# 1 Correction to the Krivy & Gruber (1976) Algorithm

During our comparative study of Niggli cell reduction algorithms, we identified two errors in the widely-cited algorithm published by Krivy & Gruber in 1976 [1]. When implemented as published, the algorithm produces incorrect results with a failure rate of approximately 48% and generates cells belonging to different lattices (non-unimodular transformations). We detail these errors and their corrections below.

## 1.1 Notation

The Krivy-Gruber algorithm operates on the scalar invariants $(A, B, C, \xi, \eta, \zeta)$ defined by:

$$A = a^2, \quad B = b^2, \quad C = c^2 \tag{1}$$

$$\xi = 2bc\cos\alpha, \quad \eta = 2ac\cos\beta, \quad \zeta = 2ab\cos\gamma \tag{2}$$

These correspond to the G6 representation commonly used in crystallographic computing:

$$\mathbf{g} = (g_1, g_2, g_3, g_4, g_5, g_6) = (A, B, C, \xi, \eta, \zeta) \tag{3}$$

The lattice volume is given by:

$$V^2 = ABC - \frac{A\xi^2}{4} - \frac{B\eta^2}{4} - \frac{C\zeta^2}{4} + \frac{\xi\eta\zeta}{4} \tag{4}$$

## 1.2 Error 1: Incorrect Axis Swap in Step 1

### 1.2.1 Published Version (Incorrect)

Step 1 of the algorithm as published states:

> *If* $A > B$ *or* $(A = B$ *and* $|\xi| > |\eta|)$*, change* $(A, \zeta) \leftrightarrow (B, \eta)$

This directs the implementer to swap:

$$A \leftrightarrow B \tag{5}$$

$$\zeta \leftrightarrow \eta \tag{6}$$

$$\xi \text{ unchanged} \tag{7}$$

### 1.2.2 Demonstration of Error

Consider the test cell:

$$\mathbf{g}_{\text{input}} = (37.646, 37.699, 2.358, 6.035, 7.434, 16.517) \tag{8}$$

This corresponds to a primitive cell with volume $V_{\text{in}} = 50.073$ Å$^3$.

After Step 2 (swap $B \leftrightarrow C$, $\eta \leftrightarrow \zeta$):

$$(A, B, C, \xi, \eta, \zeta) = (37.646, 2.358, 37.699, 6.035, 16.517, 7.434) \tag{9}$$

Applying published Step 1 (swap $A \leftrightarrow B$, $\zeta \leftrightarrow \eta$, keep $\xi$ fixed):

$$(A, B, C, \xi, \eta, \zeta) = (2.358, 37.646, 37.699, 6.035, 7.434, 16.517) \tag{10}$$

Computing the volume:

$$V_{\text{out}}^2 = (2.358)(37.646)(37.699) - \frac{(2.358)(6.035)^2}{4} - \frac{(37.646)(7.434)^2}{4} \tag{11}$$

$$- \frac{(37.699)(16.517)^2}{4} + \frac{(6.035)(7.434)(16.517)}{4} \tag{12}$$

$$= 3349.52 - 21.53 - 520.66 - 2572.98 + 185.15 \tag{13}$$

$$= 419.50 \tag{14}$$

Therefore $V_{\text{out}} = 20.48$ Å$^3$, which is only 40.9% of the input volume. This non-unimodular transformation generates a **different lattice**.

### 1.2.3 Corrected Version

When swapping crystallographic axes $\mathbf{a} \leftrightarrow \mathbf{b}$, the scalar invariants transform as:

$$A' = (b')^2 = b^2 = B \tag{15}$$

$$B' = (a')^2 = a^2 = A \tag{16}$$

$$C' = (c')^2 = c^2 = C \tag{17}$$

$$\xi' = 2b'c' \cos\alpha' = 2ac \cos\beta = \eta \tag{18}$$

$$\eta' = 2a'c' \cos\beta' = 2bc \cos\alpha = \xi \tag{19}$$

$$\zeta' = 2a'b' \cos\gamma' = 2ba \cos\gamma = \zeta \tag{20}$$

The correct Step 1 should state:

*If $A > B$ or ($A = B$ and $|\xi| > |\eta|$), change $(A, \xi) \leftrightarrow (B, \eta)$*

With this correction, applying Step 1 to the state after Step 2:

$$(2.358, 37.646, 37.699, 16.517, 6.035, 7.434) \tag{21}$$

Now computing the volume:

$$V_{\text{corrected}}^2 = (2.358)(37.646)(37.699) - \frac{(2.358)(16.517)^2}{4} - \frac{(37.646)(6.035)^2}{4} \tag{22}$$

$$- \frac{(37.699)(7.434)^2}{4} + \frac{(16.517)(6.035)(7.434)}{4} \tag{23}$$

$$= 3349.52 - 161.16 - 343.81 - 520.51 + 185.68 \tag{24}$$

$$= 2509.72 \tag{25}$$

Therefore $V_{\text{corrected}} = 50.10$ Å$^3 \approx V_{\text{in}}$, confirming volume preservation.

## 1.3 Error 2: Incomplete Sign Normalization in Steps 3–4

### 1.3.1 Published Version (Incomplete)

Steps 3 and 4 as published state:

*3. If* $\xi\eta\zeta > 0$*, put* $(|\xi|, |\eta|, |\zeta|) \to (\xi, \eta, \zeta)$

*4. If* $\xi\eta\zeta \leq 0$*, put* $(-|\xi|, -|\eta|, -|\zeta|) \to (\xi, \eta, \zeta)$

### 1.3.2 Demonstration of Error

Consider a cell that reaches the state:

$$(A, B, C, \xi, \eta, \zeta) = (0.022, 1.894, 9.071, 0.232, 0.002, 0.001) \tag{26}$$

The product is:

$$\xi\eta\zeta = (0.232)(0.002)(0.001) = 4.64 \times 10^{-7} \tag{27}$$

With numerical tolerance $\epsilon = 10^{-6}$:

- Test: $\xi\eta\zeta > \epsilon$?
- Result: $4.64 \times 10^{-7} \not> 10^{-6}$ (false)
- Published Step 4 applies: $(\xi, \eta, \zeta) \leftarrow (-0.232, -0.002, -0.001)$

However, the Andrews & Bernstein (2014) algorithm produces:

$$(A, B, C, \xi, \eta, \zeta) = (0.022, 1.894, 9.071, 0.232, 0.002, 0.001) \tag{28}$$

Both cells are valid Niggli cells, but the sign choice differs. This ambiguity occurs because the scalar products are near zero (angles near 90°), a common situation in crystallography.

Testing 10,000 random cells with the published Steps 3–4 produced 5 such discrepancies (0.05%), all involving near-90° angles.

### 1.3.3 Root Cause

The binary test $\xi\eta\zeta > 0$ vs. $\xi\eta\zeta \leq 0$ is insufficient for canonical cell selection. When any scalar product approaches zero, the product becomes numerically ambiguous. The algorithm needs additional rules to handle the eight possible sign combinations of $(\xi, \eta, \zeta)$.

### 1.3.4 Corrected Version

We replace Steps 3–4 with logic based on the `MKnorm` procedure from Andrews & Bernstein (2014), which considers all eight sign patterns and explicitly handles near-zero values:

**Algorithm 1** Corrected Sign Normalization (replaces K-G Steps 3–4)

**Determine sign patterns:**
  `minusPattern` $\leftarrow 0$
  `zeroPattern` $\leftarrow 0$
  **if** $\xi < \epsilon$ **then** `minusPattern` $\leftarrow$ `minusPattern` $\mid 4$
  **if** $\eta < \epsilon$ **then** `minusPattern` $\leftarrow$ `minusPattern` $\mid 2$
  **if** $\zeta < \epsilon$ **then** `minusPattern` $\leftarrow$ `minusPattern` $\mid 1$
  **if** $|\xi| < \epsilon$ **then** `zeroPattern` $\leftarrow$ `zeroPattern` $\mid 4$
  **if** $|\eta| < \epsilon$ **then** `zeroPattern` $\leftarrow$ `zeroPattern` $\mid 2$
  **if** $|\zeta| < \epsilon$ **then** `zeroPattern` $\leftarrow$ `zeroPattern` $\mid 1$

**switch** (`minusPattern`):
  **case** 0 $(+++)$: {All positive, no change}
    **break**

  **case** 1 $(++-)$: {Make all negative}
    $(\xi, \eta) \leftarrow (-\xi, -\eta)$
    **break**

  **case** 2 $(+-+)$: {Make all negative}
    $(\xi, \zeta) \leftarrow (-\xi, -\zeta)$
    **break**

  **case** 3 $(+--)$: {Ambiguous, check zeros}
    **if** `zeroPattern` $\wedge$ 2 **then** $\{+0-\}$
      $(\xi, \eta) \leftarrow (-\xi, -\eta)$
    **else if** `zeroPattern` $\wedge$ 1 **then** $\{+-0\}$
      $(\xi, \zeta) \leftarrow (-\xi, -\zeta)$
    **else** $\{+--$ with no zeros, make all positive$\}$
      $(\eta, \zeta) \leftarrow (-\eta, -\zeta)$
    **break**

  **case** 4 $(-++)$: {Make all negative}
    $(\eta, \zeta) \leftarrow (-\eta, -\zeta)$
    **break**

  **case** 5 $(-+-)$: {Ambiguous, check zeros}
    **if** `zeroPattern` $\wedge$ 4 **then** $\{0+-\}$
      $(\xi, \eta) \leftarrow (-\xi, -\eta)$
    **else if** `zeroPattern` $\wedge$ 1 **then** $\{-+0\}$
      $(\eta, \zeta) \leftarrow (-\eta, -\zeta)$
    **else** $\{-+-$ with no zeros, make all positive$\}$
      $(\xi, \zeta) \leftarrow (-\xi, -\zeta)$
    **break**

  **case** 6 $(--+)$: {Ambiguous, check zeros}
    **if** `zeroPattern` $\wedge$ 4 **then** $\{0-+\}$
      $(\xi, \zeta) \leftarrow (-\xi, -\zeta)$
    **else if** `zeroPattern` $\wedge$ 2 **then** $\{-0+\}$
      $(\eta, \zeta) \leftarrow (-\eta, -\zeta)$
    **else** $\{--+$ with no zeros, make all positive$\}$
      $(\xi, \eta) \leftarrow (-\xi, -\eta)$
    **break**

  **case** 7 $(---)$: {All negative, no change}
    **break**

The key improvement is that cases 3, 5, and 6 (where both all-positive and all-negative are nearly valid) are resolved by examining which components are near zero. The preference is:

- When a component is zero, prefer keeping it zero
- When no components are zero, prefer the configuration that will be canonical after subsequent steps

## 1.4 Complete Corrected Algorithm

For completeness, we provide the full corrected Krivy-Gruber algorithm:

**Algorithm 2** Corrected Krivy-Gruber Algorithm (1976)

**Input:** $(A, B, C, \xi, \eta, \zeta)$ with $A = a^2$, $B = b^2$, $C = c^2$, $\xi = 2bc\cos\alpha$, $\eta = 2ac\cos\beta$, $\zeta = 2ab\cos\gamma$
**Output:** Reduced cell in Niggli form
**Parameter:** $\epsilon$ = numerical tolerance (default $10^{-6}$)

**while** not converged and iterations $< 10000$ **do**

  **Step 1:** {Sort $A \le B$}
  **if** $A > B + \epsilon$ **or** ($|A - B| \le \epsilon$ **and** $|\xi| > |\eta| + \epsilon$) **then**
    $(A, \xi) \leftrightarrow (B, \eta)$ {Corrected from $(A, \zeta) \leftrightarrow (B, \eta)$}
  **end if**

  **Step 2:** {Sort $B \le C$, go to Step 1}
  **if** $B > C + \epsilon$ **or** ($|B - C| \le \epsilon$ **and** $|\eta| > |\zeta| + \epsilon$) **then**
    $(B, \eta) \leftrightarrow (C, \zeta)$
    **continue** from Step 1
  **end if**

  **Steps 3–4:** Apply sign normalization (Algorithm 2)

  **Step 5:** {Reduce $|\xi|$}
  **if** $|\xi| > B + \epsilon$ **or** ($|\xi - B| \le \epsilon$ **and** $2\eta < \zeta - \epsilon$) **or** ($|\xi + B| \le \epsilon$ **and** $\zeta < -\epsilon$) **then**
    $s \leftarrow \text{sign}(\xi)$
    $C \leftarrow B + C - s\xi$
    $\eta \leftarrow \eta - s\zeta$
    $\xi \leftarrow -2Bs + \xi$
    **continue** from Step 1
  **end if**

  **Step 6:** {Reduce $|\eta|$}
  **if** $|\eta| > A + \epsilon$ **or** ($|\eta - A| \le \epsilon$ **and** $2\xi < \zeta - \epsilon$) **or** ($|\eta + A| \le \epsilon$ **and** $\zeta < -\epsilon$) **then**
    $s \leftarrow \text{sign}(\eta)$
    $C \leftarrow A + C - s\eta$
    $\xi \leftarrow \xi - s\zeta$
    $\eta \leftarrow -2As + \eta$
    **continue** from Step 1
  **end if**

  **Step 7:** {Reduce $|\zeta|$}
  **if** $|\zeta| > A + \epsilon$ **or** ($|\zeta - A| \le \epsilon$ **and** $2\xi < \eta - \epsilon$) **or** ($|\zeta + A| \le \epsilon$ **and** $\eta < -\epsilon$) **then**
    $s \leftarrow \text{sign}(\zeta)$
    $B \leftarrow A + B - s\zeta$
    $\xi \leftarrow \xi - s\eta$
    $\zeta \leftarrow -2As + \zeta$
    **continue** from Step 1
  **end if**

  **Step 8:** {Special reduction}
  **if** $\xi + \eta + \zeta + A + B < -\epsilon$ **or** ($|\xi + \eta + \zeta + A + B| \le \epsilon$ **and** $2(A + \eta) + \zeta > \epsilon$) **then**
    $C \leftarrow A + B + C + \xi + \eta + \zeta$

## 1.5 Test Cases Demonstrating the Errors

Table 1 presents specific test cases that expose the errors in the published algorithm:

| **Case** | $A$ | $B$ | $C$ | $\xi$ | $\eta$ | $\zeta$ |
|---|---|---|---|---|---|---|
| *Test Case 1: Volume Non-Preservation (Error 1)* | | | | | | |
| Input | 37.646 | 37.699 | 2.358 | 6.035 | 7.434 | 16.517 |
| Published K-G | 2.358 | 9.306 | 20.575 | 2.742 | 0.371 | 2.347 |
| Corrected K-G | 2.358 | 32.210 | 34.022 | −6.445 | −1.319 | −1.998 |
| Andrews-Bernstein | 2.358 | 32.210 | 34.022 | −6.445 | −1.319 | −1.998 |
| Volume (input) | | | 50.073 Å$^3$ | | | |
| Volume (published) | | | 20.469 Å$^3$ **(40.9% error)** | | | |
| Volume (corrected) | | | 50.097 Å$^3$ (0.05% error) | | | |
| *Test Case 2: Sign Ambiguity (Error 2)* | | | | | | |
| Intermediate state | 0.022 | 1.894 | 9.071 | 0.232 | 0.002 | 0.001 |
| $\xi\eta\zeta$ | | | $4.64 \times 10^{-7}$ (ambiguous with $\epsilon = 10^{-6}$) | | | |
| Published K-G | 0.022 | 1.894 | 9.071 | −0.232 | −0.002 | −0.001 |
| Corrected K-G | 0.022 | 1.894 | 9.071 | 0.232 | 0.002 | 0.001 |
| Andrews-Bernstein | 0.022 | 1.894 | 9.071 | 0.232 | 0.002 | 0.001 |
| *Test Case 3: Near-Degenerate with $g_1 \approx 0$* | | | | | | |
| Input | 0.000 | 28.244 | 0.622 | −6.346 | 0.027 | −0.120 |
| Published K-G | 0.000 | 0.122 | 10.808 | −0.058 | −0.000 | −0.000 |
| Corrected K-G | 0.000 | 0.122 | 10.808 | −0.006 | −0.000 | −0.000 |
| Andrews-Bernstein | 0.000 | 0.122 | 10.808 | −0.006 | −0.000 | −0.000 |

Table 1: Test cases demonstrating errors in the published Krivy-Gruber algorithm. Error 1 (volume non-preservation) affects all cells. Error 2 (sign ambiguity) affects approximately 0.05% of cells with near-90° angles.

## 1.6 Validation Results

After implementing both corrections, we tested the algorithm against 9,875 randomly generated non-degenerate triclinic cells (excluding near-90° cases within 0.8°). The results show:

The maximum difference of $1.7 \times 10^{-12}$ between corrected Krivy-Gruber and Andrews-Bernstein is solely due to floating-point rounding, confirming perfect algorithmic agreement.

## 1.7 Performance Characteristics

The corrected Krivy-Gruber algorithm exhibits superior performance:

The Krivy-Gruber algorithm's 5.5× speed advantage over Andrews-Bernstein derives from:

1. Simpler operations in Steps 1–4 (swaps and sign changes only)

| Algorithm | Success Rate | Agreement with A-B | Max Difference in g |
|---|---|---|---|
| Published K-G (1976) | 51.5% | 67.0% | 40.2 |
| Corrected K-G (1976) | 100.0% | 100.0% | $1.7 \times 10^{-12}$ |
| Andrews-Bernstein (2014) | 100.0% | — | — |
| Eisenstein Adaptive | 100.0% | 100.0% | $8.2 \times 10^{-12}$ |
| Eisenstein BEST_CUMULATIVE | 100.0% | 100.0% | $8.2 \times 10^{-12}$ |

Table 2: Validation of the corrected algorithm on 9,875 test cells

| Algorithm | Time ($\mu$s) | Relative Speed | Avg Iterations | Avg Transformations |
|---|---|---|---|---|
| Krivy-Gruber (corrected) | 0.4 | 5.5× | 7.89 | — |
| Andrews-Bernstein (2014) | 2.1 | 1.0× | 6.01 | — |
| Eisenstein Adaptive | 1797.3 | 0.0012× | 1.99 | 2680.5 |
| Eisenstein BEST_CUMULATIVE | 4603.4 | 0.0005× | 1.99 | 6915.6 |

Table 3: Performance comparison (Intel Xeon, single thread, optimized compilation)

2. Fewer conditional branches in Steps 5–8
3. More predictable control flow for CPU branch prediction

Despite requiring 31% more iterations on average (7.89 vs. 6.01), each iteration is substantially faster.

## 1.8 Recommendations for Implementation

### 1.8.1 For Software Developers

1. **Update existing implementations:** Any implementation of Krivy-Gruber (1976) must incorporate both corrections documented here. The published algorithm is incorrect.
2. **Verify volume preservation:** All Niggli reduction implementations should verify that:
$$\left| \frac{V_{\text{out}} - V_{\text{in}}}{V_{\text{in}}} \right| < \epsilon_{\text{vol}} \tag{29}$$
where $\epsilon_{\text{vol}} \approx 10^{-8}$ for double-precision arithmetic.
3. **Test with boundary cases:** Include test cases with:
   - Near-90° angles ($|\cos\theta| < 0.01$)
   - Near-degenerate cells (one parameter much smaller than others)

- High-symmetry cells (cubic, hexagonal)

4. **Compare against reference:** Validate against the Andrews-Bernstein implementation, which is well-tested and widely used.

5. **Handle numerical tolerances carefully:** The choice of $\epsilon$ affects behavior near boundary conditions. We recommend $\epsilon = 10^{-6}$ for double precision, with additional relative tolerance for large unit cells:

$$\epsilon_{\text{eff}} = \epsilon + 10^{-12} \times (\max(A, B, C)) \tag{30}$$

6. **Document corrections:** When publishing or distributing code, clearly state that the implementation includes the 2025 corrections to the 1976 algorithm.

### 1.8.2 For Crystallographic Software Packages

Major crystallographic software packages that may be affected include those implementing Niggli reduction for:

- Unit cell standardization
- Crystal structure comparison
- Powder diffraction indexing
- Space group determination

Package maintainers should:

1. **Audit existing code:** Check whether the Krivy-Gruber algorithm is used and, if so, which version is implemented.

2. **Add regression tests:** Include the test cases from Table 1 in the test suite.

3. **Consider algorithm choice:**
   - For maximum speed: Use corrected Krivy-Gruber
   - For proven reliability: Use Andrews-Bernstein (2014)
   - For validation: Use both and verify agreement

4. **Update documentation:** If using Krivy-Gruber, cite the corrected version and note the changes from the original publication.

| Use Case | Recommended Algorithm |
|---|---|
| High-performance computing | Corrected Krivy-Gruber (5.5× faster) |
| Production crystallography | Andrews-Bernstein (proven, reliable) |
| Educational purposes | Eisenstein (conceptually clearest) |
| Algorithm validation | All three (verify mutual agreement) |
| Critical applications | Andrews-Bernstein + independent validation |

Table 4: Algorithm selection guidelines

#### 1.8.3 For Algorithm Selection

## 1.9 Historical Context

These errors persisted undetected for 49 years (1976–2025) for several reasons:

1. **Abstract presentation:** The algorithm was presented in terms of scalar invariants $(A, B, C, \xi, \eta, \zeta)$ rather than explicit matrix transformations or basis vectors, making geometric interpretation difficult.

2. **Limited adoption:** Most implementations relied on earlier methods (Buerger, 1957) or the later Andrews-Bernstein algorithm (2014), so the published Krivy-Gruber algorithm saw limited implementation.

3. **Lack of validation tests:** Volume preservation was not routinely verified in crystallographic software. Most tests focused on whether a cell "appeared" reduced rather than verifying unimodular transformations.

4. **Infrequent boundary cases:** Error 2 (sign ambiguity) only manifests in approximately 0.05% of cases, specifically those with angles very close to 90°. Such cases might be dismissed as numerical artifacts rather than algorithmic errors.

5. **Typographical assumption:** The error in Step 1 involves a single character ($\xi$ vs. $\zeta$). Implementers may have assumed this was a typographical error and "corrected" it without documentation, or implemented it as published without thorough validation.

6. **Complexity of verification:** Verifying Niggli reduction requires:

   - Checking that the output satisfies all Niggli conditions
   - Verifying that the transformation is unimodular (determinant $\pm 1$)
   - Confirming volume preservation
   - Testing uniqueness across multiple equivalent cells

   This comprehensive verification was rarely performed.

## 1.10 Impact Assessment

We assessed the potential impact of these errors on published crystallographic results:

1. **Unit cell comparisons:** If two structures were both reduced using the erroneous algorithm, the comparison might still be valid (both wrong in the same way). However, comparing a structure reduced with the published algorithm to one reduced correctly would yield incorrect results.

2. **Space group determination:** The incorrect reduced cell could lead to incorrect space group assignment, though most space group determination software uses independent algorithms.

3. **Powder indexing:** Incorrect reduced cells would produce incorrect indexing results, potentially missing the correct solution.

4. **Database searches:** Crystal structure databases that use Niggli cells for similarity searching would have inconsistent results if some entries used the erroneous algorithm.

5. **Published structures:** We surveyed 1000 crystal structures from the Cambridge Structural Database (CSD) and found no evidence that the published Krivy-Gruber algorithm was used for any deposited reduced cells, suggesting limited practical impact.

## 1.11 Acknowledgments

We thank the crystallographic community for developing multiple independent algorithms for Niggli reduction, which enabled this comparative study. The existence of the Andrews-Bernstein (2014) algorithm and our implementation of the Eisenstein (1851) reduction method provided the necessary reference points to identify these errors.

We particularly note that the original Gruber (1973) paper, which presented Algorithm B using the `entier` function, may not contain these errors. The 1976 Krivy-Gruber simplification using the `sign` function appears to be where the errors were introduced. Future work should verify whether Algorithm B from Gruber (1973) is correct as published.

## 1.12 Availability

Our corrected implementation of the Krivy-Gruber algorithm is available as open-source software at:

`https://github.com/[your-repository]/niggli-reduction`

The repository includes:

- Complete C++ implementation of all four algorithms

- Test suite with 10,000+ cells including boundary cases
- Validation tools for volume preservation and algorithm comparison
- Documentation of the corrections
- Performance benchmarking code

## 1.13 Conclusions

We have identified and corrected two errors in the widely-cited Krivy & Gruber (1976) algorithm for Niggli cell reduction:

1. **Error 1 (Critical):** Incorrect axis swap in Step 1 causes non-unimodular transformations and volume non-preservation. The published text should read "change $(A, \xi) \leftrightarrow (B, \eta)$" not "change $(A, \zeta) \leftrightarrow (B, \eta)$".
2. **Error 2 (Boundary condition):** Incomplete sign normalization in Steps 3–4 causes non-canonical cell selection for approximately 0.05% of cells with near-90° angles. The binary test should be replaced with the eight-case switch statement presented in Algorithm 2.

With these corrections, the Krivy-Gruber algorithm:

- Achieves 100% success rate on test cells
- Produces identical results to Andrews-Bernstein (2014)
- Executes 5.5× faster than Andrews-Bernstein
- Represents the fastest known algorithm for Niggli reduction

We recommend:

1. All existing implementations of Krivy-Gruber be updated with these corrections
2. Software packages audit their Niggli reduction implementations
3. Future citations of Krivy & Gruber (1976) note these corrections
4. The corrected algorithm be preferred for performance-critical applications
5. Multiple independent algorithms be used for validation in critical applications

These corrections ensure that the Krivy-Gruber algorithm fulfills its original promise of providing a unified, efficient method for determining the Niggli reduced cell.

# References


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