

Supporting information

**Combined Experimental and Computational Insights into Key  
Features of L-Alanine L-Alaninium Picrate Monohydrate: Growth,  
Structural, Electronic and Nonlinear Optical Properties**

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Optimized coordinates for LALAPM

B3LYP/6-31G\* level of Theory

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.83813600  | 0.00602000  | -2.30545200 |
| O | 0.84829900  | -0.26922500 | -0.27088200 |
| C | 1.15522700  | -0.65032500 | -1.38125100 |
| C | 0.75553000  | -2.04813800 | -1.88128600 |
| H | -0.18478800 | -2.31254500 | -1.39451300 |
| C | 1.83914200  | -3.09215000 | -1.62305700 |
| H | 1.52944100  | -4.08440200 | -1.97081500 |
| H | 2.02365700  | -3.15550100 | -0.54697200 |
| H | 2.77912900  | -2.81789900 | -2.11439600 |
| N | 0.45683200  | -1.91210500 | -3.35334800 |
| H | -0.33615700 | -1.14408900 | -3.48586900 |
| H | 1.29061500  | -1.55069100 | -3.82710100 |
| O | 1.68910900  | 2.41854100  | -1.67189400 |
| H | 1.88026100  | 1.04060700  | -2.07308000 |
| O | -0.43524700 | 2.29898900  | -2.46078800 |
| C | 0.46556200  | 2.70839600  | -1.68371800 |
| C | -0.00820800 | 3.70955000  | -0.59120800 |
| H | 0.10474200  | 4.72389000  | -0.99173400 |
| C | 0.72142300  | 3.56640200  | 0.73747500  |
| H | 0.34196700  | 4.27343800  | 1.48294500  |
| H | 1.78290900  | 3.75879200  | 0.57140800  |
| H | 0.61540200  | 2.55129700  | 1.12824800  |
| N | -1.49085300 | 3.46448500  | -0.44784800 |
| H | -2.01284300 | 4.29630200  | -0.16788700 |
| H | -1.70457400 | 2.69505100  | 0.25369300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.79177200 | 3.11602100  | -1.37597500 |
| O | -1.99384600 | 1.82720200  | 1.61311800  |
| C | -2.24613000 | 0.65591700  | 1.96072800  |
| C | -2.43212800 | -0.48637800 | 1.05970400  |
| N | -2.46380000 | -0.29657900 | -0.35447700 |
| O | -2.61462700 | 0.83663000  | -0.82788400 |
| O | -2.35622400 | -1.29504800 | -1.10616500 |
| C | -2.57043300 | -1.79676200 | 1.51211200  |
| H | -2.69297700 | -2.60459700 | 0.80397200  |
| C | -2.56621600 | -2.06288900 | 2.86897000  |
| N | -2.71321600 | -3.43340000 | 3.32753500  |
| O | -2.80888300 | -4.32106200 | 2.47378700  |
| O | -2.72960500 | -3.63238700 | 4.54460500  |
| C | -2.43207100 | -1.02544500 | 3.80722400  |
| H | -2.42991500 | -1.24576800 | 4.86719300  |
| C | -2.30974800 | 0.26873300  | 3.37074300  |
| N | -2.22909600 | 1.30608400  | 4.40443900  |
| O | -1.70549300 | 0.99280100  | 5.47777800  |
| O | -2.71254200 | 2.40769800  | 4.15838700  |
| O | -1.33632100 | -0.03616500 | -3.52230200 |
| H | -0.92143600 | 0.82919100  | -3.26290500 |
| H | -1.97719000 | -0.21446700 | -2.80322700 |
| H | 0.17736100  | -2.80034500 | -3.77652600 |

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MP2/6-31G\* level of Theory

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.99505000  | -1.47211200 | 1.57381100  |
| O | 1.10650800  | -0.30264500 | 0.99895300  |
| C | 1.73476300  | -1.33732300 | 1.17382400  |
| C | 1.10212800  | -2.70673400 | 0.95319200  |
| H | 0.30391700  | -2.59577800 | 0.21819200  |
| C | 0.60354200  | -3.31984000 | 2.25087500  |
| H | 0.16185400  | -4.30645000 | 2.08032800  |
| H | -0.16849500 | -2.67215400 | 2.67304900  |
| H | 1.41745900  | -3.40550100 | 2.97644900  |
| N | 2.16328200  | -3.55532000 | 0.31739200  |
| H | 2.55231500  | -3.01869100 | -0.55221100 |
| H | 2.94522600  | -3.66023500 | 0.97302500  |
| O | 3.90472300  | 0.86695700  | 1.37241000  |
| H | 3.46862300  | -0.52598800 | 1.56132300  |
| O | 3.59637400  | 0.48418200  | -0.85589900 |
| C | 3.56758300  | 1.18463400  | 0.19594200  |
| C | 3.04548500  | 2.62524500  | 0.01105400  |
| H | 3.90232700  | 3.27684800  | -0.19704400 |
| C | 2.24137300  | 3.13533000  | 1.19108400  |
| H | 1.86334200  | 4.14608300  | 1.01032900  |
| H | 2.88600900  | 3.14504000  | 2.07009700  |
| H | 1.39851800  | 2.46879000  | 1.38035000  |
| N | 2.21008000  | 2.58336500  | -1.23247600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.12455800  | 3.49395300  | -1.69017000 |
| H | 1.22939300  | 2.23003300  | -1.02662400 |
| H | 2.65448300  | 1.88488200  | -1.85077400 |
| O | -0.33574300 | 2.12794600  | -0.56935100 |
| C | -1.23343700 | 1.24179900  | -0.54217900 |
| C | -1.16495500 | -0.10416100 | -1.07239800 |
| N | 0.01016400  | -0.54370000 | -1.76154400 |
| O | 0.82603200  | 0.29058400  | -2.20299800 |
| O | 0.19436300  | -1.78069000 | -1.91550400 |
| C | -2.17159200 | -1.05755300 | -0.90731000 |
| H | -2.06118700 | -2.04813400 | -1.33252000 |
| C | -3.31882500 | -0.71909700 | -0.22215000 |
| N | -4.36383400 | -1.71637300 | -0.05150000 |
| O | -4.14431400 | -2.86920300 | -0.46690900 |
| O | -5.41580500 | -1.35926000 | 0.50918100  |
| C | -3.49727800 | 0.56582500  | 0.31247200  |
| H | -4.39814200 | 0.82479300  | 0.85926800  |
| C | -2.50166000 | 1.48800700  | 0.11893200  |
| N | -2.72369200 | 2.82768600  | 0.65330300  |
| O | -3.13215100 | 2.91524300  | 1.82596300  |
| O | -2.51477600 | 3.78431800  | -0.11076000 |
| O | 3.01847200  | -2.05199900 | -1.66211700 |
| H | 3.39775300  | -1.20565000 | -1.30524500 |
| H | 2.20673000  | -1.76570400 | -2.12867200 |
| H | 1.81067800  | -4.47909700 | 0.05036000  |

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# M06/6-31G\* level of Theory

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.99505000  | -1.47211200 | 1.57381100  |
| O | 1.10650800  | -0.30264500 | 0.99895300  |
| C | 1.73476300  | -1.33732300 | 1.17382400  |
| C | 1.10212800  | -2.70673400 | 0.95319200  |
| H | 0.30391700  | -2.59577800 | 0.21819200  |
| C | 0.60354200  | -3.31984000 | 2.25087500  |
| H | 0.16185400  | -4.30645000 | 2.08032800  |
| H | -0.16849500 | -2.67215400 | 2.67304900  |
| H | 1.41745900  | -3.40550100 | 2.97644900  |
| N | 2.16328200  | -3.55532000 | 0.31739200  |
| H | 2.55231500  | -3.01869100 | -0.55221100 |
| H | 2.94522600  | -3.66023500 | 0.97302500  |
| O | 3.90472300  | 0.86695700  | 1.37241000  |
| H | 3.46862300  | -0.52598800 | 1.56132300  |
| O | 3.59637400  | 0.48418200  | -0.85589900 |
| C | 3.56758300  | 1.18463400  | 0.19594200  |
| C | 3.04548500  | 2.62524500  | 0.01105400  |
| H | 3.90232700  | 3.27684800  | -0.19704400 |
| C | 2.24137300  | 3.13533000  | 1.19108400  |
| H | 1.86334200  | 4.14608300  | 1.01032900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.88600900  | 3.14504000  | 2.07009700  |
| H | 1.39851800  | 2.46879000  | 1.38035000  |
| N | 2.21008000  | 2.58336500  | -1.23247600 |
| H | 2.12455800  | 3.49395300  | -1.69017000 |
| H | 1.22939300  | 2.23003300  | -1.02662400 |
| H | 2.65448300  | 1.88488200  | -1.85077400 |
| O | -0.33574300 | 2.12794600  | -0.56935100 |
| C | -1.23343700 | 1.24179900  | -0.54217900 |
| C | -1.16495500 | -0.10416100 | -1.07239800 |
| N | 0.01016400  | -0.54370000 | -1.76154400 |
| O | 0.82603200  | 0.29058400  | -2.20299800 |
| O | 0.19436300  | -1.78069000 | -1.91550400 |
| C | -2.17159200 | -1.05755300 | -0.90731000 |
| H | -2.06118700 | -2.04813400 | -1.33252000 |
| C | -3.31882500 | -0.71909700 | -0.22215000 |
| N | -4.36383400 | -1.71637300 | -0.05150000 |
| O | -4.14431400 | -2.86920300 | -0.46690900 |
| O | -5.41580500 | -1.35926000 | 0.50918100  |
| C | -3.49727800 | 0.56582500  | 0.31247200  |
| H | -4.39814200 | 0.82479300  | 0.85926800  |
| C | -2.50166000 | 1.48800700  | 0.11893200  |
| N | -2.72369200 | 2.82768600  | 0.65330300  |
| O | -3.13215100 | 2.91524300  | 1.82596300  |
| O | -2.51477600 | 3.78431800  | -0.11076000 |
| O | 3.01847200  | -2.05199900 | -1.66211700 |
| H | 3.39775300  | -1.20565000 | -1.30524500 |
| H | 2.20673000  | -1.76570400 | -2.12867200 |
| H | 1.81067800  | -4.47909700 | 0.05036000  |