 0.52 | **$I_3$** |
| CN = | **O8** | **3.027** | **10.62** | 0.04 | 5.20 | 0 | 0.68 | **$I_3$** |
| 9+3 | **O9** | **3.039** | **12.09** | 0.04 | 5.05 | 0 | 0.61 | **$I_3$** |
| | **O2** | **3.207** | **9.79** | 0 | 4.61 | 0 | 0.63 | **$I_2$** |
| | H11C | 3.228 | 6.44 | 0 | 3.66 | 0 | 0.18 | $I_2^{agostic}$ |
| | **O11** | **3.229** | **6.27** | 0 | 3.73 | 0 | 0.21 | $I_2$ |
| | H6B | 2.323 | 4.92 | 0 | 3.25 | 0 | 0.12 | $I_2^{agostic}$ |
| | H11A | 3.345 | 3.29 | 0 | 3.28 | 0 | 0.14 | $I_2$ |
| | **O10** | **3.343** | **7.77** | 0 | 3.58 | 0 | 0.27 | **$I_2$** |
| | H6A | 3.365 | 4.07 | 0 | 3.09 | 0 | 0.10 | $I_2$ |
| | **O1** | **3.445** | **5.18** | 0 | 3.09 | 0 | 0.16 | **$I_2$** |
| | **O7** | **3.465** | **6.46** | 0 | 3.12 | 0 | 0.20 | **$I_2$** |
| | H11B | 3.669 | 3.91 | 0 | 2.40 | 0 | 0.08 | $I_2$ |
| | **O12** | **3.667** | **2.63** | 0 | 2.16 | 0 | 0.04 | **$I_2$** |
| | #H11B | 3.669 | 0.27 | 0 | 2.81 | 0 | 0.31 | $I_0$ |
| | H10B | 3.819 | 2.04 | 0 | 1.93 | 0 | 0.06 | $I_2$ |
| | #C9 | 3.888 | 0.77 | 0 | 2.03 | 0 | 0.17 | $I_0$ |
| | #O11 | 3.905 | 0.25 | 0 | 1.80 | 0 | 0.09 | $I_0$ |
| | #H2A | 3.937 | 0.36 | 0 | 1.44 | 0 | 0.01 | $I_0$ |
| | H11D' | 4.007 | 1.76 | 0 | 2.06 | 0 | 0.38 | $I_2$ |
| | #O8 | 4.760 | 0.00 | 0 | 0.52 | 0 | 0.33 | $I_0$ |
| U1 | **O1** | 1.815 | 21.41 | 0.32 | 2.54 | <0.01 | 0.68 | **$I_4$** |
| CN = 8 | **O2** | 1.819 | 21.39 | 0.32 | 2.53 | <0.01 | 0.68 | **$I_4$** |
| | **O3** | 2.420 | 10.16 | 0 | 1.10 | 0 | 0.22 | **$I_2$** |
| | **O4** | 2.451 | 10.13 | 0 | 1.07 | 0 | 0.23 | **$I_2$** |
| | **O5** | 2.500 | 9.65 | 0 | 0.98 | 0 | 0.21 | **$I_2$** |
| | **O6** | 2.537 | 8.80 | 0 | 0.89 | 0 | 0.18 | **$I_2$** |
| | **O7** | 2.491 | 9.33 | 0 | 0.97 | 0 | 0.19 | **$I_2$** |
| | **O8** | 2.494 | 9.14 | 0 | 0.96 | 0 | 0.19 | **$I_2$** |
| U2 | **O9** | 1.823 | 21.12 | 0.32 | 2.50 | 0 | 0.65 | **$I_3$** |
| CN = 7 | **O10** | 1.819 | 20.92 | 0.32 | 2.50 | 0 | 0.66 | **$I_3$** |
| | **O11** | 2.596 | 8.70 | 0 | 0.81 | 0 | 0.17 | **$I_2$** |
| | **O12** | 2.364 | 11.87 | 0 | 1.23 | 0 | 0.27 | **$I_2$** |
| | **O12'** | 2.302 | 12.83 | 0.01 | 1.38 | 0 | 0.31 | **$I_3$** |
| | **O13** | 2.459 | 11.13 | 0 | 1.11 | 0 | 0.28 | **$I_2$** |
| | **O14** | 2.317 | 12.90 | 0.01 | 1.37 | 0 | 0.33 | **$I_3$** |
| | #H12A | 2.811 | 0.15 | 0 | 0 | 0 | 0 | $I_0$ |
| | #H12A' | 2.853 | 0.32 | 0 | 0 | 0 | 0 | $I_0$ |
| | #O14 | 3.465 | 0.06 | 0 | 0 | 0 | 0 | $I_0$ |

[a] $r_s$ is the Slater radius and $R_{SD}$ is the radius of the sphere whose volume is equal to the *A* or B VD polyhedron volume; the first radius in each term is that of the central atom *A* and the second that of the B atom. The # sign marks the atoms for which the mid-point of the *A*-*B* segment does not lie on the VD polyhedron surface of the central atom. The agostic contacts are marked by superscripts.

**Table S4**. Integrated characteristics for all atoms.

| Atom | Q, e | $V_{AIM}$, Å$^3$ | $V_{VDP}$, Å$^3$ |
|---|---|---|---|
| U1 | 3.31 | 19.07 | 9.76 |
| U2 | 3.39 | 18.93 | 9.59 |
| Cs1 | 0.23 | 42.84 | 24.81 |
| O1 | -0.77 | 17.42 | 16.55 |
| O2 | -0.79 | 18.08 | 18.65 |
| O3 | -1.07 | 14.55 | 13.4 |
| O4 | -1.04 | 16.96 | 13.22 |
| O5 | -1.03 | 17.32 | 14.17 |
| O6 | -1.11 | 14.06 | 8.73 |
| O7 | -1.08 | 13.81 | 11.85 |
| O8 | -1.06 | 16.61 | 17.18 |
| O9 | -0.79 | 16.38 | 17.62 |
| O10 | -0.78 | 17.50 | 17.23 |
| O11 | -1.45 | 16.08 | 8.59 |
| O12 | -1.09 | 12.55 | 10.92 |
| O13 | -1.06 | 15.72 | 12.51 |
| O14 | -1.07 | 16.22 | 14.03 |
| C1 | 1.31 | 5.81 | 6.77 |
| C2 | 0.08 | 8.73 | 3.76 |
| C3 | 0.12 | 8.63 | 3.67 |
| C4 | 0.11 | 10.25 | 2.96 |
| C5 | 1.32 | 6.31 | 7.42 |
| C6 | 0.07 | 8.68 | 3.81 |
| C7 | 0.13 | 8.46 | 3.69 |
| C8 | 0.12 | 9.73 | 2.96 |
| C9 | 1.32 | 5.92 | 7.69 |
| C10 | 0.09 | 8.56 | 3.71 |
| C11 | 0.14 | 8.13 | 3.64 |
| C12 | 0.11 | 9.51 | 2.95 |
| C13 | 1.37 | 6.07 | 7.47 |
| C14 | 0.10 | 8.58 | 3.82 |
| C15 | 0.12 | 8.14 | 3.69 |
| C16 | 0.11 | 10.16 | 2.96 |
| H11A | 0.04 | 3.59 | 9.93 |
| H11B | 0.03 | 3.84 | 10.26 |
| H12A | 0.16 | 2.87 | 8.48 |
| H2A | 0.02 | 7.37 | 12.8 |
| H2B | 0.02 | 6.85 | 11.04 |
| H3A | -0.03 | 7.40 | 10.29 |
| H3B | -0.04 | 8.88 | 11.69 |
| H4A | -0.04 | 8.05 | 11.02 |
| H4B | -0.05 | 8.07 | 10.79 |
| H4C | -0.04 | 7.59 | 10.71 |
| H6A | 0.01 | 6.70 | 12.39 |
| H6B | 0.01 | 6.32 | 12.22 |
| H7A | -0.03 | 8.06 | 11.33 |
| H7B | -0.03 | 6.89 | 9.75 |
| H8A | -0.05 | 9.33 | 11.84 |
| H8B | -0.04 | 7.00 | 9.7 |

| | | | |
|---|---|---|---|
| H8C | -0.02 | 7.58 | 11.01 |
| H10A | 0.00 | 6.83 | 11.77 |
| H10B | 0.02 | 6.90 | 12.93 |
| H11C | 0.00 | 6.70 | 12.38 |
| H11D | -0.03 | 7.34 | 13.32 |
| H12B | -0.03 | 7.88 | 10.93 |
| H12C | -0.04 | 7.68 | 9.96 |
| H12D | -0.04 | 8.35 | 10.81 |
| H14A | -0.01 | 9.09 | 13.21 |
| H14B | 0.00 | 7.06 | 10.3 |
| H15A | -0.04 | 6.97 | 9.46 |
| H15B | -0.04 | 8.53 | 11.29 |
| H16A | -0.03 | 7.68 | 10.87 |
| H16B | -0.03 | 7.47 | 11.24 |
| H16C | -0.04 | 7.17 | 10.22 |

coordinates as taken from **1-cry** model (res file)

```
TITL a in P2(1)/c
CELL 1.54178  14.7793  21.1524   8.3971  90.000  95.071  90.000
ZERR    4.00   0.0012   0.0023   0.0008   0.000   0.005   0.000
LATT  1
SYMM -X, 0.5+Y, 0.5-Z
SFAC C H O CS U
UNIT 64 124 56 4 8
TEMP -173.000
SIZE 0.16 0.38 0.45
omit -4 130
L.S. 4
BOND $h
FMAP 2
PLAN 10
WGHT    0.100000
FVAR       0.04007
U1    5    0.126920    0.401745    0.739388    11.00000    0.04080    0.04969 =
      0.04404    0.00013    0.00548   -0.00244
U2    5    0.187908    0.763439    0.591094    11.00000    0.03781    0.04928 =
      0.04336    0.00005    0.00457    0.00135
CS1   4    0.027528    0.613177    0.766577    11.00000    0.04424    0.05003 =
      0.04968   -0.00006    0.00467   -0.00119
O1    3    0.148400    0.411011    0.529945    11.00000    0.04914    0.06353 =
      0.03519    0.00066    0.00874    0.00040
O2    3    0.101445    0.389678    0.948189    11.00000    0.04823    0.05400 =
      0.04746    0.00354   -0.00038   -0.01101
O3    3    0.166551    0.509874    0.776437    11.00000    0.05124    0.04152 =
      0.05592   -0.01368    0.00651    0.00802
O4    3    0.273130    0.444449    0.824951    11.00000    0.04714    0.03147 =
      0.08639    0.00568    0.02843   -0.00138
O5    3    0.237797    0.313419    0.764845    11.00000    0.04449    0.05851 =
      0.07798   -0.00298   -0.01410   -0.01024
O6    3    0.098625    0.283974    0.704866    11.00000    0.04466    0.05906 =
      0.03420   -0.01617    0.00061   -0.00727
O7    3   -0.029728    0.378168    0.639026    11.00000    0.05614    0.06370 =
      0.02639   -0.01039    0.00858    0.01746
O8    3   -0.006296    0.473449    0.712928    11.00000    0.05316    0.05531 =
      0.05709    0.01410    0.00965   -0.02039
O9    3    0.162687    0.843707    0.542873    11.00000    0.05410    0.06090 =
      0.04132   -0.00465    0.00640   -0.00543
O10   3    0.207321    0.682673    0.638349    11.00000    0.03686    0.06478 =
      0.05970   -0.02658    0.00136    0.00261
O11   3    0.015860    0.747618    0.567273    11.00000    0.03916    0.04915 =
      0.04866   -0.00985    0.00411   -0.00184
AFIX   3
H11A  2   -0.000280    0.783868    0.598043    11.00000   -1.50000
H11B  2   -0.018940    0.736208    0.486353    11.00000   -1.50000
AFIX   0
O12   3    0.129664    0.729424    0.334107    11.00000    0.03644    0.04907 =
      0.02356   -0.01437   -0.00237   -0.00989
```

```
AFIX   3
H12A  2    0.098574    0.695974    0.342467    11.00000   -1.50000
AFIX   0
O13   3    0.314460    0.808985    0.761082    11.00000    0.04144    0.08473 =
      0.05437    0.00136   -0.00247    0.00895
O14   3    0.315892    0.736028    0.955568    11.00000    0.04656    0.04701 =
      0.05774   -0.00558   -0.00441   -0.00455
C1    1    0.254068    0.500402    0.815227    11.00000    0.03543    0.05123 =
      0.08434   -0.00588    0.00630   -0.01286
C2    1    0.316454    0.554033    0.860766    11.00000    0.04917    0.07170 =
      0.10631   -0.03912    0.02112   -0.01305
AFIX  23
H2A   2    0.302465    0.588989    0.784128    11.00000   -1.20000
H2B   2    0.303106    0.569316    0.967640    11.00000   -1.20000
AFIX   0
C3    1    0.412248    0.540678    0.865550    11.00000    0.06604    0.09199 =
      0.12285    0.01957    0.00187   -0.00987
AFIX  23
H3A   2    0.427494    0.505137    0.939827    11.00000   -1.20000
H3B   2    0.447243    0.578187    0.905752    11.00000   -1.20000
AFIX   0
C4    1    0.439447    0.522943    0.692927    11.00000    0.07659    0.03906 =
      0.08166    0.00801    0.03888    0.00486
AFIX 137
H4A   2    0.505514    0.518007    0.696102    11.00000   -1.50000
H4B   2    0.419762    0.556656    0.617634    11.00000   -1.50000
H4C   2    0.409903    0.483187    0.658189    11.00000   -1.50000
AFIX   0
C5    1    0.179411    0.268882    0.741996    11.00000    0.03709    0.07069 =
      0.00891    0.00041    0.00108    0.00658
C6    1    0.203272    0.201174    0.770690    11.00000    0.04070    0.08178 =
      0.05282   -0.00118    0.01400    0.00228
AFIX  23
H6A   2    0.178966    0.176744    0.675820    11.00000   -1.20000
H6B   2    0.171221    0.186340    0.862381    11.00000   -1.20000
AFIX   0
C7    1    0.301915    0.185009    0.803784    11.00000    0.06543    0.06153 =
      0.04525   -0.01250   -0.00239    0.00877
AFIX  23
H7A   2    0.307002    0.144055    0.860946    11.00000   -1.20000
H7B   2    0.331229    0.217562    0.875684    11.00000   -1.20000
AFIX   0
C8    1    0.354903    0.180337    0.650983    11.00000    0.04321    0.08823 =
      0.07987    0.01585    0.00793    0.00841
AFIX 137
H8A   2    0.416736    0.165187    0.680922    11.00000   -1.50000
H8B   2    0.357516    0.222150    0.601335    11.00000   -1.50000
H8C   2    0.323653    0.150747    0.574966    11.00000   -1.50000
AFIX   0
C9    1   -0.064745    0.432225    0.669954    11.00000    0.05110    0.06896 =
      0.03529   -0.02684    0.00373   -0.01115
C10   1   -0.164291    0.444872    0.636001    11.00000    0.04927    0.07959 =
```

```
      0.03059   -0.00409   -0.00351   -0.00172
AFIX  23
H10A  2   -0.198705    0.404854    0.640559    11.00000   -1.20000
H10B  2   -0.176437    0.462926    0.527443    11.00000   -1.20000
AFIX   0
C11   1   -0.194536    0.490849    0.758866    11.00000    0.04116    0.07867 =
      0.03116    0.00901   -0.00484   -0.01313
AFIX  23
H11C  2   -0.161913    0.531359    0.749256    11.00000   -1.20000
H11D  2   -0.177563    0.473757    0.867150    11.00000   -1.20000
AFIX   0
C12   1   -0.297820    0.503549    0.740089    11.00000    0.04692    0.07379 =
      0.07817   -0.02212    0.00241    0.00064
AFIX 137
H12B  2   -0.317543    0.518165    0.842232    11.00000   -1.50000
H12C  2   -0.330041    0.464480    0.707798    11.00000   -1.50000
H12D  2   -0.311423    0.536061    0.658321    11.00000   -1.50000
AFIX   0
C13   1    0.349727    0.780897    0.875045    11.00000    0.03523    0.04233 =
      0.05343    0.00282    0.00863    0.00385
C14   1    0.442350    0.805439    0.952577    11.00000    0.06592    0.07300 =
      0.04037   -0.00928   -0.00456   -0.00599
AFIX  23
H14A  2    0.433452    0.819479    1.062574    11.00000   -1.20000
H14B  2    0.485039    0.769290    0.961768    11.00000   -1.20000
AFIX   0
C15   1    0.488066    0.859223    0.868904    11.00000    0.02595    0.07258 =
      0.06719   -0.00596    0.00334   -0.01530
AFIX  23
H15A  2    0.444790    0.894914    0.854372    11.00000   -1.20000
H15B  2    0.541011    0.873987    0.939598    11.00000   -1.20000
AFIX   0
C16   1    0.519165    0.842848    0.711881    11.00000    0.06691    0.07632 =
      0.05877   -0.00760    0.01637   -0.00409
AFIX 137
H16A  2    0.578535    0.862299    0.701462    11.00000   -1.50000
H16B  2    0.475234    0.858552    0.626792    11.00000   -1.50000
H16C  2    0.524384    0.796818    0.703094    11.00000   -1.50000
HKLF 4
END
WGHT      0.2000      0.0000
REM Highest difference peak 10.430,  deepest hole -4.067,  1-sigma level  0.724
Q1    1   0.1973  0.4026  0.7505  11.00000  0.05   10.43
Q2    1   0.1200  0.7631  0.5824  11.00000  0.05   10.41
Q3    1   0.2563  0.7639  0.6024  11.00000  0.05    9.58
Q4    1   0.0602  0.4022  0.7299  11.00000  0.05    9.23
Q5    1  -0.0378  0.6121  0.7601  11.00000  0.05    5.71
Q6    1   0.0963  0.6117  0.7759  11.00000  0.05    5.60
Q7    1   0.2607  0.4038  0.8520  11.00000  0.05    2.64
Q8    1   0.3158  0.7650  0.7207  11.00000  0.05    2.43
Q9    1   0.1368  0.4092  0.6548  11.00000  0.05    2.39
Q10   1   0.1194  0.4070  0.8471  11.00000  0.05    2.34
```

coordinates as taken from **1-calc** model

```
TITL a in P2(1)/c
CELL 1.54178  14.7793  21.1524   8.3971  90.000  95.071  90.000
ZERR    4.00   0.0000   0.0000   0.0000   0.000   0.000   0.000
LATT  1
SYMM -X, 0.5+Y, 0.5-Z
SFAC C H O CS U
UNIT 64 124 56 4 8
TEMP -173.000
WGHT    0.100000
U1   5     0.1263301710517855  0.4013700260764151  0.7406588734740844
U1   5     0.8736698289482152  0.9013700260764156  0.7593411265259156
U1   5     0.8736698289482152  0.5986299739235844  0.2593411265259167
U1   5     0.1263301710517855  0.0986299739235845  0.2406588734740828
U2   5     0.1900796187994890  0.7647590317173411  0.5913178431583030
U2   5     0.8099203812005108  0.2647590317173414  0.9086821568416970
U2   5     0.8099203812005108  0.2352409682826591  0.4086821568416971
U2   5     0.1900796187994890  0.7352409682826589  0.0913178431583029
Cs1  4     0.0268701531136484  0.6146757942348396  0.7661481276299356
Cs1  4     0.9731298468863518  0.1146757942348407  0.7338518723700644
Cs1  4     0.9731298468863518  0.3853242057651594  0.2338518723700648
Cs1  4     0.0268701531136484  0.8853242057651604  0.2661481276299347
C1   1     0.2505312830220586  0.5014345982949978  0.8189321621414366
C1   1     0.7494687169779412  0.0014345982949972  0.6810678378585634
C1   1     0.7494687169779412  0.4985654017050031  0.1810678378585632
C1   1     0.2505312830220586 -0.0014345982949971  0.3189321621414376
C2   1     0.3128068313707590  0.5564916491721554  0.8569075102661757
C2   1     0.6871931686292414  0.0564916491721547  0.6430924897338243
C2   1     0.6871931686292414  0.4435083508278453  0.1430924897338241
C2   1     0.3128068313707590  0.9435083508278446  0.3569075102661758
C3   1     0.4136050851925061  0.5411863096319217  0.8576096909305320
C3   1     0.5863949148074948  0.0411863096319222  0.6423903090694680
C3   1     0.5863949148074948  0.4588136903680782  0.1423903090694678
C3   1     0.4136050851925061  0.9588136903680783  0.3576096909305324
C4   1     0.4412311801284190  0.5260223717792001  0.6910370673442858
C4   1     0.5587688198715811  0.0260223717792010  0.8089629326557142
C4   1     0.5587688198715811  0.4739776282207993  0.3089629326557136
C4   1     0.4412311801284190  0.9739776282208000  0.1910370673442868
C5   1     0.1820043695299538  0.2686846472402495  0.7424877349190644
C5   1     0.8179956304700460  0.7686846472402504  0.7575122650809356
C5   1     0.8179956304700460  0.7313153527597496  0.2575122650809351
C5   1     0.1820043695299538  0.2313153527597503  0.2424877349190646
C6   1     0.2058358585785890  0.1999790153074693  0.7662509633669986
C6   1     0.7941641414214115  0.6999790153074682  0.7337490366330014
C6   1     0.7941641414214115  0.8000209846925318  0.2337490366330013
C6   1     0.2058358585785890  0.3000209846925311  0.2662509633669988
C7   1     0.3063358455778678  0.1838426189607557  0.8029395926060492
C7   1     0.6936641544221318  0.6838426189607559  0.6970604073939508
C7   1     0.6936641544221318  0.8161573810392441  0.1970604073939497
C7   1     0.3063358455778678  0.3161573810392447  0.3029395926060498
C8   1     0.3591984361164969  0.1811499543310516  0.6551095851847665
C8   1     0.6408015638835031  0.6811499543310517  0.8448904148152335
```

| | | | | |
|---|---|---|---|---|
| C8 | 1 | 0.6408015638835031 | 0.8188500456689483 | 0.3448904148152334 |
| C8 | 1 | 0.3591984361164969 | 0.3188500456689483 | 0.1551095851847663 |
| C9 | 1 | 0.9353857661658292 | 0.4325069206618402 | 0.6705018158140407 |
| C9 | 1 | 0.0646142338341703 | 0.9325069206618404 | 0.8294981841859593 |
| C9 | 1 | 0.0646142338341703 | 0.5674930793381596 | 0.3294981841859588 |
| C9 | 1 | 0.9353857661658292 | 0.0674930793381596 | 0.1705018158140415 |
| C10 | 1 | 0.8359909408129815 | 0.4469324766607485 | 0.6431269339858520 |
| C10 | 1 | 0.1640090591870191 | 0.9469324766607491 | 0.8568730660141480 |
| C10 | 1 | 0.1640090591870191 | 0.5530675233392509 | 0.3568730660141477 |
| C10 | 1 | 0.8359909408129815 | 0.0530675233392514 | 0.1431269339858523 |
| C11 | 1 | 0.8020917990505457 | 0.4931507901422703 | 0.7646877559046737 |
| C11 | 1 | 0.1979082009494548 | 0.9931507901422697 | 0.7353122440953263 |
| C11 | 1 | 0.1979082009494548 | 0.5068492098577303 | 0.2353122440953260 |
| C11 | 1 | 0.8020917990505457 | 0.0068492098577293 | 0.2646877559046739 |
| C12 | 1 | 0.6997833864538920 | 0.5029904147280194 | 0.7370280883448538 |
| C12 | 1 | 0.3002166135461082 | 0.0029904147280205 | 0.7629719116551462 |
| C12 | 1 | 0.3002166135461082 | 0.4970095852719795 | 0.2629719116551472 |
| C12 | 1 | 0.6997833864538920 | 0.9970095852719806 | 0.2370280883448532 |
| C13 | 1 | 0.3543806488993446 | 0.7849309106915331 | 0.8833809535623851 |
| C13 | 1 | 0.6456193511006545 | 0.2849309106915336 | 0.6166190464376149 |
| C13 | 1 | 0.6456193511006545 | 0.2150690893084666 | 0.1166190464376150 |
| C13 | 1 | 0.3543806488993446 | 0.7150690893084669 | 0.3833809535623850 |
| C14 | 1 | 0.4464471260334901 | 0.8065570916256590 | 0.9561448224093198 |
| C14 | 1 | 0.5535528739665092 | 0.3065570916256593 | 0.5438551775906802 |
| C14 | 1 | 0.5535528739665092 | 0.1934429083743408 | 0.0438551775906799 |
| C14 | 1 | 0.4464471260334901 | 0.6934429083743410 | 0.4561448224093199 |
| C15 | 1 | 0.4921343255348412 | 0.8594074528616504 | 0.8690327794314676 |
| C15 | 1 | 0.5078656744651587 | 0.3594074528616509 | 0.6309672205685324 |
| C15 | 1 | 0.5078656744651587 | 0.1405925471383490 | 0.1309672205685321 |
| C15 | 1 | 0.4921343255348412 | 0.6405925471383496 | 0.3690327794314684 |
| C16 | 1 | 0.5208931421500598 | 0.8411184308807779 | 0.7051562725023415 |
| C16 | 1 | 0.4791068578499393 | 0.3411184308807784 | 0.7948437274976585 |
| C16 | 1 | 0.4791068578499393 | 0.1588815691192221 | 0.2948437274976580 |
| C16 | 1 | 0.5208931421500598 | 0.6588815691192221 | 0.2051562725023416 |
| H11A | 2 | 0.9777337908161940 | 0.7627535804571777 | 0.6494655961085204 |
| H11A | 2 | 0.0222662091838056 | 0.2627535804571767 | 0.8505344038914796 |
| H11A | 2 | 0.0222662091838056 | 0.2372464195428229 | 0.3505344038914808 |
| H11A | 2 | 0.9777337908161940 | 0.7372464195428223 | 0.1494655961085198 |