Lactide

(Last updated 24 March 2025)



Figure . The molecular diagram of Lactide.

This molecule has two stereocentres. meso-Lactide has one centre of each type, and hence the molecule is not chiral. Both chiral molecules (LL-Lactide and DD-Lactide) and the racemic mixture of the two have determinations on the CSD. Meso-Lactide was not included in the original CSP (it is a different molecule).

# CSP studies

|  |  |
| --- | --- |
| REFCODE | BICVIS |
| Formula | C6 H8 O4 |
| Common Name | DD,LL-lactide |
| IUPAC Systematic Name | rac-3,6-dimethyl-1,4-dioxane-2,5-dione |
| CSD Refcodes | BICVIS, NAHNOZ01, TOFTIV, BEYDEO01 |
| Search identifier | A |
| Scientist | Rebecca Hylton |
| Date | 2014 |
| Publication | Buchholz HK, Hylton RK, Brandenburg JG, Seidel-Morgenstern A, Lorenz H, Stein M, Price SL, Cryst Growth Des 2017, 17 (9), 4676-4686 |
| Energy model | 1 |
| Study\_ID | 20 |
| Programs | Rigid Crystal Predictor (x), DMACRYS (2.0.8) |
| Location on S Drive | \CHEMISTRY\_CPOSS\Lactides\racemic-CrystalPredictor |
| Potential Description | CrystalPredictor + GDMA2.2(PBE0/6-31G(d,p)) + FIT |
| Energy model | 2 (published) |
| Study\_ID | 10 |
| Programs | Study\_ID=20, CrystalOptimizer (2.3), DMACRYS (2.0.8) |
| Location on S Drive | \CHEMISTRY\_CPOSS\Lactides\CrystalOptimizer |
| Potential Description | CrystalOptimizer PBE1PBE/6-31G(d,p) intramolecular + GDMA2.2(PBE1PBE/6-31G(d,p)) DMA + FIT |
| Energy model | 3 |
| Study\_ID | 30 |
| Programs | Study\_ID=10, DMACRYS (2.0.8) |
| Location on S Drive | \CHEMISTRY\_CPOSS\Lactides\PCM\_cuto15 |
| Potential Description | GDMA2.2(PCMdielectric3(PBE1PBE/6-31G(d,p))) + FIT with 15A cutoff |
| Energy model | 4 |
| Study\_ID | 31 |
| Programs | Study\_ID=10, DMACRYS (2.0.8) |
| Location on S Drive | \CHEMISTRY\_CPOSS\Lactides\PCM\_cuto30 |
| Potential Description | GDMA2.2(PCMdielectric3(PBE1PBE/6-31G(d,p))) + FIT with 30A cutoff |

A screen shot of a graph

AI-generated content may be incorrect.

Figure . Crystal energy landscape of Lactide from previous work.

# CSD structures (CSD version 5.46 with Feb 2025 update)

Table . Crystallographic information for CSD entries for Lactide. Different polymorphs are coloured differently.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| REFCODE | space group | Z’ | a / Å | b / Å | c / Å | α / ° | β / ° | γ / ° | density / g cm-3 | Form |
| BEYDEO | P21/c | 1 | 7.73 | 9.836 | 9.402 | 90 | 110.03 | 90 | 1.425 | DL Form I |
| BEYDEO01 | P21/c | 1 | 7.7308 | 9.8306 | 9.3925 | 90 | 110.039 | 90 | 1.428 | DL Form I |
| BICVIS | P21/c | 1 | 8.05 | 9.086 | 9.713 | 90 | 102.86 | 90 | 1.382 | Racemic Form I |
| BICVIS01 | P21/c | 1 | 8.046 | 9.081 | 9.711 | 90 | 103.06 | 90 | 1.385 | Racemic Form I |
| BICVIS02 | P21/c | 1 | 7.9754 | 9.1391 | 9.4798 | 90 | 106.551 | 90 | 1.445 | Racemic Form I |
| BICVIS03 | P21/c | 1 | 8.0248 | 9.0748 | 9.71 | 90 | 103.122 | 90 | 1.39 | Racemic Form I |
| NAHNOZ | P212121 | 3 | 9.329 | 13.615 | 16.822 | 90 | 90 | 90 | 1.344 | LL Form I |
| NAHNOZ01 | P212121 | 3 | 9.2439 | 13.467 | 16.669 | 90 | 90 | 90 | 1.384 | LL Form I |
| TOFTIV | P212121 | 3 | 9.3208 | 13.6137 | 16.8173 | 90 | 90 | 90 | 1.346 | DD Form I |

Table . Experimental information for CSD entries for Lactide.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| REFCODE | space group | R factor | T / K | Year | Comments |
| BEYDEO | P21/c | 8.9 | 101 | 2000 | Not mentioned. The paper was about polymerization. The sample was sublimed twice to purify it, but it was a single crystal that was measured. |
| BEYDEO01 | P21/c | 7.21 | 100 | 2009 | Recrystallization from toluene/hexane1 |
| BICVIS | P21/c | 3.8 | 295 | 1982 | Recrystallization from dry ether2 |
| BICVIS01 | P21/c | 4.89 | 295 | 1997 | Not online |
| BICVIS02 | P21/c | 3.9 | 100 | 2009 | Recrystallization from diethylether1 |
| BICVIS03 | P21/c | 6.25 | 293 | 2024 | Not mentioned. Another paper on polymerization. |
| NAHNOZ | P212121 | 2.61 | 295 | 1997 | Not online |
| NAHNOZ01 | P212121 | 2.57 | 150 | 2005 | Private Communication |
| TOFTIV | P212121 | 6.89 | 293 | 2024 | Not mentioned. Another paper on polymerization. |

BICVIS02 does not overlay very well with the other determinations of this structure. Both BICVIS and BICVIS02 were checked against structures, and the former found to match better. This was used as the reference.

# Other notes

(1) Fedushkin, I. L.; Morozov, A. G.; Chudakova, V. A.; Fukin, G. K.; Cherkasov, V. K. Magnesium(II) Complexes of the dpp-BIAN Radical-Anion: Synthesis, Molecular Structure, and Catalytic Activity in Lactide Polymerization. *European Journal of Inorganic Chemistry* **2009**, *2009* (33), 4995-5003.

(2) van Hummel, G. J.; Harkema, S.; Kohn, F. E.; Feijen, J. Structure of 3,6-dimethyl-1,4-dioxane-2,5-dione [d-,d-(l-,l-)lactide]. *Acta Crystallographica Section B* **1982**, *38* (5), 1679-1681. DOI: 10.1107/S0567740882006840.