# PES ANALYSIS TOOL

Computational Chemistry Research Lab Edition

Flask + Python | Advanced Analysis | File Upload Support

## Data Input

**Upload File**

Gaussian .log, ORCA .out, CSV, or TXT

**Manual Entry:**

Angle (°) | Energy (kJ/mol)

Add Point

| Angle (°) | Energy | Action |
|---|---|---|
| 10.0 | 30.000 | × |
| 30.0 | 12.000 | × |
| 45.0 | 50.000 | × |

Analyze | CSV | Report

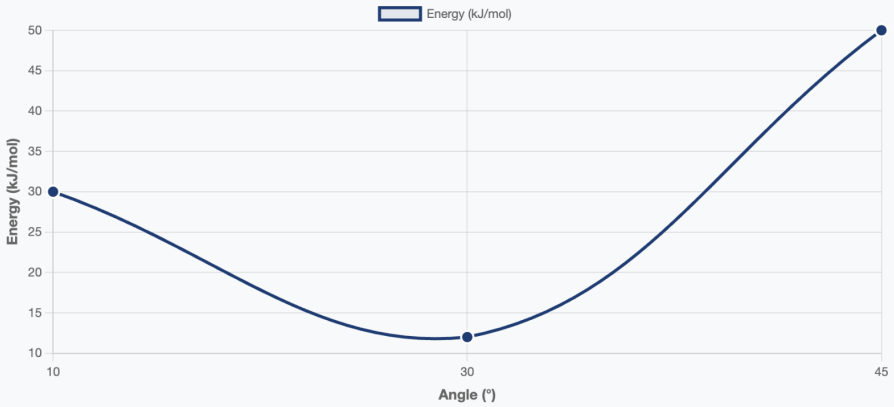
Clear

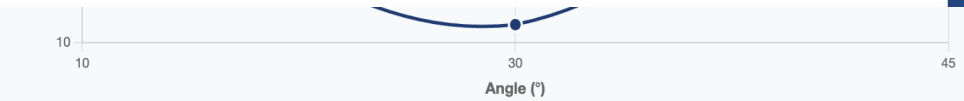
**Global Minimum**
**Energy:** 12.000000 kJ/mol
**Angle:** 30.00°

### Statistics

| 3 | 38.00 |
|---|---|
| Data Points | Energy Range (kJ/mol) |

## Interactive Visualization




## Advanced Analysis Results

**Global Minimum**
**Angle:** 30.00°
**Energy:** 12.000000 kJ/mol

### Local Minima (1)

**Minimum 1:** 30.00° | 12.000000 kJ/mol | Relative: 0.0000 kJ/mol

Generate Annotated Plot | Download Plot

## Conformational Stability

### Summary

**Most Stable Conformation:**
Angle: 30.00°
Energy: 12.000000 kJ/mol

**Least Stable Conformation:**
Angle: 45.00°
Energy: 50.000000 kJ/mol

**Stability Range:**
38.0000 kJ/mol (9.0822 kcal/mol)

### Boltzmann Population (top 3)

The populations correspond to the points in the input dataset (index starting at 0).

1. Point index 1: 99.9301 %
2. Point index 0: 0.0699 %
3. Point index 2: 0.0000 %

### Full Boltzmann Populations

| Index | Population (%) |
|---|---|
| 0 | 0.069899% |
| 1 | 99.930079% |
| 2 | 0.000022% |