

^{27}Al MASNMR spectrum of AldiEPO-1d rehydrated for 5 min by exposure to air

AldiEPO-1

1101a
Version win32 Jan 16 18:41:49 2004 Page 1

PUBTABLE

Program PUBTABLES Version win32
Generate crystal structure data tables
Distributed on Sun Nov 23 14:29:57 2003

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GENLES was run on Jan 16 18:18:17 2004 Total cycles run 370

The Current Least-Squares controls are

Maximum number of cycles is 3
I/SigI cut-off is 1.00

Anisotropic thermal factors are defined by

$$T = \exp(h^{**2}*astr^{**2}*u11+... +2*h*k*astr*bstr*u12+...)$$

Space group P -1

The lattice is centric primitive triclinic Laue symmetry 1bar

Multiplicity of a general site is 2

The symmetry of the point 0,0,0 contains 1bar

The equivalent positions are:

(1) X Y Z

Lattice constants are

a = 8.5973(10) b = 7.04996(31) c = 9.5290(4)

Alpha = 89.989(17) Beta = 104.324(8) Gamma = 114.219(11)

Cell volume = 506.99(8)

1101a
Version win32 Jan 16 18:41:49 2004 Page 2

PUBTABLE

| Name | X | Y | Z | Ui/Ue*100 | Site sym | Mult | |
|------|----------|----------|----------|-----------|----------|------|----|
| A11 | 0.481690 | 0.613693 | 0.736836 | 2.32(7) | 1 | 2 | AL |
| 1 | 1.0000 | | | | | | |
| A12 | 0.505420 | 0.124541 | 0.751961 | 2.32(7) | 1 | 2 | AL |
| 2 | 1.0000 | | | | | | |
| P1 | 0.271632 | 0.751697 | 0.906373 | 2.32(7) | 1 | 2 | P |
| 3 | 1.0000 | | | | | | |
| P2 | 0.732340 | 0.498466 | 0.593842 | 2.32(7) | 1 | 2 | P |
| 4 | 1.0000 | | | | | | |
| C1 | 0.036850 | 0.654158 | 0.824528 | 2.32(7) | 1 | 2 | C |
| 5 | 1.0000 | | | | | | |
| C2 | 0.964007 | 0.610287 | 0.677592 | 2.32(7) | 1 | 2 | C |
| 6 | 1.0000 | | | | | | |
| O1 | 0.643669 | 0.626208 | 0.643654 | 2.32(7) | 1 | 2 | O |

Page 1

AldiEPO-1

| | | | | | | | |
|-----|-----------|----------|----------|---------|---|---|---|
| 7 | 1.0000 | | | | | | |
| O2 | 0.325478 | 1.000403 | 0.848023 | 2.32(7) | 1 | 2 | O |
| 8 | 1.0000 | | | | | | |
| O3 | 0.312894 | 0.550018 | 0.582557 | 2.32(7) | 1 | 2 | O |
| 9 | 1.0000 | | | | | | |
| O4 | 0.684859 | 0.214705 | 0.916107 | 2.32(7) | 1 | 2 | O |
| 10 | 1.0000 | | | | | | |
| O5 | 0.439941 | 0.336778 | 0.777695 | 2.32(7) | 1 | 2 | O |
| 11 | 1.0000 | | | | | | |
| O6 | 0.592311 | 0.907305 | 0.736341 | 2.32(7) | 1 | 2 | O |
| 12 | 1.0000 | | | | | | |
| O7 | 0.382945 | 0.635946 | 0.874706 | 2.32(7) | 1 | 2 | O |
| 13 | 1.0000 | | | | | | |
| O8 | 0.676462 | 0.232839 | 0.645408 | 2.32(7) | 1 | 2 | O |
| 14 | 1.0000 | | | | | | |
| O9 | 0.665915 | 0.702278 | 0.940382 | 2.32(7) | 1 | 2 | O |
| 15 | 1.0000 | | | | | | |
| O10 | 0.309779 | 0.005581 | 0.554262 | 2.32(7) | 1 | 2 | O |
| 16 | 1.0000 | | | | | | |
| H1 | -0.021600 | 0.495900 | 0.847700 | 2.50 | 1 | 2 | H |
| 17 | 1.0000 | | | | | | |
| H2 | -0.022500 | 0.713900 | 0.866600 | 2.50 | 1 | 2 | H |
| 18 | 1.0000 | | | | | | |
| H3 | 0.032800 | 0.564500 | 0.636600 | 2.50 | 1 | 2 | H |
| 19 | 1.0000 | | | | | | |
| H4 | 0.016300 | 0.773500 | 0.655400 | 2.50 | 1 | 2 | H |
| 20 | 1.0000 | | | | | | |

Thermal parameters multiplied by 100.0 are

| Name | U11 | U22 | U33 | U12 | U13 | U23 |
|------|---------|------|------|------|------|------|
| A11 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| A12 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| P1 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| P2 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| C1 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| C2 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O1 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O2 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O3 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O4 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O5 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O6 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O7 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O8 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O9 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| O10 | 2.32(7) | 2.32 | 2.32 | 0.00 | 0.00 | 0.00 |
| H1 | 2.50 | 2.50 | 2.50 | 0.00 | 0.00 | 0.00 |

AldiEPO-1

| | | | | | | |
|----|------|------|------|------|------|------|
| H2 | 2.50 | 2.50 | 2.50 | 0.00 | 0.00 | 0.00 |
| H3 | 2.50 | 2.50 | 2.50 | 0.00 | 0.00 | 0.00 |
| H4 | 2.50 | 2.50 | 2.50 | 0.00 | 0.00 | 0.00 |

Bond distances and angles are

| | | | | | |
|-----|-----|-------------|---|--------|---|
| A11 | O1 | 1.80181(17) | . | 1.555 | N |
| A11 | O3 | 1.69672(24) | . | 1.555 | N |
| A11 | O5 | 1.89357(16) | . | 1.555 | N |
| A11 | O6 | 1.89110(20) | . | 1.555 | N |
| A11 | O7 | 1.76989(13) | . | 1.555 | N |
| A11 | O9 | 2.08073(30) | . | 1.555 | N |
| A12 | O2 | 1.89385(25) | . | 1.545 | N |
| A12 | O4 | 1.79788(28) | . | 1.555 | N |
| A12 | O5 | 1.83722(13) | . | 1.555 | N |
| A12 | O6 | 1.97977(14) | . | 1.545 | N |
| A12 | O8 | 1.89567(23) | . | 1.555 | N |
| A12 | O10 | 2.08729(35) | . | 1.555 | N |
| P1 | C1 | 1.79941(28) | . | 1.555 | N |
| P1 | O2 | 1.74894(20) | . | 1.555 | N |
| P1 | O4 | 1.63459(12) | . | -1.667 | N |
| P1 | O7 | 1.56733(14) | . | 1.555 | N |
| P1 | H1 | 2.3437(4) | . | 1.555 | N |
| P1 | H2 | 2.36266(29) | . | 1.555 | N |
| P2 | C2 | 1.77505(29) | . | 1.555 | N |
| P2 | O1 | 1.53622(14) | . | 1.555 | N |
| P2 | O3 | 1.63133(14) | . | -1.666 | N |
| P2 | O8 | 1.83233(19) | . | 1.555 | N |
| P2 | H3 | 2.35543(31) | . | 1.655 | N |
| P2 | H4 | 2.3392(4) | . | 1.655 | N |
| C1 | P1 | 1.79941(28) | . | 1.555 | N |
| C1 | C2 | 1.36223(14) | . | 1.455 | N |
| C1 | H1 | 1.06813(13) | . | 1.555 | N |
| C1 | H2 | 0.93599(9) | . | 1.555 | N |
| C1 | H3 | 1.88656(20) | . | 1.555 | N |
| C1 | H4 | 1.82125(24) | . | 1.555 | N |
| C2 | P2 | 1.77505(29) | . | 1.555 | N |
| C2 | C1 | 1.36223(14) | . | 1.655 | N |
| C2 | H1 | 1.80977(23) | . | 1.655 | N |
| C2 | H2 | 1.90223(22) | . | 1.655 | N |
| C2 | H3 | 0.93679(9) | . | 1.655 | N |
| C2 | H4 | 1.09241(12) | . | 1.655 | N |
| O1 | A11 | 1.80181(17) | . | 1.555 | N |
| O1 | P2 | 1.53622(14) | . | 1.555 | N |
| O2 | A12 | 1.89385(25) | . | 1.565 | N |
| O2 | P1 | 1.74894(20) | . | 1.555 | N |
| O3 | A11 | 1.69672(24) | . | 1.555 | N |
| O3 | P2 | 1.63133(14) | . | -1.666 | N |
| O4 | A12 | 1.79788(28) | . | 1.555 | N |
| O4 | P1 | 1.63459(12) | . | -1.667 | N |
| O5 | A11 | 1.89357(16) | . | 1.555 | N |
| O5 | A12 | 1.83722(13) | . | 1.555 | N |
| O6 | A11 | 1.89110(20) | . | 1.555 | N |
| O6 | A12 | 1.97977(14) | . | 1.565 | N |
| O7 | A11 | 1.76989(13) | . | 1.555 | N |
| O7 | P1 | 1.56733(14) | . | 1.555 | N |
| O8 | A12 | 1.89567(23) | . | 1.555 | N |
| O8 | P2 | 1.83233(19) | . | 1.555 | N |
| O9 | A11 | 2.08073(30) | . | 1.555 | N |
| O10 | A12 | 2.08729(35) | . | 1.555 | N |
| H1 | P1 | 2.3437(4) | . | 1.555 | N |

AldiEPO-1

| | | | | | |
|----|----|-------------|---|-------|---|
| H1 | C1 | 1.06813(13) | . | 1_555 | N |
| H1 | C2 | 1.80977(23) | . | 1_455 | N |
| H1 | H2 | 1.55083(9) | . | 1_555 | N |
| H2 | P1 | 2.36266(29) | . | 1_555 | N |
| H2 | C1 | 0.93599(9) | . | 1_555 | N |
| H2 | C2 | 1.90223(22) | . | 1_455 | N |
| H2 | H1 | 1.55083(9) | . | 1_555 | N |
| H3 | P2 | 2.35543(31) | . | 1_455 | N |
| H3 | C1 | 1.88656(20) | . | 1_555 | N |
| H3 | C2 | 0.93679(9) | . | 1_455 | N |
| H3 | H4 | 1.55158(9) | . | 1_555 | N |
| H4 | P2 | 2.3392(4) | . | 1_455 | N |
| H4 | C1 | 1.82125(24) | . | 1_555 | N |
| H4 | C2 | 1.09241(12) | . | 1_455 | N |
| H4 | H3 | 1.55158(9) | . | 1_555 | N |

| | | | | | | | |
|----|-----|-----|--------------|--------|---|--------|---|
| 01 | A11 | 03 | 94.849(8) | 1_555 | . | 1_555 | N |
| 01 | A11 | 05 | 91.716(12) | 1_555 | . | 1_555 | N |
| 01 | A11 | 06 | 81.486(13) | 1_555 | . | 1_555 | N |
| 01 | A11 | 07 | 162.002(4) | 1_555 | . | 1_555 | N |
| 01 | A11 | 09 | 92.997(8) | 1_555 | . | 1_555 | N |
| 03 | A11 | 05 | 97.038(18) | 1_555 | . | 1_555 | N |
| 03 | A11 | 06 | 99.895(19) | 1_555 | . | 1_555 | N |
| 03 | A11 | 07 | 102.893(8) | 1_555 | . | 1_555 | N |
| 03 | A11 | 09 | 171.8406(13) | 1_555 | . | 1_555 | N |
| 05 | A11 | 06 | 162.2082(28) | 1_555 | . | 1_555 | N |
| 05 | A11 | 07 | 89.126(14) | 1_555 | . | 1_555 | N |
| 05 | A11 | 09 | 84.950(18) | 1_555 | . | 1_555 | N |
| 06 | A11 | 07 | 92.376(15) | 1_555 | . | 1_555 | N |
| 06 | A11 | 09 | 79.048(19) | 1_555 | . | 1_555 | N |
| 07 | A11 | 09 | 69.164(8) | 1_555 | . | 1_555 | N |
| 02 | A12 | 04 | 95.134(10) | 1_545 | . | 1_555 | N |
| 02 | A12 | 05 | 77.469(10) | 1_545 | . | 1_555 | N |
| 02 | A12 | 06 | 103.601(10) | 1_545 | . | 1_545 | N |
| 02 | A12 | 08 | 175.9960(12) | 1_545 | . | 1_555 | N |
| 02 | A12 | 010 | 88.035(10) | 1_545 | . | 1_555 | N |
| 04 | A12 | 05 | 93.631(16) | 1_555 | . | 1_555 | N |
| 04 | A12 | 06 | 82.123(15) | 1_555 | . | 1_545 | N |
| 04 | A12 | 08 | 88.022(10) | 1_555 | . | 1_555 | N |
| 04 | A12 | 010 | 174.5549(9) | 1_555 | . | 1_555 | N |
| 05 | A12 | 06 | 175.6829(9) | 1_555 | . | 1_545 | N |
| 05 | A12 | 08 | 104.832(10) | 1_555 | . | 1_555 | N |
| 05 | A12 | 010 | 91.377(15) | 1_555 | . | 1_555 | N |
| 06 | A12 | 08 | 74.352(10) | 1_545 | . | 1_555 | N |
| 06 | A12 | 010 | 92.838(15) | 1_545 | . | 1_555 | N |
| 08 | A12 | 010 | 88.630(10) | 1_555 | . | 1_555 | N |
| C1 | P1 | 02 | 95.700(13) | 1_555 | . | 1_555 | N |
| C1 | P1 | 04 | 110.267(11) | 1_555 | . | -1_667 | N |
| C1 | P1 | 07 | 122.295(12) | 1_555 | . | 1_555 | N |
| 02 | P1 | 04 | 106.415(18) | 1_555 | . | -1_667 | N |
| 02 | P1 | 07 | 115.664(7) | 1_555 | . | 1_555 | N |
| 04 | P1 | 07 | 105.541(11) | -1_667 | . | 1_555 | N |
| C2 | P2 | 01 | 111.560(13) | 1_555 | . | 1_555 | N |
| C2 | P2 | 03 | 111.806(11) | 1_555 | . | -1_666 | N |
| C2 | P2 | 08 | 98.897(14) | 1_555 | . | 1_555 | N |
| 01 | P2 | 03 | 114.623(11) | 1_555 | . | -1_666 | N |
| 01 | P2 | 08 | 118.570(7) | 1_555 | . | 1_555 | N |
| 03 | P2 | 08 | 99.961(18) | -1_666 | . | 1_555 | N |
| P1 | C1 | C2 | 122.476(10) | 1_555 | . | 1_455 | N |
| P1 | C1 | H1 | 106.851(14) | 1_555 | . | 1_555 | N |
| P1 | C1 | H2 | 115.840(13) | 1_555 | . | 1_555 | N |
| C2 | C1 | H1 | 95.496(20) | 1_455 | . | 1_555 | N |

| AldiEPO-1 | | | | | | | |
|-----------|----|-----|-------------|-------|---|--------|---|
| C2 | C1 | H2 | 110.348(10) | 1_455 | . | 1_555 | N |
| H1 | C1 | H2 | 101.192(9) | 1_555 | . | 1_555 | N |
| P2 | C2 | C1 | 123.653(10) | 1_555 | . | 1_655 | N |
| P2 | C2 | H3 | 117.190(12) | 1_555 | . | 1_655 | N |
| P2 | C2 | H4 | 106.904(14) | 1_555 | . | 1_655 | N |
| C1 | C2 | H3 | 108.881(9) | 1_655 | . | 1_655 | N |
| C1 | C2 | H4 | 95.165(20) | 1_655 | . | 1_655 | N |
| H3 | C2 | H4 | 99.463(10) | 1_655 | . | 1_655 | N |
| A11 | O1 | P2 | 143.382(6) | 1_555 | . | 1_555 | N |
| A12 | O2 | P1 | 122.876(10) | 1_565 | . | 1_555 | N |
| A11 | O3 | P2 | 141.598(6) | 1_555 | . | -1_666 | N |
| A12 | O4 | P1 | 142.644(6) | 1_555 | . | -1_667 | N |
| A11 | O5 | A12 | 142.991(4) | 1_555 | . | 1_555 | N |
| A11 | O6 | A12 | 131.076(6) | 1_555 | . | 1_565 | N |
| A11 | O7 | P1 | 137.872(8) | 1_555 | . | 1_555 | N |
| A12 | O8 | P2 | 118.436(11) | 1_555 | . | 1_555 | N |
| C1 | H1 | H2 | 36.304(4) | 1_555 | . | 1_555 | N |
| C1 | H2 | H1 | 42.505(9) | 1_555 | . | 1_555 | N |
| C2 | H3 | H4 | 43.986(9) | 1_455 | . | 1_555 | N |
| C2 | H4 | H3 | 36.551(4) | 1_455 | . | 1_555 | N |

AldiEPO-1d

lwowater
Version win32 Jan 16 17:02:20 2004 Page 1

PUBTABLE

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Program PUBTABLES Version win32
Generate crystal structure data tables
Distributed on Fri Jan 16 17:02:20 2004
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GENLES was run on Jan 16 16:37:49 2004 Total cycles run 241

The Current Least-Squares controls are

Maximum number of cycles is 3
I/SigI cut-off is 1.00Anisotropic thermal factors are defined by
 $T = \exp(h^{**2}astr^{**2}u11+... +2*h*k*astr*bstr*u12+...)$

Space group C 2/c

The lattice is centric C-centered monoclinic Laue symmetry 2/m

Multiplicity of a general site is 8

The unique axis is b

The symmetry of the point 0,0,0 contains 1bar

The equivalent positions are:

(1) X Y Z (2) -X Y 1/2-Z

Lattice constants are

a = 15.3723(21) b = 6.7613(8) c = 9.7374(13)

Alpha = 90 Beta = 102.392(9) Gamma = 90

Cell volume = 988.49(23)

| Name | X | Y | Z | Ui/Ue*100 | Site | sym | Mult | |
|-----------------|----------|----------|----------|-----------|------|-----|------|--|
| Type Seq Fractn | | | | | | | | |
| AL1 | 0.231716 | 0.396528 | 0.706419 | 2.56(12) | 1 | 8 | AL | |
| 1 1.0000 | | | | | | | | |
| P1 | 0.132202 | 0.661400 | 0.901643 | 2.56(12) | 1 | 8 | P | |
| 2 1.0000 | | | | | | | | |
| C1 | 0.010869 | 0.669403 | 0.826681 | 2.56(12) | 1 | 8 | C | |
| 3 1.0000 | | | | | | | | |
| O1 | 0.320737 | 0.361895 | 0.630950 | 2.56(12) | 1 | 8 | O | |
| 4 1.0000 | | | | | | | | |
| O2 | 0.143364 | 0.378836 | 0.567002 | 2.56(12) | 1 | 8 | O | |
| 5 1.0000 | | | | | | | | |
| O3 | 0.231650 | 0.166356 | 0.802096 | 2.56(12) | 1 | 8 | O | |
| 6 1.0000 | | | | | | | | |
| O4 | 0.162616 | 0.475104 | 0.825273 | 2.56(12) | 1 | 8 | O | |
| 7 1.0000 | | | | | | | | |
| H1 | 0.029800 | 0.560000 | 0.658100 | 2.50 | 1 | 8 | H | |

Page 1

AldiEPO-1d

8 1.0000
 H2 0.026300 0.789300 0.656900 2.50 1 8 H
 9 1.0000
 lwowater
 Version win32 Jan 16 17:02:20 2004 Page 2 PUBTABLE

Thermal parameters multiplied by 100.0 are

| Name | U11 | U22 | U33 | U12 | U13 | U23 |
|------|----------|------|------|------|------|------|
| AL1 | 2.56(12) | 2.56 | 2.56 | 0.00 | 0.00 | 0.00 |
| P1 | 2.56(12) | 2.56 | 2.56 | 0.00 | 0.00 | 0.00 |
| C1 | 2.56(12) | 2.56 | 2.56 | 0.00 | 0.00 | 0.00 |
| O1 | 2.56(12) | 2.56 | 2.56 | 0.00 | 0.00 | 0.00 |
| O2 | 2.56(12) | 2.56 | 2.56 | 0.00 | 0.00 | 0.00 |
| O3 | 2.56(12) | 2.56 | 2.56 | 0.00 | 0.00 | 0.00 |
| O4 | 2.56(12) | 2.56 | 2.56 | 0.00 | 0.00 | 0.00 |
| H1 | 2.50 | 2.50 | 2.50 | 0.00 | 0.00 | 0.00 |
| H2 | 2.50 | 2.50 | 2.50 | 0.00 | 0.00 | 0.00 |

Bond distances and angles are

| | | | | |
|-----|-----|-------------|---------|---|
| AL1 | P1 | 3.0582(4) | -2.565 | N |
| AL1 | P1 | 2.99255(28) | 102.546 | N |
| AL1 | O1 | 1.70269(20) | 1.555 | N |
| AL1 | O2 | 1.70603(23) | 1.555 | N |
| AL1 | O3 | 1.81392(17) | 1.555 | N |
| AL1 | O3 | 1.91636(21) | 102.556 | N |
| AL1 | O4 | 1.81042(19) | 1.555 | N |
| P1 | AL1 | 3.0582(4) | -2.566 | N |
| P1 | AL1 | 2.99255(28) | 102.556 | N |
| P1 | C1 | 1.85209(26) | 1.555 | N |
| P1 | O1 | 1.60009(15) | 102.556 | N |
| P1 | O2 | 1.60546(22) | -2.566 | N |
| P1 | O4 | 1.58348(14) | 1.555 | N |
| C1 | P1 | 1.85209(26) | 1.555 | N |
| C1 | C1 | 1.45862(20) | 2.556 | N |
| C1 | H1 | 1.87924(21) | 1.555 | N |
| C1 | H1 | 0.99987(9) | 2.556 | N |
| C1 | H2 | 1.90129(21) | 1.555 | N |
| C1 | H2 | 1.02391(9) | 2.556 | N |
| O1 | AL1 | 1.70269(20) | 1.555 | N |
| O1 | P1 | 1.60009(15) | 102.546 | N |
| O2 | AL1 | 1.70603(23) | 1.555 | N |
| O2 | P1 | 1.60546(22) | -2.565 | N |
| O3 | AL1 | 1.81392(17) | 1.555 | N |
| O3 | AL1 | 1.91636(21) | 102.546 | N |
| O4 | AL1 | 1.81042(19) | 1.555 | N |
| O4 | P1 | 1.58348(14) | 1.555 | N |
| H1 | C1 | 1.87924(21) | 1.555 | N |
| H1 | C1 | 0.99987(9) | 2.556 | N |
| H1 | H2 | 1.55125(18) | 1.555 | N |
| H2 | C1 | 1.90129(21) | 1.555 | N |
| H2 | C1 | 1.02391(9) | 2.556 | N |
| H2 | H1 | 1.55125(18) | 1.555 | N |

AldiEPO-1d

loop_

| | _geom_angle_atom_site_label_1 | | | | | | |
|-----|-------------------------------|-----|--------------|---------|---|---------|---|
| | _geom_angle_atom_site_label_2 | | | | | | |
| | _geom_angle_atom_site_label_3 | | | | | | |
| | _geom_angle | | | | | | |
| | _geom_angle_site_symmetry_1 | | | | | | |
| | _geom_angle_site_symmetry_2 | | | | | | |
| | _geom_angle_site_symmetry_3 | | | | | | |
| | _geom_angle_publ_flag | | | | | | |
| O1 | AL1 | O2 | 102.899(11) | 1_555 | . | 1_555 | N |
| O1 | AL1 | O3 | 101.114(5) | 1_555 | . | 1_555 | N |
| O1 | AL1 | O3 | 80.874(4) | 1_555 | . | 102_556 | N |
| O1 | AL1 | O4 | 162.2530(24) | 1_555 | . | 1_555 | N |
| O2 | AL1 | O3 | 105.096(6) | 1_555 | . | 1_555 | N |
| O2 | AL1 | O3 | 102.9133(30) | 1_555 | . | 102_556 | N |
| O2 | AL1 | O4 | 93.047(11) | 1_555 | . | 1_555 | N |
| O3 | AL1 | O3 | 150.640(5) | 1_555 | . | 102_556 | N |
| O3 | AL1 | O4 | 81.857(7) | 1_555 | . | 1_555 | N |
| O3 | AL1 | O4 | 88.078(5) | 102_556 | . | 1_555 | N |
| C1 | P1 | O1 | 110.917(5) | 1_555 | . | 102_556 | N |
| C1 | P1 | O2 | 106.383(9) | 1_555 | . | -2_566 | N |
| C1 | P1 | O4 | 102.241(6) | 1_555 | . | 1_555 | N |
| O1 | P1 | O2 | 112.763(4) | 102_556 | . | -2_566 | N |
| O1 | P1 | O4 | 112.901(9) | 102_556 | . | 1_555 | N |
| O2 | P1 | O4 | 110.943(6) | -2_566 | . | 1_555 | N |
| P1 | C1 | C1 | 113.177(9) | 1_555 | . | 2_556 | N |
| P1 | C1 | H1 | 121.924(6) | 1_555 | . | 2_556 | N |
| P1 | C1 | H2 | 120.671(5) | 1_555 | . | 2_556 | N |
| C1 | C1 | H1 | 97.966(6) | 2_556 | . | 2_556 | N |
| C1 | C1 | H2 | 98.450(6) | 2_556 | . | 2_556 | N |
| H1 | C1 | H2 | 100.077(10) | 2_556 | . | 2_556 | N |
| AL1 | O1 | P1 | 129.9092(31) | 1_555 | . | 102_546 | N |
| AL1 | O2 | P1 | 134.865(7) | 1_555 | . | -2_565 | N |
| AL1 | O3 | AL1 | 139.640(6) | 1_555 | . | 102_546 | N |
| AL1 | O4 | P1 | 143.7570(20) | 1_555 | . | 1_555 | N |
| C1 | H1 | H2 | 40.532(5) | 2_556 | . | 1_555 | N |
| C1 | H2 | H1 | 39.391(5) | 2_556 | . | 1_555 | N |

energyminimised_coordinates

AldiEPO-1

a=8.686, b=7.065, c=9.605

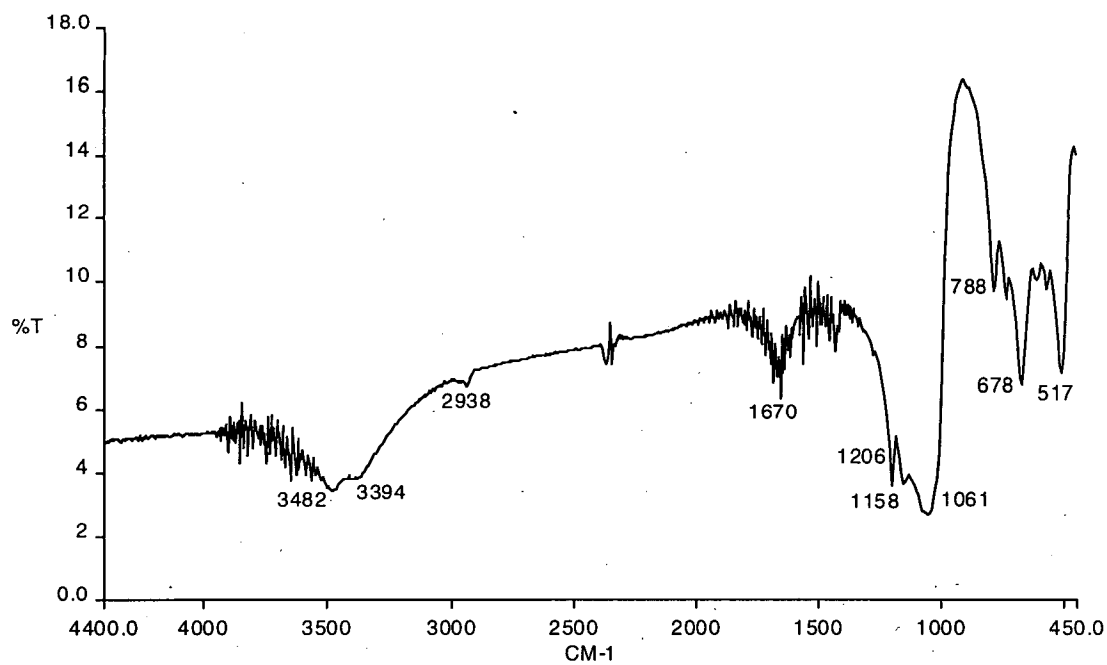
alpha=90.154, beta=104.617, gamma=114.057

| Element | Atom number | Fractional coordinates after optimization step | | | Forces in cartesian (eV/A) before optimization step | | |
|---------|-------------|--|---------|---------|---|---------|---------|
| | | u | v | w | Fx | Fy | Fz |
| Al | 1 | .48433 | .61239 | .73692 | .00246 | .00323 | -.00132 |
| Al | 2 | .51567 | .38760 | .26308 | -.00246 | -.00323 | .00132 |
| Al | 3 | .51554 | .12785 | .76587 | -.01793 | .00396 | .00104 |
| Al | 4 | .48446 | .87214 | .23413 | .01792 | -.00396 | -.00104 |
| P | 1 | .26677 | .75584 | .90022 | .01876 | -.02575 | -.00842 |
| P | 2 | .73323 | .24416 | .09978 | -.01878 | .02574 | .00841 |
| P | 3 | .72971 | .48592 | .60062 | -.01834 | .00285 | .01881 |
| P | 4 | .27029 | .51407 | .39938 | .01834 | -.00284 | -.01881 |
| C | 1 | .03287 | .64806 | .83315 | -.00205 | .00388 | .01458 |
| C | 2 | .96713 | .35194 | .16685 | .00204 | -.00388 | -.01458 |
| C | 3 | .96351 | .60712 | .66838 | .02103 | .00460 | -.00950 |
| C | 4 | .03649 | .39287 | .33162 | -.02103 | -.00461 | .00950 |
| O | 1 | .66096 | .62922 | .65556 | -.00369 | -.00871 | -.00164 |
| O | 2 | .33904 | .37078 | .34444 | .00369 | .00873 | .00164 |
| O | 3 | .34269 | -.02645 | .85410 | -.01881 | -.00302 | .00109 |
| O | 4 | .65731 | .02645 | .14590 | .01880 | .00303 | -.00109 |
| O | 5 | .31365 | .54063 | .56216 | -.02704 | -.01330 | .01028 |
| O | 6 | .68635 | .45936 | .43784 | .02704 | .01330 | -.01028 |
| O | 7 | .69060 | .23717 | .93687 | .00221 | .00696 | -.01836 |
| O | 8 | .30940 | .76283 | .06313 | -.00222 | -.00695 | .01836 |
| O | 9 | .43422 | .33517 | .76540 | .02541 | .00013 | -.00194 |
| O | 10 | .56578 | .66483 | .23460 | -.02541 | -.00014 | .00194 |
| O | 11 | .56612 | .90098 | .73826 | -.05967 | .00690 | -.00052 |
| O | 12 | .43388 | .09902 | .26174 | .05968 | -.00689 | .00052 |
| O | 13 | .32495 | .60796 | .83575 | -.00766 | -.00262 | .00679 |
| O | 14 | .67505 | .39203 | .16425 | .00767 | .00263 | -.00679 |
| O | 15 | .66515 | .27254 | .65569 | .00514 | .00210 | .00363 |
| O | 16 | .33485 | .72745 | .34431 | -.00514 | -.00210 | -.00363 |
| O | 17 | .66805 | .69070 | .93649 | -.00481 | -.01748 | -.00298 |
| O | 18 | .33194 | .30929 | .06351 | .00487 | .01749 | .00298 |
| O | 19 | .32688 | .01393 | .56801 | -.00365 | .02841 | -.01178 |
| O | 20 | .67312 | .98607 | .43199 | .00361 | -.02841 | .01177 |
| H | 1 | .68800 | .73283 | .23670 | .03986 | .00336 | -.00149 |
| H | 2 | .31200 | .26717 | .76330 | -.03986 | -.00335 | .00150 |
| H | 3 | .31251 | .04447 | .26231 | -.03198 | .01099 | -.00365 |
| H | 4 | .68749 | .95553 | .73769 | .03198 | -.01100 | .00365 |
| H | 5 | -.01115 | .24736 | .38028 | .00358 | .00749 | .00377 |
| H | 6 | .01115 | .75263 | .61972 | -.00357 | -.00750 | -.00377 |
| H | 7 | .98724 | .49455 | .37350 | -.00091 | -.01688 | .00033 |
| H | 8 | .01277 | .50544 | .62651 | .00091 | .01687 | -.00032 |
| H | 9 | .98047 | .50205 | .88001 | .00464 | .00338 | .00174 |
| H | 10 | .01953 | .49795 | .11999 | -.00465 | -.00337 | -.00174 |
| H | 11 | -.01256 | .75308 | .87651 | .00498 | -.01197 | -.00221 |
| H | 12 | .01256 | .24692 | .12349 | -.00498 | .01198 | .00221 |
| H | 13 | .66715 | .57818 | -.00416 | -.03547 | .02422 | -.01175 |
| H | 14 | .33285 | .42181 | .00416 | .03549 | -.02424 | .01175 |
| H | 15 | .33220 | .19828 | .00299 | .05329 | -.00797 | -.00943 |
| H | 16 | .66780 | .80171 | -.00299 | -.05329 | .00798 | .00943 |
| H | 17 | .33726 | .90930 | .50827 | -.00897 | -.01929 | -.01187 |
| H | 18 | .66274 | .09070 | .49173 | .00899 | .01929 | .01186 |
| H | 19 | .66692 | .87114 | .48967 | -.00217 | .01943 | -.00672 |
| H | 20 | .33308 | .12886 | .51033 | .00218 | -.01944 | .00671 |

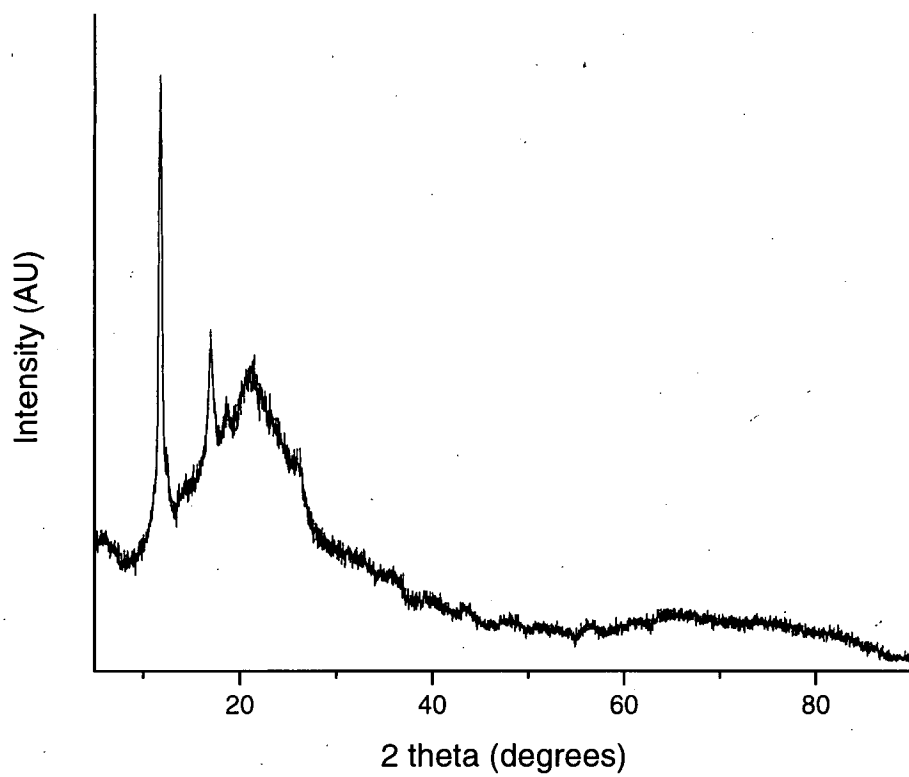
 energyminimised_coordinates

AldiEPO-1d
 a=8.490 b=6.788 c=9.822
 alpha=89.935, beta=102.343, gamma=113.393

| Element | Atom number | Fractional coordinates after optimization step | | | Forces in cartesian (eV/A) before optimization step | | |
|---------|-------------|--|---------|--------|---|---------|---------|
| | | u | v | w | Fx | Fy | Fz |
| Al | 1 | .45926 | .60104 | .71098 | -.00918 | .00076 | -.01178 |
| Al | 2 | .54074 | .39896 | .28902 | .00918 | -.00076 | .01177 |
| Al | 3 | .53971 | .13967 | .79146 | .00906 | .00321 | -.00905 |
| Al | 4 | .46029 | .86033 | .20854 | -.00906 | -.00321 | .00905 |
| P | 1 | .26123 | .74905 | .89103 | .00574 | .01049 | .00992 |
| P | 2 | .73877 | .25095 | .10897 | -.00574 | -.01049 | -.00992 |
| P | 3 | .73313 | .48058 | .60708 | -.01158 | -.00888 | .00779 |
| P | 4 | .26687 | .51942 | .39292 | .01158 | .00887 | -.00779 |
| C | 1 | .02749 | .64493 | .83074 | -.00794 | -.00442 | .00511 |
| C | 2 | .97251 | .35507 | .16926 | .00794 | .00442 | -.00511 |
| C | 3 | .96625 | .60680 | .67123 | -.00171 | .00078 | -.00955 |
| C | 4 | .03375 | .39320 | .32877 | .00171 | -.00078 | .00955 |
| O | 1 | .65769 | .62950 | .65448 | -.01935 | -.01032 | .00317 |
| O | 2 | .34231 | .37050 | .34552 | .01935 | .01032 | -.00317 |
| O | 3 | .33737 | -.03067 | .83816 | -.00144 | .00474 | .01252 |
| O | 4 | .66263 | .03067 | .16184 | .00144 | -.00474 | -.01252 |
| O | 5 | .30332 | .54814 | .55061 | -.00478 | -.01271 | -.00777 |
| O | 6 | .69668 | .45186 | .44939 | .00479 | .01271 | .00777 |
| O | 7 | .69774 | .23554 | .95098 | .01296 | .01482 | .00451 |
| O | 8 | .30226 | .76446 | .04902 | -.01296 | -.01482 | -.00451 |
| O | 9 | .43950 | .33713 | .76727 | -.00277 | .00554 | -.00982 |
| O | 10 | .56050 | .66287 | .23273 | .00277 | -.00554 | .00982 |
| O | 11 | .56724 | .89431 | .74510 | .01307 | .00271 | -.01055 |
| O | 12 | .43276 | .10569 | .25490 | -.01307 | -.00271 | .01055 |
| O | 13 | .32251 | .59360 | .83207 | .02944 | .00919 | -.00260 |
| O | 14 | .67749 | .40640 | .16793 | -.02944 | -.00919 | .00260 |
| O | 15 | .66785 | .26466 | .66721 | -.01561 | .01922 | -.01190 |
| O | 16 | .33215 | .73534 | .33279 | .01561 | -.01922 | .01190 |
| H | 1 | .65404 | .70963 | .18290 | .00490 | -.00578 | .00552 |
| H | 2 | .34596 | .29037 | .81710 | -.00490 | .00578 | -.00552 |
| H | 3 | .33132 | .06155 | .29588 | .03047 | -.01228 | .00648 |
| H | 4 | .66868 | .93845 | .70412 | -.03047 | .01228 | -.00647 |
| H | 5 | -.01401 | .24141 | .37713 | .00112 | .00413 | .00515 |
| H | 6 | .01401 | .75859 | .62287 | -.00112 | -.00414 | -.00515 |
| H | 7 | .97879 | .49591 | .36864 | -.00380 | .01146 | .00335 |
| H | 8 | .02121 | .50409 | .63136 | .00380 | -.01146 | -.00335 |
| H | 9 | .97085 | .49423 | .87791 | .00862 | .00445 | .00416 |
| H | 10 | .02915 | .50577 | .12209 | -.00862 | -.00445 | -.00416 |
| H | 11 | -.01697 | .75831 | .87223 | -.00797 | .00739 | .00053 |
| H | 12 | .01697 | .24169 | .12777 | .00796 | -.00739 | -.00053 |



IR spectrum of AldiEPO-1



XRD pattern of AldiEPO-1 heated to 400 °C